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An Exact Solution to the Classical, Anisotropic Heisenberg Model with Long-Range Kac Interactions

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A rigorous derivation is given for the "constant-magnetization" free energy density of the classical, anisotropic Heisenberg model with long-range Kac interactions. The derivation involves bounding arguments similar to those used for a classical fluid by Lebowitz and Penrose. The present work is carried out in a constant-magnetization ensemble. The free energy density is determined exactly under a quadruple-limiting process. The limits involved are a Lebowitz–Penrose type of triple-limiting process, followed by a final limit, $\chi \to 0$, where χ is a parameter which represents the range over which each component of the net spin density can vary. Explicit equations of state are determined for the special case of zero short-range interactions plus pure Kac-type long-range interactions.

KEY WORDS: Statistical mechanics; ferromagnet; constant magnetization ensemble; thermodynamics; equations of state; phase transitions.

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1. INTRODUCTION

The objective of this work is to study the thermodynamics of the classical, anisotropic Heisenberg model with long-range Kac interactions. Such a study represents an attempt to contribute to the understanding of the effects of anisotropy on thermodynamic behavior. The effects of anisotropy are illustrated dramatically by the fact that the two-dimensional, isotropic (quantum) Heisenberg model with finite-range interactions does not exhibit a spontaneous magnetization for any nonzero temperature,[(1)] in contradistinction with the well-known ferromagnetic phase transition of the corresponding (fully anisotropic) Ising model.[(2)] Such effects indicate that further rigorous investigations of the thermodynamic behavior of systems with anisotropic couplings are of interest.

In this article, the second of a two-article[(3)] sequence, an exact solution is given to the classical, anisotropic Heisenberg model[4] with long-range Kac interactions. It is seen that the constant-magnetization ensemble[(3)] is a "natural" ensemble for such a calculation. The technique employed, which is analogous to that used by Lebowitz and Penrose[(5)] for a classical fluid, is to obtain upper and lower bounds on the constant-magnetization free energy density $f_m(\boldsymbol{\rho}, \chi, N, \gamma)$. These bounds are established by dividing the lattice into P cells, each containing n lattice sites. The bounds on $f_m(\boldsymbol{\rho}, \chi, N, \gamma)$ involve the free energy density of each cell and an estimate of the long-range intercell interactions. Under the Lebowitz–Penrose[(5)] limiting process and the additional limit as $\chi \to 0$, the upper and lower bounds coalesce, determining the free energy density exactly. The parameter χ which arises in the constant-magnetization ensemble[(3)] represents the range over which each component of the net spin density can vary.

The Lebowitz–Penrose limiting process involves three separate limits.

1. The first limit is the thermodynamic limit of the entire lattice. This limit is taken such that the number of cells P becomes infinite (in all directions) while the number of sites in a cell n remains fixed.
2. The long-range limit, $\gamma \to 0$, is the second limit performed.
3. The final limit is the thermodynamic limit of each cell, i.e., the limit $n \to \infty$.

Section 2 contains a discussion of the Kac potential and the free energies arising in this problem. In Sections 3 and 4 upper and lower bounds are established for the constant-magnetization free energy density. Sections 5 and 6 consist in a determination of the convex envelope construction for the constant-magnetization free energy density and a discussion of the equations

[4] For a discussion of the classical Heisenberg model as the classical limit of the quantum model see Ref. 4a. For a discussion of the classical, anisotropic Heisenberg model with short-range interactions see Ref. 4b.

of state[5] for the classical, anisotropic Heisenberg model with long-range Kac interaction but no short-range interactions.

2. THE KAC POTENTIAL AND FREE ENERGY DENSITIES

We assume that each coupling coefficient in the Hamiltonian[6] for the classical, anisotropic Heisenberg model can be written as the sum of two terms as follows:

$$J_{i,kl} = q_{i,kl} + w_{i,kl} \tag{1}$$

for $i = x, y, z$. Here $q_{x,kl}$, $q_{y,kl}$, and $q_{z,kl}$ are the short-range contributions to the coupling coefficients and $w_{x,kl}$, $w_{y,kl}$, and $w_{z,kl}$ are the long-range "Kac" contributions to the coupling coefficients. The latter coefficients depend upon γ, the Kac parameter, which is described below. We assume that $q_{x,kl}$, $q_{y,kl}$, and $q_{z,kl}$ satisfy the inequality

$$|q_{i,kl}| \leqslant D_2/r_{kl}^{\nu+\epsilon_2} \tag{2}$$

for $i = x, y, z$ where ν is the dimensionality of the lattice and where D_2 and ϵ_2 are finite, positive constants. The functions $w_{x,kl}$, $w_{y,kl}$, and $w_{z,kl}$ are assumed to be of the Kac form,[(5)] i.e.,

$$w_{i,kl} = \gamma^\nu \phi_i(\gamma r_{kl}) \tag{3}$$

for $i = x, y, z$ (the label γ is suppressed in $w_{i,kl}$ for convenience). We assume the following bounds for $\phi_i(t)$:

$$|\phi_i(t)| \leqslant A \tag{4a}$$

and

$$|\phi_i(t)| \leqslant D_3/t^{\nu+\epsilon_3} \tag{4b}$$

for $i = x, y, z$, where both sets of inequalities hold for all t. D_3, ϵ_3, and A are finite, positive constants.

We note that the conditions (1)–(4) are consistent with those of Section 2.4 of Ref. 3, which were sufficiency conditions for the equivalence of the canonical and constant-magnetization ensembles. Conditions (4a) and (4b) establish the existence of the quantities α_x, α_y, and α_z, defined by

$$\alpha_i = \gamma^\nu \int d^\nu r \, \phi_i(\gamma r) \tag{5}$$

for $i = x, y, z$. The integrals in (5) extend over all space. We note that the quantities α_x, α_y, and α_z are independent of γ.

[5] Some of the thermodynamic results have been compiled in Ref. 6.
[6] See Eq. (2) of Ref. 3.

The constant-magnetization partition function for a lattice of N spin sites is written as follows:

$$Q_m(\mathbf{M}, \Delta, N, \gamma) = \exp[-\beta N f_m(\boldsymbol{\rho}, \chi, N, \gamma)] \tag{6a}$$

where

$$\boldsymbol{\rho} = \mathbf{M}/N \tag{6b}$$

$$\chi = \Delta/N \tag{6c}$$

and $f_m(\boldsymbol{\rho}, \chi, N, \gamma)$ is the corresponding free energy density. The parameter Δ represents the interval over which each component of the net spin can vary in this ensemble (see Section 2.2 of Ref. 3). A superscript "0" is used to denote a function which corresponds to a system with zero long-range Kac interactions, i.e., $w_{i,kl} = 0$ for $i = x, y, z$ and all sites k and l. But from (3)

$$\lim_{\gamma \to 0} w_{i,kl} = 0 \tag{7}$$

for $i = x, y, z$, so that the superscript "0" is equivalent to taking the limit $\gamma \to 0$ *before* the thermodynamic limit. Thus

$$f_m{}^0(\boldsymbol{\rho}, \chi, N) = \lim_{\gamma \to 0} f_m(\boldsymbol{\rho}, \chi, N, \gamma) \tag{8a}$$

We define two free energy densities in the thermodynamic limit, namely

$$f_m{}^0(\boldsymbol{\rho}, \chi) = \lim_{N \to \infty} f_m{}^0(\boldsymbol{\rho}, \chi, N) \tag{8b}$$

and

$$f_m(\boldsymbol{\rho}, \chi, \gamma) = \lim_{N \to \infty} f_m(\boldsymbol{\rho}, \chi, N, \gamma) \tag{9a}$$

The former represents an infinite system with zero long-range interactions, while the latter represents a system with nonzero long-range Kac interactions.

The long-range limit $\gamma \to 0$ is then defined by

$$f_m(\boldsymbol{\rho}, \chi) = \lim_{\gamma \to 0} f_m(\boldsymbol{\rho}, \chi, \gamma) \tag{9b}$$

assuming this limit exists. For the classical Heisenberg model we must take the additional limit $\chi \to 0$. In Ref. 3 the equivalence of the constant-magnetization ensemble to the canonical ensemble is established provided the limit $\chi \to 0$ was taken *after* the thermodynamic limit. Further, as mentioned in Section 1, we obtain bounds on $f_m(\boldsymbol{\rho}, \chi, N, \gamma)$ in terms of the free energies of the individual cells. We therefore take the limit $\chi \to 0$ *after* the thermodynamic limit of each cell, i.e., the limit $\chi \to 0$ is the last limit taken. We then define

$$f_m{}^0(\boldsymbol{\rho}) = \lim_{\chi \to 0} f_m{}^0(\boldsymbol{\rho}, \chi) \tag{10a}$$

and

$$f_m(\rho) = \lim_{\chi \to 0} f_m(\rho, \chi) \tag{10b}$$

In this article the existence of this last limit is proved and $f_m(\rho)$ is determined explicitly for the case of zero short-range interactions plus Kac-type long-range interactions.

3. UPPER BOUND ON THE FREE ENERGY

Consider a (regular-linear, square, cubic) lattice of spin sites for $\nu = (1, 2, 3)$. Divide the lattice into P identical (regular-linear, square, cubic) cells, each containing n lattice sites. The division is made so that each site is contained in one and only one cell. For any possible configuration of the system we denote the net spin of the λth cell by $\mathbf{m}_\lambda$ (Greek letters will be used to label cells). We therefore have the relations

$$nP = N \tag{11a}$$

and

$$\sum_{\lambda=1}^{P} \mathbf{m}_\lambda = \mathbf{M} \tag{11b}$$

Note that we restrict N to values satisfying (11a).

We now divide the Hamiltonian $\mathscr{H}_N^{(s)}$ into the sum of two terms,

$$\mathscr{H}_N^{(s)} = T + \tilde{\mathscr{H}}_N^{(s)} \tag{12}$$

$\tilde{\mathscr{H}}_N^{(s)}$ is itself a sum of two terms:

$$\tilde{\mathscr{H}}_N^{(s)} = \mathscr{H}' + \mathscr{H}'' \tag{13}$$

The term $\mathscr{H}'$ contains all intracell, short-range interactions,

$$\mathscr{H}' = \sum_{\lambda=1}^{P} \mathscr{H}_\lambda' \tag{14}$$

where

$$\mathscr{H}_\lambda' = -\tfrac{1}{2} \sum_{i=x,y,z} \sum_{\substack{k \neq l \\ k\in\lambda; l\in\lambda}}^{n} q_{i,kl} s_{i,k} s_{i,l} \tag{15}$$

The first summation in (15) is over $i = x, y, z$, and the second summation is over all sites k and l such that both sites k and l are contained in cell λ. The term $\mathscr{H}''$ is a "measure" of the long-range, cell–cell interaction, given by

$$\mathscr{H}'' = -\tfrac{1}{2} \sum_{i=x,y,z} \sum_{\lambda \neq \tau}^{P} w_{i,\lambda\tau} m_{i,\lambda}' m_{i,\tau}' \tag{16}$$

where the first summation on i is over x, y, and z, and the second summation is over all cells λ and τ. The terms $w_{x,\lambda\tau}$, $w_{y,\lambda\tau}$, and $w_{z,\lambda\tau}$ are defined by

$$w_{i,\lambda\tau} = \operatorname*{Max}_{k\in\lambda;l\in\tau} w_{i,kl} \tag{17a}$$

Similarly, define

$$\tilde{w}_{i,\lambda\tau} = \operatorname*{Min}_{k\in\lambda;l\in\tau} w_{i,kl} \tag{17b}$$

where $i = x, y, z$, and where site k is contained in cell λ and site l is contained in cell τ. The term T then contains all terms of $\mathscr{H}_N^{(s)}$ that are not contained in $\bar{\mathscr{H}}_N^{(s)}$.

We write T as the sum of three terms,

$$T = T_1 + T_2 + T_3 \tag{18}$$

where

$$T_1 = -\tfrac{1}{2} \sum_{i=x,y,z} \sum_{\lambda\neq\tau}^{P} \sum_{\substack{k,l \\ k\in\lambda;l\in\tau}}^{n} q_{i,kl} s_{i,k} s_{i,l} \tag{19}$$

$$T_2 = -\tfrac{1}{2} \sum_{i=x,y,z} \sum_{\lambda\neq\tau}^{P} \sum_{\substack{k,l \\ k\in\lambda;l\in\tau}}^{n} [w_{i,kl} - w_{i,\lambda\tau}] s_{i,k} s_{i,l} \tag{20}$$

and

$$T_3 = -\tfrac{1}{2} \sum_{i=x,y,z} \sum_{\lambda=1}^{P} \sum_{\substack{k\neq l \\ k\in\lambda;\, l\in\lambda}}^{n} w_{i,kl} s_{i,k} s_{i,l} \tag{21}$$

The term T_1 can be interpreted as the Hamiltonian for short-range intercell interactions; T_2 as the Hamiltonian for intercell, long-range interactions with coupling coefficients $[w_{x,kl} - w_{x,\lambda\tau}]$, $[w_{y,kl} - w_{y,\lambda\tau}]$, and $[w_{z,kl} - w_{z,\lambda\tau}]$; and T_3 is the Hamiltonian for long-range, intracell interactions.

We can think of T_1 as the interaction of the λth cell with all other cells summed over $\lambda = 1, 2, \ldots, P$. We find a bound on $|T_1|$ by determining an upper bound for the magnitude of the interaction of a reference cell with each other cell. Since we deal with the sum of magnitudes and are interested in an upper bound, we may allow the reference cell to be imbedded in an infinite lattice. This yields a weaker, but nevertheless useful, upper bound. This, multiplied by P, is a bound for $|T_1|$.

We first pick a reference cell and obtain an upper bound on the short-range interactions between the reference cell and all other cells except those $3^\nu - 1$ cells that are immediately adjacent to the reference cell. We consider the interaction of the reference cell with a (linear, square, cubic) shell for $\nu = (1, 2, 3)$ centered at the reference cell. The kth shell is made up of $(2k + 3)^\nu - (2k + 1)^\nu$ cells and is separated from the reference cell by at least k cells.

Using (2), the short-range interaction of the reference cell with the kth shell is bounded by

$$3D_2 n^2[(2k+3)^\nu - (2k+1)^\nu]/(kn^{1/\nu})^{\nu+\epsilon_2}$$

Therefore a bound for the short-range interaction of the reference cell with all other cells except the $3^\nu - 1$ adjacent cells is given by

$$3D_2 n^{(1-\epsilon_2/\nu)} \sum_{k=1}^{\infty} \{[(2k+3)^\nu - (2k+1)^\nu]/k^{\nu+\epsilon_2}\}$$

An upper bound on the magnitudes of the short-range interactions between the reference cell and the $3^\nu - 1$ adjacent cells is obtained by arguments completely analogous to those leading to inequality (37) of Ref. 3. We thus find that an upper bound to the magnitude of the short-range interactions between the reference cell and the $3^\nu - 1$ adjacent cells is given by

$$3^{\nu+1}\nu t n^{(\nu-1)/\nu} D_2[5^\nu + (\nu 2^\nu/\epsilon_2)] + 3^{\nu+1} D_2(n^2/t^{\nu+\epsilon_2})$$

where t is the width of a corridor within a cell, as described in Section 3.2 of Ref. 3. Combining these terms and multiplying by P, we obtain the bound

$$|T_1| \leqslant N[B_1(1/n^{\epsilon_2/\nu}) + B_2(t/n^{1/\nu}) + B_3(n/t^{\nu+\epsilon_2})] \tag{22}$$

where

$$B_1 = 3D_2 \sum_{k=1}^{\infty} \{[(2k+3)^\nu - (2k+1)^\nu]/k^{\nu+\epsilon_2}\} \tag{23a}$$

$$B_2 = 3^{\nu+1}\nu D_2[5^\nu + (\nu 2^\nu/\epsilon_2)] \tag{23b}$$

$$B_3 = 3^{\nu+1} D_2 \tag{23c}$$

An upper bound on $|T_2|$ is easily found by using (17a) and (17b),

$$|T_2| \leqslant \tfrac{1}{2}Pn^2 \sum_{\tau=2}^{\infty} (\Delta w_{x,1\tau} + \Delta w_{y,1\tau} + \Delta w_{z,1\tau}) \tag{24}$$

where

$$\Delta w_{i,\lambda\tau} = w_{i,\lambda\tau} - \tilde{w}_{i,\lambda\tau} \tag{25}$$

for $i = x, y, z$. Similarly, an upper bound on $|T_3|$ is found to be

$$|T_3| \leqslant \tfrac{1}{2}Pn^2(w_{x,11} + w_{y,11} + w_{z,11}) \tag{26}$$

where

$$w_{i,11} = \operatorname*{Max}_{k\in 1;\, l\in 1} w_{i,kl} \tag{27}$$

for $i = x, y, z$.

From Eq. (11) of Ref 3, and (12), we can write the constant-magnetization partition function as

$$Q_m(\mathbf{M}, P\Delta, N, \gamma)$$
$$= \int_\Omega d\mathbf{s}_1' \cdots \int_\Omega d\mathbf{s}_N' [\exp(-\beta T - \beta \mathscr{H}_N^{(s)})] \Theta(\mathbf{M}', \mathbf{M}, P\Delta)$$
$$\geqslant [\exp(-\beta T_{\max})] \int_\Omega d\mathbf{s}_1' \cdots \int_\Omega d\mathbf{s}_N' [\exp(-\beta \mathscr{H}_N^{(s)})] \Theta(\mathbf{M}', \mathbf{M}, P\Delta) \qquad (28)$$

We have used $P\Delta$ as the interval over which M_x', M_y', and M_z' can range. We allow m_x', m_y', and m_z' for each cell to range over an interval Δ. By such a convention, the parameter χ for the total system of N sites is the same as the χ parameter for each cell of n sites, i.e.,

$$\chi_{\text{total system}} = P\Delta/N = \Delta/n = \chi_{\text{single cell}} \qquad (29)$$

A weakened form of inequality (28) is then

$$Q_m(\mathbf{M}, P\Delta, N, \gamma) \geqslant (\exp - \beta T_{\max}) \left[\prod_{\tau=1}^{P} \int_\Omega d\mathbf{s}_1' \cdots \int_\Omega d\mathbf{s}_n' \; \Theta(\mathbf{m}_\tau', \mathbf{m}_\tau, \Delta) \right]$$
$$\times (\exp - \beta \mathscr{H}') \exp - \beta \mathscr{H}'' \qquad (30)$$

where we have restricted the net spin of each cell to a particular set of values $\{\mathbf{m}_\lambda\}$ such that

$$\sum_{\lambda=1}^{P} \mathbf{m}_\lambda = \mathbf{M} \qquad (31a)$$

and

$$nP = N \qquad (31b)$$

Equation (13) has been used to obtain the integrand of (30). Now, $\mathscr{H}''$ can be bounded in terms of $\{\mathbf{m}_\lambda\}$ and Δ. We represent such a bound by $\mathscr{H}''_{\max}(\{\mathbf{m}_\lambda\}, \Delta)$. This bound is determined explicitly in (42) below. Inequality (30) is now written as

$$Q_m(\mathbf{M}, P\Delta, N, \gamma)$$
$$\geqslant (\exp - \beta T_{\max}) \{\exp[-\beta \mathscr{H}''_{\max}(\{\mathbf{m}_\lambda\}, \Delta)]\}$$
$$\times \prod_{\tau=1}^{P} \left[\int_\Omega d\mathbf{s}_1' \cdots \int_\Omega d\mathbf{s}_n' (\exp - \beta \mathscr{H}_\tau') \Theta(\mathbf{m}_\tau', \mathbf{m}_\tau, \Delta) \right]$$
$$= (\exp - \beta T_{\max}) \{\exp[-\beta \mathscr{H}_{\max}(\{\mathbf{m}_\lambda\}, \Delta)]\} \prod_{\tau=1}^{P} Q_m{}^0(\mathbf{m}_\tau, \Delta, n) \qquad (32)$$

where (14) and (15) have been used. The superscript "0" indicates a partition function for a system with *no* long-range interactions, i.e.,

$$\begin{aligned} Q_m{}^0(\mathbf{m}_\tau, \Delta, n) &= \int_\Omega d\mathbf{s}_1{}'\cdots\int_\Omega d\mathbf{s}_n{}' \,(\exp -\beta\mathscr{H}_\tau{}')\,\Theta(\mathbf{m}_\tau{}', \mathbf{m}_\tau, \Delta) \\ &= \exp[-\beta n f_m{}^0(\mathbf{m}_\tau/n, \Delta/n, n)] \end{aligned} \tag{33}$$

Using (6) and (33), inquality (32) can be written as

$$f_m\left(\frac{\mathbf{M}}{N}, \frac{P\Delta}{N}, N, \gamma\right) \leqslant \frac{1}{N} T_{\max} + \frac{1}{N}\mathscr{H}''_{\max}(\{\mathbf{m}_\lambda\}, \Delta) + \frac{1}{P}\sum_{\tau=1}^{P} f_m{}^0\left(\frac{\mathbf{m}_\tau}{n}, \frac{\Delta}{n}, \right)n \tag{34}$$

subject to (31a) and (31b). Since (34) is valid for any set $\{\mathbf{m}_\lambda\}$ satisfying the constraints, it is expedient to choose

$$\mathbf{m}_\lambda = \mathbf{m}_\tau, \qquad \tau, \lambda = 1, 2,..., P \tag{35}$$

Such a choice implies

$$\boldsymbol{\rho} = \mathbf{m}_\lambda/n = \mathbf{M}/N \tag{36}$$

for all λ. Since the free energy density in the constant-magnetization ensemble has the symmetry property given by Eq. (16) of Ref. 3, we can assume all three components of $\boldsymbol{\rho}$ are positive. Inequality (34) can then be written as

$$f_m(\boldsymbol{\rho}, \chi, N, \gamma) \leqslant (1/N)T_{\max} + (1/N)\mathscr{H}''_{\max}(\{n\boldsymbol{\rho}\}, \Delta) + f_m{}^0(\boldsymbol{\rho}, \chi, n) \tag{37}$$

where

$$\chi = P\Delta/N = \Delta/n \tag{38}$$

We now take the limit $P \to \infty$ of (37), to obtain

$$f_m(\boldsymbol{\rho}, \chi, \gamma) \leqslant \lim_{P\to\infty} \frac{1}{N} T_{\max} + \lim_{P\to\infty} \frac{1}{N}\mathscr{H}''_{\max}(\{n\boldsymbol{\rho}\}, \Delta) + f_m{}^0(\boldsymbol{\rho}, \chi, n) \tag{39}$$

We wish to obtain an upper bound on (16) where the $\{\mathbf{m}_\lambda{}'\}$ is evaluated in the region

$$n\rho_i \leqslant m'_{i,\lambda} \leqslant n\rho_i + \Delta \tag{40}$$

for $i = x, y, z$ and for all $\lambda = 1, 2,..., P$. In this region we note that

$$\begin{aligned} w_{x,\lambda\tau} m'_{x,\lambda} m'_{x,\tau} &\geqslant w_{x,\lambda\tau} n^2 \rho_x{}^2 - |w_{x,\lambda\tau}|(2\Delta n\rho_x + \Delta^2) \\ &\geqslant w_{x,\lambda\tau} n^2 \rho_x{}^2 - |w_{x,\lambda\tau}|(2\Delta n + \Delta^2) \end{aligned} \tag{41}$$

and similarly for the y and z terms. We can now write the upper bound for $\mathscr{H}''$,

$$\mathscr{H}'' \leqslant -\tfrac{1}{2}n^2 \sum_{i=x,y,z} \sum_{\lambda\neq\tau}^{P} w_{i,\lambda\tau}\rho_i^2 + \tfrac{1}{2}\Delta(2n+\Delta) \sum_{i=x,y,z} \sum_{\lambda\neq\tau}^{P} |w_{i,\lambda\tau}| \tag{42}$$

Dividing by N, we obtain

$$(1/N)\mathscr{H}'' \leqslant -\tfrac{1}{2}n \sum_{i=x,y,z} \rho_i^2\left[(1/P)\sum_{\lambda\neq\tau}^{P} w_{i,\lambda\tau}\right] + \tfrac{1}{2}\chi n(2+\chi) \sum_{i=x,y,z}\left[(1/P)\sum_{\lambda\neq\tau}^{P} |w_{i,\lambda\tau}|\right] \tag{43}$$

We can now use Lemma 2.14 of Ref. 5 to take the limit $P\to\infty$ of (43),

$$\lim_{P\to\infty} (1/N)\mathscr{H}''_{\max}(\{n\boldsymbol{\rho}\},\Delta) \leqslant -\tfrac{1}{2} \sum_{i=x,y,z} \rho_i^2\left[n\sum_{\lambda=2}^{\infty} w_{i,1\lambda}\right] + \tfrac{1}{2}\chi(2+\chi) \sum_{i=x,y,z}\left[n\sum_{\lambda=2}^{\infty} |w_{i,1\lambda}|\right] \tag{44}$$

Combining (39) and (44), we find

$$f_m(\boldsymbol{\rho},\chi,\gamma) \leqslant f_m^{0}(\boldsymbol{\rho},\chi,n) - \tfrac{1}{2}\sum_{i=x,y,z}\rho_i^2\left[n\sum_{\lambda=2}^{\infty} w_{i,1\lambda}\right] + \lim_{P\to\infty}(1/N)T_{\max} + \tfrac{1}{2}\chi(2+\chi)\sum_{i=x,y,z}\left[n\sum_{\lambda=2}^{\infty}|w_{i,1\lambda}|\right] \tag{45}$$

In Ref. 3 it is proved that $f_m(\boldsymbol{\rho},\chi,\gamma)$ exists and is a convex function of $\boldsymbol{\rho}$. However, at this point we do *not* know if the limit as $\gamma\to 0$ of $f_m(\boldsymbol{\rho},\chi,\gamma)$ exists. We choose a fixed sequence $\{\gamma_k\}$ of positive numbers approaching zero. For such a sequence (45) represents an upper bound on $f_m(\boldsymbol{\rho},\chi,\gamma_k)$, so that we can conclude that the quantity[7] $\lim_k \sup f_m(\boldsymbol{\rho},\chi,\gamma_k)$ is either finite or equal to minus infinity. If $\lim_k \sup f_m(\boldsymbol{\rho},\chi,\gamma_k)$ is finite, i.e.,

$$|\lim_k \sup f_m(\boldsymbol{\rho},\chi,\gamma_k)| < \infty \tag{46}$$

then it is always possible to choose an infinite subsequence of $\{\gamma_k\}$, say $\{\delta_j\}$, approaching zero, such that the sequence $f_m(\boldsymbol{\rho},\chi,\delta_j)$ converges to the limit superior of the sequence $f_m(\boldsymbol{\rho},\chi,\gamma_k)$, i.e.,

$$\lim_{j\to\infty} f_m(\boldsymbol{\rho},\chi,\delta_j) = \lim_k \sup f_m(\boldsymbol{\rho},\chi,\gamma_k) \tag{47}$$

[7] For a discussion of the concepts of limit superior and limit inferior see Ref. 7.

We then use the sequence $\{\delta_j\}$ in (45) to obtain

$$\lim_{j\to\infty} f_m(\boldsymbol{\rho}, \chi, \delta_j) \leqslant f_m{}^0(\boldsymbol{\rho}, \chi, n) - \tfrac{1}{2} \sum_{i=x,y,z} \rho_i{}^2 \lim_{j\to\infty} \left[n \sum_{\lambda=2}^{\infty} w_{i,1\lambda}(\delta_j) \right] + \lim_{\delta\to 0} \lim_{P\to\infty} (1/N) T_{\max} + \tfrac{1}{2}\chi(2+\chi) \sum_{i=x,y,z} \lim_{j\to\infty} \left[n \sum_{\lambda=2}^{\infty} |w_{i,1\lambda}(\delta_j)| \right] \tag{48}$$

But it has been shown in Section 2 of Ref. 5 that

$$\lim_{j\to\infty} \left[n \sum_{\lambda=2}^{\infty} w_{i,1\lambda}(\delta_j) \right] = \alpha_i \tag{49}$$

for $i = x, y, z$, where α_x, α_y, and α_z are defined by (5). We define the quantity $\bar{\alpha}$, which by similar arguments is equal to

$$\bar{\alpha} = \sum_{i=x,y,z} \delta^{\nu} \int d^{\nu}r \, |\phi_i(\delta r)| = \sum_{i=x,y,z} \lim_{\delta\to 0} \left[n \sum_{\lambda=2}^{\infty} |w_{i,1\lambda}(\delta)| \right] \tag{50}$$

Expressions (3) and (4) guarantee that $\bar{\alpha}$ is finite. Combining (48)–(50), we obtain

$$\lim_{j\to\infty} f_m(\boldsymbol{\rho}, \chi, \delta_j) \leqslant f_m{}^0(\boldsymbol{\rho}, \chi, n) - \tfrac{1}{2} \sum_{i=x,y,z} \alpha_i \rho_i{}^2 + \lim_{\delta\to 0} \lim_{P\to\infty} (1/N) T_{\max} + \tfrac{1}{2}\chi(2+\chi)\bar{\alpha} \tag{51}$$

provided $\lim_k \sup f_m(\boldsymbol{\rho}, \chi, \gamma_k)$ is finite. But for this case, since $f_m(\boldsymbol{\rho}, \chi, \delta_j)$ is a convex function and the sequence converges to a limit, the quantity $\lim_{j\to\infty} f_m(\boldsymbol{\rho}, \chi, \delta_j)$ must also be convex. We can then improve the bound, (51), as

$$\lim_{j\to\infty} f_m(\boldsymbol{\rho}, \chi, \delta_j) \leqslant \text{C.E.}\left\{ f_m{}^0(\boldsymbol{\rho}, \chi, n) - \tfrac{1}{2} \sum_{i=x,y,z} \alpha_i \rho_i{}^2 + \lim_{\delta\to 0} \lim_{P\to\infty} (1/N) T_{\max} + \tfrac{1}{2}\chi(2+\chi)\bar{\alpha} \right\} \tag{52}$$

The object C.E. is the convex envelope with respect to $\boldsymbol{\rho}$, where C.E.$\{f(\boldsymbol{\rho})\}$ means, for any function $f(\boldsymbol{\rho})$, the maximal convex function not exceeding $f(\boldsymbol{\rho})$. Now using (47) and the fact that the last two terms in the brackets in (52) are independent of $\boldsymbol{\rho}$, we obtain

$$\lim_k \sup f_m(\boldsymbol{\rho}, \chi, \gamma_k) \leqslant \text{C.E.}\left\{ f_m{}^0(\boldsymbol{\rho}, \chi, n) - \tfrac{1}{2} \sum_{i=x,y,z} \alpha_i \rho_i{}^2 \right\} + \lim_{\delta\to 0} \lim_{P\to\infty} (1/N) T_{\max} + \tfrac{1}{2}\chi(2+\chi)\bar{\alpha} \tag{53}$$

provided $\lim_k \sup f_m(\boldsymbol{\rho}, \chi, \gamma_k)$ is finite. The other possibility for $\lim_k \sup f_m(\boldsymbol{\rho}, \chi, \gamma_k)$ is

$$\lim_k \sup f_m(\boldsymbol{\rho}, \chi, \gamma_k) = -\infty \tag{54}$$

However, since (53) is valid for this case as well, we conclude that (53) is valid in general.

We now take the limit as $n \to \infty$. We have already shown (Section 3.7 of Ref. 3) that the thermodynamic limit of $f_m{}^0(\boldsymbol{\rho}, \chi, n)$ converges uniformly, so that by Lemma 4.23 of Ref. 5 we can interchange the objects $\lim_{n\to\infty}$ and C.E. in the limit as $n \to \infty$ of (53). Further, we can define a sequence, similar to that used in Section 3.3 of Ref. 3, such that as $k \to \infty$

$$n_k \to \infty, \qquad t_k \to \infty \tag{55a}$$

but

$$\frac{t_k}{n_k^{1/\nu}} \to 0 \qquad \text{and} \qquad \frac{n_k}{t_k^{\nu+\epsilon_2}} \to 0 \tag{55b}$$

By (22)–(27) we then find that

$$\lim_{n\to\infty} \lim_{\delta\to 0} \lim_{P\to\infty} (1/N)T_{\max} = 0 \tag{56}$$

The limit $n \to \infty$ of (53) then yields

$$\lim_k \sup f_m(\boldsymbol{\rho}, \chi, \gamma_k) \leqslant \text{C.E.}\left\{ f_m{}^0(\boldsymbol{\rho}, \chi) - \tfrac{1}{2} \sum_{i=x,y,z} \alpha_i \rho_i{}^2 \right\} + \tfrac{1}{2}\chi(2 + \chi)\bar{\alpha} \tag{57}$$

We have one last limit to take, the limit $\chi \to 0$. We choose a fixed sequence $\{\chi_l\}$ of positive numbers, approaching zero. At this point we do not know if the limit as $l \to \infty$ of $\lim_k \sup f_m(\boldsymbol{\rho}, \chi_l, \gamma_k)$ exists. However, (57) represents an upper bound to the sequence $\lim_k \sup f_m(\boldsymbol{\rho}, \chi_l, \gamma_k)$. Therefore we conclude that either $\lim_l \sup \lim_k \sup f_m(\boldsymbol{\rho}, \chi_l, \gamma_k)$ is finite or equal to minus infinity. Let us suppose it is finite, i.e.,

$$|\lim_l \sup \lim_k \sup f_m(\boldsymbol{\rho}, \chi_l, \gamma_k)| < \infty \tag{58}$$

For this case it is always possible to choose an infinite subsequence of $\{\chi_l\}$, call it $\{\eta_j\}$, such that the sequence $\lim_k \sup f_m(\boldsymbol{\rho}, \eta_j, \gamma_k)$ converges to the limit superior,

$$\lim_{j\to\infty} \lim_k \sup f_m(\boldsymbol{\rho}, \eta_j, \gamma_k) = \lim_l \sup \lim_k \sup f_m(\boldsymbol{\rho}, \chi_l, \gamma_k) \tag{59}$$

Using the sequence $\{\eta_j\}$ in (57), we find

$$\lim_{j\to\infty} \lim_k \sup f_m(\boldsymbol{\rho}, \eta_j, \gamma_k) \leqslant \lim_{j\to\infty} \text{C.E.}\left\{ f_m{}^0(\boldsymbol{\rho}, \eta_j) - \tfrac{1}{2} \sum_{i=x,y,z} \alpha_i \rho_i{}^2 \right\} \tag{60}$$

where we have used

$$\lim_{\eta\to 0} \tfrac{1}{2}\eta(2+\eta)\bar{\alpha} = 0 \tag{61}$$

But we have already shown in Section 3.11 of Ref. 3 that $f_m{}^0(\boldsymbol{\rho}, \eta_j)$ converges uniformly to $f_m{}^0(\boldsymbol{\rho})$. We can therefore use Lemma 4.23 of Ref. 5 to interchange the objects $\lim_{j\to\infty}$ and C.E. in (60), to obtain

$$\lim_{j\to\infty} \lim_k \sup f_m(\boldsymbol{\rho}, \eta_j, \gamma_k) \leqslant \text{C.E.}\left\{ f_m{}^0(\boldsymbol{\rho}) - \tfrac{1}{2} \sum_{i=x,y,z} \alpha_i \rho_i{}^2 \right\} \tag{62}$$

But by (59) this is just

$$\lim_l \sup \lim_k \sup f(\boldsymbol{\rho}, \chi_l, \gamma_k) \leqslant \text{C.E.}\left\{ f_m{}^0(\boldsymbol{\rho}) - \tfrac{1}{2} \sum_{i=x,y,z} \alpha_i \rho_i{}^2 \right\} \tag{63}$$

provided (58) holds. If (58) does not hold, then

$$\lim_l \sup \lim_k \sup f_m(\boldsymbol{\rho}, \chi_l, \gamma_k) = -\infty \tag{64}$$

and (63) obviously holds. We therefore conclude that (63) is valid in general.

4. LOWER BOUND ON THE FREE ENERGY

We start by dividing the lattice into P cells as discussed in Section 3. We also divide the spin–spin portion of the Hamiltonian into a sum of two terms, as in (12). By arguments similar to those leading to (28), we can bound the constant-magnetization partition function from above by

$$\begin{aligned} &Q_m(\mathbf{M}, P\Delta, N, \gamma) \\ &\quad\leqslant (\exp \beta T_{\max}) \int_\Omega d\mathbf{s}_1' \cdots \int_\Omega d\mathbf{s}_N' \,(\exp -\beta \mathscr{H}_N^{(s)})\, \Theta(\mathbf{M}', \mathbf{M}, P\Delta) \end{aligned} \tag{65}$$

In terms of the net spin of each cell, we only weaken inequality (65) by enlarging the domain of integration. Therefore

$$\begin{aligned} &Q_m(\mathbf{M}, P\Delta, N, \gamma) \\ &\quad\leqslant (\exp \beta T_{\max}) \sum_{\{\mathbf{m}_\tau\}}{}' \prod_{\lambda=1}^{P} \left[\int_\Omega d\mathbf{s}_1' \cdots \int_\Omega d\mathbf{s}_n' \; \Theta(\mathbf{m}_\lambda', \mathbf{m}_\lambda, \Delta) \right] \exp -\beta \mathscr{H}_N^{(s)} \end{aligned} \tag{66}$$

where the summation is over $m_{i,\tau} = k\Delta$, $k = 0, \pm 1, \pm 2, \ldots$, for $i = x, y, z$. The prime on the summation indicates the constraint $M_i - P\Delta \leqslant \sum m_{i,\tau} \leqslant M_i + P\Delta$. We examine the domains of the spin space indicated in (65) and (66) to verify that we have indeed enlarged the domain of integration. Let D denote the domain in spin space consistent with $M_i \leqslant M_i' \leqslant M_i + P\Delta$, for $i = x, y, z$. Here D is the domain of integration in (65). Let $D'(\{\mathbf{m}_\tau\})$ be the domain of spin space consistent with $m_{i,\tau} \leqslant m'_{i,\tau} \leqslant m_{i,\tau} + \Delta$ for $i = x, y, z$ and $\tau = 1, 2, \ldots, P$. Define $\tilde{D}$ to be

$$\tilde{D} = \bigcup_{\{\mathbf{m}_\tau\}} D'(\{\mathbf{m}_\tau\})$$

subject to the constraint $M_i - P\Delta \leqslant \sum_{\tau=1}^{P} m_{i,\tau} \leqslant M_i + P\Delta$ for $i = x, y, z$. For *all* $\{\mathbf{m}_\tau\}$ not included in this constraint, i.e., for $\sum_{\tau=1}^{P} m_{i,\tau} + P\Delta < M_i$ and $M_i + P\Delta < \sum_{\tau=1}^{P} m_{i,\tau}$ for $i = x, y, z$, the condition $M_i \leqslant M_i' \leqslant M_i + P\Delta$ is nowhere satisfied. This statement follows since $\sum_{\tau=1}^{P} m_{i,\tau} \leqslant M_i' \leqslant \sum_{\tau=1}^{P} m_{i,\tau} + P\Delta$ for $i = x, y, z$. (Note that while $\sum_{\tau=1}^{P} m'_{i,\tau} = m_i'$, it is *not* necessarily true that $\sum_{\tau=1}^{P} m_{i,\tau} = M_i$, for $i = x, y, z$.) We therefore conclude that D is contained in $\tilde{D}$. From its definition $\tilde{D}$ is the domain of integration in spin space indicated in (66). Thus (66) does indeed follow from (65).

Now for each cell there are at most $\{2[(n/\Delta) + 1]\}^3 = (2\chi + 2)^3$ different values of $\mathbf{m}_\tau$. Therefore in the summation in (66) there are at most $(2\chi + 2)^{3P}$ terms. Since each term in the summation is positive, we weaken the inequality (66) by

$$Q_m(\mathbf{M}, P\Delta, N, \gamma) \leqslant (2\chi + 2)^{3P}(\exp \beta T_{\max}) \times \operatorname{Max}'_{\{\mathbf{m}_\tau\}}\left\{\prod_{\lambda=1}^{P}\left[\int_\Omega d\mathbf{s}_1'\cdots\int_\Omega d\mathbf{s}_n'\ \Theta(\mathbf{m}_\lambda', \mathbf{m}_\lambda, \Delta)\right] \exp -\beta\tilde{\mathscr{H}}_N^{(s)}\right\} \tag{67}$$

for $i = x, y, z$ and where $\operatorname{Max}'_{\{\mathbf{m}_\tau\}}$ refers to the maximum of a function with respect to the set $\{\mathbf{m}_\tau\}$ such that the constraint $M_i - P\Delta \leqslant \sum m_{i,\tau} \leqslant M_i + P\Delta$ is satisfied. Decomposing $\tilde{\mathscr{H}}_N^{(s)}$ according to (13), $\mathscr{H}''$ [see (16)] can be bounded in terms of $\{\mathbf{m}_\tau\}$ and Δ. We represent such a bound by $\mathscr{H}''_{\min}(\{\mathbf{m}_\tau\}, \Delta)$. This bound is determined explicitly by (73). Using (13) and (14), inequality (67) can then be written as

$$\begin{aligned} Q_m(\mathbf{M}, P\Delta, N, \gamma) &\leqslant (2\chi + 2)^{3P}(\exp \beta T_{\max}) \operatorname{Max}'_{\{\mathbf{m}_\tau\}}\Big\{(\exp[-\beta\mathscr{H}''_{\min}(\{\mathbf{m}_\tau\}, \Delta)]) \\ &\quad \times \prod_{\lambda=1}^{P}\Big[\int_\Omega d\mathbf{s}_1'\cdots\int_\Omega d\mathbf{s}_n'\,(\exp -\beta\mathscr{H}_\lambda')\ \Theta(\mathbf{m}_\lambda', \mathbf{m}_\lambda, \Delta)\Big]\Big\} \\ &= (2\chi + 2)^{3P}\,(\exp \beta T_{\max}) \\ &\quad \times \operatorname{Max}'_{\{\mathbf{m}_\tau\}}\Big\{(\exp[-\beta\mathscr{H}''_{\min}(\{\mathbf{m}_\tau\}, \Delta)]) \prod_{\lambda=1}^{P} Q_m{}^0(\mathbf{m}_\lambda, \Delta, n)\Big\} \end{aligned} \tag{68}$$

for $i = x, y, z$. Using (6), we obtain

$$-\beta N f_m\left(\frac{\mathbf{M}}{N}, \frac{P\Delta}{N}, N, \gamma\right)$$
$$\leqslant 3P \, ln(2\chi + 2) + \beta T_{\max}$$
$$+ \, ln \operatorname*{Max'}_{\{\mathbf{m}_\tau\}}\left\{(\exp[-\beta \mathscr{H}''_{\min}(\{\mathbf{m}_\tau\}, \Delta)]) \prod_{\lambda=1}^{P} \exp\left[-\beta n f_m{}^0\left(\frac{\mathbf{m}_\lambda}{n}, \frac{\Delta}{n}, n\right)\right]\right\} \tag{69}$$

But since the logarithm is a monotonically increasing function, we can write (69) as

$$f_m\left(\frac{\mathbf{M}}{N}, \frac{P\Delta}{N}, N, \gamma\right)$$
$$\geqslant -3\beta^{-1}\frac{1}{n} ln(2\chi + 2) - \frac{1}{N} T_{\max}$$
$$+ \operatorname*{Min'}_{\{\mathbf{m}_\tau\}}\left\{\frac{1}{N}\mathscr{H}''_{\min}(\{\mathbf{m}_\tau\}, \Delta) + \frac{1}{P}\sum_{\lambda=1}^{P} f_m{}^0\left(\frac{\mathbf{m}_\lambda}{n}, \frac{\Delta}{n}, n\right)\right\} \tag{70}$$

for $i = x, y, z$.

We now examine the term $(1/N)\mathscr{H}''_{\min}(\{\mathbf{m}_\tau\}, \Delta)$; i.e., we seek a lower bound on (16), where $\{\mathbf{m}_\lambda'\}$ is such that

$$m_{i,\lambda} \leqslant m'_{i,\lambda} \leqslant m_{i\lambda,} + \Delta \tag{71}$$

for $i = x, y, z$. In this region we note that

$$w_{x,\lambda\tau} m_{x}{}'_{,\lambda} m_{x}{}'_{,\tau} \leqslant w_{x,\lambda\tau} m_{x,\lambda} m_{x,\tau} + |w_{x,\lambda\tau}|[2\Delta n + \Delta^2] \tag{72}$$

and similarly for the y and z terms. We can now write the lower bound for $\mathscr{H}''$,

$$\mathscr{H}'' \geqslant -\tfrac{1}{2}\sum_{j=x,y,z}\sum_{\lambda\neq\tau}^{P} w_{i,\lambda\tau} m_{i,\lambda} m_{i,\tau}$$
$$-\tfrac{1}{2}\sum_{i=x,y,z}\Delta(2n + \Delta)\sum_{\lambda\neq\tau}^{P}|w_{i,\lambda\tau}| \tag{73}$$

Using this in (70), we find

$$f_m\left(\frac{\mathbf{M}}{N}, \frac{P\Delta}{N}, N, \gamma\right) \geqslant -3\beta^{-1}\frac{1}{n} ln(2\chi + 2) - \frac{1}{N} T_{\max}$$
$$-\tfrac{1}{2}\frac{\Delta}{n}(2n + \Delta)\frac{1}{P}\sum_{j=x,y,z}\sum_{\lambda\neq\tau}^{P}|w_{j,\lambda\tau}|$$
$$+ \operatorname*{Min'}_{\{\mathbf{m}_\tau\}}\left\{-\frac{1}{2n}\frac{1}{P}\sum_{j=x,y,z}\sum_{\lambda\neq\tau}^{P} w_{j,\lambda\tau} m_{j,\lambda} m_{j,\tau}\right.$$
$$\left. + \frac{1}{P}\sum_{\lambda=1}^{P} f_m{}^0\left(\frac{\mathbf{m}_\lambda}{n}, \frac{\Delta}{n}, n\right)\right\} \tag{74}$$

for $i = x, y, z$. To obtain (74), we have used the fact that the second term in (73) is independent of the set $\{\mathbf{m}_\tau\}$.

We now restrict the class of long-range interactions by requiring

$$w_{i,\lambda\tau} \geqslant 0 \tag{75}$$

for $i = x, y, z$ and for all λ and τ. Using this restriction and the inequality

$$m_\lambda m_\tau \leqslant \tfrac{1}{2}m_\lambda{}^2 + \tfrac{1}{2}m_\tau{}^2 \tag{76}$$

we find

$$\begin{aligned} -\sum_{\lambda\neq\tau}^{P} w_{x,\lambda\tau} m_{x,\lambda} m_{x,\tau} & \\ \geqslant -\sum_{\lambda\neq\tau}^{P} w_{x,\lambda\tau}(\tfrac{1}{2}m_{x,\lambda}^2 + \tfrac{1}{2}m_{x,\tau}^2) & \\ = -\sum_{\lambda\neq\tau}^{P} w_{x,\lambda\tau} m_{x,\lambda}^2 = -\sum_{\lambda=1}^{P} m_{x,\lambda}^2 \sum_{\tau=1;\lambda\neq\tau}^{P} w_{x,\lambda\tau} & \end{aligned} \tag{77}$$

If we extend the sum on τ to be over an infinite lattice, the inequality (77) is further weakened. Thus

$$-\sum_{\lambda\neq\tau}^{P} w_{x,\lambda\tau} m_{x,\lambda} m_{x,\tau} \geqslant -\sum_{\lambda=1}^{P} m_{x,\lambda}^2 \left[\sum_{\tau=2}^{\infty} w_{x,1\tau}\right] \tag{78}$$

We have used the fact that $\sum_{\lambda=1;\lambda\neq\tau}^{\infty} w_{x,\lambda\tau}$ is independent of λ and can therefore be referred to any reference cell, say number one. Similar expressions hold for y and z interactions, so that (74) becomes

$$\begin{aligned} f_m(\boldsymbol{\rho}, \chi, N, \gamma) \geqslant\ & -3\beta^{-1}(1/n)\, ln(2\chi + 2) - (1/N)T_{\max} \\ & - \tfrac{1}{2}\chi n(2 + \chi) \sum_{j=x,y,z} \sum_{\tau=2}^{\infty} |w_{j,1\tau}| \\ & + \operatorname*{Min'}_{\{\boldsymbol{\rho}_\tau\}}\left\{(1/P)\sum_{\lambda=1}^{P}\left[f_m{}^0(\boldsymbol{\rho}_\lambda, \chi, n)\right.\right. \\ & \left.\left. - \tfrac{1}{2}\sum_{j=x,y,z} \rho_{j,\lambda}^2\left(n\sum_{\tau=2}^{\infty} w_{j,1\tau}\right]\right)\right\} \end{aligned} \tag{79}$$

for $i = x, y, z$, where

$$\boldsymbol{\rho} = \mathbf{M}/N \tag{80a}$$

$$\boldsymbol{\rho}_\lambda = \mathbf{m}_\lambda/n \tag{80b}$$

and

$$\chi = \Delta/n = P\Delta/N \tag{80c}$$

We have extended the summation on τ to an infinite lattice to obtain the third term on the right-hand side of (79).

We now examine the bracketed term in (79). Since the convex envelope of a function is always less than or equal to the function itself, we find

$$(1/P) \sum_{\lambda=1}^{P} \left[f_m{}^0(\boldsymbol{\rho}_\lambda, \chi, n) - \tfrac{1}{2} \sum_{j=x,y,z} \rho_{j,\lambda}^2 \left(n \sum_{\tau=2}^{\infty} w_{j,1\tau} \right) \right]$$
$$\geqslant (1/P) \sum_{\lambda=1}^{P} \text{C.E.} \left[f_m{}^0(\boldsymbol{\rho}_\lambda, \chi, n) - \tfrac{1}{2} \sum_{j=x,y,z} \rho_{j,\lambda}^2 \left(n \sum_{\tau=2}^{\infty} w_{j,1\tau} \right) \right] \qquad (81)$$

But by definition the function C.E., $f(\boldsymbol{\rho})$ is a convex function. Therefore

$$(1/P) \sum_{\lambda=1}^{P} \text{C.E.} \left[f_m{}^0(\boldsymbol{\rho}_\lambda, \chi, n) - \tfrac{1}{2} \sum_{j=x,y,z} \rho_{j,\lambda}^2 \left(n \sum_{\tau=2}^{\infty} w_{j,1\tau} \right) \right]$$
$$\geqslant \text{C.E.} \left[f_m{}^0(\tilde{\boldsymbol{\rho}}, \chi, n) - \tfrac{1}{2} \sum_{j=x,y,z} \tilde{\rho}_j{}^2 \left(n \sum_{\tau=2}^{\infty} w_{j,1\tau} \right) \right] \qquad (82)$$

where

$$\tilde{\rho}_j = (1/P) \sum_{\lambda=1}^{P} \rho_{j,\lambda} \qquad (83a)$$

for $j = x, y, z$. The constraint listed below (67) then reduces to

$$\rho_j - \chi \leqslant \tilde{\rho}_j \leqslant \rho_j + \chi \qquad (83b)$$

Inequality (79) can now be written as

$$f_m(\boldsymbol{\rho}, \chi, N, \gamma)$$
$$\geqslant -3\beta^{-1}(1/n) \ln(2\chi + 2) - (1/N) T_{\max}$$
$$- \tfrac{1}{2}\chi n(2 + \chi) \sum_{j=x,y,z} \sum_{\tau=2}^{\infty} |w_{j,1\tau}|$$
$$+ \text{Min}' \, \text{C.E.} \left[f_m{}^0(\tilde{\boldsymbol{\rho}}, \chi, n) - \tfrac{1}{2} \sum_{j=x,y,z} \tilde{\rho}_j{}^2 \left(n \sum_{\tau=2}^{\infty} w_{j,1\tau} \right) \right] \qquad (84)$$

for $i = x, y, z$, where the minimum is taken subject to the constraint (83b).

According to Section 3.7 of Ref. 3, $f_m{}^0(\boldsymbol{\rho}, \chi, n)$ converges uniformly to $f_m{}^0(\boldsymbol{\rho}, \chi)$. Defining $\epsilon(\boldsymbol{\rho}, \chi, n)$ by

$$f_m{}^0(\boldsymbol{\rho}, \chi, n) = f_m{}^0(\boldsymbol{\rho}, \chi) + \epsilon(\boldsymbol{\rho}, \chi, n) \qquad (85a)$$

we are guaranteed that there exists an $\epsilon(n, \chi)$,

$$\epsilon(n, \chi) = \operatorname*{Max}_{\boldsymbol{\rho}} |\epsilon(\boldsymbol{\rho}, \chi, n)| \qquad (85b)$$

such that

$$\lim_{n \to 0} \epsilon(n, \chi) = 0 \qquad (85c)$$

Also, by Section 3.11 of Ref. 3, $f_m{}^0(\boldsymbol{\rho}, \chi)$ converges uniformly to $f_m{}^0(\boldsymbol{\rho})$, and therefore there exists $\delta(\boldsymbol{\rho}, \chi)$ and $\delta(\chi)$ defined by

$$f_m{}^0(\boldsymbol{\rho}, \chi) = f_m{}^0(\boldsymbol{\rho}) + \delta(\boldsymbol{\rho}, \chi) \tag{86a}$$

and

$$\delta(\chi) = \operatorname*{Max}_{\boldsymbol{\rho}} |\delta(\boldsymbol{\rho}, \chi)| \tag{86b}$$

such that

$$\lim_{\chi \to 0} \delta(\chi) = 0 \tag{86c}$$

Since $\epsilon(n, \chi)$ and $\delta(\chi)$ are independent of $\tilde{\boldsymbol{\rho}}$, (84) can be written as

$$\begin{aligned} f_m(\boldsymbol{\rho}, \chi, N, \gamma) \geqslant\ & -3\beta^{-1}(1/n)\, ln(2\chi + 2) - (1/N)T_{\max} - \epsilon(n, \chi) - \delta(\chi) \\ & - \tfrac{1}{2}\chi n(2 + \chi) \sum_{j=x,y,z} \sum_{\tau=2}^{\infty} |w_{j,1\tau}| \\ & + \text{Min}'\ \text{C.E.}\Big[f_m{}^0(\tilde{\boldsymbol{\rho}}) - \tfrac{1}{2} \sum_{j=x,y,z} \tilde{\rho}_j{}^2\Big(n \sum_{\tau=2}^{\infty} w_{j,1\tau}\Big)\Big] \end{aligned} \tag{87}$$

for $i = x, y, z$. Now, by Eq. (16) of Ref. 3, the last term on the right-hand side of (87) has an argument which is completely symmetric with respect to the transformations $\rho_j \to -\rho_j$ for $j = x, y, z$. Therefore the convex envelope of this argument must have the same symmetry property. By the same arguments used in Section 3.8 and Appendix C of Ref. 3, the minimum of the last term in (87) occurs at the value of $\boldsymbol{\rho}$ closest to the origin. For $\boldsymbol{\rho}$ with all positive components, the minimum occurs at $\tilde{\rho}_i = \rho_i - \chi$ for $i = x, y, z$. Using this result and taking the limit of (87) as $P \to \infty$, we obtain

$$\begin{aligned} f_m(\boldsymbol{\rho}, \chi, \gamma) \geqslant\ & -3\beta^{-1}(1/n)\, ln(2\chi + 2) - \lim_{P \to \infty} (1/N)T_{\max} - \epsilon(n, \chi) - \delta(\chi) \\ & - \tfrac{1}{2}\chi(2 + \chi) \sum_{j=x,y,z} \Big[n \sum_{\tau=2}^{\infty} |w_{j,1\tau}|\Big] \\ & + \Big\{\text{C.E.}\Big[f_m{}^0(\tilde{\boldsymbol{\rho}}) - \tfrac{1}{2} \sum_{j=x,y,z} \tilde{\rho}_j{}^2\Big(n \sum_{\tau=2}^{\infty} w_{j,1\tau}\Big)\Big]\Big\}_{\tilde{\rho}_i = \rho_i - \chi} \end{aligned} \tag{88}$$

for $i = x, y, z$.

We now take the limit as $\gamma \to 0$. But there is no guarantee that the quantity $\lim_{\gamma \to 0} f_m(\boldsymbol{\rho}, \chi, \gamma)$ exists. Choose a fixed sequence $\{\gamma_k\}$ of positive numbers approaching zero. Since (88) represents a lower bound and (63) an upper bound to the sequence $f_m(\boldsymbol{\rho}, \chi, \gamma_k)$, we conclude that the quantity

$$\lim_k \inf f_m(\boldsymbol{\rho}, \chi, \gamma_k)$$

is finite. Then we can always choose an infinite subsequence of $\{\gamma_k\}$, call it $\{\delta_j\}$, for which $f_m(\boldsymbol{\rho}, \chi, \delta_j)$ converges to the limit inferior, i.e.,

$$\lim_{j\to\infty} f_m(\boldsymbol{\rho}, \chi, \delta_j) = \lim_k \inf f_m(\boldsymbol{\rho}, \chi, \gamma_k) \tag{89}$$

Choosing the sequence $\{\delta_j\}$, [not necessarily the same sequence used in Section 3] we find, following an analysis similar to that leading to (53),

$$\begin{aligned} &\lim_k \inf f_m(\boldsymbol{\rho}, \chi, \gamma_k) \\ &\quad \geqslant -3\beta^{-1}(1/n)\, ln(2\chi + 2) - \lim_{\delta\to 0}\lim_{P\to\infty}(1/N)T_{\max} - \epsilon(n, \chi) \\ &\quad\quad - \delta(\chi) - \tfrac{1}{2}\chi(2+\chi)\bar{\alpha} + \left\{\mathrm{C.E.}\left[f_m{}^0(\tilde{\boldsymbol{\rho}}) - \tfrac{1}{2}\sum_{j=x,y,z}\alpha_j\tilde{\rho}_j{}^2\right]\right\}_{\tilde{\rho}_i=\rho_i-\chi} \end{aligned} \tag{90}$$

for $i = x, y, z$. Now taking the limit $n \to \infty$ as described in (55), and using (85), we obtain

$$\begin{aligned} &\lim_k \inf f_m(\boldsymbol{\rho}, \chi, \gamma_k) \\ &\quad \geqslant -\delta(\chi) - \tfrac{1}{2}\chi(2+\chi)\bar{\alpha} + \left\{\mathrm{C.E.}\left[f_m{}^0(\boldsymbol{\rho}) - \tfrac{1}{2}\sum_{j=x,y,z}\alpha_j\tilde{\rho}_i{}^2\right]\right\}_{\tilde{\rho}_i=\rho_i-\chi} \end{aligned} \tag{91}$$

for $i = x, y, z$.

Finally, we take the limit $\chi \to 0$. Let $\{\chi_l\}$ be a fixed sequence of positive numbers, approaching zero. Since each term in the sequence

$$\lim_k \inf f_m(\boldsymbol{\rho}, \chi_l, \gamma_k)$$

is bounded above and below by (63) and (91), respectively, we know that the quantity

$$\lim_l \inf \lim_k \inf f_m(\boldsymbol{\rho}, \chi_l, \gamma_k)$$

is finite. We can then always choose an infinite subsequence of $\{\chi_l\}$, call it $\{\eta_i\}$ (not necessarily the same subsequence used in Section 3), such that $\lim_k \inf f_m(\boldsymbol{\rho}, \eta_i, \gamma_k)$ converges to the limit inferior, i.e.,

$$\lim_{i\to\infty}\lim_k \inf f_m(\boldsymbol{\rho}, \eta_i, \gamma_k) = \lim_l \inf \lim_k \inf f_m(\boldsymbol{\rho}, \chi_l, \gamma_k) \tag{92}$$

We can carry out an analysis similar to that leading to (63) to obtain

$$\lim_l \inf \lim_k \inf f_m(\boldsymbol{\rho}, \chi_l, \gamma_k) \geqslant \mathrm{C.E.}\left[f_m{}^0(\boldsymbol{\rho}) - \tfrac{1}{2}\sum_{j=x,y,z}\alpha_j\rho_j{}^2\right] \tag{93}$$

The inequalities (63) and (93) together imply the existence of the quantity

$$\lim_{\chi\to 0}\lim_{\gamma\to 0} f_m(\boldsymbol{\rho}, \chi, \gamma) = f_m(\boldsymbol{\rho}) \tag{94}$$

and that

$$f_m(\rho) = \text{C.E.}\left\{f^0(\rho) - \tfrac{1}{2} \sum_{j=x,y,z} \alpha_i \rho_i^2\right\} \tag{95}$$

The lower bound, (93), has only been carried out for the case of all long-range coupling constants being purely ferromagnetic, according to (75). Presumably, this bound can be proved for a more general class of coupling constants by a method similar to that carried out for a classical fluid in Section 5 of reference 5.

5. CONVEX ENVELOPE CONSTRUCTION FOR SYSTEMS WITH ZERO SHORT-RANGE INTERACTIONS

5.1. The Free Energy Density

The free energy density $f_m{}^0(\rho)$ with zero long-range Kac interactions can be determined indirectly by evaluating the Helmholtz free energy density $f_c{}^0(\mathbf{H}^0)$ using the canonical ensemble and employing Eq. (106) of Ref. 3, i.e.,

$$f_m{}^0(\rho) = \mu\mathbf{H}^0\cdot\rho + f_c{}^0(\mathbf{H}^0) \tag{96}$$

where $\rho(\mathbf{H}^0)$ is given by

$$\rho_i = -\mu^{-1}\, \partial f_c{}^0(H_x{}^0, H_y{}^0, H_z{}^0)/\partial H_i{}^0 \tag{97}$$

for $i = x, y, z$. Here $\mathbf{H}^0$ is a fictitious magnetic field associated with a system with zero long-range Kac interactions. For the case of zero short-range interactions

$$\begin{aligned} Q_c{}^0(\mathbf{H}^0) &= \left[\int_\Omega d\mathbf{s}\, \exp(\beta\mu\mathbf{H}^0\cdot\mathbf{s})\right]^N \\ &= \left[\int_0^{2\pi} d\phi \int_0^\pi d\theta\, (\sin\theta) \exp(\beta\mu H^0 \cos\theta)\right]^N \\ &= [(4\pi/\beta\mu H^0)\sinh(\beta\mu H^0)]^N \end{aligned} \tag{98}$$

or

$$f_c{}^0(\mathbf{H}^0) = \beta^{-1}\, ln(\beta\mu H^0/4\pi) - \beta^{-1}\ln[\sinh(\beta\mu H^0)] \tag{99a}$$

where

$$H^0 = [H_x^{02} + H_y^{02} + H_z^{02}]^{1/2} \tag{99b}$$

Using (96) and (97), we obtain

$$f_m{}^0(\rho) = \mu\mathbf{H}^0\cdot\rho + \beta^{-1}\ln(\beta\mu H^0/4\pi) - \beta^{-1}\ln[\sinh(\beta\mu H^0)] \tag{100}$$

where from Eq. (7) of Ref. 3

$$\rho(\mathbf{H}^0) = [\coth(\beta\mu H^0) - (1/\beta\mu H^0)]\mathbf{H}^0/H^0 \tag{101}$$

Combining (95), (100), and (101), we find

$$f_m(\boldsymbol{\rho}) = \text{C.E.}\left\{f_m{}^0(\boldsymbol{\rho}) - \tfrac{1}{2} \sum_{i=x,y,z} \alpha_i \rho_i{}^2\right\} \tag{102}$$

where

$$\boldsymbol{\rho}(\mathbf{H}^0) = L(\beta\mu H^0)\mathbf{H}^0/H^0 \tag{103}$$

The term $L(t)$ is the Langevin function,

$$L(t) = \coth t - (1/t) \tag{104}$$

Taking the scalar product of (103) with itself, we find

$$\rho = |\boldsymbol{\rho}| = L(\beta\mu H^0) \tag{105}$$

In determining the convex envelope construction, it is convenient to introduce a function equal to the bracket term in (102),

$$f_m{}^*(\boldsymbol{\rho}) = f_m{}^0(\boldsymbol{\rho}) - \tfrac{1}{2} \sum_{i=x,y,z} \alpha_i \rho_i{}^2 \tag{106}$$

$f_m{}^*(\boldsymbol{\rho})$ so defined is equal to $f_m(\boldsymbol{\rho})$ *except* in those regions where the convex envelope construction is employed. In examining the free energy density, the following properties of the Langevin function are helpful:

$$L(0) = 0 \tag{107a}$$

$$L'(0) = \tfrac{1}{3} \tag{107b}$$

$$L'(t) \leqslant (1/t)L(t) \tag{107c}$$

5.2. The Convex Envelope Construction

We consider the case of general anisotropy, for which α_x, α_y, and α_z are in general not equal. Suppose α_z is the largest of α_x, α_y, α_z, i.e.,

$$\alpha_z \geqslant \alpha_x, \alpha_y; \qquad \alpha_x, \alpha_y, \alpha_z \geqslant 0 \tag{108}$$

We first show the property:

(i) If $\alpha_z\beta \leqslant 3$, then $f_m{}^*(\boldsymbol{\rho})$ is a convex function of $\boldsymbol{\rho}$.

To verify property (i), it is sufficient[8] to show that

$$g(t) = f_m{}^*(\rho_x{}' + \rho_x''t, \rho_y{}' + \rho_y''t, \rho_z{}' + \rho_z''t) \tag{109}$$

[8] A function of several variables $f(\mathbf{r})$ is said to be convex in $\mathbf{r}$ if the inequality $f(\alpha\mathbf{r}_1 + \beta\mathbf{r}_2) \leqslant \alpha f(\mathbf{r}_1) + \beta f(\mathbf{r}_2)$ is satisfied everywhere for $\alpha, \beta \geqslant 0$ and $\alpha + \beta = 1$. An equivalent definition of convexity is that the function $g(t)$, defined by $g(t) = f(\mathbf{r}_1{}' + t\mathbf{r}_2{}')$, be a convex function of t for *all* $\mathbf{r}_1{}'$ and $\mathbf{r}_2{}'$. To verify that these definitions are equivalent, choose $\mathbf{r}_1 = \mathbf{r}_1{}' + t_1\mathbf{r}_2{}'$ and $\mathbf{r}_2 = \mathbf{r}_1{}' + t_2\mathbf{r}_2{}'$. See, for example, Ref. 8.

is a convex function of t for any p_i' and ρ_i'', $i = x, y, z$. From (105), (106), and (109), it follows that

$$\frac{d^2g(t)}{dt^2} = \left(\frac{\mu H^0}{\rho} - \alpha_z\right)\rho''^2 + (\alpha_z - \alpha_x)\rho_x''^2 + (\alpha_z - \alpha_y)\rho_y''^2 + \mu\left(\frac{\partial H^0}{\partial\rho} - \frac{H^0}{\rho}\right) \times \left[\frac{\rho_x''(\rho_x' + \rho_x''t) + \rho_y''(\rho_y' + \rho_y''t) + \rho_z''(\rho_z' + \rho_z''t)}{\rho}\right]^2 \quad (110a)$$

where

$$\rho'' = (\rho_x''^2 + \rho_y''^2 + \rho_z''^2)^{1/2} \quad (110b)$$

and

$$\rho = [(\rho_x' + \rho_x''t)^2 + (\rho_y' + \rho_y''t)^2 + (\rho_z' + \rho_z''t)^2]^{1/2} \quad (110c)$$

From (105) and (107c) we observe that $[(\partial H^0/\partial\rho) - (H^0/\rho)]$ is nonnegative. The terms $(\alpha_z - \alpha_x)$ and $(\alpha_z - \alpha_y)$ were chosen to be positive. By (105), (107b), and (107c), $[(\mu H^0/\rho) - \alpha_z]$ is nonnegative, provided $\alpha_z\beta \leqslant 3$. We thus conclude that for $\alpha_z\beta \leqslant 3$ each coefficient in (110a) is nonnegative. Therefore $g(t)$ is a convex function[9] of t. This in turn implies that for $\alpha_z\beta \leqslant 3$, $f_m^*(\boldsymbol{\rho})$ is a convex function in $\boldsymbol{\rho}$. We have thus proved property (i).

We examine the extrema of $f_m^*(\boldsymbol{\rho})$, for $\alpha_z\beta > 3$, in a plane determined by $\rho_x, \rho_y = \text{const}$. To determine the extrema of $f_m^*(\rho_x = \text{const}, \rho_y = \text{const}, \rho_z)$, we set $\partial f_m^*(\rho_x, \rho_y, \rho_z)/\partial\rho_z = 0$. This condition is always satisfied for $\rho_z = 0$ and sometimes satisfied for $|\rho_z| > 0$. We define $\tilde{\rho}(\rho_x, \rho_y)$ as the maximal solution of

$$0 \leqslant \tilde{\rho} = L(\beta\alpha_z\tilde{\rho}) \quad (111a)$$

Correspondingly, we define $\tilde{\rho}_z$ by

$$\tilde{\rho}_z = (\tilde{\rho}^2 - \rho_x^2 - \rho_y^2)^{1/2} \quad (111b)$$

From (105) and (107) we find the properties

(iia) If $\alpha_z\beta > 3$ and $(\rho_x^2 + \rho_y^2)^{1/2} \geqslant \tilde{\rho}$, then $f_m^*(\rho_x = \text{const}, \rho_y = \text{const}, \rho_z)$ has one extremum, at $\rho_z = 0$. Also $\partial^2 f_m^*(\rho_x, \rho_y, \rho_z)/\partial\rho_z^2 \geqslant 0$. The minimum at $\rho_z = 0$ is an absolute minimum.

(iib) If $\alpha_z\beta > 3$ and $(\rho_x^2 + \rho_y^2)^{1/2} < \tilde{\rho}$, then $f_m^*(\rho_x = \text{const}, \rho_y = \text{const}, \rho_z)$ has three extrema. The extremum at $\rho_z = 0$ is a relative maximum. The other extrema are at $\rho_z = \pm\tilde{\rho}_z$, defined by (111). Also

[9] This follows from the theorem: Suppose $f(t)$ and $df(t)/dt$ are continuous. Then $f(t)$ is convex in t if $df(t)/dt$ is a nondecreasing function of t. See Ref. 8.

$\partial^2 f_m^*(\rho_x, \rho_y, \rho_z)/\partial \rho_z^2 \geqslant 0$ for $|\rho_z| \geqslant \tilde{\rho}_z$. The minima at $\rho_z = \pm\tilde{\rho}_z$ are absolute minima and $f_m^*(\rho_x, \rho_y, \tilde{\rho}_z) = f_m^*(\rho_x, \rho_y, -\tilde{\rho}_z)$.

From (i) and (ii) we conclude:

(1) If $\alpha_z\beta \leqslant 3$, then $f_m^*(\rho_x, \rho_y, \rho_z)$ is convex in $\boldsymbol{\rho}$ and is therefore equal to $f_m(\boldsymbol{\rho})$.

(2) If $\alpha_z\beta > 3$, then for fixed ρ_x and ρ_y, $f_m^*(\rho_x, \rho_y, \rho_z)$ is *not* everywhere convex[10] in ρ_z.

We now surmise the construction for $\alpha_z\beta > 3$ and then verify that it is indeed the correct construction.

From property (ii) it is concluded that if we look in any plane determined by ρ_x and ρ_y being constant, the maximal function which is convex in ρ_z is the constant $f_m^*(\rho_x, \rho_y, \tilde{\rho}_z)$ for $\rho < \tilde{\rho}$. This suggests the construction:

(2′) If $\alpha_z\beta > 3$, then $f_m(\rho_x, \rho_y, \rho_z) = f_m^*(\rho_x, \rho_y, \tilde{\rho}_z)$ provided $\rho < \tilde{\rho}$. If $\rho \geqslant \tilde{\rho}$, then $f_m(\rho_x, \rho_y, \rho_z) = f_m^*(\rho_x, \rho_y, \rho_z)$.

To verify that (2′) is the correct construction, we show that $f_m(\boldsymbol{\rho})$ so defined is a convex function of $\boldsymbol{\rho}$.

From (106) and (111) we find that for $\boldsymbol{\rho}$ interior to the construction region defined above

$$f_m(\boldsymbol{\rho}) = f_m{}^0(\tilde{\rho}) - \tfrac{1}{2}\alpha_z\tilde{\rho}^2 - \tfrac{1}{2}(\alpha_x - \alpha_z)\rho_x{}^2 - \tfrac{1}{2}(\alpha_y - \alpha_z)\rho_y{}^2 \tag{112}$$

for $0 \leqslant \rho < \tilde{\rho}$ and $\alpha_z\beta > 3$. To verify that $f_m(\rho_x, \rho_y, \rho_z)$ is everywhere convex, we show that

$$g(t) = f_m(\rho_x{}' + \rho_x''t, \rho_y{}' + \rho_y''t + \rho_z{}' + \rho_z''t) \tag{113}$$

is a convex function of t for *any* $\rho_i{}'$, ρ_i'' $(i = x, y, z)$. From (105), (106), (112), and (113) we find for $\alpha_z\beta > 3$

$$\begin{aligned} dg(t)/dt \\ &= (\alpha_z - \alpha_x)\rho_x''(\rho_x{}' + \rho_x''t) + (\alpha_z - \alpha_y)\rho_y''(\rho_y{}' + \rho_y''t), \qquad \text{for} \quad \rho < \tilde{\rho} \\ &= (\mu H^0 - \alpha_z\rho)[\rho_x''(\rho_x{}' + \rho_x''t) + \rho_y''(\rho_y{}' + \rho_y''t) + \rho_z''(\rho_z{}' + \rho_z''t)]\rho^{-1} \\ &\quad + (\alpha_z - \alpha_x)\rho_x''(\rho_x{}' + \rho_x''t) + (\alpha_z - \alpha_y)\rho_y''(\rho_y{}' + \rho_y''t), \qquad \text{for} \quad p \geqslant \tilde{\rho} \end{aligned} \tag{114a}$$

where

$$\rho = [(\rho_x{}' + \rho_x''t)^2 + (\rho_y{}' + \rho_y''t)^2 + (\rho_z{}' + \rho_z''t)^2]^{1/2} \tag{114b}$$

We thus observe that at $\rho = \tilde{\rho}$ (which is the condition determining the onset of the construction region) $dg(t)/dt$ is continuous [see (111a)]. From (112) and from (110) and the argument following (110) we note that $d^2g(t)/dt^2$ is everywhere nonnegative. [In (110a), $(\mu H^0/\rho) - \alpha_z$ is nonnegative for

[10] Note that if $f(\mathbf{r})$ is convex in $\mathbf{r} = (x, y, z)$, then $f(x, y, z)$ is also convex in x.

$\alpha_z\beta > 3$ if $p \geqslant \tilde{\rho}$. This follows from (107b) and (105)]. We therefore conclude (see footnote 9) that the function $f_m(\boldsymbol{\rho})$ is indeed a convex function of $\boldsymbol{\rho}$.

This construction was defined such that in any plane determined by ρ_x and ρ_y being fixed, the construction is the maximal convex function of ρ_z. Therefore the construction in all three variables cannot exceed this construction. But we have shown that this construction is convex in $\boldsymbol{\rho}$. We thus conclude that this construction is the desired convex construction and that $f(\boldsymbol{\rho}) = \text{C.E.}\{f_m{}^*(\boldsymbol{\rho})\}$ is determined by construction (2′).

6. EQUATIONS OF STATE

We discuss the equations of state for the general anisotropic Heisenberg model. We have noted that for $\alpha_z\beta > 3$ there is always a region ($\rho < \tilde{\rho}$) over which a convex construction is necessary. Interior to this construction region $f_m(\boldsymbol{\rho})$ has a different functional form than in the region exterior to the construction. It is then reasonable to associate $\tilde{\rho}$ with the onset of a phase transition. The validity of this association is borne out by an examination of the equations of state. While a convex construction is necessary if $\alpha_z\beta > 3$, no such construction need be employed if $\alpha_z\beta \leqslant 3$. The critical temperature is then defined by

$$\alpha_z\beta^c = 3 \tag{115}$$

An expression for $\tilde{\rho}$ is obtained by combining (111a) and (105). $\tilde{\rho}$ is the maximal ($\tilde{\rho} \geqslant 0$) solution of

$$\tilde{\rho} = L(\beta\alpha_z\tilde{\rho}) \tag{116}$$

We note that $\tilde{\rho}$ is a function of temperature only. A plot of $\tilde{\rho}$ vs. T/T^c is shown

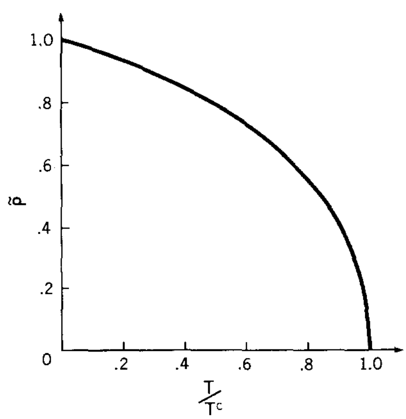

Fig. 1. Plot of $\tilde{\rho}$ vs. T/T^c for a classical Heisenberg model. This plot is a phase boundary curve for a region ($T < T^c$ and $\rho < \tilde{\rho}$) requiring a convex construction and a region ($\rho > \tilde{\rho}$) not requiring a construction.

in Fig. 1. This is interpreted as a phase boundary curve for a region ($T < T^c$ and $\rho < \tilde{\rho}$) in which a convex construction is necessary and a region ($\rho > \tilde{\rho}$) in which no construction is employed.

The net spin per lattice $\boldsymbol{\rho}$ as a function of the magnetic field is determined by Eq. (18) of Ref. 3. From (106) we find that for $\alpha_z\beta \leqslant 3$, or $\alpha_z\beta > 3$ but $\rho \geqslant \tilde{\rho}$,

$$\mu H_i = \mu H_i^0 - \alpha_i \rho_i \qquad (i = x, y, z) \tag{117}$$

subject to (101). From (112) we find that for $\alpha_z\beta > 3$ and $p < \tilde{\rho}$

$$\mu H_x = (\alpha_z - \alpha_x)\rho_x \tag{118a}$$

$$\mu H_y = (\alpha_z - \alpha_y)\rho_y \tag{118b}$$

$$H_z = 0 \tag{118c}$$

Equations (101) and (117) constitute a mean field-type equation of state. Equations (118) arise due to the convex envelope construction. Since the general equations of state are not transparent, we examine several special cases.

Case a:

$$H_x = H_y = 0 \tag{119}$$

Equations (101) and (117) for this case imply

$$\rho_x = \rho_y = 0 \tag{120a}$$

and

$$\rho_z = L(\beta\mu H_z + \beta\alpha_z\rho_z) \tag{120b}$$

for $\alpha_z\beta \leqslant 3$, or $\alpha_z\beta > 3$ but $\rho \geqslant \tilde{\rho}$. Equations (118) imply

$$H_z = 0 \tag{121a}$$

and

$$\rho_x = \rho_y = 0, \qquad |\rho_z| < \tilde{\rho} \tag{121b}$$

if $\alpha_z\beta > 3$ and $p < \tilde{\rho}$. Equation (120b) is a mean field solution for a classical Ising model, and (121b) is a Maxwell-type construction for this solution. Figure 2 is a plot of ρ_z vs. $\mu H_z/\alpha_z$ for this case. Curves are shown for temperatures above and below the critical temperature.

Case b:

$$H_y = H_z = 0 \tag{122}$$

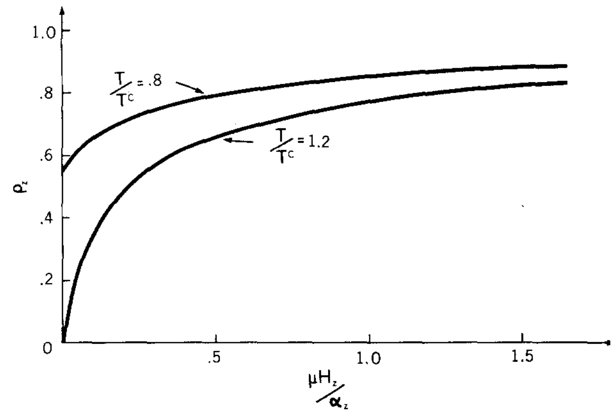

Fig. 2. Plot of ρ_z vs. $\mu H_z/\alpha_z$ for the classical Heisenberg model (ρ_z, $H_z \geqslant 0$). Plots are drawn for case a: $\alpha_z > \alpha_x$, α_y; $H_x = H_y = 0$. For this case $\rho_x = \rho_y = 0$. Shown are isotherms for temperatures above and below the critical temperature.

Equations (101) and (117) for this case imply

$$\rho_y = \rho_z = 0 \tag{123a}$$

$$\rho_x = L(\beta\mu H_x + \beta\alpha_x\rho_x) \tag{123b}$$

if $\alpha_z\beta \leqslant 3$, or $\alpha_z\beta > 3$ but $\rho \geqslant \tilde{\rho}$. Equations (118) imply

$$\mu H_x = (\alpha_z - \alpha_x)\rho_x \tag{124a}$$

and

$$\rho_y = 0, \qquad (\rho_x^2 + \rho_z^2)^{1/2} < \tilde{\rho} \tag{124b}$$

if $\alpha_z\beta > 3$ and $\rho < \tilde{\rho}$. Equation (123b) is a mean field equation for all $\boldsymbol{\rho}$ exterior to the construction region. Equation (124a) indicates a linear behavior between ρ_x and H_x for $\boldsymbol{\rho}$ interior to the construction region. Also indicated is that ρ_z can take on any value satisfying (124b) for $\boldsymbol{\rho}$ interior to the construction region. This nonzero transverse (to the magnetic field) component of the net spin per lattice site is consistent with the discussion of dominant transverse coupling for the quantum Heisenberg ferromagnet given by Fisher[9]. From (124) the magnetic field $\tilde{H}_x$ corresponding to $\tilde{\rho}$ at the onset of the phase transition is given by

$$\mu\tilde{H}_x = (\alpha_z - \alpha_x)\tilde{\rho} \tag{125}$$

$\tilde{\rho}$ is already plotted in Fig. 1. Figure 3 is a plot of ρ_x vs. $\mu H_x/\alpha_x$ for this case, where we have chosen $2\alpha_x = \alpha_z$. Plots are shown for temperatures above and below the critical temperature.

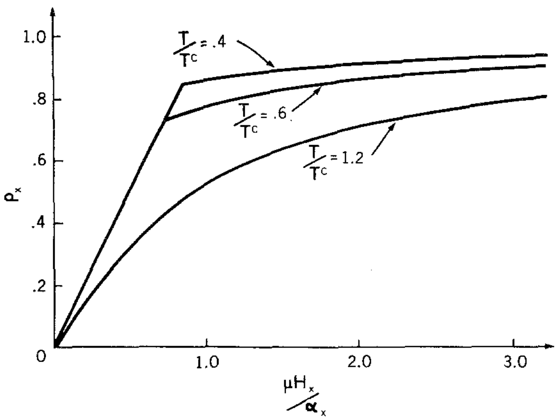

Fig. 3. Plot of ρ_x vs. $\mu H_x/\alpha_x$ for the classical Heisenberg model (ρ_x, $H_x \geqslant 0$). Plots are drawn for case b: $\alpha_z > \alpha_x$, α_y; $H_y = H_z = 0$; with $\alpha_z = 2\alpha_x$. For this case $\rho_y = \rho_z = 0$ over the nonlinear portion of the curves. Over the linear portion of the curves ρ_z can take on any value such that $(\rho_x^2 + \rho_z^2)^{1/2} \leqslant \tilde{\rho}$. Shown are isotherms above and below the critical temperature.

The specific heats at constant magnetic field and at constant magnetization are defined, respectively, by

$$C_H = -T[\partial^2 f_c(T, H)/\partial T^2]_{\mathbf{H}} \tag{126a}$$

and

$$C_\rho = -T[\partial^2 f_m(T, \rho)/\partial T^2]_\rho \tag{126b}$$

Since $f_c(T, \mathbf{H})$ and $f_m(T, \rho)$ are related by a Legendre transformation [see Eq. (106) of Ref. 3], we obtain the relation

$$C_H = C_\rho - \mu T \sum_{i=x,y,z} (\partial H_i/\partial T)_\rho (\partial \rho_i/\partial T)_{\mathbf{H}} \tag{127}$$

From (101), (102), (126b), and the convex envelope construction [(111) and (112)] we find

$$C_\rho/k = \begin{cases} \left(3\tilde{\rho}\dfrac{T^c}{T}\right)^2 \dfrac{(T/3\tilde{\rho}T^c)^2 - \operatorname{csch}^2(3\tilde{\rho}T^c/T)}{1 - (3T^c/T)[(T/3\tilde{\rho}T^c)^2 - \operatorname{csch}^2(3\tilde{\rho}T^c)/T]} \\ \text{if} \quad T < T^c \quad \text{and} \quad \rho < \tilde{\rho} \\ 0 \quad \text{otherwise} \end{cases} \tag{128}$$

where k is Boltzmann's constant. Similarly we find that

$$-(\mu T/k) \sum_{i=x,y,z} (\partial H_i/\partial T)_\rho (\partial \rho_i/\partial T)_{\mathbf{H}} = 0 \qquad \text{if} \quad T < T^c \quad \text{and} \quad \rho < \tilde{\rho} \tag{129}$$

(that is, if ρ is interior to the construction region). We examine this term for ρ exterior to the construction region in the two cases described above.

Case a:

$$H_x = H_y = 0 \tag{130}$$

From (101) and (102) we find

$$-\frac{\mu T}{k}\sum_{i=x,y,z}\left(\frac{\partial H_i}{\partial T}\right)_{\rho}\left(\frac{\partial \rho_i}{\partial T}\right)_{\mathbf{H}} = u^2\frac{u^{-2}-\operatorname{csch}^2 u}{1-(3T^c/T)(u^{-2}-\operatorname{csch}^2 u)} \tag{131a}$$

subject to

$$(T/3T^c)u - r_z = L(u) \tag{131b}$$

where

$$r_z = \mu H_z/\alpha_z \tag{131c}$$

Equations (131) are valid for $T > T^c$, and for $T < T^c$ but $\rho > \tilde{\rho}$. Figure 4 is a plot of C_H/k vs. T/T^c for this case. Illustrations are shown for zero and nonzero H_z. From (127) we note that if $H_z = 0$, then $C_\rho = C_H$ for $\rho < \tilde{\rho}$. For $\rho \geqslant \tilde{\rho}$, $C_\rho = 0$.

Case b:

$$H_y = H_z = 0 \tag{132}$$

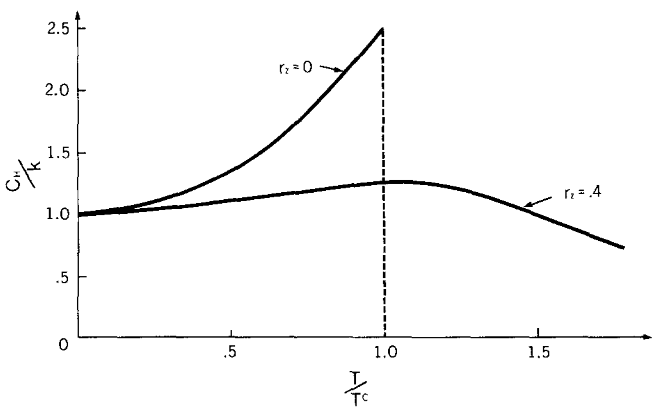

Fig. 4. Plot of C_H/k vs. T/T^c for the classical Heisenberg model. Plots are drawn for case a: $\alpha_z > \alpha_x, \alpha_y$; $H_x = H_y = 0$. Shown are curves for zero and nonzero H_z ($r_z = \mu H_z/\alpha_z$). The plot for $H_z = 0$ ($r_z = 0$) is equal to C_ρ/k for $|\rho| < \tilde{\rho}$. For $|\rho| \geqslant \tilde{\rho}$, $C_\rho = 0$.

From (101) and (102) we find

$$-\frac{\mu T}{k}\sum_{i=x,y,z}\left(\frac{\partial H_i}{\partial T}\right)_{\rho}\left(\frac{\partial \rho_i}{\partial T}\right)_{\mathbf{H}} = v^2\,\frac{v^{-2} - \operatorname{csch}^2 v}{1 - (3T^c/T)(\alpha_x/\alpha_z)(v^{-2} - \operatorname{csch}^2 v)} \tag{133a}$$

subject to

$$(\alpha_z/\alpha_x)(T/3T^c)v - r_x = L(v) \tag{133b}$$

where

$$r_x = \mu H_x/\alpha_x \tag{133c}$$

Equations (133) are valid for $T > T^c$, or $T < T^c$ but $\rho > \tilde{\rho}$. Figure 5 is a plot of C_H/k vs. T/T^c for this case, where we have chosen $\alpha_z = 2\alpha_x$. Curves are shown for zero and nonzero H_x. We note that there is always a discontinuity in C_H at the temperature corresponding to the phase transition.

For this case the fact that C_H is independent of the applied magnetic field if $\alpha_z\beta > 3$ and $\rho < \tilde{\rho}$ follows [as an alternative to the arguments leading to (128)] from the Maxwell relation (S being the entropy per lattice site)

$$\left(\frac{\partial S}{\partial H_x}\right)_{T,H_y,H_z} = \mu\left(\frac{\partial \rho_x}{\partial T}\right)_{\mathbf{H}} \tag{134}$$

For $H_y = H_z = 0$ (124a) implies that the right-hand side of (134) is zero if $\alpha_z\beta > 3$ and $\rho < \tilde{\rho}$. We thus conclude that for this case the entropy is independent of the applied field. This in turn implies that C_H is independent of the applied field.

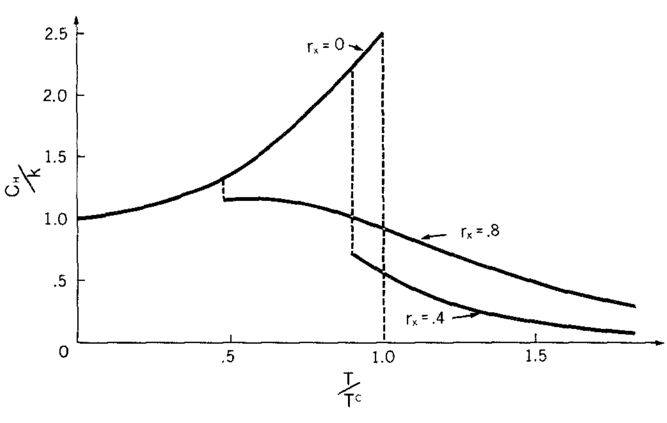

Fig. 5. Plot of C_H/k vs. T/T^c for the classical Heisenberg model. Plots are drawn for case b: $\alpha_z > \alpha_x, \alpha_y$; $H_y = H_z = 0$; with $\alpha_z = 2\alpha_x$. Shown are curves for zero and nonzero H_x ($r_x = \mu H_x/\alpha_x$). There is always a discontinuity at the temperature corresponding to the phase transition.

7. CONCLUDING REMARKS

In this article we have presented an exact solution to the classical anisotropic Heisenberg model with long-range Kac interactions. For the special case of zero short-range interactions we have analyzed in detail (see Section 6) the thermodynamics of this model. The thermodynamic behavior of the long-range anisotropic Heisenberg model was found to be highly sensitive to the degree of anisotropy. In particular, the qualitative features of the thermodynamics depend dramatically on whether the dominant coupling coefficient (all coupling coefficients nonnegative) is parallel to or transverse to the magnetic field. Qualitatively, the results can be summarized in the following way. If the coupling coefficient parallel to the magnetic field is larger than the coupling coefficients in the plane perpendicular to the magnetic field, the usual Ising-type mean field results are recovered (see Figs. 2 and 4). If, however, the dominant coupling coefficient is in the plane perpendicular to the magnetic field, the thermodynamic behavior is quite different. For this latter case the magnetization is a continuous function of the magnetic field and there is no spontaneous magnetization (see Fig. 3). There is, however, a phase transition, which manifests itself by a discontinuity in the magnetic susceptibility and specific heat (see Figs. 3 and 5). For the special case of the isotropic Heisenberg model these two cases degenerate to a single case characteristic of an Ising-type mean field result. As one would expect from a model with long-range Kac interaction, the above results are independent of the dimensionality of the system. This independence of dimensionality emphasizes an important distinction between models with long-range Kac interactions and models with short-range interactions. The above results for the isotropic Heisenberg model with long-range interactions must be contrasted with the fact that the one- and two-dimensional (quantum) Heisenberg models with nearest-neighbor interactions do *not* exhibit a spontaneous magnetization.

We also wish to take particular note of the form of the constant-magnetization free energy density for the classical Heisenberg [see (95)] spin systems with long-range Kac interactions. This type of solution also arises in the solution of the quantum Ising model with long-range Kac interactions.[10] The constant-magnetization free energy density is found to be equal to the convex envelope of the sum of two terms. These terms are (1) the free energy density for a system with *no* long-range interactions and (2) term(s) involving the product of a "characteristic" long-range coupling parameter with the square of a net spin density. The analysis can then be thought of as "decoupling" the long- and short-range interactions into the sum of two terms. These terms constitute the argument of the convex envelope in the expression for the constant-magnetization free energy.

This form for the free energy density for systems with long-range Kac interactions appears to be quite general. Lebowitz and Penrose[5] have solved the problem of a classical fluid with long-range Kac interactions. Their analysis was carried out in the canonical ensemble. The Helmholtz free energy density $a(\rho)$ there obtained is given by

$$a(\rho) = \text{C.E.}\{a^0(\rho) + \tfrac{1}{2}\alpha\rho^2\} \tag{135}$$

where ρ in this case is the particle density, $a^0(\rho)$ is the Helmholtz free energy density for a system with *no* long-range interactions, and α is a "characteristic" coupling parameter. The work of Lebowitz and Penrose was extended to quantum fluids by Lieb[11]. The formal solution to the quantum problem is also given by (135). The solution is valid for Boltzmann, Bose, or Fermi statistics. The different statistics enter $a^0(\rho)$ and do *not* appear in the long-range term $\frac{1}{2}\alpha\rho^2$.

On the basis of these results for classical and quantum fluids it is tempting to speculate that the formal solution to the quantum Heisenberg model with long-range Kac interactions is the same as that of the corresponding classical system [see (95)]. Furthermore, it is known that this is in fact the case for Heisenberg systems with constant interaction potentials whose strengths are proportional to N^{-1}. This has been demonstrated in the canonical ensemble[6]. However, this framework does not appear to be useful with regard to Heisenberg systems with Kac potentials. Unfortunately, an appropriate definition for the constant-magnetization ensemble is complicated by the fact that the components M_x, M_y, and M_z ($M_i = \sum_{k=1}^{N} s_{i,k}$ for $i = x, y, z$) of the total spin operator do not commute with each other. A potential way of circumventing this difficulty is to employ an ensemble for which one component of the total spin and the magnitude of the total spin are held fixed. At present a complete solution is still lacking.

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