

Spherical Models with a Gates–Penrose-Type Phase Transition

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Gates and Penrose have given criteria under which classical gases with weak long-range interactions fail to be described by the van der Waals equation with Maxwell's rule. Unfortunately, examples of equations of state for such systems have not yet been produced. This paper examines the Gates–Penrose class of interactions—i.e., $U_\gamma(r) = q(r) + \gamma\Phi(\gamma r)$, in the limit $\gamma \rightarrow 0$, where the Fourier transform $\hat{\Phi}(p)$ has a minimum at a nonzero value of p —for the spherical model on a one-dimensional lattice. Free energy and magnetization isotherms are computed; it is seen that there is a phase transition, but that the zero-field spontaneous magnetization is always zero (a parahelical phase). However, the pair-correlation function may exhibit either long-range order or the appearance of oscillation.

KEY WORDS: Equation of state; phase transition; spherical model; nonferromagnetic; correlations; van der Waals; Maxwell's rule; Kac limit.

1. GATES–PENROSE CONDITIONS

In the third of a series of articles on the van der Waals limit for classical systems,^(2–4) Gates and Penrose (GP henceforth) have found that for a certain class of interactions, systems of classical particles will exhibit first-order phase transitions which do not correspond to the van der Waals–Maxwell isotherms. GP studied continuous systems in d dimensions ($d \geq 1$) with two-body potentials of the form

$$U_\gamma(r) = q(r) + \gamma^d \Phi(\gamma r) \quad (1)$$

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where $r \in \mathbb{R}^d$ and $\gamma > 0$, which satisfy the conditions

$$q(r) = q(-r) \tag{2a}$$

$$q(r) = +\infty \quad \text{for } |r| \leq 2r_0 \quad (\text{hard core}) \tag{2b}$$

$$|q(r)| < C_1 |r|^{-d-\epsilon} \quad \text{for } |r| > 2r_0 \quad (\epsilon > 0) \tag{2c}$$

$$\Phi(r) = \Phi(-r) \tag{3a}$$

$$|\Phi(0)| < \infty \tag{3b}$$

$$|\Phi(r)| < C_2 |r|^{-d-\epsilon} \tag{3c}$$

$$\int_{\mathbb{R}^d} |\Phi(r)| dr < \infty \tag{3d}$$

Let

$$\hat{\Phi}(p) = \int_{\mathbb{R}^d} ds \Phi(s) \exp(2\pi i p \cdot s)$$

be the Fourier Transform of $\Phi(r)$, and let $\psi_0(\rho, \beta)$ be the free energy density at particle density ρ and temperature $(k\beta)^{-1}$ of the reference system, i.e., a system with two-body potential $q(r)$ alone. (Here $0 \leq \rho \leq \rho_c \equiv$ maximum particle density, and $0 \leq \beta < \infty$.) For any function f , define

$$\text{CE}(f) \equiv \text{maximal convex function not exceeding } f \\ (\text{called the convex envelope of } f)$$

and

$$\text{ME}(f)(\rho) = \inf_h \left(\frac{1}{2} [f(\rho + h) + f(\rho - h)] \right) \\ (\text{called the midpoint envelope of } f)$$

Define the generalized van der Waals free energy for a system with potential $U_\gamma(r)$ as

$$\psi_w(\rho, \beta) \equiv \text{CE}(\psi_0(\rho, \beta) + \frac{1}{2} \hat{\Phi}(0) \rho^2)$$

In one dimension, if $q(r)$ is a strict hard core, [$q(r) = 0$, for $|r| > 2r_0$] then

$$\psi_0(\rho, \beta) = \frac{\rho}{\beta} \log \frac{\rho}{\rho_c - \rho}$$

and the van der Waals pressure is given by

$$p_w(\rho, \beta) \equiv \left(\rho \frac{\partial}{\partial \rho} - 1 \right) \psi_w(\rho, \beta) = \frac{\rho}{\beta(1 - \rho/\rho_c)} + \frac{1}{2} \hat{\Phi}(0) \rho^2$$

with the equal area rule when $\hat{\Phi}(0) < 0$ and $\beta > 27/4 |\hat{\Phi}(0)| \rho_c$.

If $\psi(\rho, \beta, \gamma)$ is the free energy density for the system with potential $U_\gamma(r)$ and $\psi_0(\rho, \beta) \equiv \lim_{\gamma \rightarrow 0} \psi(\rho, \beta, \gamma)$ is the free energy density in the weak long-range limit, GP found that if

$$\inf_p \hat{\Phi}(p) < \min(0, 2\hat{\Phi}(0)) \tag{4}$$

then $\psi(\rho, \beta) < \psi_w(\rho, \beta)$ for all values of (ρ, β) for which either

$$\psi_0(\rho, \beta) + \frac{1}{2} \hat{\Phi}(0) \rho^2 > \text{CE}[\psi_0(\rho, \beta) + \frac{1}{2} \hat{\Phi}(0) \rho^2] \tag{5a}$$

or

$$\psi_0(\rho, \beta) + \frac{1}{4} \inf_p \hat{\Phi}(p) \rho^2 > \text{ME}(\psi_0(\rho, \beta) + \frac{1}{4} \inf_p \hat{\Phi}(p) \rho^2) \tag{5b}$$

In particular, if either (5a) or (5b) occurs in conjunction with (4), then the system has a first-order phase transition which is not described by the van der Waals equation of state with the Maxwell rule.

If a one-dimensional system with a strict hard-core reference potential $q(x)$ satisfies condition (4), then

$$\psi_0(\rho, \beta) + \frac{1}{4} \inf_p \hat{\Phi}(p) \rho^2 = \frac{\rho}{\beta} \log \frac{\rho}{\rho_c - \rho} - b\rho^2$$

where $-b = \frac{1}{4} \inf_p \hat{\Phi}(p) < 0$. For $\beta > 27/8\rho_c b$, this expression is not convex in ρ , which implies that condition (5b) can be satisfied in this case.

However, GP did not actually give an example of what an equation of state might be for such a system; even in one dimension, examples are difficult to compute. One can attempt to adapt the “transfer matrix” methods of K.U.H.⁽⁸⁾ to such a computation⁽⁹⁾ by constructing a potential which satisfies condition (4), of the form

$$\gamma\Phi(\gamma x) = \gamma A e^{-\gamma\alpha|x|} - \gamma R e^{-\gamma r|x|}$$

Such a potential gives rise to a family $K(\gamma)$ of integral operators, and the pressure at each γ can be derived from the spectral radius,

$$\lim_{N \rightarrow \infty} |\text{Tr}(K^N(\gamma))|^{1/N}$$

Previous investigators have evaluated the spectral radius in the weak long-range limit by interchanging the limit $N \rightarrow \infty$ with the limit $\gamma \rightarrow 0$, which simplifies the computation enormously.^(8,11) However, this procedure always results in the van der Waals equation with Maxwell's rule, even for potentials which satisfy condition (4), and is thus not even heuristically useful.

2. A BRIEF REVIEW OF THE SPHERICAL MODEL AND THE MEAN SPHERICAL MODEL

We may begin to understand the differences between the Gates–Penrose transition and the van der Waals–Maxwell transition by contrasting transitions produced by GP-type interactions with ferromagnetic transitions in the spherical model.⁽¹⁾ In an N -site spherical model, each site k ($k = 1, \dots, N$) is given a real-valued spin variable, σ_k . Admissible states are sets

$$\left\{ \sigma_k: k = 1, \dots, N, \sum_{k=1}^N \sigma_k^2 = N \right\}$$

The energy of each state is

$$H_N(\sigma) = - \left(\sum_{1 \leq k < l \leq N} I_{kl} \sigma_k \sigma_l + \sum_{k=1}^N h_k \sigma_k \right) \quad (6)$$

where I_{kl} is the interaction strength between the spins σ_k and σ_l , and h_k is the external field. For a one-dimensional model, the distance between points k and l is just $|k - l|$; we consider only interactions of the form $I_{kl} = J(|k - l|)$ and external fields of uniform strength: $h_k = h$ for all k .

The canonical partition function is given by

$$Z_N(\beta, h) = \frac{1}{A_N} \int \exp[-\beta H_N(\sigma)] d\mu_N(\sigma) \quad (7)$$

where $d\mu_N(\sigma)$ is the uniform measure on the sphere $\sum_{k=1}^N \sigma_k^2 = N$, and

$$A_N = \int d\mu_N(\sigma) = \frac{2\pi^{N/2} N^{(N-1)/2}}{\Gamma(N/2)}$$

The infinite-volume free energy density is given by

$$F(\beta, h) = - \lim_{N \rightarrow \infty} \left(\frac{\log Z_N(\beta, h)}{\beta N} \right)$$

Let

$$g(\theta) \equiv \sum_{k=-\infty}^{\infty} J(|k|) e^{ik\theta}$$

Then, a steepest descent computation,⁽⁹⁾ followed by a use of Szegő’s theorem,⁽⁵⁾ yields the result

$$F(\beta, h) = \frac{1}{2} \left(\frac{1 + \log \beta}{\beta} - [s - J(0)] - \frac{h^2}{s - g(0)} + \frac{1}{2\pi\beta} \int_0^{2\pi} d\theta \log[s - g(\theta)] \right) \tag{8}$$

when a solution s exists to the equation

$$1 = \frac{h^2}{[s - g(0)]^2} + \frac{1}{2\pi\beta} \int_0^{2\pi} \frac{d\theta}{s - g(\theta)} \tag{9}$$

In particular,

$$s \geq g_m \tag{10}$$

where $g_m \equiv \sup_{0 \leq \theta < 2\pi} g(\theta)$

Nonexistence of a solution to equation (9) can occur only if

$$\frac{1}{2\pi} \int_0^{2\pi} \frac{d\theta}{g_m - g(\theta)} = \beta_c < \infty \tag{11}$$

Then, if β is large enough ($\beta > \beta_c$) and $|h|$ is small enough, Eq. (9) has no solution; in this case the system has a phase transition, i.e., a loss of analyticity of $F(\beta, h)$. We will discuss this case further in Section 4.

The magnetization is defined as

$$m(\beta, h) = - \frac{\partial F}{\partial h}(\beta, h)$$

It follows from Eqs. (8) and (9) that

$$m(\beta, h) = \frac{h}{s - g(0)} \tag{12}$$

For the purposes of calculation, it is often useful to consider the Mean Spherical model. The Mean Spherical partition function corresponding to Eq. (7) is

$$Q_N(s_N, \beta, h) = \frac{1}{A_N} \int_{\mathbb{R}^N} d\sigma \exp \left(\left(-\frac{s_N \beta}{2} \right) \sum_{k=1}^N \sigma_k^2 + \beta \left[\frac{1}{2} \sum_{k=1}^N \sum_{l=1}^N J(|k - l|) \sigma_k \sigma_l + h \sum_{k=1}^N \sigma_k \right] \right) \tag{13}$$

subject to the condition that

$$E_N^M \left(\sum_{k=1}^N \sigma_k^2 \right) = N \tag{14}$$

where $E_N^M(\)$ is the expectation with respect to the Q_N distribution. Equation (14) determines s_N . Furthermore, as $N \rightarrow \infty$, the value of s_N which satisfies Eq. (14) approaches the value of s which satisfies Eq. (9).

The Mean Spherical model can be used to compute the spin correlations in the Spherical model.⁽⁷⁾ The zero-field pair-correlation in the Mean Spherical model is given by taking the limit $N \rightarrow \infty$ of

$$E_N^M(\sigma_k \sigma_l) = \frac{1}{A_N Q_N(s_N, \beta, 0)} \int_{\mathbb{R}^N} d\sigma \sigma_k \sigma_l \exp \left[\left(-\frac{\beta s_N}{2} \right) \sum_{j=1}^N \sigma_j^2 + \beta \left(\frac{1}{2} \sum_{j,n=1}^N J(|n-j|) \sigma_j \sigma_n \right) \right] \tag{15a}$$

$$= \frac{1}{\beta} (s_N - \tilde{J}_N)_{kl}^{-1} \tag{15b}$$

The right-hand side of equation (15b) is the (k, l) element of the inverse of the matrix $\beta(s_N - \tilde{J}_N)$. If the limiting value of the s_N is greater than the supremum of $g(\theta)$, and if the limit $N \rightarrow \infty$ of $E_N^M(\sigma_k \sigma_l)$ is taken so that k, l are not close to the boundary of the lattice on which they lie, then the limit of $E_N^M(\sigma_k \sigma_l)$ will depend only on the distance $|k - l|$, and by Szegő's theorem⁽⁵⁾

$$E^M(|k - l|, \beta) \equiv \lim_{N \rightarrow \infty} E_N^M(\sigma_k \sigma_l) = \frac{1}{2\pi\beta} \int_0^{2\pi} \frac{\exp i(|k - l| \theta)}{s - g(\theta)} d\theta \tag{16}$$

The symmetry of the interaction implies that $g(\theta) = g(2\pi - \theta)$, and we can then rewrite Eq. (16) as

$$E^M(|k - l|, \beta) = \frac{1}{\beta\pi} \int_0^\pi \frac{\cos(|k - l| \theta)}{s - g(\theta)} d\theta \tag{17}$$

3. THE SPHERICAL MODEL IN THE WEAK, LONG-RANGE LIMIT

In the Spherical model, the lattice spacing between points acts as a hard-core potential. The interaction $-J(|k - l|)$ corresponds to the long-range potential Φ of the gas [Eq. (1)]. Let

$$g_\gamma(\theta) \equiv \gamma \sum_{k=-\infty}^{\infty} J(\gamma k) e^{ik\theta}$$

If J is sufficiently regular, then

$$\lim_{\gamma \rightarrow 0} g_\gamma(2\pi\gamma\phi) = \tilde{J}(\phi)$$

for any real number ϕ , where $\hat{J}(\phi)$ is the Fourier transform of $J(k)$, as defined above; furthermore,

$$\lim_{\gamma \rightarrow 0} \sup_{\theta \in [0, 2\pi]} g_\gamma(\theta) = \sup_{\phi \in [0, \infty)} \hat{J}(\phi) = - \inf_{\phi \in [0, \infty)} [-\hat{J}(\phi)] \quad (18)$$

Let

$$\hat{J}_m \equiv \sup_{\phi \in [0, \infty)} \hat{J}(\phi)$$

Note that if the interaction is ferromagnetic, i.e., $J(k) \geq 0$ for all k , then $\hat{J}_m = \hat{J}(0)$. For the potentials that we consider here, note that $\hat{J}_m \geq 0$.

In the Spherical model, as previously noted, it is possible to have a phase transition for fixed $\gamma > 0$ [see Eq. (11) ff., and Section 4].² If, however, J is continuously differentiable and

$$|J(k)| \leq C |k|^{-2-\epsilon}$$

then $g_\gamma(\theta)$ will be continuously differentiable in θ for all $\gamma > 0$, and hence there will be no phase transition for $\gamma > 0$ [since β_c , defined in Eq. (11), will be $+\infty$].

A phase transition may nevertheless be obtained by taking $\gamma \rightarrow 0$. The existence and nature of the phase transition in this limit are determined entirely by the constant \hat{J}_m .

There are three cases to consider:

- i. $\hat{J}_m = 0$
- ii. $\hat{J}_m = J(0) > 0$
- iii. $\hat{J}_m > \max[0, \hat{J}(0)]$

For any fixed $\theta \in (0, 2\pi)$

$$\lim_{\gamma \rightarrow 0} g_\gamma(\theta) = 0$$

Thus, if $\hat{J}_m = 0$, as $\gamma \rightarrow 0$ the solution $s(\gamma)$ of Eq. (9) approaches continuously the solution s of the equation

$$1 = \frac{h^2}{[s - \hat{J}(0)]^2} + \frac{1}{\beta s} \quad (19)$$

for all values of h and all $\beta > 0$. Hence, there is no loss of analyticity and no phase transition in the limit $\gamma \rightarrow 0$ when $\hat{J}_m = 0$.

² This cannot occur in the classical continuum gas: if the potentials satisfy conditions (3a)–(3d), there is never a phase transition for fixed $\gamma > 0$. Phase transitions occur only after the limit $\gamma \rightarrow 0$ is taken.⁽²⁾

If $\hat{J}_m > 0$, as $\gamma \rightarrow 0$, requirement (10) and Eq. (18) force $s \geq \hat{J}_m$ always, so that the solution of Eq. (9) cannot approach the solution of Eq. (19) for all values of h and all $\beta > 0$. However, if $\beta < \hat{\beta}$, where

$$\hat{\beta} = \frac{1}{\hat{J}_m}$$

then $s(\gamma)$ does approach the solution of Eq. (19) as $\gamma \rightarrow 0$, and the free energy and magnetization are smooth functions of h . The magnetization is zero at zero field strength, i.e., $m(\beta, 0) = 0$, as expected above the critical temperature. Figure 1 depicts a magnetization isotherm for $\beta < \hat{\beta}$ when $\gamma = 0$. (For $\gamma > 0$, there is no critical β , and all magnetization isotherms appear as smooth as the curve in Fig. 1. This is also the case for $\gamma = 0$ when $\hat{J}_m = 0$.)

The zero-field pair-correlations can also be computed in the limit $\gamma \rightarrow 0$. Applying the above discussion to Eq. (17), it follows that for $\beta < \hat{\beta}$ (all $\beta > 0$ when $\hat{J}_m = 0$)

$$E^M(|k-l|, \beta) = \delta_{kl}$$

i.e., the spins are completely uncorrelated above the critical temperature.

We now summarize the results for the magnetization and zero-field pair-correlations when $\beta > \hat{\beta}$ (followed by a sketch of the derivation).

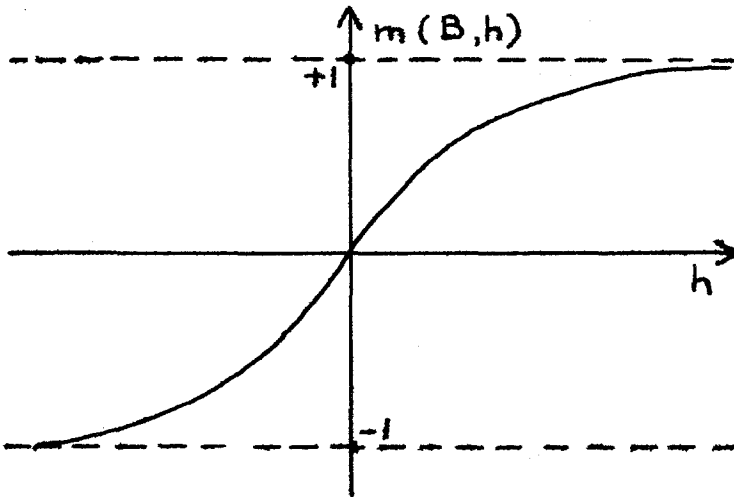


Fig. 1. $m(\beta, h)$ for $\beta < \hat{\beta}$ (at $\gamma = 0$).

(a) In case (ii)

$$\lim_{h \rightarrow 0^\pm} m(\beta, h) = \pm \left(1 - \frac{\hat{\beta}}{\beta}\right)^{1/2}$$

(See Fig. 2.)

(b) In case (iii), when $|h| < \hat{h}(\beta)$, where

$$\hat{h}(\beta) = [\hat{J}_m - \hat{J}(0)] \left(1 - \frac{\hat{\beta}}{\beta}\right)^{1/2}$$

$$m(\beta, h) = \frac{h}{\hat{J}_m - \hat{J}(0)}$$

(See Fig. 3.)

(c) In both cases (i) and (ii)

$$E^M(|k-l|, \beta) = \begin{cases} 1, & |k-l| = 0 \\ 1 - \hat{\beta}/\beta, & |k-l| \neq 0 \end{cases}$$

i.e., long-range order.

In case (ii), which includes the ferromagnetic case, $s(\gamma)$ approaches the solution $s > \hat{J}(0)$ of Eq. (19) for any $h \neq 0$. If $h \rightarrow 0$, then $s \rightarrow \hat{J}(0)$ in such a way that

$$\lim_{h \rightarrow 0} \frac{h^2}{[s - \hat{J}(0)]^2} = 1 - \frac{1}{\beta \hat{J}(0)}$$

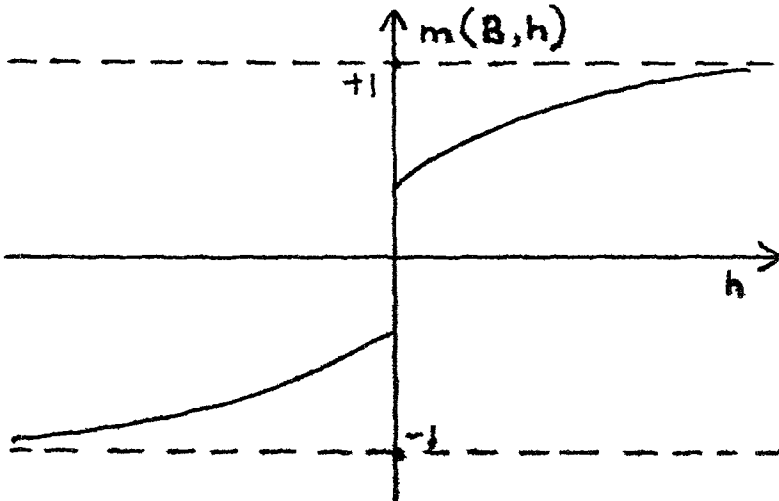


Fig. 2. $m(\beta, h)$ for $\beta > \hat{\beta} = [\hat{J}(0)]^{-1}$ at $\gamma = 0$.

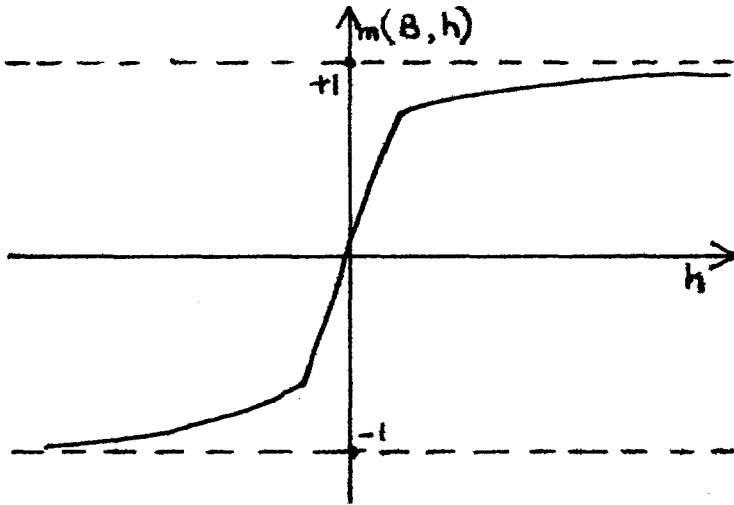


Fig. 3. $m(\beta, h)$ for $\beta > \hat{\beta} = (\hat{J}_m)^{-1} < [\hat{J}(0)]^{-1}$ at $\gamma = 0$.

and result (a), which is well known,⁽⁶⁾ follows from Eq. (12)

In case (iii), $s(\gamma)$ approaches the solution $s > \hat{J}_m$ of Eq. (19) when $|h| > \hat{h}(\beta)$. If $|h| < \hat{h}(\beta)$, then

$$\lim_{\gamma \rightarrow 0} s(\gamma) = \hat{J}_m$$

and result (b) again follows from Eq. (12). Hence, in this case, the magnetization isotherms are continuous in h for all $\beta > 0$, but they each develop a linear region when $|h| < \hat{h}(\beta)$. Since $m(\beta, 0) = 0$, there is no residual net magnetization, although the lattice cannot be considered disordered.

To obtain result (c), observe that for $|k - l| \neq 0$, as $\gamma \rightarrow 0$

$$\frac{1}{\beta\pi} \int_{\delta}^{\pi} \frac{\cos(|k - l|\theta)}{s(\gamma) - g_{\gamma}(\theta)} d\theta = O(\delta)$$

and

$$\left| \frac{1}{\beta\pi} \int_0^{\delta} \frac{\cos(|k - l|\theta)}{s(\gamma) - g_{\gamma}(\theta)} d\theta - \frac{1}{\beta\pi} \int_0^{\delta} \frac{d\theta}{s(\gamma) - g_{\gamma}(\theta)} \right| = O(\delta^2) \quad (20)$$

In order to satisfy Eq. (9), the second integral in Eq. (20) must approach

$$1 - \frac{1}{\beta\hat{J}_m} + O(\delta)$$

and the formula for the mean-spherical zero-field pair correlation follows. Application of the Kac–Thompson transformation between mean-spherical and spherical correlations⁽¹⁷⁾ to this model reveals that the spherical pair correlations equal $E^M(|k - l|, \beta)$ for all β .

Since $E^M(|k - l|, \beta)$ is independent of $|k - l|$ and nonzero for $\beta > \beta_c$, this demonstrates the existence of long-range order whenever the weak, long-range limit is taken for sufficiently smooth interactions. While long-range order is expected in the ferromagnetic case, it is surprising to observe long-range order in case (iii), when the zero-field spontaneous magnetization is zero. Note that case (iii) includes the Gates–Penrose conditions (4). An example of a smooth function $J(x)$ which falls under case (iii) is

$$J(x) = Ae^{-a|x|} - Re^{-r|x|}$$

where

$$\frac{a}{r} > \frac{R}{A} > \left(\frac{r}{a}\right)^3$$

4. FURTHER INVESTIGATIONS ON THE SPHERICAL MODEL (FIXED $\gamma > 0$)

As previously noted, the Spherical model may have phase transitions for potentials satisfying conditions (3a)–(3d) without introducing the weak, long-range limit parameter γ . A potential $J(|k - l|)$ will exhibit a spherical phase transition when the Fourier series

$$g(\theta) = \sum_{k=-\infty}^{\infty} J(k) e^{ik\theta}$$

satisfies condition (11). For such interactions, a phase transition occurs when $\beta > \beta_c$.

Although Eq. (9) cannot be satisfied when $\beta > \beta_c$, and $h^2 < h_c^2$, where

$$h_c^2 \equiv [g_m - g(0)]^2 \left(1 - \frac{\beta_c}{\beta}\right)$$

$F(\beta, h)$ exists⁽⁹⁾ and is given by

$$F(\beta, h) = \frac{1}{2} \left(\frac{1 + \log \beta}{\beta} - [g_m - J(0)] - \frac{h^2}{g_m - g(0)} + \frac{1}{2\pi\beta} \int_0^{2\pi} d\theta \log [g_m - g(\theta)] \right)$$

[which is obtained by setting $s = g_m$ in Eq. (8)]. Then the magnetization exists and is given by

$$m(\beta, h) = \begin{cases} \frac{h}{s - g(0)}, & h > h_c \text{ or } \beta < \beta_c, \quad s \text{ satisfies Eq. (9)} \\ \frac{h}{g_m - g(0)}, & h < h_c, \quad \beta > \beta_c, \quad g_m > g(0) \end{cases}$$

If $g_m = g(0)$, then

$$\lim_{h \rightarrow 0^\pm} m(\beta, h) = \pm \left(1 - \frac{\beta_c}{\beta}\right)^{1/2}$$

Hence, the magnetization isotherms are qualitatively identical to the case of the weak, long-range limit discussed in Section 3. Note that the weak long-range limit can be taken for interactions satisfying condition (11). If this is done, it is found that $\lim_{\gamma \rightarrow 0} \beta_c(\gamma) = \beta_c$, $\lim_{\gamma \rightarrow 0} h_c(\beta, \gamma) = h_c(\beta)$, so that the weak long-range limit does not introduce a "new" phase-transition.

However, a difference appears in the pair-correlations. For $\beta < \beta_c$, the zero-field correlations are given by Eq. (17). When $\beta > \beta_c$, the continuous version of Szegő's theorem does not suffice to evaluate the thermodynamic limit for $E_N^M(\sigma_k \sigma_l)$.

Let $\lambda_{N,j}$, $j = 1, \dots, N$ be the eigenvalues of J_N , listed in descending order of magnitude (counting multiplicity), with respective (orthonormalized) eigenvectors

$$\psi_{N,j} = (\psi_{N,j}(1), \psi_{N,j}(2), \dots, \psi_{N,j}(N))$$

The mean spherical condition [Eq. (14)] can be rewritten as

$$1 = \frac{1}{\beta N} \sum_{j=1}^N (s_N - \lambda_{N,j})^{-1} \quad (21)$$

and the N -particle pair correlation is given by

$$E_N^M(\sigma_k \sigma_l) = \frac{1}{\beta} \sum_{j=1}^N \frac{\overline{\psi_{N,k}(j)} \psi_{N,l}(j)}{(s_N - \lambda_{N,j})}$$

From results known about the spectrum of Toeplitz matrices,⁽⁵⁾ it seems reasonable to believe that for a $g(\theta)$ as pictured in Fig. 4 [note that $g(\theta) = g(2\pi + \theta) = g(-\theta)$], the two largest eigenvalues correspond to $g(\theta_0)$ and $g(-\theta_0) = g_m$ and Szegő's theorem applies to give

$$\frac{1}{\beta N} \sum_{j=3}^N \frac{1}{(s_N - \lambda_{N,j})} \rightarrow \frac{1}{2\pi\beta} \int_{-\pi}^{\pi} \frac{d\theta}{g_m - g(\theta)} = \frac{\beta_c}{\beta} \quad (22)$$

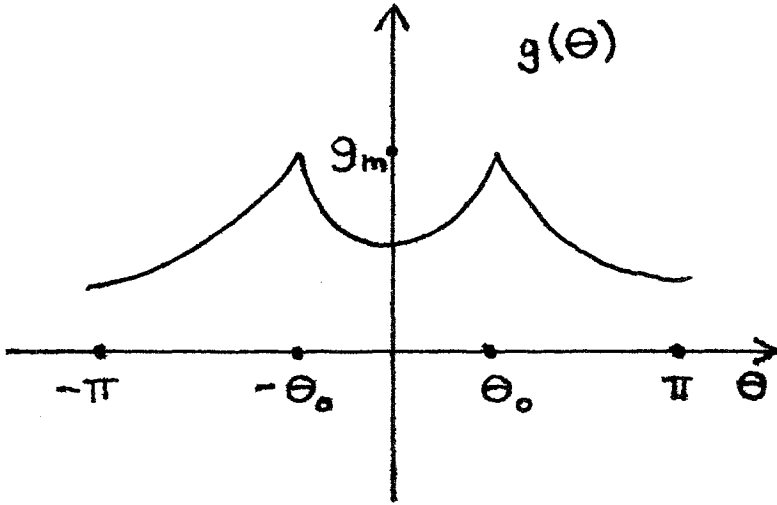


Fig. 4. Example of a $g(\theta)$ from a potential which has a spherical phase transition near θ_0 ,
 $g(\theta) = g(\theta_0) - c|\theta - \theta_0|^\varepsilon + o(|\theta - \theta_0|^\varepsilon)$, $\varepsilon < 1$.

as $N \rightarrow \infty$. This leads us to further conjecture that, as $N \rightarrow \infty$,

$$\frac{1}{\beta} \sum_{j=3}^N \frac{\overline{\psi_{N,k}(j)} \psi_{N,i}(j)}{s_N - \lambda_{N,j}} \rightarrow \frac{1}{2\pi\beta} \int_{-\pi}^{\pi} \frac{\exp[i|k-l|\theta] d\theta}{g_m - g(\theta)} \quad (23)$$

Equations (21) and (22) imply that, as $N \rightarrow \infty$,

$$\frac{1}{\beta N} \sum_{j=1}^2 \frac{1}{s_N - \lambda_{N,j}} \rightarrow 1 - \frac{\beta_c}{\beta}$$

If the $N \rightarrow \infty$ limit for the pair correlations is taken so that $|k-l|$ is constant, but k and l are kept away from the ends of the lattice, then we are led to believe that in this limit

$$\frac{1}{\beta} \sum_{j=1}^2 \frac{\overline{\psi_{N,k}(j)} \psi_{N,i}(j)}{s_N - \lambda_{N,j}} \rightarrow \left(1 - \frac{\beta_c}{\beta}\right) \cos(|k-l|\theta_0) \quad (24)$$

Combining (23) and (24) gives

$$E^M(|k-l|, \beta) = \left(1 - \frac{\beta_c}{\beta}\right) \cos(|k-l|\theta_0) + \frac{1}{\beta\pi} \int_0^\pi \frac{\cos(|k-l|\theta) d\theta}{g_m - g(\theta)} \quad (25)$$

The Kac–Thompson transformation again gives equality between spherical and mean-spherical pair correlations for all temperatures if Eq. (25) is

correct. Equation (25) demonstrates long-range order for $\theta_0 = 0$ [the ferromagnetic case], and long-range oscillatory behavior of the pair correlation as $|k - l| \rightarrow \infty$ for $\theta_0 \neq 0$. Presumably, if $g(\theta)$ has several cusplike maxima, there would be long-range oscillatory terms for all the cusps of steepest order (i.e., smallest ε for cusps of the type in Fig. 4).

In three or more dimensions, the spherical model can exhibit phase transitions for short-range interactions. In this case, the free energy and magnetization show the same behavior as above. However, the correlation functions do not exist in general for $\beta > \beta_c$.⁽¹⁰⁾

For a treatment of other aspects of some nonferromagnetic spherical models which may have some relevance to this model, see Ref. 12.

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