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1995 J. Phys. A: Math. Gen. 28 3389

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First-order phase transition and metastability in the critical two-dimensional Ising model

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Received 9 December 1994

Abstract. The fermionic version of the two-dimensional Ising model in a uniform magnetic field is studied. Its approximate but rather accurate solution was obtained recently in a variational procedure based on the BCS ansatz for the ground state. Here, this solution is continued analytically into the complex H -plane in the vicinity of the origin. In the ferromagnetic phase an essential singularity in the free-energy is observed at the point $H = 0$ of the type predicted by the droplet condensation theory. Simple phenomenological estimates for the radius of the critical droplet and for the rate of decay of metastable states are confirmed by microscopic calculations.

1. Introduction

The problem of analytical continuation of thermodynamic functions into the metastable region beyond the point of the first-order phase transition has been of considerable interest for many years. Traditionally it is concerned with the Ising-like models of a ferromagnet or lattice gas.

Two main approaches have been widely discussed in literature.

(i) In the van der Waals and equivalent approximate theories, the thermodynamic functions are analytical in the line of the first-order phase transition $H = +0$, $T < T_C$. Their analytical continuation to negative magnetic fields is associated with metastable states; it is terminated by the spinodal line, where the magnetic susceptibility diverges.

(ii) Qualitatively different predictions are given by the droplet, or cluster theory of condensation. In phenomenological form the theory was put forward by Frenkel [1], Band [2] and Bijl [3] after stimulating Mayer's analysis [4] of the high-order cluster integrals. In the droplet theory the metastable state has a finite lifetime and its relaxation is caused by the fluctuating appearance and subsequent growth of a critical droplet of the stable phase. Droplets are treated as spheres with free-energies determined by their radii.

The droplet model was reviewed critically and extended by Essam and Fisher [5], and in more detail by Fisher [6]. Considering an 'ideal gas' of isolated clusters of different size and shape, Fisher constructed an approximate 'mimic' partition function. The main conclusions arising from this work are as follows.

(i) At the point $H = +0$ the free-energy has a very weak essential singularity which prevents it from analytical continuation through the point $H = 0$ into the metastable phase† $H < 0$.

† This result was obtained independently by Andreev [7].

(ii) In the stable region $H > 0$ the radius of convergence of the activity series (in magnetic terminology the activity μ is given by $\mu = \exp[-2H/k_B T]$) is determined by the above mentioned singularity at $\mu = 1$.

(iii) The free-energy can be analytically continued from positive to negative magnetic fields by passing around the singularity in the complex H -plane. In the half-line $H < 0$ the free-energy continuation has a non-zero imaginary part.

It should be noted that Fisher's treatment ignores the interaction between clusters. This approximation is reasonable in the so-called dilute limit, where the density of clusters is small, i.e. at temperatures well below the Curie point T_C .

A further strong support to the droplet model was given by Isakov [8]. He proved rigorously that the free-energy of the d -dimensional Ising model has an essential singularity at the point $H = 0$ for small enough temperatures. An important insight into the mathematical nature of the droplet theory was made by Langer [9]. He studied a certain one-dimensional quantum model with a Hamiltonian simulating the transfer matrix of the 2D Ising model in a uniform magnetic field. In microscopic analysis, Langer reproduced all the main features of the droplet model. Furthermore, he demonstrated in his model that the Hamiltonian ground state continuation in the metastable region became unstable due to the effect of quantum tunnelling. Langer then conjectured that the imaginary part of the free-energy in the line $HM < 0$ 'ought to be identified with the rate of decay of the metastable state under some suitable stochastic process'. Subsequent investigations supported this conjecture, though its domain of validity is not completely clear (for more detail see [10, 11] and references therein). For low enough temperatures $T \leq 0.8T_C$ droplet theory predictions were confirmed in extensive numerical studies by Rikvold with collaborators [10–12].

Thus, the droplet theory of condensation now has a reliable microscopic foundation in the dilute limit. In contrast, the situation is less certain in the scaling region. Direct extrapolation of Fisher's partition function into the scaling region discussed in [6] seems problematic. Domb [13] proposed a modification of Fisher's treatment to take into account the effect of the interaction between droplets and to extend the class of configurations considered. His suggestion is that the droplet model is applicable in the dilute limit only, while at higher temperatures the system exhibits behaviour of the van der Waals type. Enting and Baxter [14] investigated the critical thermodynamics by studying the high-field series for the 2D Ising model. They conclude that their results 'are consistent with the predictions of the droplet model, rather than indicating the existence of spinodal'. Abraham and Upton [15] came to the same conclusion upon analysis of the correlation function structure.

The present study is based on the recent analysis [16, 17] of a simple fermionic model, which is equivalent in the critical region to the 2D Ising model in a uniform magnetic field. The model small- H thermodynamics was described rather accurately by an approximate variational procedure, being very similar to that of the famous article by Bardeen, Cooper and Schrieffer [18] where they explain the nature of superconductivity. Here we examine analytical properties of the solution obtained in [16] near the line of the first-order phase transition $H = 0$, $T < T_C$ for complex values of a magnetic field H . Though we are primarily interested in the scaling region, the dilute limit is also considered to make a useful link with well known results.

The paper is organized as follows. In section 2 we review the droplet theory predictions for the radius of the critical droplet and for the rate of decay of metastable states in the critical 2D Ising model. A simple fermionic realization of the Ising model in a non-zero magnetic field and its approximate solution [16, 17] are described briefly in section 3. Sections 4 and 5 give asymptotical analysis of the above mentioned solution for small complex values of a magnetic field in the dilute and scaling limits respectively. In both limits we find

an essential singularity at the origin $H = 0$ of the type predicted by the droplet model, and Langer's conjecture is verified in the scaling region. Concluding remarks are given in section 6.

2. Phenomenological estimates in the critical region

In this section we review some predictions of the droplet theory in the 2D Ising model. We leave details of the theory to [10, 11] and references therein.

Consider the Ising model on the square lattice with lattice constant a and with equal pair energies $J \equiv J_1 = J_2$. The notation H_1 will be used for the magnetic field in the Ising model. Throughout this section we concentrate on the critical region $|\lambda - 1| \ll 1$, where $\lambda(T) \equiv \sinh^2(2J/k_B T)$ is the standard temperature-like parameter which takes the unit value at the Curie point $\lambda(T_C) = 1$.

Let us now discuss how a very small magnetic field $H_1 < 0$ effects the ferromagnetic state ($T < T_C$) with positive average magnetization M_0 given by the Onsager formula [19]

$$M_0 = (1 - \lambda^{-2})^{1/8} \cong [2(\lambda - 1)]^{1/8}. \quad (2.1)$$

If we are considering the droplet model we expect that this state will be destroyed in a finite time τ_c as a result of the fluctuational appearance of a critical cluster; the cluster is understood to be a compact region of size R_c where average magnetization is negative. We expect further, that for a given temperature $T < T_C$ the size of the critical cluster goes to infinity in the limit $H_1 \rightarrow -0$. So, for small enough values of $|H_1|$ the critical cluster becomes large compared with the zero-field correlation length $\xi(T)$: $R_c \gg \xi$. Several conclusions follow from this notation.

(i) We can average over 'small-scale' fluctuations of size of the order of $\xi(T)$ and consider the ferromagnet as a continuous medium with magnetization $-M_0$ inside the cluster, and $+M_0$ beyond it.

(ii) There is only a very small chance of such large clusters occurring, so they can be treated as being well separated from one another.

(iii) The surface tension \mathcal{S} associated with the cluster boundary can be taken from the equilibrium statistical mechanics [19]

$$\mathcal{S} \cong (\lambda - 1)k_B T_C / (2^{1/2} a). \quad (2.2)$$

It should be mentioned that in [19] the lattice is rotated by the angle $\pi/4$, and the lattice constant value chosen is $a = 2^{-1/2}$.

(iv) After averaging over 'small-scale' fluctuations one only needs to consider the spherical clusters.

The free-energy \mathcal{F} of such a cluster with radius R is given by the phenomenological condensation theory [20]

$$\mathcal{F}(R) = 2\pi R\mathcal{S} - 2|H_1|M_0\pi R^2/a^2. \quad (2.3)$$

† Usually these fluctuations are known as long-scale fluctuations. We shall reserve this name for the size of the critical droplet R_c which is assumed to be much larger than the correlation length $\xi(T)$.

It has a maximum in the radius R_c of the critical cluster

$$R_c = \frac{Sa^2}{2|H_1|M_0} = \frac{k_B T_C (\lambda - 1)}{|H_1|M_0} \frac{1}{2^{3/2}} a. \quad (2.4)$$

Such a cluster appears with probability $P(R_c)$ proportional to the rate of decay τ_c^{-1} of the metastable state. They are both characterized by the Boltzmann factor [10, 11]

$$P(R_c) \sim \tau_c^{-1} \sim \exp \left[-\frac{\mathcal{F}(R_c)}{k_B T_C} \right] = \exp \left[-\frac{\pi k_B T_C (\lambda - 1)^{15/8}}{|H_1|} \frac{1}{2^{17/8}} \right]. \quad (2.5)$$

Phenomenological estimates (2.4) and (2.5) will be reproduced in section 5 using the transfer-matrix technique.

3. Low-field equation of state in the BCS approximation

We now study the fermionic realization of the Ising model

$$\mathcal{H} = \int_0^L dx \left\{ \Omega_0 \psi^+ \psi + s \frac{d\psi^+}{dx} \frac{d\psi}{dx} + \frac{i\Gamma}{2} \left(\frac{d\psi^+}{dx} \psi^+ + \frac{d\psi}{dx} \psi \right) \right\} - HLM. \quad (3.1)$$

Here operators $\psi(x)$ and $\psi^+(x)$ describe a spinless fermionic field obeying the standard anticommutational relations

$$\begin{aligned} \{\psi(x), \psi(x')\} &= \{\psi^+(x), \psi^+(x')\} = 0 \\ \{\psi(x), \psi^+(x')\} &= \delta(x - x'). \end{aligned}$$

Magnetization $M \geq 0$ is the square root of the operator

$$\begin{aligned} M^2 &= L^{-2} \int_0^L dx_1 dx_2 \hat{\sigma}(x_1) \hat{\sigma}(x_2) \\ \hat{\sigma}(x_1) \hat{\sigma}(x_2) &= \exp \left\{ i\pi \int_{x_1}^{x_2} dx \psi^+(x) \psi(x) \right\}. \end{aligned} \quad (3.2)$$

L denotes the system length in the x -direction, H is the magnetic field, parameter Ω_0 is proportional to the reduced temperature: $\Omega_0 = -\varkappa t$, $\varkappa > 0$, $t = (T - T_C)/T_C$. The latter relation in (3.2) defines the product of two Ising spin operators $\hat{\sigma}(x_1)$ and $\hat{\sigma}(x_2)$ in terms of the fermionic field $\psi(x)$.

The Hamiltonian (3.1) corresponds to the extreme anisotropic limit of the ferromagnetic Ising model on the square lattice in a uniform magnetic field: \mathcal{H} can be obtained directly from the Ising-model transfer matrix by use of sequential duality [21] and Jordan–Wigner [22] transformations followed by the formal continuous limit procedure. Correspondence with coupling constants $J_1, J_2 > 0$ and magnetic field H_1 of the Ising model in the extreme anisotropic limit $J_1/J_2 \gg 1$ is given by [17]

$$\Omega_0 = 2(\lambda - 1) \quad s = a^2 \quad \Gamma = 2a \quad H = \frac{H_1}{a\tau k_B T_C} \quad (3.3)$$

where

$$\tau = \exp[-2J_1/(k_B T_C)] \ll 1$$

$$\lambda = \sinh[2J_1/(k_B T)] \sinh[2J_2/(k_B T)] \approx J_2/(\tau k_B T)$$

and a is the lattice constant.

The above fermionic model, being equivalent in the critical region to the Ising model, has by itself a very clear interpretation. Operators $\psi^+(x)$ and $\psi(x)$ create and annihilate, respectively, a domain wall at a point x . More precisely, fermion trajectories correspond to the domain-wall lines in the (x, y) -plane. Such a wall separates regions with Ising spin values $\sigma(x, y) = +1$ and $\sigma(x, y) = -1$ (see figure 1). The last term on the right-hand side of (3.1) permits us to describe finite-size domains. Relation (3.2) means, simply, that spins at the points x_1, x_2 are the same or opposite if the number of domain walls between these two points is even or odd respectively. As is implied by the fermion analogy, the free energy of two-dimensional classical system is proportional to the ground-state energy of the quantum one-dimensional Hamiltonian (3.1).

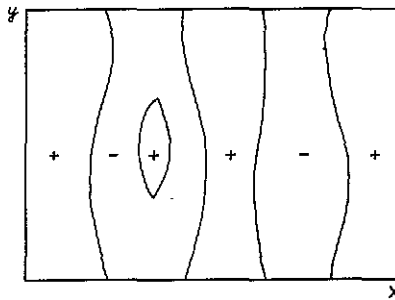


Figure 1. A typical configuration of domain walls and Ising spins described by the Hamiltonian (3.1).

The equation of state of the model (3.1) has been studied recently [16, 17]. We shall summarize the main results which will be used in the following sections.

If $H = 0$, the Hamiltonian can be diagonalized by the Bogoliubov transformation. Its ground state has the BCS-like form

$$|\Phi\rangle = \exp \left\{ \frac{1}{2} \int dx_1 dx_2 \psi^+(x_1) \psi^+(x_2) G(x_1 - x_2) \right\} |0\rangle \tag{3.4}$$

where

$$G(x) = \int \frac{dp}{2\pi} \exp(ipx) \tan[\varphi_0(p)]$$

denotes the ‘wavefunction of the Cooper pair’, and with $\varphi_0(p)$ being the angle of Bogoliubov transformation

$$\tan[\varphi_0(p)] = \frac{\Omega_0 + sp^2 - \sqrt{(\Omega_0 + sp^2)^2 + (\Gamma p)^2}}{\Gamma p}$$

In the case of a small positive magnetic field $H \geq 0$ the ground state and the equation of state were obtained by an approximate variational procedure. The ground state was approximated by the BCS vector $\Phi[\varphi]$, like (3.4), where the angle $\varphi_0(p)$ was replaced by some unknown function $\varphi(p)$. It was determined by minimizing the system's energy

$$E[\varphi] \equiv L^{-1} \frac{\langle \Phi | \mathcal{H} | \Phi \rangle}{\langle \Phi | \Phi \rangle} = \int \frac{dp}{4\pi} \{ (\Omega_0 + sp^2)[1 - \cos 2\varphi(p)] + \Gamma p \sin 2\varphi(p) \} - HM[\varphi] \quad (3.5)$$

where

$$M[\varphi] = \exp \left\{ \frac{1}{2\pi^2} \int_{-\infty}^{\infty} dp \varphi(p) \int_{-\infty}^{\infty} \frac{dq}{q-p} \frac{d\varphi(q)}{dq} \right\}. \quad (3.6)$$

The notation f is used for the integral as understood in the sense of the Cauchy principal value.

The variational equation $\delta E / \delta \varphi(p) = 0$ reads as

$$(\Omega_0 + sp^2) \sin 2\varphi(p) + \Gamma p \cos 2\varphi(p) = \frac{2MH}{\pi} \int_{-\infty}^{\infty} \frac{dq}{(q-p)} \frac{d\varphi(q)}{dq}. \quad (3.7)$$

In the critical region the equation of state following from (3.6) and (3.7) has the scaling form

$$H = CM^{15} h(x_s)$$

where $C = \Gamma^3 / (32s^2)$ and x_s is the familiar scaling variable

$$x_s = \frac{t}{M^8} \frac{4\kappa s}{\Gamma^2} \quad (3.8)$$

that lies in the interval $-1 < x_s < \infty$ for equilibrium states. It should be noted that the critical asymptote of the zero-field magnetization in the ferromagnetic phase is

$$M_0(t) = (4\Omega_0 s / \Gamma^2)^{1/8}. \quad (3.9)$$

The scaling function $h(x_s)$ in the adopted BCS approximation is given by the following construction.

Denote by $\varphi(p; y_s)$ the solution of the equation

$$-\text{sign}(t) \sin 2\varphi(p) + p \cos 2\varphi(p) = \frac{y_s}{\pi} \int_{-\infty}^{\infty} \frac{dq}{(q-p)} \frac{d\varphi(q)}{dq} \quad (3.10)$$

with the boundary conditions $\varphi(-\infty; y_s) = -\varphi(\infty; y_s) = \pi/4$. The parameter y_s is given by

$$y_s = \frac{2MH\Gamma}{\Omega_0^2}. \quad (3.11)$$

The scaling variables x_s and y_s are connected by the relation

$$x_s(y_s) = \text{sign}(t) \exp \left\{ \frac{4}{\pi^2} \int_{-\infty}^{\infty} dp [\varphi_0(p) - \varphi(p; y_s)] \int_{-\infty}^{\infty} \frac{dq}{q-p} \frac{\partial}{\partial q} [\varphi_0(q) + \varphi(q; y_s)] \right\} \quad (3.12)$$

where $\varphi_0(p) = -\frac{1}{2} \arctan p$. The inverse function $y_s(x_s)$ with prefactor x_s^2 gives the scaling function

$$h(x_s) = x_s^2 y_s(x_s). \tag{3.13}$$

It is analytical in the whole interval $-1 < x_s < \infty$ and leads to correct values of the critical exponents $\beta = 1/8$ and $\delta = 15$, $\gamma = -\gamma' = 7/4$. Perturbation theory analysis of equation (3.7) in the limit $H \rightarrow +0$ yields

$$\frac{\partial M}{\partial H} \Big|_{H=+0} = \begin{cases} C_- (-t)^{-7/4} (1+4v)^{3/4} I(v) & t < 0 \\ C_+ t^{-7/4} & t > 0 \end{cases} \tag{3.14}$$

where

$$C_- = \frac{(2\Gamma)^{1/2} s^{1/4}}{6\pi \kappa^{7/4}} \tag{3.15}$$

$$C_+ = 12\pi C_- \tag{3.16}$$

$$I(v) = \frac{3}{2} \int_{-\infty}^{\infty} \frac{p^2 dp}{[(1+vp^2)^2 + p^2]^{5/2}} \underset{v \rightarrow 0}{\approx} \frac{1}{v} - 3v + \frac{15}{2} v^2 \ln v$$

$$v = (\Omega_0 s / \Gamma^2).$$

In the critical region, formulae (3.14) can be rewritten in terms of the parameters λ , τ , and $\chi \equiv \partial M / \partial H|_{H=0}$ of the initial extreme anisotropic Ising model by use of (3.3):

$$k_B T_C \chi = \frac{|2(\lambda - 1)|^{-7/4}}{3\pi \tau} \quad \text{for } t < 0 \tag{3.17}$$

and the same expression multiplied by a factor of 12π for $t > 0$.

Exact calculation of the zero-field magnetic susceptibility for the critical 2D Ising model was reported by Barouch *et al* [23]. In particular, their formula (14) describes how the critical amplitudes depend on the pair energies J_1 , J_2 . Applying their formula to (3.17) we extrapolate our estimate from the extreme anisotropic limit to the point $J_1 = J_2 = 1$. Obtained in such a way, critical amplitudes for the Ising model with unit pair energies have the form

$$k_B T_C \chi = C_{0\pm}^{(0)} |t|^{-7/4} \tag{3.18}$$

$$C_{0+}^{(0)} = 2^{-3/8} [\ln(1 + \sqrt{2})]^{-7/4} = 0.961\,797\,62 \tag{3.19a}$$

$$C_{0-}^{(0)} = C_{0+}^{(0)} / (12\pi) = 0.025\,512\,474. \tag{3.19b}$$

The upper index (0) in the above estimates for the critical amplitudes is written to distinguish them from the exact values C_{0+} , C_{0-} given in [23]

$$C_{0+} = 0.962\,581\,7322 \quad C_{0-} = 0.025\,536\,9719. \tag{3.20}$$

† The initial claim [16, 17] that the scaling function (3.13) is also analytical at the point $x_s = -1$ is incorrect. As was supposed by Fisher its essential singularity lies at $x_s = -1$ (see section 5).

Guttman has recently† pointed out that estimates (3.19) are not new. This ‘rather accurate approximate result’ was reported by Tracy and McCoy [24] (see the last sentence in their paper before the acknowledgments). They derived (3.19) in quite a different way by using leading terms of certain series for the zero-field correlation functions.

To conclude this section let us present a useful critical asymptote for the scaling variable y_s , which expresses it in terms of universal quantities in the vicinity of the line $T < T_C$, $H \rightarrow 0$. In this region the magnetization M in (3.11) can be replaced by its zero-field value (3.9). Combining (3.11) with (3.9), (3.14), (3.15) and (3.18)–(3.20), in the scaling region for $T < T_C$ we can write

$$y_s = 12\pi \frac{H(\partial M/\partial H)|_{H=0}}{M_0} W^{-1}. \quad (3.21)$$

The numerical factor

$$W = C_{0-}/C_{0-}^{(0)} = 1.00096\dots \quad (3.22)$$

was introduced in order to improve formula (3.15) by making it agree exactly with result (3.20). After replacing $H \rightarrow H_1$ one can extrapolate the universal relation (3.21) to the Ising model with arbitrary value of anisotropy ratio J_1/J_2 , though it was derived in the limit $J_1/J_2 \rightarrow \infty$. In particular, in the case of equal coupling constants $J_1 = J_2$ formula (3.21) takes the form

$$y_s = 2^{17/8}(\lambda - 1)^{-15/8}(H_1/k_B T_C) \quad H_1 \rightarrow 0. \quad (3.23)$$

4. The dilute limit

The most unambiguous and reliable results obtained in the framework of the droplet (cluster) picture are related to the dilute limit. It corresponds to the ferromagnetic phase well below the Curie point where the density of clusters of the opposite phase is small. In our scheme the dilute limit is characterized by the small angle of the Bogoliubov transformation $|\varphi(p)| \ll 1$. This allows us to linearize (3.5) and (3.7) with respect to $\varphi(p)$:

$$E[\varphi] = \int \frac{dp}{2\pi} \{(\Omega_0 + sp^2)\varphi^2(p) + \Gamma p\varphi(p)\} - H \left\{ 1 + \frac{1}{2\pi^2} \int_{-\infty}^{\infty} dp \varphi(p) \int_{-\infty}^{\infty} \frac{dq}{q-p} \frac{d\varphi(q)}{dq} \right\} \quad (4.1)$$

$$(\Omega_0 + sp^2)\varphi(p) + \frac{\Gamma p}{2} = \frac{H}{\pi} \int_{-\infty}^{\infty} \frac{dq}{(q-p)} \frac{d\varphi(q)}{dq}. \quad (4.2)$$

† The author was kindly informed by Professor B Nienhuis about this unpublished notation of Professor A J Guttman.

4.1. *The coordinate representation*

Equation (4.2) has a very clear interpretation in the coordinate representation

$$\left(-s \frac{d^2}{dx^2} + \Omega_0\right) \varphi(x) + H|x|\varphi(x) = \frac{i\Gamma}{2} \frac{d\delta(x)}{dx} \tag{4.3}$$

where $x \in (-\infty, +\infty)$ and

$$\varphi(x) = (2\pi)^{-1} \int dp \varphi(p) \exp(ipx).$$

This is a Schrödinger-like equation describing relative motion of two domain walls bounding a cluster. They are coupled by the linear potential $H|x|$ and have a source at the origin.

For positive Ω_0 and H equation (4.3) has a bound-state solution given by

$$\varphi(x; H) = -i \frac{\Gamma}{4s} \text{sign}(x) \frac{\text{Ai} \left[\left(|x| + \frac{\Omega_0}{H} \right) \left(\frac{H}{s} \right)^{1/3} \right]}{\text{Ai} \left[\frac{\Omega_0}{H} \left(\frac{H}{s} \right)^{1/3} \right]} \tag{4.4}$$

where

$$\text{Ai}(u) = \pi^{-1/2} \int_0^\infty dv \cos(uv + \frac{1}{3}v^3)$$

is the Airy function; however, if H becomes negative, no localized solutions of (4.3) exist. One can obtain two linearly independent delocalized solutions $\varphi_\pm(x; H) \equiv \varphi(x; H \pm i0)$ by performing an analytical continuation of (4.4) in the complex H -plane from the point $H_0 > 0$ along the paths $H(\alpha) = H_0 \exp(\pm i\alpha)$, $0 \leq \alpha < \pi$.

The minimal value of function (4.1) can be written as

$$E = -H - \frac{\Gamma^2}{8s} \frac{d}{dx} \Big|_{x \rightarrow +0} [\ln \varphi(x)] + \text{constant}. \tag{4.5}$$

The constant on the right-hand side corresponds to a divergent integral which does not depend on temperature or magnetic field and, therefore, can be omitted. Inserting (4.4) into (4.5) and using well known properties of the Airy function we find the $|H| \rightarrow 0$ asymptote of the ground-state energy for both positive and negative values of the magnetic field:

$$H > 0 \quad E = \frac{\Gamma^2}{8s} (\Omega_0/s)^{1/2} - H \left(1 - \frac{\Gamma^2}{32s\Omega_0} \right) + \dots \tag{4.6}$$

$$H = -|H| \pm i0$$

$$E = \frac{\Gamma^2}{8s} (\Omega_0/s)^{1/2} - H \left(1 - \frac{\Gamma^2}{32s\Omega_0} \right) + \dots \pm i \frac{\Gamma^2}{8s^{3/2}} \Omega_0^{1/2} \exp \left[-\frac{4}{3} \frac{\Omega_0^{3/2}}{|H|s^{1/2}} \right]. \tag{4.7}$$

The asymptote has the essential singularity at the point $H = 0$.

Unfortunately, a straightforward transfer of the above analysis into the scaling region is impossible; the ‘kinetic energy term’ in (4.3) becomes non-local in the latter case (see section 5.2). To facilitate further analysis of the scaling limit, we shall consider the dilute limit directly in the momentum representation.

4.2. The momentum representation

Rewrite equation (4.2) as

$$(\Omega_0 + sp^2)\zeta(p) = \frac{H}{\pi} \int_{-\infty}^{\infty} \frac{dq}{(q-p)} \frac{d}{dq} [\varphi_0(q) + \zeta(q)] \quad (4.8)$$

where $\zeta(p) \equiv \varphi(p) - \varphi_0(p)$ and $\varphi_0(p) = -\Gamma p / [2(\Omega_0 + sp^2)]$. Let us define two functions $g_{\pm}(p)$ of the complex variable p as

$$g_{\pm}(p) = \pi^{-1} \int_{-\infty}^{+\infty} dq \zeta(q) (q-p)^{-1} \quad \text{Im } p \gtrless 0 \quad (4.9)$$

which are analytic in the upper and lower half-planes respectively. Using the Plemel formulae, one obtains from (4.8) two equations in the real p -axis:

$$dg_+(p)/dp - dg_-(p)/dp = 2i d\zeta(p)/dp \quad (4.10)$$

$$H \left[\frac{dg_+(p)}{dp} + \frac{dg_-(p)}{dp} + \frac{2}{\pi} \int \frac{dq}{(q-p)} \frac{d\varphi_0(q)}{dq} \right] = (\Omega_0 + sp^2)\zeta(p). \quad (4.11)$$

Adding (4.10) to (4.11) we have

$$-iH d\zeta(p)/dp = (\Omega_0 + sp^2)\zeta(p) + H\rho(p) \quad (4.12)$$

where

$$\rho(p) = \rho_0(p) - dg_+(p)/dp \quad (4.13)$$

$$\rho_0(p) = -\pi^{-1} \int_{-\infty}^{+\infty} dq (q-p)^{-1} d\varphi_0(q)/dq = \frac{\Gamma p (s\Omega_0)^{1/2}}{(\Omega_0 + sp^2)^2}. \quad (4.14)$$

Let us imagine for a while that we know the function $\rho(p)$ in equation (4.12). Its formal general solution is then given by

$$\zeta(p) = i \int_{p_0}^p dq \rho(q) \exp \left\{ \frac{i}{H} [f(p) - f(q)] \right\} \quad (4.15)$$

where $f(p) \equiv \Omega_0 p + \frac{1}{3} sp^3$.

It is clear that in the case $\text{Im } H > 0$ we must put $p_0 = +\infty$ in (4.15), whereas for $\text{Im } H < 0$ we have to assign $p_0 = -\infty$. Only such a choice permits us to prevent divergency in integral (4.15) and to obtain a solution going to zero as $p \rightarrow \pm\infty$. In the half-line $\text{Im } H = 0, \text{Re } H > 0$ these two functions must coincide, since a unique bound-state solution is expected in this case; however, for $\text{Im } H = 0, \text{Re } H < 0$ we have two different solutions $\zeta_{\pm}(p; H) \equiv \zeta(p; H \pm i0)$ given by

$$\zeta_{\pm}(p; H) = i \int_{\pm\infty}^p dq \rho(q) \exp \left\{ \frac{i}{H} [f(p) - f(q)] \right\}. \quad (4.16)$$

Continuing (4.16) from the real p -axis into the upper half-plane $\text{Im } p > 0$, we can neglect the term $dg_+(p)/dp$ in (4.13) and replace $\rho(p)$ by $\rho_0(p)$ in (4.16) for small enough values of $|H|$. Therefore, for the difference

$$\Delta\zeta(p; H) \equiv \zeta(p; H + i0) - \zeta(p; H - i0) \quad (4.17)$$

we have the asymptotic relation

$$\Delta\zeta(p; H) \cong -D(H) \exp[if(p)/H] \tag{4.18}$$

valid under conditions $\text{Im } p > 0, \text{Im } H = 0, \text{Re } H < 0$ and $|H| \rightarrow 0$. Here

$$D(H) = \int_{-\infty}^{+\infty} dq \rho_0(q) \sin[f(q)/H] \cong (\Gamma/2) \left(\frac{\pi \Omega_0^{1/2}}{|H|s^{3/2}} \right)^{1/2}$$

Recalling that $\zeta(p; H)$ is an odd function of p , one can immediately write down the similar relation for $\text{Im } p < 0$:

$$\Delta\zeta(p; H) \cong D(H) \exp[-if(p)/H].$$

So, in the whole p -plane including the real axis we can write

$$\Delta\zeta(p; H) \cong -2iD(H) \sin[f(p)/H]. \tag{4.19}$$

Inserting (4.19) into the relation

$$\Delta E(H) \equiv E(H + i0) - E(H - i0) = \frac{H}{2\pi} \int_{-\infty}^{+\infty} dp \rho_0(p) \Delta\zeta(p) \tag{4.20}$$

following directly from (4.1) and (4.2), we have finally for $H < 0, |H| \rightarrow 0$

$$\Delta E(H) = \frac{i}{\pi} |H| D^2 = i \frac{\Gamma^2 \Omega_0^{1/2}}{4s^{3/2}} \exp\left(-\frac{4}{3} \frac{\Omega_0^{3/2}}{|H|s^{1/2}}\right) \tag{4.21}$$

in agreement with our previous result (4.7).

5. The scaling limit

In the critical region, thermodynamics is determined by fluctuations with momenta p small compared with Ω_0/s . So, we can drop the term sp^2 in the energy function (3.5). Then, after regularization, it becomes

$$\text{Reg } E = \int \frac{dp}{4\pi} \{ \Omega_0 [\cos 2\varphi_0(p) - \cos 2\varphi(p)] + \Gamma p [\sin 2\varphi(p) - \sin 2\varphi_0(p)] \} - HM \tag{5.1}$$

where

$$\begin{aligned} \text{Reg } E(H, T) &\equiv E(H, T) - E(0, T) \\ M[\varphi] &= M_0 \exp \left\{ \frac{1}{2\pi^2} \int_{-\infty}^{\infty} dp \zeta(p) \int_{-\infty}^{\infty} \frac{dq}{q-p} \frac{d}{dq} [\zeta(q) + 2\varphi_0(q)] \right\}. \end{aligned}$$

As in the previous section, $\varphi_0(p)$ and $\zeta(p)$ denote the zero-field solution and field-induced deviation respectively:

$$\varphi_0(p) = -\frac{1}{2} \arctan[\Gamma p / \Omega_0] \quad \zeta(p) = \varphi(p) - \varphi_0(p).$$

The zero-field magnetization M_0 is given by (3.9).

As we are interested in the case of extremely small magnetic fields, we can linearize the first term in function (5.1) with respect to $\zeta(p)$:

$$\text{Reg } E \cong \int \frac{dp}{2\pi} \zeta^2(p) [\Omega_0^2 + (\Gamma p)^2]^{1/2} - HM. \tag{5.2}$$

5.1. The momentum representation

The variational equation following from (5.2) reads

$$[\Omega_0^2 + (\Gamma p)^2]^{1/2} \zeta(p) = \frac{HM}{\pi} \int_{-\infty}^{\infty} \frac{dq}{q-p} \frac{d}{dq} [\zeta(q) + \varphi_0(q)]. \quad (5.3)$$

Its asymptotical analysis for small magnetic fields H is almost the same as that given in section 4.2 for the dilute limit. We restrict ourselves to sketching the principal points.

Using notation (4.9) we obtain

$$\begin{aligned} -iMH \, d\zeta(p)/dp &= [\Omega_0^2 + (\Gamma p)^2]^{1/2} \zeta(p) \\ &+ MH \left[-dg_+(p)/dp - \pi^{-1} \int_{-\infty}^{\infty} \frac{dq}{q-p} d\varphi_0(q)/dq \right]. \end{aligned} \quad (5.4)$$

It is convenient to rewrite the above equation in terms of the new independent variable $u = \operatorname{arcsinh}(\Gamma p/\Omega_0)$:

$$-iy_s \, d\zeta(u)/du = 2\zeta(u) \cosh^2 u + y_s \rho(u) \quad (5.5)$$

where y_s is the familiar scaling parameter (3.11) proportional to the magnetic field, and

$$\begin{aligned} \rho(u) &= \rho_0(u) - dg_+(u)/du \\ \rho_0(u) &= -\frac{dp/du}{\pi} \int_{-\infty}^{\infty} \frac{dq}{q-p} d\varphi_0(q)/dq = -\frac{1}{2} \tanh u. \end{aligned}$$

The formal solution of (5.5) is given by

$$\zeta(u; y_s) = i \int_{u_0}^u dv \rho(v) \exp \left\{ \frac{i}{y_s} [f(u) - f(v)] \right\} \quad (5.6)$$

where $f(u) = u + \frac{1}{2} \sinh 2u$. As in the dilute limit, we must choose $u_0 = +\infty$ for $\operatorname{Im} y_s > 0$, and $u_0 = -\infty$ for $\operatorname{Im} y_s < 0$. Consider now the case of a negative magnetic field, i.e. $y_s < 0$. In complete analogy with (4.19) we have

$$\begin{aligned} \Delta\zeta(u; y_s) &\equiv \zeta(u; y_s + i0) - \zeta(u; y_s - i0) \\ &\cong -2iD(y_s) \sin[f(u)/y_s] \end{aligned} \quad (5.7)$$

where

$$D(y_s) = \int_{-\infty}^{+\infty} dv \rho_0(v) \sin[f(v)/y_s]. \quad (5.8)$$

The latter integral is given in the limit $y_s \rightarrow -0$ by the asymptotical formula

$$D(y_s) \cong (\pi/6)^{1/2} \exp \left[\frac{1}{3} - \frac{\pi}{2|y_s|} \right] \quad (5.9)$$

describing the contribution of the saddle point $v_0 = i[\frac{\pi}{2} - |\frac{y_s}{2}|^{1/3}]$ of the integrand.

A representation analogous to (4.20) can be written as

$$\Delta E(H) = \frac{|H|M_0}{2\pi^2} \int_{-\infty}^{+\infty} dp \Delta \zeta(p; H) \oint_{-\infty}^{\infty} \frac{dq}{q-p} d\varphi_0(q)/dq. \quad (5.10)$$

Inserting (5.7) and (5.9) into (5.10) for $H < 0$, $|H| \rightarrow 0$, we finally obtain

$$\Delta E(H) = i \frac{|H|M_0}{\pi} D^2 \cong i \frac{|H|M_0}{6} \exp \left[\frac{2}{3} - \frac{\pi}{|y_s|} \right]. \quad (5.11)$$

Thus, in both dilute and scaling limits we observe similar behaviour of the free-energy: it has branching and essential singularities at the point $H = 0$, in agreement with the predictions of the droplet model.

Rewriting (5.11) by use of (3.21) in terms of the initial Ising model gives

$$\text{Im } F(-|H_1| \pm i0) = \pm \frac{|H_1|M_0}{12} \exp \left[\frac{2}{3} - \frac{M_0}{12|H_1|\chi} W \right]. \quad (5.12)$$

Here F is the free-energy per unit site, $W = 1.00096\dots$ is the numerical constant (3.22) and the magnetic susceptibility χ is taken at the zero field.

Though relation (5.12) was derived in the extreme anisotropic limit, it appears to be independent on the anisotropy ratio J_1/J_2 , as implied by the universality hypothesis in the critical region. For the case $J_1 = J_2$ we have

$$\text{Im } F(-|H_1| \pm i0) = \pm \frac{|H_1|[2(\lambda - 1)]^{1/8}}{12} \exp \left[\frac{2}{3} - \frac{\pi k_B T_C (\lambda - 1)^{15/8}}{|H_1| 2^{17/8}} \right]. \quad (5.13)$$

Formulae (2.1) and (3.23) have been taken into account. Apart from the prefactor, the result (5.13) coincides with the droplet model phenomenological estimate (2.5) for the rate of decay of the metastable state. Linear dependence on the magnetic field of the prefactor in (5.13) is also in agreement with predictions of the droplet theory. Such a behaviour is commonly associated with the contribution of the Goldstone excitations on the droplet surface [9, 25]. Thus, we have given a strong support to the applicability of the droplet model in the critical region and to Langer's conjecture cited in the introduction.

5.2. The coordinate representation

In the critical region the coordinate representation is not as convenient as in the dilute limit. Nevertheless, it provides a better insight into the nature of the metastable state. Throughout this section the case of a small negative magnetic field $H < 0$ is considered.

First, let us note that for the arbitrary probe function $\varphi(p)$, function (3.5) gives an exact upper bound for the ground-state energy of the Hamiltonian (3.1). Rewriting (5.2) in the coordinate representation, we obtain the inequality

$$E(H, T) - E(H, 0) \geq \int dx_1 dx_2 \zeta^*(x_1) \zeta(x_2) L(x_1 - x_2) - HM_0 \times \exp \left\{ - \int dx |x| \zeta^*(x) [\zeta(x) + 2\varphi_0(x)] \right\} \quad (5.14)$$

where

$$L(x) = \int \frac{dp}{2\pi} [\Omega_0^2 + (\Gamma p)^2]^{1/2} \exp(ipx).$$

Now let us choose the trial function $\zeta(x)$ as

$$\zeta(x) = C \frac{\text{sign}(x)}{(2d)^{1/2}(2\pi)^{1/4}} \exp\left[-\frac{(|x| - x_0)^2}{4d^2}\right]. \quad (5.15)$$

For $x_0, d \gg \Gamma/\Omega_0$ and small enough constant C the right-hand side in (5.14) reduces to

$$|C|^2 \Omega_0 - HM_0 \exp\{-x_0|C|^2\}. \quad (5.16)$$

The BCS-like state Φ corresponding to (5.15) has an obvious interpretation; it describes the zero-field ferromagnetic vacuum with $2(L/l) = L|C|^2$ extra domain walls intersecting the interval $(0, L)$ of the x -axis. The extra domain-walls bound L/l large-scale clusters of size x_0 . If $(x_0/l) \ll 1$ then these clusters do not intersect with each other and (5.16) transforms into

$$|H|M_0 + (2/l)(\Omega_0 - |H|M_0x_0). \quad (5.17)$$

The first term gives the energy of the ferromagnetic metastable 'ground state'; the second term corresponding to large-scale clusters becomes negative for $x_0 > x_c$. The size of the critical cluster x_c is given by

$$x_c = \frac{\Omega_0}{|H|M_0} = \frac{1}{|y_s|} \frac{2\Gamma}{\Omega_0}. \quad (5.18)$$

Let us map this result to the Ising model. In the extreme anisotropic limit using (3.3) we obtain

$$x_c = \frac{1}{|y_s|} \frac{2a}{(\lambda - 1)}. \quad (5.19)$$

As is known, critical fluctuations in the Ising model with arbitrary J_1, J_2 become isotropic and universal if one describes them in terms of the scaling coordinate $r(m, n)$ given by [26]:

$$r = |z_1 z_2 + z_1 + z_2 - 1| \left\{ \frac{n^2}{z_2(1 - z_1^2)} + \frac{m^2}{z_1(1 - z_2^2)} \right\}^{1/2}. \quad (5.20)$$

Here n and m denote the column and row of a site in the square lattice and

$$z_1 = \tanh(J_1/k_B T_C) \quad z_2 = \tanh(J_2/k_B T_C).$$

For $n = x_c/a$ and $m = 0$, formula (5.20) reduces to

$$r = (x_c/a)|\lambda - 1|$$

in the extreme anisotropic limit $J_1/J_2 \gg 1$, and to

$$r = (x_c/a)|\lambda - 1|/\sqrt{2}$$

for $J_1 = J_2$. Therefore, we obtain an extra factor $\sqrt{2}$ in the latter case:

$$x_c = \frac{1}{|y_s|} \frac{2\sqrt{2}a}{(\lambda - 1)}.$$

By use of (2.1) and (3.23) we rewrite the above formula as ($J_1 = J_2$ is supposed)

$$x_c = \frac{k_B T_C}{|H_1|M_0} \frac{(\lambda - 1)}{2^{1/2}} a = 2R_c \quad (5.21)$$

where R_c is given by (2.4). We see that the size of the critical cluster resulting from the above transfer-matrix analysis is the same as the diameter of the spherical critical droplet given by the phenomenological condensation theory.

6. Conclusions

The present analysis of the 2D Ising model and related fermionic theory supports the droplet theory of condensation in both dilute and scaling limits.

(i) In both cases we observed a very weak essential singularity in the free-energy at the origin $H = 0$.

(ii) When the free-energy is continued analytically into the half-line $H < 0$ it gains a non-zero imaginary part. For the critical Ising model this imaginary part coincides, apart from some prefactor, with the rate of decay of the metastable state estimated in the frame of the phenomenological droplet condensation theory.

(iii) For $H < 0$, $T < T_C$ the metastable 'ground state' of the transfer matrix becomes unstable. In the fermionic analogy it looks like quantum tunnelling of a particle from a potential-well through a barrier of finite size and width. The width of the barrier coincides with the diameter of the critical droplet estimated phenomenologically.

It should be pointed out that in our analysis we have followed the ideology of Langer's paper [9]. However, in contrast to [9] we considered the quantum Hamiltonian (3.1) derived directly from the Ising model transfer matrix. This allowed us to make a quantitative comparison of our results with predictions of the droplet model.

We emphasize once again that we have used the approximate evaluational procedure based on the BCS ansatz for the ground state of the transfer matrix. An important question remaining, is to what extent the results obtained depend on the above approximation? It is unlikely, however, that the main results will change in the exact treatment. The droplet picture can be taken to imply that there exists a path (or paths) in the configurational space that links the metastable state with thermodynamically more preferable configurations. This enables the system to relax in a finite time. The 'narrow throat' of the relaxation is just the critical cluster. In sections 2 and 5 we demonstrated, from different points of view, that in the critical region such paths can be associated with spherical clusters (droplets). If some others paths are also important then they could only give additional channels of relaxation which would increase the rate of decay. Thus, the main conclusions of the droplet model will hold.

Acknowledgments

The author wishes to thank Professor M E Fisher for correspondence introducing the problem of the condensation-point singularity, and also wishes to thank Professor B Nienhuis for helpful discussion, and Professor P A Rikvold for supplying reprints of his works.

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