

FERROMAGNETISM IN TWO DIMENSIONS—SOME MODELS AND APPLICATIONS

by Michael Schick

ABSTRACT

Several physical realizations of two-dimensional models of ferromagnetism are discussed in the context of adsorbed systems. An exact renormalization group treatment of the simplest of these models, the Ising model, is described.

I. INTRODUCTION

I have been interested in phase transitions in lower dimensional systems since studying superconductivity in one dimension as a graduate student of Felix Bloch. This interest has developed at the University of Washington, where I am fortunate to have colleagues expert in both theoretical and experimental Surface Physics. It is in this connection that I have encountered models of ferromagnetism in two dimensions. These models are studied for several reasons. In some cases, the models are intrinsically difficult, such as those that possess a continuous symmetry, and their solution provides insights into other areas encountering similar difficulties. Furthermore, there are interesting experimental systems that can be related in various ways to ferromagnetic models. These systems often provide experimental tests of our understanding of phase transitions that can be obtained nowhere else. Last, there is at least one model that, in addition to being intrinsically difficult and descriptive of real systems, can be solved exactly and thereby serves as a standard against which new theories and methods in Statistical Mechanics can be compared. This is, of course, the two-dimensional Ising model. In what follows, I shall try to illustrate these reasons with a brief discussion of several areas of current activity.

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II. THE PLANAR ROTATOR OR x - y MODEL

In his famous paper of 1930, "Zur Theorie des Ferromagnetismus,"¹ Bloch showed the existence of spin-wave excitations in an isotropic Heisenberg ferromagnet. The excitation of these waves with temperature leads to a decrease of the magnetization, which, for a three-dimensional simple cubic system at low temperature, can be written

$$M(T, \alpha) \cong N\mu \left[1 - \frac{1}{4\pi^2 K^{3/2}} \int_0^\infty \frac{u^{1/2} du}{e^{u+\alpha} - 1} \right],$$

where K is the exchange interaction in units of kT and α is the magnetic energy also in units of kT . In the limit of zero applied field, α vanishes and the integral is simply a constant. The result is the Bloch $T^{3/2}$ law for the decrease of the spontaneous magnetization with temperature. In the two-dimensional Heisenberg model on a quadratic lattice, Bloch noted that the analogous expression is

$$M(T, \alpha) \cong N\mu \left[1 - \frac{1}{2\pi K} \int_0^\infty \frac{du}{e^{u+\alpha} - 1} \right].$$

In the limit of zero applied field the integral diverges so that "no ferromagnetism exists." Similar arguments were thereafter employed by Peierls² to show that there could be no two-dimensional crystalline order at any finite temperature. These results have been strengthened³ and generalized to other systems. In particular one can show that there exists no Bose-Einstein condensation in two dimensions at any finite temperature.⁴ All of these results rest on the existence of a continuous symmetry. The planar model, whose spins have only two components as contrasted to the three components of the Heisenberg spins, is invariant under the continuous symmetry of the two-dimensional rotation group. Thus it has no spontaneous magnetization either.

For years it was inferred from these results that there were no phase transitions in such systems. But in 1966 Stanley and Kaplan⁵ found that high temperature series expansions for the two-dimensional planar model indicated a phase transition at which the magnetic susceptibility would diverge at a finite temperature. The low temperature phase of this system was investigated⁶ using the kind of spin wave analysis Bloch had introduced in 1930. It was found that at low temperatures the magnetization varied as a temperature-dependent power of the applied field. Because at high temperatures the magnetization and field are linearly related, a phase transition was

again indicated. In 1973, Kosterlitz and Thouless,⁷ in a remarkable paper, elucidated the nature of this unusual transition. They showed that whereas one kind of excitation, the spin wave, played the role of destroying any spontaneous magnetization, another kind of excitation was responsible for the transition. This excitation is the vortex, a circular pattern of the planar magnetization completely analogous to the vortex in a fluid. At high temperatures such vortices can be created individually, whereas at low temperatures they appear bound to another vortex of opposite circulation. The presence or absence of free vortices substantially alters the properties of the phase. For example, in a two-dimensional fluid, free vortices will cause a flow to dissipate, whereas bound vortex pairs will not. Thus, the system can exhibit superfluidity at low temperatures although there is no Bose condensation. In the two-dimensional solid the analogues of the vortices are dislocations. Free dislocations move under the application of a shear stress and the system behaves like a liquid. At low temperatures the dislocations are bound and the system possesses a finite shear modulus, although there is no long range crystalline order.

The solution of the problem of interacting vortices was carried out by Kosterlitz and Thouless in an approximate way in 1973. The following year Kosterlitz⁸ applied Renormalization Group methods.

It is quite in keeping with the spirit of this Festschrift to note that a completely different path to the solution of the planar model taken by Luther and Scalapino⁹ employs a method that goes back to another paper by Felix Bloch.

Luther and Scalapino noted that the interacting vortex problem is equivalent to the problem of a one-dimensional Fermi gas with interactions such that electrons can scatter from one side of the Fermi sea to the other. To solve this problem, they employed a method originated by Bloch in 1934 and later developed by Tomonaga.¹⁰ In the paper "Inkohärente Röntgenstreuung in entarteten Fermigas,"¹¹ Bloch argued that as the incoherent scattering of x rays from a Fermi gas was due to its excitations, which were simply density fluctuations, one should be able to treat this problem in a manner analogous to Rayleigh scattering of light. He therefore replaced the Hamiltonian of the Fermi gas by one that describes its excitations, "sound-waves," as bosons. Proceeding with this hydrodynamic Hamiltonian, Bloch was able to obtain the correct result for the incoherent scattering of radiation from a one-dimensional electron gas. In the three-dimensional case, however, the result was in error by a factor of $\sqrt{3}/2$. This method of converting a one-dimensional Fermi gas into a boson problem was the basis for my thesis, which investigated the possibility of flux quantization in a one-dimensional superconductor. The whole subject of superconductivity in one dimension, raised originally by Little,¹² became very active again a few years ago. Luther and Peschel¹³ were able to examine several aspects of

this subject by once more employing these methods. Perhaps the greatest utility of the method, however, arises from the fact that many interesting problems, like the planar model, can be mapped onto the one-dimensional electron gas.¹⁴ Recently Luther¹⁵ has shown how to express the three-dimensional Fermi gas in terms of bosons. Presumably he should be able to calculate the incoherent scattering of x rays and emend the errant factor of $\sqrt{3}/2$.

III. MODELS OF TRANSITIONS ON SURFACES

The models discussed above are all characterized by a continuous symmetry, which is related to their lack of spontaneous magnetization. In this section I wish to describe briefly the application of these same models in the presence of various anisotropies that break the continuous symmetry and permit the appearance of a spontaneous magnetization. Consider first the planar model in the presence of an anisotropy that confines the spins to three directions given by the angles 0 , $2\pi/3$ and $4\pi/3$. The resulting Hamiltonian is that of the three-state Potts model. (A q -state Potts model describes objects that can exist in q states. If nearest-neighbor objects are in the same state, the energy of interaction is E_1 and is E_2 otherwise. The Ising model is a two-state Potts model.) Clearly there are three degenerate ground states in which the spins all point in the same direction. My interest in this problem is through order-disorder transitions on surfaces that, on first sight, appear to have no relation to ferromagnetism in the presence of anisotropies. But, "Lo and Beware"—certainly my favorite phrase of Felix's—there is such a relation. Consider a substrate that presents a triangular array of adsorption sites, graphite for example. Now adsorb upon it an atom that is somewhat larger than one site, so that it costs energy to put two atoms on adjacent sites. An ordered ground state of such a system is shown in figure 1. A glance at this figure reveals that there are in fact three degenerate ground states, just as in the three-state Potts model. It is argued¹⁶ on the basis of symmetry that the critical properties of this order-disorder transition will be identical to those of the ferromagnetic three-state Potts model. The particular system of helium adsorbed on graphite has been well studied, particularly by my colleagues at the University of Washington, Greg Dash and Oscar Vilches, and their students.¹⁷ Recent measurements by Bretz¹⁸ appear to substantiate the identification above.

Other kinds of order-disorder transitions are related to other models of anisotropic ferromagnets by the same arguments of symmetry. The examples that follow are drawn from a complete list I prepared in collaboration with Eytan Domany, James Walker, and Robert Griffiths.¹⁹

Consider the planar model in a four-fold anisotropy; i.e., angles 0 , $\pi/2$, π , $3\pi/2$. Clearly there are four degenerate ground states. Now consider

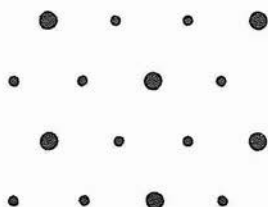


FIG. 1. ONE OF THREE DEGENERATE GROUND STATES of a system of atoms adsorbed on a substrate that presents a triangular array of adsorption sites, and in which the atoms interact via a nearest-neighbor repulsion. Large dots represent occupied sites, small dots unoccupied ones.

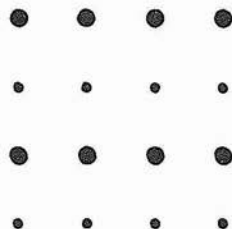


FIG. 2. ONE OF FOUR DEGENERATE GROUND STATES that can be realized by a system adsorbed on a substrate that presents a square array of adsorption sites.

the ground state of an adsorbed system shown in figure 2. In such a system there are also four degenerate ground states; two in which columns are occupied and two in which rows are occupied. The symmetries of these two systems are the same and thus their critical properties are predicted to be the same.^{20,21}

Other transitions of interest correspond to a two-dimensional Heisenberg model in the presence of anisotropy. Consider first one that causes the spins to align in one of four directions that point to the vertices of a tetrahedron. It is easily seen that the Hamiltonian of this system is just that of the four-state Potts model, because the interaction energy of two adjacent spins $S_i \cdot S_j$ is either S^2 , if the spins are in the same state, and $-S^2/2$ otherwise. There are four degenerate ground states, as in the planar model with a four-fold anisotropy, but the symmetry relations among these states are clearly quite different. This new symmetry is, however, identical to that of the four degenerate ground states that can be constructed from figure 3a. Thus adsorbed systems that undergo a transition into such an ordered array are expected to display the critical properties of the four-state Potts model. A second anisotropy of interest is the cubic anisotropy, which causes the Heisenberg spins to align along three mutually perpendicular axes. There are six degenerate ground states and the symmetry relations between them are the same as among the six states that can be obtained from figure 3b. The critical properties of these two-dimensional models, the four-state Potts model and the Heisenberg model with cubic anisotropy, are believed to be different from one another and from the models mentioned previously. This belief can be tested by experiments on physical realizations of these models provided by adsorbed systems.

It should not be thought that the transition to just any ordered structure yields different critical behavior. To the contrary, it is predicted

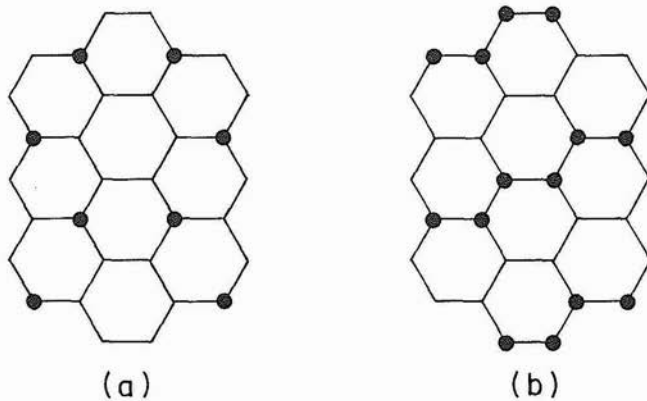


FIG. 3. TWO DIFFERENT KINDS OF GROUND STATES that can be realized by a system adsorbed on a substrate that presents a hexagonal array of sites. Which ground states are realized depends upon the interactions. The degeneracies of the ground states are (a) four, (b) six.

that all critical behavior of such transitions will either be discontinuous or fall into one of a small number of classes, those of the four models above and a few others. One of these is the model of ferromagnetism in the limit of extreme axial anisotropy, the Ising model. The simple symmetry of the two ground states of the ferromagnetic Ising model is shared by several order-disorder transitions. The ground states of two of them are shown in figure 4. These two cases illustrate the idea that different transitions can manifest identical critical properties.

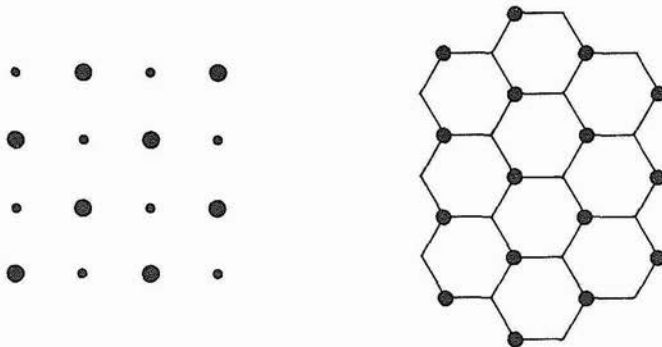


FIG. 4. POSSIBLE GROUND STATES on square or hexagonal arrays of adsorption sites. Each ground state is doubly degenerate.

IV. THE ISING MODEL AND ITS INFINITESIMAL RENORMALIZATION GROUP TRANSFORMATION

My interest in the Ising Model stems from the desire to describe the ordering transition shown by helium adsorbed on graphite, which was discussed above. An obvious Hamiltonian to describe this system is that of a lattice gas in which an atom can exist only on adsorption sites and nowhere else. As a site is either occupied or it is not, there is clearly a simple mapping from this Hamiltonian to that of an Ising model in which a spin at each site is either up or down. The repulsive interaction between atoms translates into an antiferromagnetic interaction between spins. This antiferromagnetic Ising model is, like the ferromagnetic one, exactly soluble only in zero magnetic field, which corresponds to zero magnetization. In the lattice gas analogy this corresponds to the experimentally inaccessible region of a gas density of one atom for every two adsorption sites. At the time at which the experiments on helium were performed that measured the variation of the transition temperature with coverage, there were no approximate solutions of the model described above that predicted this quantity. The few mean-field calculations that had been performed gave incorrect results at the coverage of one-half where the exact result was known. I decided to learn something about the Renormalization Group ideas of Ken Wilson²² by applying them to this problem.²³ Let me recall a few of the relevant ideas here.

In principle, the aim of a calculation in Statistical Mechanics is to obtain the partition function

$$Z = \sum_S e^{-H(K, S)} \quad , \quad (1)$$

where for definiteness I consider the Hamiltonian of a set of spins S with interactions $\{K\}$. The factor of $1/kT$ is absorbed into the Hamiltonian. On calculating the partition function, one knows the free energy and all its singularities. Unfortunately, the trace in Eq. (1) can rarely be performed. Traditional mean-field methods for approximating the sum yield singularities in the approximate free energy that differ significantly from the true singularities. The idea of the Renormalization Group (RG) is to carry out the infinite reduction of the degrees of freedom in Eq. (1) in an infinite number of identical steps. Thus in each step the system of spins S is mapped onto another system of fewer spins S' by means of a projection operator $P(S', S)$; i.e., Eq. (1) is rewritten

$$Z = \sum_{S'} \sum_S P(S', S) e^{-H(K, S)} \quad (2)$$

The partition function is unchanged provided that the projection operator satisfies

$$\sum_{S'} P(S', S) = 1 \quad . \quad (3)$$

The sum over spin S configurations in Eq. (2) produces an operator that depends only on the spins S' . A renormalized Hamiltonian $H'(\{K'\}, S')$ that has the same functional form as $H(\{K\}, S)$, but in which the interaction strengths are renormalized, is defined by

$$e^{-H'(\{K'\}, S')} = \sum_S P(S', S) e^{-H(\{K\}, S)} \quad , \quad (4)$$

so that Eq. (2) takes the form

$$Z = \sum_{S'} e^{-H'(\{K'\}, S')} \quad , \quad (5)$$

analogous to Eq. (1). Thus, starting with H , we obtain a renormalized Hamiltonian H' , which has fewer degrees of freedom. We can apply the projection operator again and obtain the entire trace by iteration. The transformation on the Hamiltonians given by Eq. (4) can also be viewed as a transformation on the set of interactions $\{K\}$ and be written symbolically as

$$\{K'\} = R\{K\} \quad (6)$$

where R is the RG (renormalization group) operator. As the entire trace emerges from repeated application of Eq. (6), these recursion relations contain all the information about the singularities of the partition function. The methods for extracting this information are well known.²² In particular, phase transitions are associated with fixed point solutions $\{K^*\}$ of the nonlinear recursion relations defined by $\{K^*\} = R\{K^*\}$. The critical exponents characterizing the singularities at the transition are obtained from the eigenvalues of the operator R linearized about the fixed point. It is characteristic of RG methods that by focusing on the recursion relations, Eq. (6), they produce information about critical properties first. Other information, such as the behavior of the thermodynamic functions away from the critical region, emerges later.

The great advantage of the RG approach is that the non-analyticities in the free energy emerge from the infinite number of applications of the RG transformation. The recursion relations themselves, however, are in general

analytic. As such they can, if necessary, be more safely approximated without doing great violence to the non-analyticities in the partition function.

A particular RG transformation is determined by specifying the projection operator $P(S', S)$. As an example of a projection operator that maps one spin system in position space onto another, I shall employ one drawn from the original work of 'Dorus Niemeyer and Hans van Leeuwen, who introduced these real space methods.²⁴

Consider an Ising model on a triangular lattice and group all the spins into cells as shown in figure 5. Each spin is assigned to only one cell. The projection operator $P(S', S)$ is written as a product over all cells

$$P(S', S) = \prod_i p(S_1^i, S_2^i, S_3^i; S_i') \quad (7)$$

where the cell projection operator is given by

$$p(S_1, S_2, S_3; S') = \frac{1}{2} [1 + \frac{1}{2} (S_1 + S_2 + S_3 - S_1 S_2 S_3) S'] \quad (8)$$

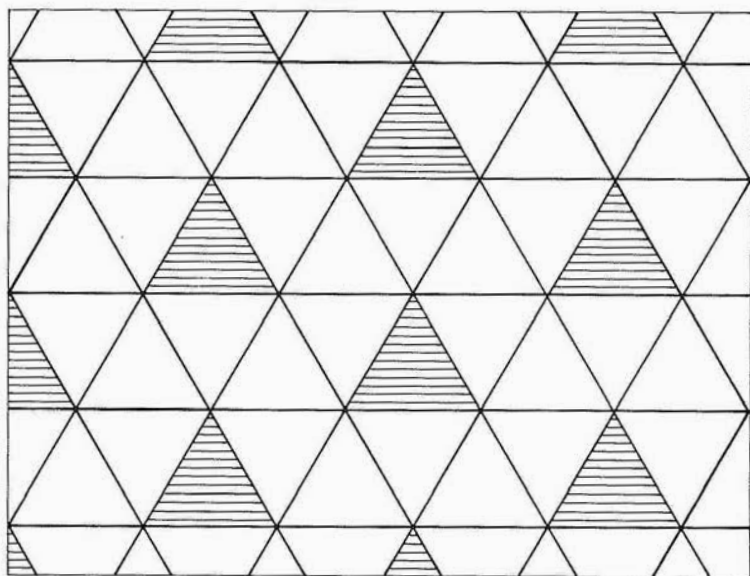


FIG. 5. AN ASSIGNMENT OF SPINS TO CELLS. The cells are shown shaded.

It is easily seen that p maps any configuration of a cell in which a majority of spins are up to the state in which S' is up. As there is one cell spin S' for each three site spins S , the Hamiltonian H' will contain one-third as many degrees of freedom as H . Therefore, the recursion relations Eq. (6) will be finite difference equations. Unfortunately, when Eqs. (7) and (8) are substituted into Eq. (4), the sum can not be carried out, and approximations are necessary.²⁵ As noted earlier, however, the entire procedure ensures that the results of these approximations will, in general, be superior to mean-field methods.

In 1977-78 I spent six months visiting the Technische Hogeschool in Delft, Holland, in order to improve my understanding of the RG via discussions with Hans van Leeuwen and Henk Hilhorst. For all of the considerable success of the position space RG methods, Hans was dissatisfied that, by their very nature, the cell-spin approach decreased the degrees of freedom by a finite amount and led to difference equations. Ideally, one would like to perform an infinitesimal transformation. In such a case the content of the recursion relations would be expressed in the canonical language of theoretical physics, partial differential equations. Such infinitesimal transformations can be carried out in principle by working in momentum space, i.e., with a Hamiltonian expressed in terms of spin Fourier components. Traces are then integrations in momentum space, and, by integrating over an infinitesimal shell of momenta, one can reduce the degrees of freedom infinitesimally. In practice one can not carry out the integration explicitly and approximation methods must be employed.

Henk and Hans and I were able to formulate an infinitesimal RG transformation in real space by proceeding as follows: We considered a two-dimensional triangular lattice of Ising spins, which has a lattice constant a and the shape of an equilateral triangle with side of length L (the unprimed system). This system is mapped onto a similar triangular lattice also of length L but with one fewer lattice site along each edge (the primed system). The lattice constant of the primed system is therefore larger than that of the unprimed one by the fractional amount $\delta a/a = a/L - a$. The number of spins in the two systems differs by a fraction of order a/L , which is infinitesimal in the thermodynamic limit. Figure 6 shows the primed and unprimed system denoted by crosses and circles respectively. We found it convenient to rewrite the basic RG equations, (3) and (4), by introducing the combined Hamiltonian of the S and S' system defined by

$$e^{-H_c(S',S)} \equiv P(S',S)e^{-H(S)}$$

Then Eqs. (3) and (4) can be rewritten in the more symmetric form

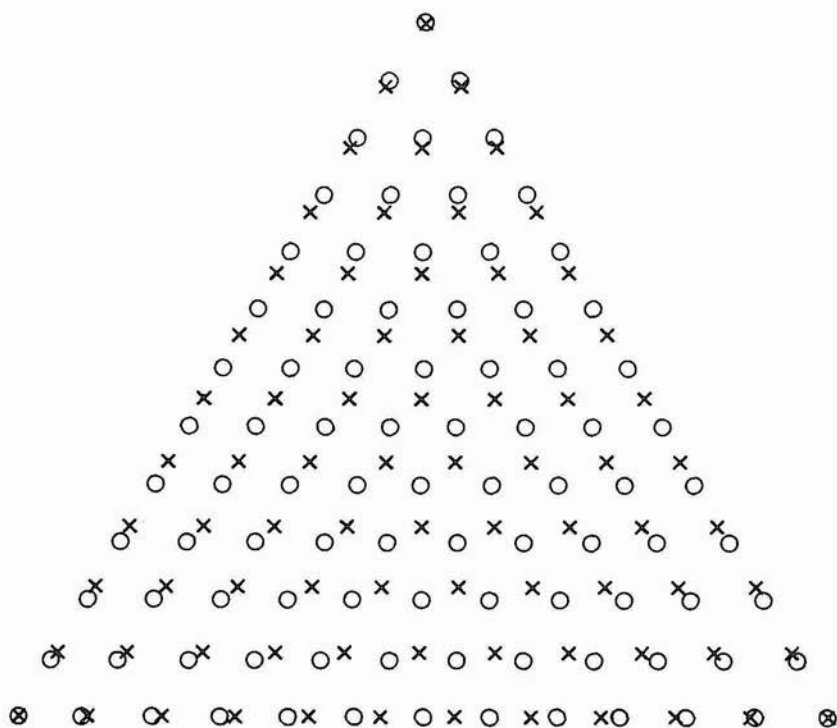


FIG. 6. THE TRIANGULAR SYSTEM OF OPEN CIRCLES IS MAPPED TO THE TRIANGULAR SYSTEM OF CROSSES BY THE RENORMALIZATION GROUP TRANSFORMATION.

$$e^{-H(S)} = \sum_{S'} e^{-H_c(S',S)} \quad , \quad (9)$$

$$e^{-H'(S')} = \sum_S e^{-H_c(S',S)} \quad . \quad (10)$$

The form of $H_c(S',S)$ was at our disposal and we chose a local Hamiltonian that couples nearby spins S and S' . Intuitively we expected that pairs of primed and unprimed spins that are quite close to one another, such as occur near the vertices in figure 6, should be coupled more strongly by H_c than pairs that are not so close as in the center. Thus we expected the coupling constants in H_c to be spatially dependent.

From Eqs. (9) and (10) it is clear that if $H_c(S', S)$ were symmetric in S and S' then H' would equal H and the RG transformation would reduce to the identity. However, if H_c fails infinitesimally from being symmetric, it will generate an infinitesimal difference between H and H' as desired. It turns out that the infinitesimal deviation from symmetry that is needed is provided precisely by the spatial gradients of the coupling constants. When the couplings vary appreciably only over distances of the order L , then $H' - H$ is of the order a/L and therefore infinitesimal in the limit of infinite L . The spatial dependence of H_c led us to consider spatially dependent Hamiltonians H and H' . We all vigorously resisted being led down such a path. It is one thing to consider one-particle interactions that vary with position, as in the case of an inhomogeneous applied magnetic field. It is quite another to consider two-particle interactions that so vary! When we finally yielded, however, we found to our delight that we were able to carry out all operations explicitly and thereby obtain exact RG equations for the Ising model with nearest-neighbor interactions. As we had desired, our recursion relations were non-linear first-order partial differential equations. They appear to be too complicated to solve in general, but we were able to locate the fixed point governing the phase transition. We then linearized the recursion relations about this fixed point and obtained the eigenvalue that demonstrates the logarithmically singular specific heat.²⁶

Henk, Hans, and I spent a morning in Leiden talking with mathematicians about our non-linear partial differential equation. They informed us that little was known about this kind of equation. One thing could be said, however. The solutions of such equations often tended to develop very abrupt changes over very short distances. I smiled as I mused to myself that such solutions of non-linear equations are very "hot" currently. They go by the name of "solitons." The simplest example of a soliton that I know of occurs in ferromagnetic systems. It is called a Bloch wall.²⁷

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