Abstract

We consider the three-dimensional Ising model slightly below its critical temperature, with boundary conditions leading to the presence of an interface. We show how the interface and its fluctuations originate from the fundamental degrees of freedom of the continuum description, namely the particle modes of the underlying field theory. The product of the surface tension and the correlation length yields the particle density along the string whose propagation spans the interface. We also exactly determine the order parameter and energy density profiles across the interface, and show that they are in complete agreement with Monte Carlo simulations we perform. The variance of the interface fluctuations expressed in terms of the correlation length is half of that in two dimensions.
1 Introduction

The notion of interface plays an important role in different areas of physics. In statistical systems the separation of different phases is characterized through the formation of an interface. In particle physics, the simplest description of confinement is in terms of a flux tube (a string) that connects the quarks and whose time propagation spans an interface. Lattice discretization establishes a direct connection between the two problems when duality relates a spin model to a lattice gauge theory, with the Ising model providing the basic example \[1\]. Effective descriptions adopting interfacial fluctuations as the basic degrees of freedom result into capillary wave theory \[2\] on one side, and effective string actions \[3, 4, 5\] on the other.

There must be, however, a deeper level at which the interface and its fluctuations appear as the result of the truly fundamental degrees of freedom of the continuum description, namely the particle modes of the underlying field theory. In this paper we show analytically how this mechanism takes place, taking the three-dimensional Ising model as the natural example where to illustrate the general ideas. The theory accounts for the intrinsic large distance nature of interfacial phenomena, unveils the role of boundary states and of the connectedness structure in momentum space, and constrains the low energy behavior of matrix elements in the field theory.

In the next section, after considering the partition function and the surface tension, we extend our analysis to one-point functions, and the magnetization profile across the interface is one of the results we obtain exactly. In section 3 we present Monte Carlo simulations of the Ising model on the cubic lattice and show that the results we derived analytically are in complete agreement with the numerical data. Finally, in section 4 we discuss several implications of our results and point out lines of further development.

2 From particles to the interface

We consider the Ising model with reduced Hamiltonian

\[
\mathcal{H} = -\frac{1}{T} \sum_{\langle i,j \rangle} s_i s_j ,
\]

where \( s_i = \pm 1 \) is the spin variable located at the site \( i \) of a cubic lattice, and the sum is performed over all pairs of nearest neighboring sites. We focus on the case \( T < T_c \) in which the spin reversal \( \mathbb{Z}_2 \) symmetry of the Hamiltonian is spontaneously broken, i.e.

\[
M \equiv |\langle s_i \rangle| \neq 0 ;
\]

as usual, \( \langle \cdots \rangle \) denotes the average over spin configurations weighted by \( e^{-\mathcal{H}} \). More precisely, we restrict our attention to the temperature range slightly below \( T_c \), where the correlation length \( \xi \) becomes large and the system is described by a Euclidean field theory, which in turn is the continuation to imaginary time of a quantum field theory in \( (2+1) \) dimensions. In the continuum we will denote by \( r = (x, y, z) \) a point in Euclidean space, \( z \) being the imaginary time direction,
Figure 1: Geometry considered for the Ising model below $T_c$, with $L \to \infty$ in the theoretical analysis. Boundary spins on the top and bottom surfaces are fixed to 1 (red) for $x < 0$ and to $-1$ (blue) for $x > 0$, and left free for $x = 0$, so that an interface (one configuration is shown) runs between the axes $x = 0$ on these surfaces.

and by $s(r)$ the spin field. We refer to this translationally and rotationally invariant theory as the bulk theory.

We then focus on the case in which the system is finite in the $z$ direction, with $z \in (-R/2, R/2)$ and $R \gg \xi$. The boundary conditions at $z = \pm R/2$ are chosen in such a way that $s_i = 1$ for $x < 0$ and $s_i = -1$ for $x > 0$; the spins are left unconstrained for $x = 0$. It follows that for $z = 0$ and $R$ large, the magnetization $\langle \sigma(r) \rangle_{++}$ tends to the bulk value $M$ as $x \to -\infty$, and to $-M$ as $x \to \infty$; we denote by $\langle \cdots \rangle_{++}$ configurational averages with the boundary conditions we have fixed. The two pure phases for $x$ large and negative and $x$ large and positive are separated around $x = 0$ by an interfacial region spanned by the fluctuations of an interface running between the straight lines $x = 0$ at $z = \pm R/2$ (Figure 1). It is our goal to determine the one-point function $\langle \Phi(x, y, 0) \rangle_{++}$ of a field $\Phi(r)$.

The boundary conditions at $z = \pm R/2$ correspond in the field theory to boundary states $|B(\pm R/2)\rangle = e^{\pm \frac{R}{2}H}|B(0)\rangle$ of the Euclidean time evolution, with $H$ denoting the Hamiltonian of the quantum system. The boundary states can be expanded on the basis of asymptotic particle states of the quantum field theory. Since they correspond to an excitation localized at $x = 0$ but extending for all values of $y$ (a string), the states in the expansion involve $N \to \infty$ particles,
and this limit will be understood in the following. We then write

\[ |B(\pm R/2)\rangle = \frac{1}{\sqrt{N!}} \int \prod_{i=1}^{N} d\mathbf{p}_{i} (2\pi)^2 E_{\mathbf{p}_{i}} \delta\left(\sum_{i=1}^{N} p_{y,i}\right) |\mathbf{p}_{1}, \ldots, \mathbf{p}_{N}\rangle + \ldots, \]

(3)

where \( \mathbf{p} = (p_x, p_y) \) is the momentum of a particle, \( E_{\mathbf{p}} = \sqrt{p_x^2 + m^2} \) its energy, \( f(\mathbf{p}_1, \ldots, \mathbf{p}_N) \) an amplitude, particle states are normalized as \( \langle \mathbf{p}'|\mathbf{p}\rangle = (2\pi)^2 E_{\mathbf{p}} \delta(\mathbf{p} - \mathbf{p}') \), and the delta function enforces translation invariance in the \( y \) direction. \( m \) is the mass of the lightest particle in the spectrum of the spontaneously broken phase of the bulk field theory. It enters the large distance decay of the spin-spin correlator as \( \langle s(r)s(0)\rangle \sim e^{-m|\mathbf{r}|} \). Comparison with the definition of the correlation length yields

\[ \xi = 1/m. \]

(4)

States involving heavier particles also enter the expansion (3) in the part that we do not write explicitly; they produce only subleading corrections in large \( R \) limit we are interested in. Then we have

\[ Z_{++} = \langle B(R/2)|B(-R/2)\rangle = \langle B(0)|e^{-RH}|B(0)\rangle \]

\[ \sim \frac{L}{2\pi} |f_0|^2 \int \prod_{i=1}^{N} d\mathbf{p}_{i} (2\pi)^2 m \delta\left(\sum_{i=1}^{N} p_{y,i}\right) e^{-R\left(\sum_{i=1}^{N} p_{x,i}^2 + \frac{p_y^2}{2m}\right)} \]

\[ = \frac{L|f_0|^2 e^{-RM\xi}}{(2\pi)^{2(N+1)}} \left(\frac{2\pi}{R}\right)^N \sqrt{\frac{2\pi R}{N}} , \]

(5)

where we used the fact that the large \( R \) limit forces all momenta to be small, defined \( f_0 = f(0, \ldots, 0) \), exploited \( 2\pi\delta(p) = f e^{ipx} du \), and regularized \( \delta(0) \) as \( L/2\pi \), so that in the following \( L \rightarrow \infty \) is the size of the system in the \( y \) direction. Here and below the symbol \( \sim \) indicates omission of terms subleading for large \( R \).

The surface tension is the contribution, for \( R \rightarrow \infty \) and per unit area, to the free energy coming from the presence of the interface. It is then given by

\[ \sigma = -\lim_{R \rightarrow \infty} \frac{1}{LR} \ln Z_{++} = \kappa m^2 = \frac{\kappa}{\xi^2} , \]

(6)

where

\[ \kappa = \frac{N\xi}{L} \]

(7)

is a universal (i.e. lattice independent) number, and \( N/L = \sigma \xi \) is the number of particles per unit length along the string.

The one-point functions are given by

\[ G_{\Phi}(x) \equiv \langle \Phi(x, y, 0)|_{++} = \frac{1}{Z_{++}} \langle B(R/2)|\Phi(x, y, 0)|B(-R/2)\rangle \]

\[ \sim \frac{|f_0|^2}{Z_{++} N!} \prod_{i=1}^{N} \left(\frac{d\mathbf{p}_{i}}{(2\pi)^2 m} \frac{d\mathbf{q}_{i}}{(2\pi)^2 m}\right) \delta\left(\sum_{i=1}^{N} p_{y,i}\right) \delta\left(\sum_{i=1}^{N} q_{y,i}\right) \]

\[ \times \langle \Phi|_{++} \left(\sum_{i=1}^{N} (p_{x,i}^2 + \frac{q_y^2}{2m})\right)^{+\xi} \sum_{i=1}^{N} (p_{x,i} - q_{x,i}) \rangle , \]

(8)
where the matrix element
\[ F_\Phi(p_1, \ldots, p_N|q_1, \ldots, q_N) = \langle p_1, \ldots, p_N|\Phi(0)\rangle\langle q_1, \ldots, q_N \rangle \]
\[ = \langle p_1, \ldots, p_N|\Phi(0)\rangle\langle q_1, \ldots, q_N \rangle_c + (2\pi)^2 m \delta(p_1 - q_1)\langle p_2, \ldots, p_N|\Phi(0)\rangle\langle q_2, \ldots, q_N \rangle_c + \ldots \]
is evaluated for small momenta. In the second line we take into account its decomposition in connected and disconnected parts, the latter originating from annihilation of particles on the left with particles on the right; the subscript \( c \) denotes connected matrix elements, and the dots indicate that all possible annihilations have to be included. It follows from (8) that each power of momentum in the integral contributes a factor \( R^{-1/2} \) to the one-point function. Since each annihilation in (9) produces a delta function \( \delta(p_i - q_j) \), and then a factor \( R \), the leading contribution to (8) for large \( R \) is obtained maximizing the number of annihilations. Since \( N \) annihilations leave an \( x \)-independent term \( C_\Phi \), the interesting term is that with \( N - 1 \) annihilations. Taking also into account that there are \( N!N \) ways of performing \( N - 1 \) annihilations, we finally obtain
\[ G_\Phi(x) \sim C_\Phi + \frac{\kappa R}{(2\pi)^2 m} \int dp dq \delta(p_y - q_y) F_\Phi(p|q) c^{-\frac{R}{4m}(p^2 + q^2) + i x(p_x - q_x)} . \]
If \( F_\Phi(p|q) \equiv \langle p|\Phi(0)\rangle\langle q \rangle_c \) behaves as momentum to the power \( \alpha \), the \( x \)-dependent part of (10) behaves as
\[ R^{-(1+\alpha)/(2)} . \]
We also have that the integral term in (10) is even (resp. odd) in \( x \) when \( F_\Phi(p|q)|_{p_y = q_y} \) is even (resp. odd) under exchange of \( p_x \) and \( q_x \).

The fact that the magnetization profile \( G_s(x) \) has to be an odd function of \( x \) interpolating between \( M \) and \( -M \) fixes \( C_s = 0 \) and \( \alpha_s = -1 \). This leads to
\[ F_s^c(p|q) = c_s \left[ (p - q)^2 \right]^{-1/2} . \]
Upon insertion in (10) the delta function leaves a pole in \( p_x - q_x \) that is conveniently canceled by differentiation with respect to \( x \). Performing the momentum integrations and integrating back in \( x \) yields
\[ G_s(x) = -M \text{ erf}(\eta) , \]
\[ \eta = \sqrt{\frac{2}{R \xi}} x , \]
and \( c_s = -2iM/\kappa \).

The energy density profile \( G_\epsilon(x) \) has to be an even function of \( x \), but the value of \( \alpha_\epsilon \) is not obvious a priori and remains as a parameter. We then write
\[ F_\epsilon^c(p|q) = c_\epsilon \left[ (p + q)^2 \right]^{\alpha_\epsilon/2} . \]
The integrations in (10) are easily performed passing to the variables \( p \pm q \) and yield the result
\[ G_\epsilon^c(x) \equiv G_\epsilon(x) - C_\epsilon \propto \frac{\xi - \xi_x}{(R/\xi)^{(1+\alpha_\epsilon)/2}} e^{-\eta^2} , \]
where \( X_\epsilon \) is the scaling dimension of \( \epsilon(x) \), so that the proportionality constant we omit is dimensionless.
3 Comparison with Monte Carlo simulations

We now compare the theoretical predictions with Monte Carlo simulations of the Ising model on the cubic lattice. The numerical data for the bulk quantities entering our analysis are all already contained in [6] within an accuracy sufficient for our purposes. In particular, we have $1/T_c = 0.2216544(3)$ (corresponding to $T_c \approx 4.51153$), $\nu = 1/(3 - X_e) = 0.6310(15)$, $\beta = 0.3270(6)$. The critical exponents $\nu$ and $\beta$ rule the behavior of the correlation length and spontaneous magnetization for $T \to T_c^-$ as (see e.g. [1])

$$\xi \simeq \xi_0 (T_c - T)^{-\nu},$$

$$M \simeq B (T_c - T)^\beta,$$

respectively. The critical amplitude $\xi_0$ can be obtained from a fit of the data listed in Table 3 of [6] and reads $\xi_0 \approx 0.668$. Subleading corrections to (18) are not completely negligible in the temperature range we consider below, and then we use Eq. (40) of [6] that takes them into account.

We can then focus on the numerical determination of the profiles for the magnetization and the energy density for which we derived the analytic expressions (13) and (16). The system is simulated in the volume $x \in (-L/2, L/2)$, $y \in (-L/2, L/2)$, $z \in (-R/2, R/2)$, with $L$ sufficiently larger than $R$ in order to take into account that the theory we want to compare with refers to $L \to \infty$. The boundary spins are fixed as previously described for $z = \pm R/2$, and are left free on the other boundaries. Lattice sizes with $L$ up to 121 and $R$ up to 41 are considered; lengths entering simulations are expressed in units of the lattice spacing. Technical details of the simulations are similar to those of our recent studies of two-dimensional Potts models [7] and of the three-dimensional XY model [8]. In particular, the standard Metropolis algorithm [9] is used. Thermal averages are computed over a few realizations with different sets of random numbers, with each run being of length $10^7$ Monte Carlo steps per site. Error bars normally do not exceed the size of the symbols in figures 2 and 3 below, and are not depicted in those figures.

The profiles are determined along the axis $y = z = 0$. Figure 2 shows that the Monte Carlo data we obtain for the magnetization for different values of $T$ and $R$ collapse on a single profile once divided by $M$ and plotted as a function of the scaling variable (14). The figure also shows that this numerically determined profile agrees very well with the analytical result $-\text{erf}(\eta)$, see (13). It is worth stressing that the comparison contains no free parameter.

For the energy density, which on the lattice corresponds to $\epsilon_i = \sum_{j \sim i} s_i s_j$, with the sum running over the nearest neighbors of site $i$, we consider the profile $G_\epsilon(x)$, which we obtain subtracting the constant term we read from the data. Figure 2 shows that the Monte Carlo data for $G_\epsilon(x)/G_\epsilon(0)$ exhibit the expected collapse when plotted against $\eta$; agreement with the analytic result $e^{-\eta^2}$ is also very good, again without free parameters. From the $R$-dependence of the data for $G_\epsilon(0)$ we estimate $(1 + \alpha_\epsilon)/2 \approx 0.27$ for the exponent appearing in (16).

We also recall that the universal number $\kappa$ appearing in (6) has been numerically determined.
Figure 2: Analytic result (13) for the magnetization profile (continuous curve) and the corresponding Monte Carlo results (data points). The latter are obtained for $T = 4.2, R = 17, L = 55$ (squares), $T = 4.3, R = 31, L = 91$ (circles), and $T = 4.4, R = 41, L = 121$ (pentagons). The scaling variable $\eta$ is given by (14). In the literature. The Monte Carlo result $\kappa = 0.1084(11)$ was obtained in [10].

4 Discussion

In this paper we have considered the three-dimensional Ising model slightly below the critical temperature $T_c$, with boundary conditions enforcing the presence of an interface running between two straight lines separated by a distance $R$ much larger than the bulk correlation length $\xi$. We have shown analytically how the interface emerges from the study of the bulk field theory supplemented with the required boundary conditions. In particular, we showed how the string whose imaginary time propagation spans the interface is related to the particle modes of the field theory, and how the surface tension is expressed in terms of the particle density along the string. We then exactly determined the order parameter and energy density profiles, and exhibited the complete agreement of these analytical results with Monte Carlo simulations we performed.

Our theoretical derivation shows that the interface exhibits Gaussian fluctuations that are not due to displacements of the interface as a whole (which would require an infinite amount of energy), but to localized excitations that, at leading order in $1/R$, involve single particle modes. These particles propagate in the $(2+1)$-dimensional space (both momentum components $p_x$ and $p_y$ are non-zero), but the configurational average distributes them along the surface in such a way to finally yield the translational invariance of the profiles in the $y$ direction required by the boundary conditions.

This mechanism, which essentially involves the connectedness structure of the matrix ele-

\footnote{Multi-particle modes yielding subleading terms in $1/R$ can also be derived from [8].}
ments of local fields on particle states, effectively implements a form of dimensional reduction in the large $R$ limit of the configurational average. This is why the magnetization profile (13) is analogous to that in two dimensions, i.e. in absence of the $y$ axis in Figure 1. The profile in two dimensions was obtained from the lattice solution of the Ising model in [11] (see also [12]), and more recently in field theory in [13]. The dimensional interplay holds up to an important difference: the factor $\sqrt{2}$ in (14) is absent in two dimensions. The origin of this difference is clear in field theory. In two dimensions the particles below $T_c$ have a topological nature – they are kinks – and the spin field couples only to topologically neutral states, of which the kink-antikink state is the lightest. This is why in two dimensions the relation (4) is replaced by $\xi = 1/2m$. It follows that in three dimensions the variance of the interfacial fluctuations expressed in terms of $\xi$ – the measurable length scale of the statistical system – is half of that in two dimensions.

The light that the results of this paper shed about these mechanisms is particularly interesting, since it implies the relevance in three dimensions of results recently obtained in two dimensions. These include those of [13] for the relation between subleading corrections in $1/R$ and the internal structure of the interface, those of [14, 15] for interfacial wetting [16], those of [17, 18, 19] for the effects of system geometry, and those of [20] for the long range correlations induced by the presence of the interface. The detailed investigation of these points will provide relevant directions of development of the exact theory of interfaces in three dimensions introduced in this paper.

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