Non-equilibrium Dynamics of Finite Interfaces

D. B. Abraham, T. J. Newman and G. M. Schütz

Department of Physics, University of Oxford,
Theoretical Physics, 1 Keble Road, OX1 3NP, U.K.

We present an exact solution to an interface model representing the dynamics of a domain wall in a two-phase Ising system. The model is microscopically motivated, yet we find that in the scaling regime our results are consistent with those obtained previously from a phenomenological, coarse-grained Langevin approach.

PACS numbers: 75.40.Gb, 05.50.+q, 05.70.Ln
The study of the magnetisation profile between coexistent phases in models of subcritical uniaxial ferromagnets (and their analogues) has generated important and unexpected theoretical advances. A typical example is the existence of spatial fluctuations of the interface location so large that they diverge with system size. Phenomenologically speaking, these fluctuations are generated by capillary waves described in a continuum theory of an interface which is a sharp dividing surface between oppositely magnetised phases, controlled by a somewhat arbitrary short range spatial cutoff [1]. Against this, one has to set the density functional theories going back to van der Waals and Maxwell [2] which do not give divergent spatial interface fluctuations. It is fortunate that both exact and rigorous results are available for the planar Ising model which resolve the conflict in favour of the large spatial fluctuations [3], but have yet to resolve the problem of local interface structure. The conclusions of the exact calculation were recaptured in a Helmholtz fluctuation theory for the phase separating surface [4] which brings in the concept of interfacial stiffness and which is valid in a spatially coarse-grained sense, much as in Widom scaling theory [5]. These fluctuations are an essential ingredient in the statistical mechanics of a number of surface phase transition phenomena [6]. In this letter we focus on dynamical aspects of these fluctuations by studying an exactly solvable model on a finite lattice.

First, we recall an equilibrium result which helps motivate the model itself and an earlier phenomenological treatment. Suppose in a zero-field planar Ising ferromagnetic model, the interface between coexistent phases is established and localised in laboratory-fixed axes by specifying the boundary spins as shown in Fig. 1. The straight line of length $2L$ connecting the spin-flip points is the Wulff shape for the interface. It is convenient to define coordinates parallel and perpendicular to this line, with origin at its centre. Let the thermodynamic limit of infinite strip length be taken first. Then denoting the magnetisation at $(x, y)$ by $m(x, y/L)$ we have for $-1 < \alpha < 1$
\[
\tilde{m}(\alpha, \beta) = \lim_{L \to \infty} m(\alpha L, \beta L^\delta / L) = m^* \Phi \left( \frac{b(\vartheta, T) \beta}{\sqrt{1 - \alpha^2}} \right) \quad (\delta = 1/2) \quad (1)
\]

where \( m^* \) is the spontaneous magnetisation, \( \Phi(x) \) is the error function \( \text{erf}(x) \) and \( b(\vartheta, T) = \sigma(\vartheta) + \sigma''(\vartheta) \) is the surface stiffness. (Here \( \sigma(\vartheta) \) is the angle-dependent surface tension.) On the other hand, one has \( \tilde{m}(\alpha, \beta) = 0 \) \( (m^* \text{ sign}(\beta)) \) for \( \delta < 1/2 \) \( (> 1/2) \).

In this letter we study the dynamical case with a new exact result. In order to generalise to the dynamical case we need to define a model with dynamics appropriate to the physical system described above. We shall see that our model reproduces the equilibrium result (1) in the infinite time scaling limit. To motivate our model, note that as \( T \to 0 \), \( b(\vartheta) > 0 \) (strictly) provided \( \vartheta \neq 0, \pm \pi/2 \); for \( \vartheta = 0, \pm \pi/2 \), \( b(\vartheta, T) \to 0 \) as \( T \to 0 \). This is a primitive example of facetting. At \( T = 0 \), the Peierls contours reduce to paths connecting \((-L, 0)\) to \((L, 2L \tan \vartheta)\) which either step to the right or upwards \((\tan \vartheta > 0)\); all such paths are degenerate. They separate regions of opposite magnetisation; since \( T = 0 \), this magnetisation is of unit magnitude. In this case, the theorem is related to normal fluctuations in coin tossing. Let us now concentrate on the case \( \tan \vartheta = 1 \), with an initial sawtooth configuration as shown in Fig. 2. For later convenience we have rotated the system by 45 degrees.

At \( T = 0 \), any minimum energy path can be represented as a sequence \( S = \{n_{-L+1}, n_{-L+2}, \ldots, n_L\} \) of \( 2L \) binary numbers \( n_k \) where \( n_k = 1 \) if the \( k^{th} \) segment of the interface steps upwards \((\text{in an angle of 45 degrees})\) and \( n_k = 0 \) if the steps goes downwards \( (\text{see Fig. 2})\). One can think of \( n_k \) as an occupation number which is related to the interface height \( h_k \) in the rotated system by \( 2n_k - 1 = h_k - h_{k-1} \). The configuration at any time \( t \) is then given as a time-slice \( S(t) = \{n_k(t) : k = -L + 1, \ldots, L\} \) and the dynamics are
given by specifying rules connecting $S(t+1)$ to $S(t)$.

We take particle-hole exchange on neighbouring lattice sites with probability $p$, but leave pairs of particles or holes unchanged. This corresponds to single spin-flips at local extrema of the interface. The nearest neighbour interaction makes it advisable to update on alternating sublattices at subsequent time-steps. This updating scheme turns our model into a cellular automaton which is related to the six vertex model on a lattice oriented at 45 degrees: take $n_k = 1$ (resp. $=0$) to be an upwards (resp. downwards) pointing arrow as in Fig. 3 where we show the ice-vertices, the corresponding dynamical events and their weights in the particle-hole picture. With $0 \leq p \leq 1$, the two row-to-row transfer matrices in the $(1,1)$ direction generate a stochastic time evolution satisfying local detailed balance.

The transfer matrix can be written as

$$T = T^{\text{even}} T^{\text{odd}} = \prod_{j=-L+1}^{L-1} T_{2j} \prod_{j=-L+1}^{L} T_{2j-1}$$  \hspace{1cm} (2)

with $T_j = 1 - pe_j$, $e_j = (\sigma^x_j \sigma^x_{j+1} + \sigma^y_j \sigma^y_{j+1} + \sigma^z_j \sigma^z_{j+1} - 1)/2$, the $\sigma^{x,y,z}$ being the Pauli matrices. We choose $n_k = (1 - \sigma^z_k)/2$, a vacuum $|0\rangle$ with $n_k|0\rangle = 0$.

The initial state is the $L$-particle state $|v\rangle = (|1,0,1,0,\ldots\rangle + |0,1,0,1,\ldots\rangle)/2$.

The displacement of the interface at $(x,t)$ is thus

$$h(x,t) = \sum_{k=-L+1}^{x} (1 - 2n_k(t))$$  \hspace{1cm} (3)

with zero mean by spin-reversal symmetry, but with

$$w^2(x,t) = \langle (h(x,t))^2 \rangle = 4 \sum_{k,j=-L}^{x} \langle L|n_k n_j T^t |v\rangle - (x + L)^2 .$$  \hspace{1cm} (4)

Here $\langle L |$ is the out state which sums over all eigenstates of the $n_k$ with
particle number \( N = L \), giving each such state equal weight. Evidently

\[
\langle L \rangle = (L!)^{-1/2} \langle 0 | (S^+)^L \rangle \tag{5}
\]

where \( S^\pm = \sum s_k^\pm \) and \( s_k^\pm = (\sigma_k^x \pm i\sigma_k^y)/2 \). Using the commutator

\[
[(S^+)^L, n_k] = L s_k^+(S^+)^{L-1} \tag{6}
\]

and the \( SU(2) \) symmetry of \( T \), (5) and (6) together with (4) give

\[
w^2(x, t) = 4 \sum_{k,l=\pm 1}^L \sum_{p,q=-L+1}^L M_1(k, l; p, q|t) M_2(p, q) + 2(x + L) - (x + L)^2 \tag{7}
\]

where

\[
M_1(k, l; p, q|t) = \langle 0 | s_k^+ s_l^+ T^t s_p^- s_q^- | 0 \rangle \tag{8}
\]

is a matrix element in the 2-particle sector and

\[
M_2(p, q) = \langle 0 | s_p^+ s_q^+(S^+)^{L-2} | v \rangle / (L - 2)!
\]

contains the information coming from the initial condition. Using (3) and the expression for \( | v \rangle \) above, it follows that \( M_2(p, q) = 1/2 \) for \( (p - q) \) even and =0 otherwise. Thus

\[
w^2(x, t) = 2 \sum_{k,l=\pm 1}^L \sum_{p,q=-L+1}^L M_1(k, l; p, q|t) + 2(x + L) - (x + L)^2 \tag{10}
\]

which is an enormous simplification of (4). Expressions for higher moments can be obtained in a similar way.

We study first the infinite-time limit, thus deriving the static magnetisation \( m(x, y) = 1 - 2\langle \Theta(h(x) - y) \rangle \) where \( \Theta(s) \) is the Heavyside step function. The (normalised) \( L \)-particle steady state of the system is \( | L \rangle / B(2L, L) \) with
the binomial coefficient \( B(m, n) = m!/(n!(m-n)!) \). A short calculation yields

\[
m(x, y) = \frac{\text{sign}(y)}{B(2L, L)} \sum_{k=-y+1}^{y-1} B(L - x, \frac{L - x}{2} - k) B(L + x, \frac{L + x}{2} + k) \quad . \tag{11}
\]

In the scaling limit \( x = \alpha L \) and \( y = \beta L^\delta / L \) one obtains again the scaling form (\text{I}) with surface stiffness \( b = 1 \) and \( m^* = 1 \).

Now we turn to the dynamics. For an exact calculation of the transition amplitudes (\text{8}) one may either derive difference equations in \( t \) and \( x \) as in (\text{I}) or use the Bethe ansatz (\text{10}). It simplifies matters if (a) we pass to a continuous-time formulation by taking the limit \( p \to 0 \) and \( t \to \infty \) such that \( \tau = 2tp \) remains fixed and (b) by taking periodic boundary conditions (i.e. by studying the transfer matrix \( T_P = T_L T \) instead of \( T \)). Neither of these simplifications is expected to be of physical relevance to the system (8, 9).

Note, however, that \( w^2(x, \tau) \) now measures fluctuations in the height differences \( h(x, \tau) - h(-L, \tau) \). By taking this infinite time limit the evolution operator \( T_P \) becomes the evolution operator \( \exp(-H\tau) \) of the symmetric simple exclusion process (\text{11}), but defined on a finite lattice with \( 2L \) sites.

\( H = -\frac{1}{2} \sum_{k=-L+1}^{L} e_k \) is the quantum Hamiltonian of the isotropic ferromagnetic Heisenberg model in one dimension.

In order to derive an exact expression for the height fluctuations (\text{10}) as a function of \( x \) and \( \tau \) we define the translationally invariant states

\[
|0, r\rangle = \frac{1}{\sqrt{2L}} \sum_{k=-L+1}^{L} s_k^+ s_{k+r}^+ |0\rangle \quad (1 \leq r \leq L) \quad . \tag{12}
\]

Note that \( |r\rangle, |-r\rangle \) and \( |r + 2L\rangle \) are identical and \( \langle r|r\rangle = 1 + \delta_{r,L} \). Using
translational invariance of $H$ one can write with these conventions

$$w^2(x, t) = 2 \sum_{r=-L+1}^{L-1} \sum_{R=1}^{x-1} (L+x-r)\langle 0, r|\exp (-H\tau)|0, 2R\rangle + 2(x+L)-(x+L)^2$$

(13)

The matrix elements $c_R(r, \tau) = \langle 0, r|\exp (-H\tau)|0, R\rangle$ satisfy the differential-difference equation

$$\frac{\partial}{\partial \tau} c_R(r, \tau) = c_R(r + 1, \tau) + c_R(r - 1, \tau) - 2c_R(r, \tau) \quad (r > 1)$$

$$\frac{\partial}{\partial \tau} c_R(r, \tau) = c_R(r + 1, \tau) - c_R(r, \tau) \quad (r = 1)$$

(14)

with initial condition $c_R(r, 0) = \delta_{r,R}(1 + \delta_{R,L})$. We note in passing that one may obtain these equations of motion directly from a master equation formulation of the problem [12], indicating that the usual stochastic formulation of the exclusion process is isomorphic to the continuous-time limit of the model defined above. Taking into account the periodicity and reflection properties of the states $|0, r\rangle$ one finds

$$c_R(r, \tau) = e^{-2\tau} \sum_{m=-\infty}^{\infty} \left( I_{r-R+(2L-1)m}(2\tau) + I_{r+R-1+(2L-1)m}(2\tau) \right)$$

(15)

where $I_p(x)$ are modified Bessel functions. With (13) and

$$\sum_{m=-\infty}^{\infty} I_{p+mN}(z) = \frac{1}{N} \sum_{k=0}^{N-1} e^{z \cos (2\pi k/N)} e^{-2\pi i kp/N}$$

(16)

we finally obtain

$$w^2(x, \tau) = \frac{4}{2L-1} \sum_{k=1}^{2L-1} \left( 1 - (-1)^k \frac{\cos 2\pi k x/(2L-1)}{\cos \pi k/(2L-1)} \right) \frac{1 - e^{-2(1-\cos 2\pi k/(2L-1))\tau}}{1 - \cos 2\pi k/(2L-1)^2} + \epsilon(x)$$

(17)

where $\epsilon(x) = 0 \ (1)$ for $x$ even (odd).

It is instructive to compare this exact result with that obtained from a phenomenological approach based on a Langevin description [13] - the dy-
namics of the interface are assumed to be described by the following additive noise Langevin equation

$$\partial_t h_j = \frac{1}{2}(h_{j-1} + h_{j+1} - 2h_j) + \eta_j(t)$$  \hspace{1cm} (18)

where $\eta_j(t)$ is the usual gaussian white noise. One easily obtains

$$w^2(x, \tau) = \frac{4}{2L} \sum_{k=1}^{2L} \left(1 - (-1)^k \cos 2\pi k x/(2L)\right) \frac{1 - e^{-2(1-\cos 2\pi k/(2L))\tau}}{1 - \cos 2\pi k/(2L)} .$$  \hspace{1cm} (19)

The similarity between the two expressions (17) and (19) is striking, considering the vast simplifications inherent in the phenomenological Langevin model.

It is interesting to take the scaling limit of the above expressions, i.e. we take $x, \tau, L \to \infty$ with $\alpha \equiv x/L$ and $u \equiv \tau/L^2$ fixed. We then find from both (17) and (19).

$$\lim_{L \to \infty} \frac{w^2(\alpha, u)}{2L} = 2 \int_0^u ds \left(\theta_3(0) - \theta_3(\pi(\alpha - 1)/2))\right)$$  \hspace{1cm} (20)

where $\theta_3(v) \equiv \theta_3(v, q)$ is the theta function with nome $q = \exp(-\pi^2 u)$. We obtain the following asymptotic forms of the scaling function: for arbitrary $\alpha$ and $u \to \infty$ we have

$$\lim_{L \to \infty} \frac{w^2(\beta, u)}{L} = \frac{1}{4}(1 - \alpha^2) - \frac{2}{\pi^2}(1 + \cos \pi \alpha) e^{-\pi^2 u}$$  \hspace{1cm} (21)

and for $\alpha = 0$ and $u \ll 1$ we have

$$\lim_{L \to \infty} \frac{w^2(0, u)}{L} = 2 \sqrt{u/\pi} .$$  \hspace{1cm} (22)

The fact that the scaling function evaluated from the exact dynamics is
identical to that obtained from the Langevin description (18) is very surprising, since the latter approach completely neglects the strong dynamical constraints of the original model, i.e. the restricted possible values of neighbouring height differences.

We may gain some insight into this result by considering the corresponding particle dynamics for the Langevin description (18). The appropriate particle picture is one of symmetric diffusion with no exclusion, the particles to be interpreted as units of height gradient. One may derive an exact Langevin equation for this non-exclusive particle process which then may be mapped to (18) in the height variables. This is done by Taylor expanding the master equation for the distribution $P(\{n_j\},t)$ (where $n_j$ is the unrestricted occupation number at site $j$), thus deriving a Fokker-Planck equation in the Stratonovich representation. The corresponding Langevin equation for the occupation numbers may then be mapped to the original height variables reproducing (18). It is of interest to compare this to an exact Langevin equation for the exclusion case that we have studied in this paper. Using the stochastic Grassmann variables introduced in [12] one may derive an exact Langevin equation for the ‘height’ variables $\{f_j\}$ of the form

$$\partial_t f_j = \frac{1}{2} (f_{j-1} + f_{j+1} - 2f_j)(1 + 2^{1/2}\eta_j(t))$$

(23)

(These variables are of Grassmann type, but are simply related to the original height variables $\{h_j\}$). The essential difference between this exact Langevin equation and that given in (18) is the appearance of multiplicative noise, which appears to be irrelevant in the scaling regime. Therefore the equivalence between the scaling functions for the restricted and unrestricted interface models may be thought of as an equivalence between symmetric diffusion with or without exclusion - even for non-zero values of the scaling variable $u$. 

8
We have yet to derive a full dynamical version of the magnetisation \((1)\) for our model, as was done in \([13]\) for the Langevin dynamics with additive noise. To this end, one has to calculate all higher even moments of the height fluctuations. (The odd moments all vanish due to spin reversal symmetry.) As regards our model and the phenomenological model of Ref. \([13]\), it is unclear whether the identity in the scaling forms of the height fluctuations derived above persists beyond the second moments. However, having shown that in the scaling limit both the static magnetisation \(m(x, y)\) and \(w^2(x, t)\) coincide, we conclude that the simplified Langevin dynamics with additive noise represent a qualitatively and quantitatively adequate approach to this problem in large but finite systems in the scaling region.

We note that our discussion of the dynamics is limited to the continuous time limit defined above. One expects no difference in the scaling form \((20)\) for non-zero hopping rate \(p\) (except that the natural scaling variable is now \(t/L^2\) as opposed to \(\tau/L^2\). However, the continuous time limit defined by \((1-p) \to 0, t \to \infty\) with \(\tau' = t(1-p)\) fixed has qualitatively distinct scaling behaviour since it corresponds to a ‘relativistic’ limit of the dynamics \([9]\). The behaviour of the interface fluctuations for this case will be discussed elsewhere \([14]\).

In summary, we have investigated a particular stochastic model of a finite interface for which the dynamics act on the microscopic degrees of freedom, rather than on the phenomenologically specified, coarse-grained microscopic variables as is the case in Langevin theories. Nevertheless, results obtained so far for our model agree with the earlier Langevin theory, encouraging its continued use in appropriate contexts where the truly microscopic theories are not analytically amenable.

The authors acknowledge financial support from the SERC, and the hos-
pitality and stimulating environment of both the Isaac Newton Institute, Cambridge and the Weizmann Institute. They thank E. Domany, P. Ferrari, C. Kipnis and E. Presutti for encouraging remarks.
References

[1] F. P. Buff, R. A. Lovett and F. H. Stillinger, Phys. Rev. Lett., 15, 621 (1965).

[2] S. Fisk and B. Widom, J. Chem. Phys. 50, 3219 (1969).

[3] D. B. Abraham and P. Reed, Phys. Rev. Lett. 33, 377 (1974); Comm. Math. Phys. 49, 35 (1976).

[4] D.S. Fisher, M.P.A. Fisher and J.D. Weeks, Phys. Rev. Lett. 48, 369 (1982).

[5] B. Widom, J. Chem. Phys. 43, 3892 and 3898 (1965).

[6] M. E. Fisher, J. Stat. Phys. 34, 667 (1984).

[7] D. B. Abraham and P. J. Upton, Phys. Rev. B 37RC, 3835 (1988).

[8] D. Kandel, E. Domany and B. Nienhuis, J. Phys. A, 23, L755 (1990).

[9] G. M. Schütz and S. Sandow Phys. Rev. E to appear.

[10] C. Destri and H. J. de Vega, Nucl. Phys. B 290, 363 (1987).

[11] T. Ligget, ”Interacting Particle Systems”, New York, Springer Verlag (1985).

[12] S. E. Esipov and T. J. Newman, J. Stat. Phys. 70, 691, (1992).

[13] D. B. Abraham and P. J. Upton, Phys. Rev. B 39, 736 (1989).

[14] D. B. Abraham, T. J. Newman and G. M. Schütz (in preparation)
List of Figure Captions

Fig. 1: The Wulff profile separating regions of opposite magnetisation. The lower (upper) region has negative (positive) magnetisation.

Fig. 2: The mapping between the restricted interface and the particle exclusion process. In a) we indicate the initial condition of a flat interface corresponding to alternating sites in the particle model being occupied. In b) we show a possible interface configuration at some later time and the corresponding particle occupancies. The indicated flips in the interface correspond to particles hopping on the lattice.

Fig. 3: Allowed vertex configurations in the six-vertex model and their Boltzmann weights. Up-pointing arrows correspond to particles, down-pointing arrows represent vacant sites. In the dynamical interpretation of the model the Boltzmann weights give the transition probability of the state represented by the pair of arrows below the vertex to that above the vertex.