

FROM MICROSCOPIC TO MACROSCOPIC MODELS FOR PHASE TRANSITIONS

Markos A. Katsoulakis (M. A. カツオウラキス)

Department of Mathematics and Statistics

University of Massachusetts (マサチューセッツ大学)

Amherst, MA 01003, USA

In this note we present some recent results on the mesoscopic and macroscopic behavior of stochastic Ising models with long range interactions and general spin flip dynamics. We derive a mean field equation as the interaction range tends to infinity, we study its asymptotic behavior and we show that it yields a front (interface), separating two distinct phases and moving with normal velocity which is an anisotropic function of its principal curvatures. This function is given by a Green-Kubo-type formula which also specifies the relationship between the mobility and the surface tension of the moving interface. We conclude with some results on macroscopic limits for the interacting particle system describing the dynamics of the Ising model. We show that, for a continuum of appropriate scalings, the particle system yields in the limit a front moving with the same normal velocity as the one governing the asymptotics of the mean field equation. These results illustrate the relationship between the *phenomenological* and *microscopic* theories of phase transitions in a setting where anisotropies are present. They may also be thought as providing a theoretical justification for the Monte-Carlo simulations performed by physicists to compute moving fronts.

First we briefly discuss some of the phase transition theories for non-conservative, two-phase systems. The modelling of such phenomena is mainly approached by either phenomenological or microscopic theories.

In the phenomenological approach, models are roughly divided in two categories. First, sharp interface models derived by rigorous continuum mechanics arguments where interfaces are represented as smooth $(N - 1)$ dimensional hypersurfaces in $\mathbf{R}^N$, evolving with prescribed normal velocity

$$(1) \quad V = \alpha(x, t, n, \kappa_1, \dots, \kappa_{N-1}).$$

(see Gurtin [14] and references therein). Here n is the normal and $\kappa_1, \dots, \kappa_{N-1}$ are the principal curvatures of the evolving interface Γ_t . An example arising in the isotropic, isothermal case and capturing many important features of this class of

hypersurface evolutions, is the *motion by mean curvature*, i.e. when the normal velocity V of Γ_t is proportional to the mean curvature,

$$(2) \quad V = -\mu\sigma\kappa = -\mu\sigma \sum_{i=1}^{N-1} \kappa_i.$$

Here σ is related to the *interfacial energy* and μ is the *mobility* of the interface.

The hypersurfaces $\{\Gamma_t\}_{t \geq 0}$ may develop singularities, change topological type and exhibit various other pathologies even when the initial set Γ_0 is smooth. A great deal of work has been done recently in order to interpret (1), *past singularities*. First Brakke [4] provided a weak formulation for the particular case of motion by mean curvature, expressing the hypersurfaces $\{\Gamma_t\}_{t \geq 0}$ as varifolds. A different approach was taken by Evans and Spruck [13] in the case of (2) and by Chen, Giga and Goto [8] for more general geometric evolutions. In both works Γ_t is represented as the zero-level set of an auxiliary function u , i.e. $\Gamma_t = \{r \in \mathbf{R}^N : u(r, t) = 0\}$ where, in the case of motion by mean curvature for example, u solves

$$(3) \quad u_t = \mu\sigma \operatorname{tr} \left(\left(I - \frac{Du \otimes Du}{|Du|^2} \right) D^2 u \right) \quad \text{in} \quad \mathbf{R}^N \times (0, \infty).$$

Nonlinear, singular, degenerate parabolic equations typically have only weak, *viscosity*, solutions, which nevertheless allows us to define a *weakly propagating interface* Γ_t as the zero level set of the viscosity solution of (3), globally in time, past possible singularities.

The second type of phenomenological models are Ginzburg-Landau type of equations, whose solution is an order parameter varying continuously between two distinct phases. In this case we do not have a sharp interface separating two different phases but rather a narrow transition region. In this framework, Allen and Cahn [1] proposed the asymptotic limit of the rescaled reaction-diffusion equation

$$(4) \quad v_t^\epsilon - \mu\sigma \Delta v^\epsilon + \frac{1}{\epsilon^2} f(v^\epsilon) = 0 \quad \text{in} \quad \mathbf{R}^N \times (0, \infty),$$

where $f(\rho) = 2\mu\rho(\rho^2 - \rho)$, as a model for the motion of antiphase boundaries in polycrystalline materials. Formal results by Allen and Cahn [1] and Rubinstein, Sternberg and Keller [22], have indicated that these interfaces move with prescribed normal velocity proportional to their mean curvature, i.e. satisfy (2). Recently, Evans, Soner and Souganidis [12] proved rigorously that, in the asymptotic limit $\epsilon \rightarrow 0$, the solutions of (4) develop interfaces moving by mean curvature in the viscosity sense, past all singularities.

Non-equilibrium statistical mechanics theories provide a microscopic approach to the modelling of phase transitions, using Interacting Particle Systems (IPS). These are Markov processes set on the lattice $\mathbf{Z}^N$, and one distinguishes stochastic Ginzburg-Landau models where the order parameter takes continuous values and Ising spin systems with either (+) or (−) spins at each lattice site. Here we only address the latter type of models. Ising systems describe phase transitions—(+)’s are converted to (−)’s and vice versa—starting from an initial state of disequilibrium; the particle system evolves towards equilibrium under the influence of spin flip and possibly spin exchange dynamics. Below we describe in more detail two such models:

1. *Glauber-Kawasaki dynamics.* The Glauber-Kawasaki (G+K) dynamics is a jump Markov process taking values in the configuration space $X = \{-1, 1\}^{\mathbf{Z}^N}$. A configuration $\sigma = \{\sigma(x) \in \{-1, 1\}, x \in \mathbf{Z}^N\}$ is updated according to a combination of spin flips (Glauber dynamics), when a spin changes sign at a site x with a rate $c(x, \sigma)$, and simple exchanges (Kawasaki dynamics), when different spins at neighboring sites x, y , exchange with a rate γ^{-2} . The generator L^γ of the G+K process is defined in $L^\infty(X; \mathbf{R})$ by $L^\gamma = \gamma^{-2}L_K + L_G$, where

$$(5) \quad L_K f(\sigma) = \sum_{x \in \mathbf{Z}^N} \sum_{i=1}^N [f(\sigma^{(x, x+e_i)}) - f(\sigma)]$$

and

$$(6) \quad L_G f(\sigma) = \sum_{x \in \mathbf{Z}^N} c(x, \sigma) [f(\sigma^{(x)}) - f(\sigma)].$$

Here $\{e_i, i = 1, \dots, N\}$ is the standard basis of $\mathbf{R}^N$,

$$\sigma^{(x,y)}(z) = \begin{cases} \sigma(x) & \text{if } z = y, \\ \sigma(y) & \text{if } z = x, \\ \sigma(z) & \text{if } z \neq x \neq y, \end{cases} \quad \text{and} \quad \sigma^{(x)}(z) = \begin{cases} -\sigma(x) & \text{if } z = x, \\ \sigma(z) & \text{if } z \neq x, \end{cases}$$

and $c(x, \sigma) = 2N - 2\chi \sum_{i=1}^N [\sigma(x)\sigma(x+e_i) + \sigma(x)\sigma(x-e_i)] + 2\chi^2 \sum_{i=1}^N \sigma(x+e_i)\sigma(x-e_i)$ with χ a constant in $[1/2, 1)$.

2. *Spin flip dynamics with long range Kač potentials.* In this case the dynamics consist only of spin flips, the generator is given by (6) with rates,

$$(7) \quad c(x, \sigma) = \Psi(-\beta h_\gamma(x) \sigma(x)),$$

where $\beta^{-1} > 0$ is identified with the temperature and $h_\gamma(x) = \sum_{y \neq x} J_\gamma(x, y) \sigma(y)$; J_γ is the Kač potential $J_\gamma(x, y) = \gamma^N J(\gamma|x - y|)$ where $x, y \in \mathbf{Z}^N$ and $\gamma^{-1} > 0$ is

the interaction range. The potential $J : \mathbf{R}^N \rightarrow [0, \infty)$ is radial, i.e. $J(r) = J(|r|)$, $r \in \mathbf{R}^N$, and has compact support. The function Ψ is nonnegative and satisfies the *detailed balance law*, $\Psi(\rho) = \Psi(-\rho)e^{-\rho}$ for all $\rho \in \mathbf{R}$. Typical choices of Ψ 's are $\Psi(\rho) = (1 + e^\rho)^{-1}$ (Glauber dynamics), $\Psi(\rho) = e^{-\rho/2}$ (Arrhenius dynamics) or $\Psi(\rho) = e^{-\rho^+}$ (Metropolis dynamics).

This process is constructed as follows: the initial configurations σ^0 are randomly distributed according to some measure μ^γ on Σ . Given a σ^0 , $\sigma_t = \sigma^0$ for an exponentially distributed waiting time with rate $\sum_y c(y, \sigma^0)$; σ_t jumps to a new configuration $\sigma^1 = \sigma^{(x)}$ with probability $c(x, \sigma^0) / \sum_y c(y, \sigma^0)$. Then $\sigma_t = \sigma^1$ for another exponentially distributed waiting time with rate $\sum_y c(y, \sigma^1)$ etc. Notice that, in view of the positivity of J , the probability of a spin flip at x is higher when the spin at x is different from most of its neighbors, than it is when the spin agrees with most of its neighbors. The construction of the G+K process is along the same lines.

Both previous models share a *mesoscopic* space scaling, giving rise through the respective BBGKY hierarchies, to deterministic equations. Such mesoscopic equations describe the limiting evolution of the average magnetization, $E\sigma_t(x)$. For G+K dynamics De Masi, Ferrari and Lebowitz [9] obtained that for given $T > 0$,

$$\lim_{\gamma \rightarrow 0} \sup_{x \in \mathbf{Z}^N} \sup_{t \in [0, T]} |E_{\mu^\gamma} \sigma_t(x) - v(\gamma x, t)| = 0,$$

where $v = v(r, t)$, $r \in \mathbf{R}^N$, solves the Ginzburg-Landau equation (4) with $\mu = \sigma = \epsilon = 1$,

$$(8) \quad v_t - \Delta v + f(v) = 0 \quad \text{in} \quad \mathbf{R}^N \times [0, \infty),$$

and initial data $v_0 = v_0(r)$, $r \in \mathbf{R}^N$, where $E_{\mu^\gamma} \sigma(x) = v_0(\gamma x)$, $x \in \mathbf{Z}^N$ with respect to the initial measure μ^γ . Furthermore $f(v) = \beta v^3 - \alpha v$ where $\alpha = 4n(2\chi - 1)$ and $\beta = 4n\chi^2$ and the stable equilibria are $\pm \frac{2\chi-1}{\chi^2}$.

In the case of pure Glauber dynamics, De Masi, Orlandi, Presutti and Triolo [10] proved that for given $T > 0$,

$$\lim_{\gamma \rightarrow 0} \sup_{x \in \mathbf{Z}^N} \sup_{t \in [0, T]} |E_{\mu^\gamma} \sigma_t(x) - m(\gamma x, t)| = 0,$$

where m is the unique solution of

$$(9) \quad m_t + m - \tanh \beta(J * m) = 0 \quad \text{in} \quad \mathbf{R}^N \times [0, \infty),$$

with initial data $m_0 = m_0(r)$, $r \in \mathbf{R}^N$. Here, $J * m$ denotes the usual convolution in $\mathbf{R}^N$. Again $E_{\mu^\gamma} \sigma(x) = m_0(\gamma x)$, $x \in \mathbf{Z}^N$, with respect to the initial measure μ^γ . In

this rescaling we essentially let the interaction range γ^{-1} of the Kač potentials tend to infinity. The passage in the limit $\gamma \rightarrow 0$ of quantities like the thermodynamical pressure, average magnetization etc. is known as the *Lebowitz-Penrose limit* (see Lebowitz and Penrose [20] and also the monograph by De Masi and Presutti [11]).

In joint works with Souganidis ([16], [17]) we rigorously derived phenomenological PDEs, describing evolving phase boundaries (e.g. (3)) past all possible singularities, from interacting particle systems. In [16], we studied an interacting particle system with Glauber-Kawasaki dynamics. In view of the relation, on the one hand between this IPS and the mesoscopic equation (8) ([9]) and on the other between the rescaled (8) (i.e. (4)) and the macroscopic equation (3) ([12]), it is reasonable to ask if there is a suitable scaling of time and space, such that in the limit the sites of the spin system separate in clusters of (+) or (−), whose boundaries move towards equilibrium according to the mean curvature rule. Indeed, in [16] we proved there is a critical ρ^* such that when $\epsilon\gamma^{-\rho^*} \rightarrow 0$, we have for any fixed $T > 0$

$$\lim_{\gamma \rightarrow 0} \sup_{x \in \mathbb{Z}^N} \sup_{t \in [0, T]} |E_{\mu\gamma} \sigma_{t\epsilon^{-2}}(x) - \frac{2\chi - 1}{\chi^2} \text{sgn}(u(\epsilon\gamma x, t))| = 0,$$

where u is the unique *viscosity* solution of (3) with constants μ and σ equal to one. Recall that $\pm \frac{2\chi-1}{\chi^2}$ are the stable equilibria of the Ginzburg-Landau equation (8). Furthermore, by choosing suitable spin flip rates, we also obtained in the appropriate scaled limit, other geometric motions including interfaces moving with constant velocity or with velocity equal to their mean curvature plus a constant. In [17] we studied the macroscopic limit of an appropriately rescaled stochastic Ising model with long range interactions, evolving with Glauber dynamics as well as rescalings of the corresponding mesoscopic equation (9). In both cases we obtained an interface evolving with normal velocity $\mu\sigma\kappa$, where κ is the mean curvature and $\theta = \mu\sigma$ is a *transport coefficient*. The novelty of the result, besides dealing with a fully nonlinear, nonlocal mesoscopic equation, is the identification of θ , through a homogenization technique, yielding an *effective Green-Kubo type formula*. The transport coefficient appears neither at the microscopic level (i.e. the particle system) nor at the level of the mesoscopic equation and it is actually the outcome of an *averaging effect* taking place during the limiting process. All results are valid globally in time, the motion of the interface being interpreted in the viscosity sense after the onset of the geometric singularities. Moreover, the “propagation of chaos” property holds globally for both models. In the case of the Glauber-Kawasaki dynamics, we obtain in addition that the resulting interfaces are varifolds evolving by their mean curvature in the

Brakke sense, thus no interface “fattening” may occur. Some analogous results were obtained earlier by Bonaventura [Bo] for the Glauber-Kawasaki dynamics and by De Masi, Orlandi, Presutti and Triolo [10] for the Glauber dynamics under the assumption that the evolving interfaces remain smooth.

We now present some recent results in collaboration with P.E. Souganidis, on how *anisotropy* is manifested in the transition from microscopic to macroscopic models. In absence of faceting phenomena, for stable (strictly convex) interfacial energies H , the evolution of the phase boundaries $\{\Gamma_t\}_{t \geq 0}$ is governed by the equation

$$(10) \quad u_t = \mu \left(\frac{Du}{|Du|} \right) \text{tr} \left[D^2 H \left(\frac{Du}{|Du|} \right) D^2 u \right] \quad \text{in } \mathbf{R}^N \times (0, \infty),$$

and

$$(11) \quad u = g \quad \text{on } \mathbf{R}^N \times \{0\},$$

where

$$\Gamma_t = \{r \in \mathbf{R}^N : u(r, t) = 0\}, \quad \Gamma_0 = \{r \in \mathbf{R}^N : g(r) = 0\}$$

and u is the viscosity solution of (10), (11) (see [8], [14] and references therein). The direction dependent scalar μ is the mobility of the interface and H is positively homogenous of degree one. Notice also that in the isotropic case ($H(e) = \sigma|e|$, $e \in S^{N-1}$), (10) simply reduces to motion by mean curvature. Our goal is to derive rigorously such equations from Ising models with Glauber dynamics and also give a Green-Kubo formula for the direction dependent *transport matrix* $A(e) = \mu(e)D^2 H(e)$, $e \in S^{N-1}$.

To account for anisotropies in the Ising model, we replace the condition of radial symmetry for the interaction potential, assuming only that J is symmetric, i.e.

$$J(r) = J(-r), \quad \text{for all } r \in \mathbf{R}^N.$$

Following the arguments of [10], we may obtain as for the isotropic case, the equation

$$(12) \quad m_t + \Phi(\beta(J * m))[m - \tanh \beta(J * m)] = 0 \quad \text{in } \mathbf{R}^N \times [0, \infty),$$

where $\Phi(\rho) = \Psi(-2\rho)(1 + e^{-2\rho})$ and Ψ defines the dynamics of the Ising system through (7). Let us briefly review some basic properties of this equation. For more details we refer to [18].

We first assume that the function

$$F(\rho) = \Phi(\rho)(m - \tanh(\rho)) \quad \text{is nonincreasing in } \rho.$$

Since $J \geq 0$, (12) admits a *comparison principle* between solutions, i.e. if w_1, w_2 solve (12), and $w_1 \leq w_2$ on $\mathbf{R}^N \times \{0\}$, then $w_1 \leq w_2$ on $\mathbf{R}^N \times (0, \infty)$. In addition, it has three steady state solutions, $\pm m^\beta$ and 0 where $m^\beta > 0$, provided $\beta \hat{J} > 1$ ($\hat{J} = \int_{\mathbf{R}^N} J(r) dr$). We will refer to the value β_{cr} , where $\beta_{cr} \hat{J} = 1$, as the *critical temperature*. Observe that the steady state solutions are equilibria of the underlying ordinary differential equation, with $\pm m^\beta$ being the stable and 0 the unstable one.

The first issue we discuss is whether solutions of (12) converge to the stable equilibria, as $t \rightarrow \infty$, and if yes, to identify the regions in $\mathbf{R}^N \times (0, \infty)$, where they converge to m^β and $-m^\beta$. We first rescale (12) by setting $r \rightarrow r/\epsilon$, $t \rightarrow t/\epsilon^2$ and obtain

$$(13) \quad m_t^\epsilon + \epsilon^{-2} \Phi(\beta(J * m^\epsilon)) [m^\epsilon - \tanh \beta(J^\epsilon * m^\epsilon)] = 0 \quad \text{in } \mathbf{R}^N \times (0, \infty),$$

where $J^\epsilon(r) = \epsilon^{-N} J(\epsilon^{-1} r)$, $r \in \mathbf{R}^N$. Formal asymptotic analysis indicates that m^ϵ has the WKB expansion,

$$(14) \quad m^\epsilon(r, t) = q\left(\frac{d(r, t)}{\epsilon}, Dd(r, t)\right) + \epsilon Q\left(\frac{d(r, t)}{\epsilon}, Dd(r, t)\right) + \Omega(\epsilon^2),$$

where $q = q(\xi, e)$, $Q(\xi, e) : \mathbf{R} \times S^{N-1} \rightarrow \mathbf{R}$ and $D \cdot$ denotes the gradient. Furthermore q is a *multidimensional travelling wave* solution $q = q(r \cdot e, e)$ of

$$(15) \quad q(\cdot, e) = \tanh[J * q(\cdot, e)] \quad \text{for all } e \in S^{N-1},$$

connecting the stable equilibria $\pm m^\beta$, and $Q = Q(\xi, e)$ solves an appropriate *cell problem*. An example of nontrivial direction dependence of the travelling wave solution of (15), is given for instance when $J(r) = \chi_{[-1,1]^2}(r)$. The formal analysis indicates that $d = d(r, t)$ is the signed distance function from a moving interface Γ_t with normal velocity,

$$V = d_t = \text{tr}\{A(Dd)D^2d\},$$

where the cell problem for the corrector Q identifies $A(e)$. In other words, we have that $\Gamma_t = \{r \in \mathbf{R}^N : u(r, t) = 0\}$, where u solves (10) and the transport matrix $A(e)$ is given by the Green-Kubo formula

$$A(e) = \mu(e)B(e),$$

where the mobility is

$$(16) \quad \mu(e) = \beta \left[\int \frac{(\dot{q}(\xi, e))^2}{\Phi(\beta J * q(\xi, e) dr) (1 - q^2(\xi, e))} d\xi \right]^{-1},$$

$D^2H(e)$ is identified with the matrix $B(e)$ and

$$(17) \quad D^2H(e) = \left(\frac{1}{2} \int \int J(r) \dot{q}(\xi, e) \dot{q}(\xi + r \cdot e, e) (r \otimes r) + D_e q(\xi + r \cdot e, e) \otimes r \right. \\ \left. + r \otimes D_e q(\xi + r \cdot e, e) \right] dr d\xi \Big) (I - e \otimes e).$$

It is expected that equation (10) formally governs the asymptotic behavior of the mesoscopic equation (13) through the WKB expansion. Indeed we have the following:

Theorem 1: *Let m^ϵ be the solution of (13) with a Lipschitz continuous initial datum,*

$$m^\epsilon = m_0^\epsilon \text{ on } \mathbf{R}^N \times \{0\}$$

and assume that there exists an open set $\Omega_0 \subset \mathbf{R}^N$ and a closed set $\Gamma_0 \subset \mathbf{R}^N$ such that $\mathbf{R}^N = \Omega_0 \cup \overline{\Omega_0} \cup \Gamma_0$,

$$\Omega_0 = \{r \in \mathbf{R}^N : m_0^\epsilon > 0\}, \quad \Gamma_0 = \{r \in \mathbf{R}^N : m_0^\epsilon = 0\}$$

and

$$\mathbf{R}^N \setminus \overline{\Omega_0} = \{r \in \mathbf{R}^N : m_0^\epsilon < 0\}.$$

Then, as $\epsilon \rightarrow 0^+$, $m^\epsilon \rightarrow m_\beta$ in $\{u > 0\}$ and $m^\epsilon \rightarrow -m_\beta$ in $\{u < 0\}$, with both limits local uniform, where u is the unique solution of (10), (11), (16)-(17), with g bounded uniformly continuous, such that

$$\Omega_0 = \{r \in \mathbf{R}^N : g(r) > 0\}, \quad \Gamma_0 = \{r \in \mathbf{R}^N : g(r) = 0\},$$

and

$$\mathbf{R}^N \setminus \overline{\Omega_0} = \{r \in \mathbf{R}^N : g(r) < 0\}.$$

The proof of this result goes along the following lines: Our first goal is to make the formal asymptotic analysis of (13) rigorous. We first construct sub- and super-solutions of (13), roughly looking like (14), as long as the interfaces Γ_t solving (10) remain smooth; thus the asymptotic behavior follows from the comparison property of (13). These arguments will appear in detail in [18]. Such a result combined with a recent work of Barles and Souganidis [2], where viscosity solutions of (10) are constructed via smooth solutions of the same equation, may yield the asymptotics

of (12), globally in time, past the possible geometric singularities of the evolution (10) (see [2] for details).

As soon as the meso/macroscopic analysis is complete, we can use it in the direct derivation of (10), (16)-(17) from the IPS, provided we first demonstrate that in a long time interval $[0, T\epsilon^{-2}]$,

$$(18) \quad E_{\mu^\gamma} \sigma_t(x) \approx m(\gamma x, t) + \text{error},$$

where m solves (12); here $t \in [0, T]$ is the macroscopic time (in say (10) or (13)) and $\epsilon = \gamma^\rho$ for some $\rho > 0$ to be determined. An important tool in this direction is the *correlation function method*, introduced by Lanford [19] for the short time derivation of the Boltzmann equation from newtonian dynamics. This technique was later extended for stochastic IPS by Caprino, DeMasi, Presutti and Pulvirenti [7]. Crudely, one first shows (18) for short times, using the correlation function method. This suggests that in order to obtain (18) in $[0, T\epsilon^{-2}]$, we should discretize in time (see among others, Bonaventura [3], De Masi, Orlandi, Presutti and Triolo [10], Katsoulakis and Souganidis [16] etc.); the errors, however, add up since the time scale is long. Nevertheless, this difficulty may be overcome by absorbing the error at each time step, using the *sharp* comparison principle for both (13) and (10), a technique successful in [16], [17]. We may accordingly conclude from (18), using the asymptotics of the mesoscopic equation. We refer to [17], [18] for the details. Before stating the relevant Theorem we define the sets,

$$\left\{ \begin{array}{l} P_t^\gamma = \{x \in \mathbf{Z}^N : u(\gamma\epsilon(\gamma)x, t) > 0\}, \quad N_t^\gamma = \{x \in \mathbf{Z}^N : u(\gamma\epsilon(\gamma)x, t) < 0\} \\ \text{and} \\ M_{\gamma,t}^n = \{\underline{x} \in \mathbf{Z}_n^N : x_i \in P_t^\gamma \cup N_t^\gamma\}. \end{array} \right.$$

where u is the viscosity solution of (10), (16)-(17). In the above notation for each $n \in \mathbf{N}$,

$$\mathbf{Z}_n^N = \{\underline{x} = (x_1, \dots, x_n) \in \mathbf{Z}^N : x_1 \neq \dots \neq x_n\}.$$

Theorem 2: Assume that the IPS defined earlier has as initial measure a product measure μ^γ such that

$$E_{\mu^\gamma}(\sigma(x)) = m_0^\epsilon(\gamma x) \quad (x \in \mathbf{Z}^N),$$

where m_0^ϵ is Lipschitz continuous. Then under the assumptions of Theorem 1 on m_0^ϵ and g , there exists a $\rho^* > 0$ such that for any $\epsilon(\gamma)$ such that $\gamma^{-\rho^*} \epsilon(\gamma) \rightarrow +\infty$, as $\gamma \rightarrow 0$, and for all $t > 0$,

$$\lim_{\gamma \rightarrow 0} \sup_{\underline{x} \in M_{\gamma,t}^n} |E_{\mu^\gamma} \prod_{i=1}^n \sigma_{t\epsilon(\gamma)^{-2}}(x_i) - (m_\beta)^n \prod_{i \in N_t^\gamma} (-1)| = 0,$$

with the limit local uniform in t .

We conclude this section with a discussion about the history of this problem as well as the meaning of our results. First, Spohn [23] derived formally Green-Kubo formulas for the mobility and the interfacial energy, using corresponding microscopic definitions. Furthermore Butta [5] proved the validity of an Einstein relation for the transport coefficient of the isotropic mean curvature evolution. To our knowledge, Theorems 1 and 2 are the first rigorous results in a non-equilibrium setting where an anisotropic macroscopic equation (10) as well as a Green-Kubo formula for the mobility (16) and the direction-dependent transport matrix (17) are derived from mesoscopic and microscopic dynamics, namely (12) and the underlying stochastic Ising model. As already mentioned earlier a result analogous to Theorem 1 was obtained for the isotropic case, i.e. when $J(r) = J(|r|)$, first under the assumption that the evolving front remains smooth in [10] and later extended past all possible singularities in [17]. In this case it turns out that the limiting motion is given by (3), where $\mu(e)D^2H(e) = \mu\sigma(I - e \otimes e) = \theta(I - e \otimes e)$, I being the unit matrix in $\mathbf{R}^N$, with the constant θ given by

$$\theta = \left(\int_{-\infty}^{\infty} \frac{\dot{q}^2(\xi)}{1 - q^2(\xi)} d\xi \right)^{-1} \frac{\beta}{2} \int_{-\infty}^{\infty} \int J(|r|) \dot{q}(\xi + e \cdot r) \dot{q}(\xi) (\hat{e} \cdot r)^2 dr d\xi,$$

with $e, \hat{e}$ are any two orthogonal vectors in S^{N-1} . Note that due to the radial symmetry of J , θ is independent of the particular choice of e and $\hat{e}$. In addition q is the direction-independent travelling wave corresponding to the symmetric J .

One may attempt to simplify (12), or in the specific case of Glauber dynamics (9), by substituting $J_2(\Delta m - m)$ for the convolution term $J * m$ (see, for example, Penrose [21], where $\bar{J}_2 = \int J(|r|)|r|^2 dr$ or even additionally linearize the hyperbolic tangent, thus obtaining a Ginzburg-Landau equation (1.1). It is known (see Jerrard [15], Evans, Soner and Souganidis [12]) that in the isotropic case, both simplified models have the same qualitative asymptotic behavior as (9) with different though transport coefficients. In the anisotropic case, however, this picture is not true anymore.

The second order approximations described earlier, still yield in the limit $\epsilon \rightarrow 0$, isotropic motion by mean curvature with a constant transport coefficient, while (9), according to our analysis should yield the anisotropic equation (10) with the Green-Kubo formulae (16), (17). It appears that anisotropy is a higher order effect which cannot be accounted for, only with second order approximating equations. This phenomenon is also pointed out by Caginalp and Fife ([6]), where depending on the type of anisotropy expected, they “correct” (4) by suitably adding higher order derivatives. Lastly we remark on the choice of dynamics for the Ising model according to (7) and the detailed balance condition; as expected, it affects only the nonequilibrium quantities, i.e. the mobility coefficient of the interface and not the surface tension.

References

- [1] S. M. ALLEN & J. W. CAHN, A macroscopic theory for antiphase boundary motion and its application to antiphase domain coarsening, *Acta Metal.* **27** (1979), 1085–1095.
- [2] G. BARLES & P. E. SOUGANIDIS, A new approach to front propagation, preprint.
- [3] L. BONAVENTURA, Mouvement par courbure dans un system de spin avec interaction, to appear.
- [4] K. A. BRAKKE, *The motion of a surface by its mean curvature*, Princeton University Press, Princeton, NJ (1978).
- [5] P. BUTTA, On the validity of an Einstein relation in models of interface dynamics, *J. Stat. Phys.* **72**, 1401–1406.
- [6] G. CAGINALP, & P. FIFE, Higher-order phase field models and detailed anisotropy, *Phys. Rev. B* **34** (1986), 4940–4943.
- [7] S. CAPRINO, A. DE MASI, E. PRESUTTI, & M. PULVIRENTI, A derivation of the Broadwell equation, *Comm. Math. Phys.*, **135** (1991), 443–465.
- [8] Y.-G. CHEN, Y. GIGA & S. GOTO, Uniqueness and existence of viscosity solutions of generalized mean curvature flow equations, *J. Diff. Geom.* **33** (1991), 749–786.
- [9] A. DE MASI, P. FERRARI & J. LEBOWITZ, Reaction-Diffusion equations for interacting particle systems, *J. Stat. Phys.* **44** (1986), 589–644.
- [10] A. DE MASI, E. ORLANDI, E. PRESUTTI & L. TRIOLO, Glauber evolution with Kač potentials: I. Mesoscopic and macroscopic limits, interface dynamics, *Nonlinearity* **7** (1994), 633–696.
- [11] A. DE MASI & E. PRESUTTI, *Mathematical Methods for Hydrodynamic Limits*, Lect. Notes in Math. 1501, Springer-Verlag, New York 1991.
- [12] L. C. EVANS, H. M. SONER & P. E. SOUGANIDIS, Phase transitions and generalized motion by mean curvature, *Comm. Pure and Appl. Math.*, **45** (1992), 1097–1123.

- [13] L. C. EVANS & J. SPRUCK, Motion of level sets by mean curvature I, *J. Diff. Geom.* **33** (1991), 635–681.
- [14] M. E. GURTIN, *Thermodynamics of Evolving Phase Boundaries in the Plane*, Oxford University Press 1993.
- [15] R. JERRARD, Fully nonlinear phase field equations and generalized mean curvature motion, *Comm. P.D.E.*, to appear.
- [16] M. A. KATSOULAKIS & P. E. SOUGANIDIS, Interacting particle systems and generalized mean curvature evolution, *Arch. Rat. Mech. Anal.*, in press.
- [17] M. A. KATSOULAKIS & P. E. SOUGANIDIS, Generalized motion by mean curvature as a macroscopic limit of stochastic Ising models with long range interactions and Glauber dynamics, *Comm. Math. Phys.* **169** (1995), 61–97.
- [18] M. A. KATSOULAKIS & P. E. SOUGANIDIS, Stochastic Ising models and anisotropic front propagation, to appear in *J. Stat. Phys.*
- [19] O. E. LANFORD, Time evolution of large classical systems. In: *Lect. Notes in Phys.* 38, ed. J. Moser, Springer, Berlin, Heidelberg 1975, 1–111.
- [20] J. LEBOWITZ & O. PENROSE, Rigorous treatment of the Van der Waals Maxwell theory of the liquid vapour transition, *J. Math. Phys.* **98** (1966), 98–113.
- [21] O. PENROSE, A mean field equation of motion for the dynamic Ising model, *J. Stat. Phys.* **63** (1991), 975–986.
- [22] J. RUBINSTEIN, P. STERNBERG & J.B. KELLER, Fast reaction, slow diffusion and curve shortening, *SIAM J. Appl. Math.* **49** (1989), 116–133.
- [23] H. SPOHN, Interface motion in models with stochastic dynamics, *J. Stat. Phys.* **71** (1993), 1081–1132.