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Microstructures and scaling limits

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ABSTRACT: *These are notes of a Colloquium given on May 30, 2005, at the Mathematical Department of the University of Roma La Sapienza. The notes based on researches of the author in statistical mechanics are intended to underline contiguities with other disciplines as probability theory, calculus of variations, geometrical measure theory, PDE's.*

1 – Introduction

The title of the talk reflects the attempt to present some of my researches in statistical mechanics in a more general frame, underlining contiguity with different areas, like variational calculus, geometric measure theory, probability and PDE's.

A crucial point of the whole approach is a "macroscopic-microscopic duality" which I will first try to explain through an example taken from every-day life. Technology is so advanced that if you go to the movies, sound and images are now so accurate and sharp that you feel you are in the middle of a real scene. Sometimes however you need more, as in Rising Sun with Sean Connery, where to investigate a homicide he was asking to magnify a frame of a movie and through this he was able to see an image of the killer in a mirror. If one takes the procedure to the extremes, he will reduce the movie to a huge sequence of 0 and 1, which to some extent is paradoxical: the whole beauty of the movie has gone, its true content is just a binary sequence! But if you look at it from the

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opposite side, here you have a dull string of digits, yet through it you can watch a nice movie!

The moral of the story is that one should be flexible, sometimes it is necessary to do a continuum limit and sometimes to go to atomistic and in both cases there are surprises.

Another key word in this talk is “microstructures”. Here I follow Stefan Müller’s terminology in his Lecture Notes at the CIME Summer School in Cetraro, [14], from where I am also borrowing the content of the next section. Thus microstructures are structures intermediate between the atomic and the macroscopic scales of which nature is a great source of examples. In many biological systems there are such structures like in leaves or, for instance, repetitive patterns in the growth of cactuses; other example can be found by examining the fine structures of rocks; some solid materials have fine phase mixtures. In all these examples the macroscopic properties of the systems depend on such structures which are sometimes responsible for enhanced stability and resistance of the body.

2 – Elastic crystals

In a certain range of values of the parameters, crystals of Cu-Al-Ni exhibit “fine twinning” at an atomic resolution, which schematically appears as a laminar pattern where two different lattice deformations alternate. The phenomenon can be explained in the context of continuum theories. In such theories the free energy of a solid body is given by a functional of the form

$$I(u) = \int_{\Omega} W(Du) \tag{2.1}$$

where $\Omega \subset \mathbb{R}^3$, $u : \Omega \to \mathbb{R}^3$ the displacement vector, Du the 3×3 displacement matrix and $W(Du) \geq 0$ the free energy density stored in the body and due to the deformation Du. To explain laminar patterns we then suppose that there are two matrices A and B such that $W(A) = W(B) = 0$ and want to investigate when they can appear in a fine mixtures with still an “infinitesimal free energy”. The analysis is beyond the purposes of this talk, thus, referring to [14] and references therein, I will just discuss here a toy model of the problem.

2.1 – The Bolza-Young functional

Let $u : [0,1] \to \mathbb{R}$, $u(0) = u(1) = 0$, and

$$I(u) = \int_0^1 (u_x^2 - 1)^2 + u^2 \,. \tag{2.2}$$

As in the previous discussion, there are two optimal slopes $u_x = \pm 1$ but also a penalty for u to detach from 0. Without such a penalty any polygonal graph with slopes ± 1 with values 0 at $x = 0, 1$ would be a minimizer. The functional (2.2) cannot be 0, because in such a case $\|u\|_2 = 0$ and the first term in (2.2) would be strictly positive. The inf over u however is 0, just consider any polygonal graph with slopes ± 1 which is contained in the strip $0 \le u \le \varepsilon$, $\varepsilon = 1/(2N)$, $N \in \mathbb{N}$. Then $I(u) \le \varepsilon^2$ and $I(u) \to 0$ as $\varepsilon \to 0$.

Thus optimality of the functional forces fast oscillations on smaller and smaller scales. To get a connection with statistical mechanics it is convenient to look further on this example trying to characterize the optimizing sequences, namely which are the common features present in all minimizing sequences. This leads us to the notion of Young measures.

2.2 – Young measures

We consider a minimizing sequence u_n, namely such that $I(u_n) \to 0$. We set $z_n = (u_n)_x$, then $u_n(x) = \int_0^x z_n(y)$. Since $I(u_n) \to 0$, $u_n \to 0$ in L^2 and consequently $z_n \to 0$ weakly. On the other hand $\int_0^1 (z_n^2 - 1)^2 \to 0$ so that polynomials of z_n converge weakly to something different that the polynomial of the weak limit of z_n. This is due to fast oscillations, microstructures, which are the object that we want to investigate and Young measures have been devised just for dealing with cases like this one.

With reference to the present context, a Young measure is a family $(\nu_x)_{x \in [0,1]}$ of probability measures on $\mathbb{R}$ such that for any $f \in C_0(\mathbb{R})$, the integral $\nu_x(f)$ is a measurable function of x.

Let z_n be a sequence of measurable functions on $[0, 1]$ and suppose that there is a positive function $w(r), r \ge 0$, $\lim_{r \to \infty} w(r) = \infty$, such that

$$\limsup_{n \to \infty} \int_0^1 w(|z_n|) < \infty \,. \tag{2.3}$$

By the Young theorem (whose validity extends the present context) there is then a subsequence z_{n_k} and a Young measure $(\nu_x)_{x \in [0,1]}$ such that

$$\lim_{n_k \to \infty} \int_0^1 \phi(x) f(z_{n_k}(x)) = \int_0^1 \phi(x) \nu_x(f) \tag{2.4}$$

for all $f \in C_0(\mathbb{R})$ and all $\phi \in L^1([0, 1])$.

Referring to the literature for a proof of the theorem (see for instance [14]) which is sketched in Appendix A in a form useful for the analysis in Section 3, I will just mention here that if we consider a piecewise constant test function ϕ, then in each interval I where ϕ is constant, we define a positive measure $\nu_{I;n}$ on

$\mathbb{R}$ given by the distribution of z_n restricted to I under the Lebesgue measure on I normalized to 1, so that $⨍_I f(z_n) = \nu_{I,n}(f)$. By (2.3), $\nu_{I;n}$ is a probability and by compactness it converges weakly by subsequences as $n \to \infty$ to a probability ν_I. The collection of all such ν_I and then a diagonalization procedure over test functions piecewise constant on finer and finer partitions of $[0, 1]$ leads in the end to the Young measure.

Let us now see how the theorem applies in the case of the Bolza functional. In such a case there is a constant c so that $\|z_n\|_4 \le c$ for all n, so that (2.3) holds with $w(r) = r^4$. Let $a > 2$, $g_a(r) = (r^2 - 1)^2$ if $|r| \le 2$, $g_a(r) = g_a(2)$ for $2 \le |r| \le a$, $g_a(r) = 0$ for $|r| \ge a + 1$ and finally $g_a(r)$ linearly interpolates between a and $a + 1$.

By (2.4) with $\phi = 1$,

$$\lim_{n_k \to \infty} \int_0^1 g_a(z_{n_k}) = \int_0^1 \nu_x(g_a) = 0$$

because $\int_0^1 g_a(z_{n_k}) \le I(z_{n_k})$ and $\lim_{n\to\infty} I(z_n) = 0$. By taking $a \to \infty$,

$$\int_0^1 \nu_x(g) = 0, \quad g(r) = \min\{(r^2 - 1)^2, 9\}$$

hence $\nu_x = \lambda(x)\delta_{-1} + (1 - \lambda(x))\delta_1$. Since $u_n(x) = \int_0^x z_n(x')$ and $u_n \to 0$ in L^2, by (2.4) with ϕ the characteristic function of $[0, x]$,

$$\int_0^x \nu_x(\{Id\}) = 0, \quad \{Id\}(r) = r, \ r \in \mathbb{R}$$

hence $\int_0^x 1 - 2\lambda(y) = 0$ for almost all x so that $\nu_x = \frac{1}{2}[\delta_{-1} + \delta_1]$.

Thus the common feature to all minimizing sequences is that their Young measure is the family of identical elements $\frac{1}{2}[\delta_{-1} + \delta_1]$. According to the heuristic considerations above, this means that in a neighborhood of each point $x \in [0, 1]$ the statistics of slopes on the elements of a minimizing sequences have a frequency of appearance of ± 1 close to $1/2$.

3 – Hydrodynamic limits

An analogue of Young measures appears in the analysis of the collective behavior of interacting particle systems. We will use the notion to establish a bridge toward Gibbs measures and statistical mechanics.

3.1 – Exclusion processes

The exclusion process is a Markov process on $\{0,1\}^{\mathbb{Z}^d}$ that we consider here in $d = 1$. An element $\eta \in \{0,1\}^{\mathbb{Z}}$ is interpreted as a configuration of particles by putting a particle at any site x where $\eta(x) = 1$ and leaving all other sites empty. We will first consider the asymmetric case, where only jumps to the right and on empty sites are allowed. The generator called L_d then acts on cylindrical functions $f(\eta)$ (i.e. $f(\eta)$ depends only on finitely many entries $\eta(x)$ of η) as

$$L_d f(\eta) = \sum_{x\in\mathbb{Z}} \eta(x)[1-\eta(x+1)]\big\{f(\eta-\delta_x+\delta_{x+1}) - f(\eta)\big\} \tag{3.1}$$

where δ_z is the element in $\{0,1\}^{\mathbb{Z}}$ equal to 1 at z and to 0 otherwise. The exclusion process is a Markov process $\{\eta(x,t), x\in\mathbb{Z}, t\geq 0\}$ where the transition probabilities are given by the semigroup generated by L_d, see [8] for instance. The well definiteness of the process is evident in the periodic version that I will consider in the sequel where $\mathbb{Z}$ is replaced by a circle with N sites or, in other words, by $\mathbb{Z}$ modulo N, N a positive integer. In such a case L_d is defined by (3.1) but with the sum over x restricted to $[1,N]$ and with $\eta(x\pm N) = \eta(x)$. Then L_d is the generator of Markov process $\{\eta(x,t), x\in[1,N], t\geq 0\}$ with state space $[0,1]^{[1/n]}$ whose law will be denoted by $P^{(N)}$ and we define $\eta(x,t)$ for all $x\in\mathbb{Z}$ by requiring that $\eta(x+N,t) = \eta(x,t)$ and eventually study the limit when $N\to\infty$.

3.2 – Continuum limit

With $S_x : \{0,1\}^{\mathbb{Z}} \to \{0,1\}^{\mathbb{Z}}$, the translation by x on particles configuration, i.e. $[S_x\eta](y) = \eta(x+y)$, for any $\phi\in C_0^\infty(\mathcal{T}\times\mathcal{R}_+)$ and any cylindrical function f on $\{0,1\}^{\mathbb{Z}}$ we define for any realization $\{\eta(x,t)\}$ of the exclusion process

$$\langle\langle\phi, f\rangle\rangle_N = \frac{1}{N}\int_0^\infty \langle\phi, f\rangle_{N,t} \tag{3.2}$$

$$\langle\phi, f\rangle_{N,t} = \frac{1}{N}\sum_{x=1}^{N} \phi\left(\frac{x}{N},\frac{t}{N}\right) f\big(S_x\eta(\cdot,t)\big) \tag{3.3}$$

The double bracket is to remind that there are two averages one in space the other in time, while the single bracket is for spatial averages only.

Calling η_x the function on $\{0,1\}^{\mathbb{Z}}$ which on η has value $\eta(x)$, as a particular case of (3.2),

$$\langle\langle\phi, \eta_0\rangle\rangle_N = \frac{1}{N}\int_0^\infty \frac{1}{N}\sum_{x=1}^{N} \phi\left(\frac{x}{N},\frac{t}{N}\right)\eta(x,t)\,. \tag{3.4}$$

The variables (3.4) are the density fields, their limits as $N \to \infty$ define the density profiles which are the quantity of interest of the continuum theory. However, as in Section 2, non linear effects force to consider as well the "non linear functions of η" defined in (3.2).

The continuum limit involves the limit distribution of these variables when $N \to \infty$. There is an analogue of the Young theorem for the limit of the variables (3.2), with the measures ν_x of the previous section replaced by measures $\nu_{x,t}$ on $\{0,1\}^{\mathbb{Z}}$. Recall however that η is random so that we will end up with random Young measures.

3.3 – A Young theorem for the exclusion process

A Young measure now is a collection $\nu = \{\nu_{x,t},\ (x,t) \in \mathcal{T} \times \mathbb{R}_+\}$, of probabilities on $\{0,1\}^{\mathbb{Z}}$ such that for any cylindrical f, $\nu_{x,t}(f)$ is a measurable function of (x,t). We call M the collection of all Young measures and equip M with the Borel structure generated by the functions

$$\nu \to X_{\phi,f}(\nu) := \int_0^\infty \int_0^1 \phi(x,t)\nu_{x,t}(f) \tag{3.5}$$

when ϕ varies in $C_0^\infty(\mathcal{T} \times \mathcal{R}_+)$ and f among the cylindrical functions. The analogue of the Young theorem is

THEOREM 3.1. *There is a subsequence N_k and a probability P on M so that for any n, any bounded continuous functions $F[r_1, \dots, r_n]$ on $\mathbb{R}^n$, any test functions $\phi_1, \dots, \phi_n$ in $C_0^\infty(\mathcal{T} \times \mathcal{R}_+)$ and any cylindrical functions $f_1, \dots, f_n$,*

$$\lim_{N_k \to \infty} P^{(N_k)}\Big(F[\dots, \langle\langle \phi_i, f_i \rangle\rangle_N, \dots]\Big) = P\Big(F[\dots, X_{\phi,f}(\nu), \dots]\Big) \tag{3.6}$$

Moreover, denoting by $\mathcal{G}$ the set of all translational invariant and stationary measures on $\{0,1\}^{\mathbb{Z}}$ (i.e. $\nu(f(\eta)) = \nu(f(S_x\eta))$ *and* $\nu(f) = \nu(L_d f)$ *for all x and all cylindrical f*)

$$P\Big((\nu \in M : \nu_{x,t} \in \mathcal{G} \text{ for almost all } x,t\Big) = 1\,. \tag{3.7}$$

The proof is essentially as in the Young theorem. The space and time invariance stated in (3.7) are the outcome of the space and time averages involved in the definitions. Some details are given in Appendix B.

3.4 – Time 0 assumptions

We will suppose convergence of the initial datum to a smooth density profile $\rho_0 \in C^\infty(\mathcal{T}, [0,1])$ in the following sense. For any $\phi \in C^\infty(\mathcal{T} \times \mathbb{R}_+)$ and any $\delta > 0$,

$$\lim_{N\to\infty} P^{(N)}\left(\left|\langle \phi, \eta_0\rangle_{N,0} - \int_0^1 \phi\rho_0\right| > \delta\right) = 0\,. \tag{3.8}$$

3.5 – A first characterization of the limit law

The purpose now is to characterize more precisely the support of the limit probability P and in this way to determine the hydrodynamic equations for the exclusion process. The starting point is a Martingale relation which is a particular example of a relation valid in general in Markov processes:

$$g\big(\eta(\cdot,t),t\big) = g\big(\eta(\cdot,0),0\big) + \int_0^t \left\{\frac{d}{ds'} g\big(\eta(\cdot,s),s'\big)\big|_{s'=s} + L_d g\big(\eta(\cdot,s),s\big)\right\} + M_t \tag{3.9}$$

$g(\eta,t)$ a bounded measurable function smooth in t and M_t a martingale. We will use (3.9) with $g\big(\eta(\cdot,t),t\big) = \langle\phi,\eta_0\rangle_{N,t}$ thus getting

$$\langle\phi,\eta_0\rangle_{N,t} = \langle\phi,\eta_0\rangle_{N,0} + \frac{1}{N}\int_0^t \{\langle\phi_s,\eta_0\rangle_{N,s} + N\langle\phi,(L_d\eta_0\rangle_{N,s}\} + M_t \tag{3.10}$$

where again M_t is a martingale. $L_d\eta_0 = \eta_{-1}[1-\eta_0] - \eta_0[1-\eta_1]$, so that after an integration by parts,

$$\begin{aligned} N\langle\phi, L_d\eta_0\rangle_{N,s} &= \langle D_N\phi, \eta_0(1-\eta_1)\rangle_{N,s}\,, \\ D_N\phi(r,t) &= N\left\{\phi\left(r+\frac{1}{N},t\right) - \phi(r,t)\right\} \end{aligned} \tag{3.11}$$

$D_N\phi$ is the discrete derivative of ϕ and it is bounded uniformly in N.

An analogous computation involving martingale calculus and then use of Doob's martingale theorem, for details see for instance [9] and Appendix B, shows that for any $\tau > 0$ and $\delta > 0$,

$$\lim_{N\to\infty} P^{(N)}\left(\left\{\sup_{t\le\tau N} |M_t| \ge \delta\right\}\right) = 0\,. \tag{3.12}$$

Since $\phi \in C_0^\infty(\mathcal{T}\times\mathcal{R}_+)$ there is $\tau > 0$ so that $\langle\phi,\eta_0\rangle_{N,t} = 0$ for $t \ge \tau N$. For such t we then get, using (3.8), (3.11) and Theorem 3.1,

$$\begin{aligned} P\Bigg(\Bigg\{&\int_0^1 \phi(x,0)\rho_0(x) \\ &+ \int_0^\tau\int_0^1 \phi_t(x,t)\nu_{x,t}(\eta_0) + \phi_x(x,t)\nu_{x,t}\big(\eta_0(1-\eta_1)\big)\Bigg\}\Bigg) = 1\,. \end{aligned} \tag{3.13}$$

To derive an equation we need to relate $\nu_{x,t}(\eta_0)$ and $\nu_{x,t}(\eta_0(1-\eta_1))$.

3.6 – The symmetric exclusion

Before proceeding further, let us examine the symmetric case which is much simpler: the process is then defined by the generator $L_0 = L_d + L_s$, where

$$L_s f(\eta) = \sum_{x\in\mathbb{Z}} \eta(x)[1-\eta(x-1)]\{f(\eta-\delta_x+\delta_{x-1})-f(\eta)\}\,.$$

By summing the contributions of L_d and L_s in (3.11) the non linear terms cancel out and we get (omitting dependence on time)

$$\begin{aligned}\langle\phi, L_0\eta_0\rangle_N &= \frac{1}{N}\sum_{x=1}^{N}[\eta(x)-\eta(x+1)]\left(\left\{\phi\left(\frac{x+1}{N}\right)-\phi\left(\frac{x}{N}\right)\right\}\right)\\ &= \frac{1}{N}\sum_{x=1}^{N}\eta(x)\left(\left\{\phi\left(\frac{x+1}{N}\right)+\phi\left(\frac{x-1}{N}\right)-2\phi\left(\frac{x}{N}\right)\right\}\right)\,.\end{aligned}\tag{3.14}$$

The last curly bracket is equal to $N^2 D_N^2\phi$, $D_N^2\phi$ the discrete laplacian of ϕ. The desired extra factor N^2 can be obtained by scaling times by N^2. We thus redefine the averages by setting

$$\langle\langle\phi,f\rangle\rangle_N = \frac{1}{N^2}\int_0^\infty \langle\phi,f\rangle\rangle_{N,t},\quad \langle\phi,f\rangle_{N,t} = \frac{1}{N}\sum_{x=1}^{N}\phi\left(\frac{x}{N},\frac{t}{N^2}\right) f\big(S_x\eta(\cdot,t)\big)\tag{3.15}$$

and, with such a new terminology,

$$\langle\phi,\eta_0\rangle_{N,t} = \langle\phi,\eta_0\rangle_{N,0} + \frac{1}{N^2}\int_0^t \{\langle\phi_t,\eta_0\rangle_{N,s} + N^2\langle\phi, D_N^2\eta_0\rangle_{N,s}\} + M_t\,.\tag{3.16}$$

Taking $t=\tau N^2$ we have for τ large enough

$$P\left(\left\{\int_0^1 \phi(x,0)\rho_0(x) + \int_0^\tau\int_0^1 \phi_t(x,t)\nu_{x,t}(\eta_0)+\phi_{xx}(x,t)\nu_{x,t}(\eta_0)\right\}\right)=1\,.\tag{3.17}$$

Calling $\rho(x,t) := \nu_{x,t}(\eta_0)$,

$$P\left(\left\{\int_0^1 \phi(x,0)\rho_0(x) + \int_0^\tau\int_0^1 \phi_t(x,t)\rho(x,t)+\phi_{xx}(x,t)\rho(x,t)\right\}\right)=1\tag{3.18}$$

deducing that P is actually supported by Young measures ν such that

$$\rho_t = \rho_{xx},\quad \rho(x,0)=\rho_0(x)\tag{3.19}$$

(3.19) is the hydrodynamic equation associated to the symmetric simple exclusion, which is thus a model for the heat equation.

3.7 – Gradient systems and propagation of chaos

We call "gradient" the interacting particle systems where the analogue of the computations (3.11) or (3.14) can be carried out getting respectively a first or a second discrete derivative: in the former case the system is called hyperbolic, in the latter parabolic. Thus the asymmetric exclusion is a hyperbolic gradient system, the symmetric exclusion a parabolic gradient systems. For gradient systems in general the above procedure applies and in this way several other systems in dimensions $d \geq 1$ have been studied deriving relations of the form (3.13) or (3.18) if the system is parabolic.

Let us now go back to the asymmetric exclusion process for which we have deduced (3.13). To obtain the hydrodynamic equations it is necessary to specify further the support of P. The first step is the ergodic problem: determine the set $\mathcal{G}$ of all stationary, translational invariant measures. $\mathcal{G}$ is a convex set, which for the exclusion process has been completely characterized, see [8]. The collection $\mathcal{G}_{\text{extr}}$ of its extremal elements is in fact the set of all the Bernoulli measures $\mu_p, p \in [0,1]$, $\mu_p(\{\eta(x) = 1, x \in X\}) = p^{|X|}$. Thus any $\mu \in \mathcal{G}$ is of the form $\mu = \int_0^1 \mu_p \lambda(dp)$, λ a probability on $[0,1]$.

Definition 3.1. P is a local equilibrium measure and propagation of chaos holds, if P is supported by Young measures ν such that for almost all x, t, $\nu_{x,t} \in \mathcal{G}_{\text{extr}}$, i.e. in the case of the exclusion process, if $\nu_{x,t}$ is Bernoulli.

Failure of local equilibrium may occur due to fast oscillations on a mesoscopic scale intermediate between macroscopic and lattice. The averages involved in the definition of Young measures may then pick up different extremal measures which after averaging give rise to a non extremal one. Such a possibility has been ruled out in some parabolic systems by proving the absence of such oscillations (the two block estimates in [9]), and/or supposing some good properties of the initial law.

Propagation of chaos has been proved to hold for the exclusion process, see [8]. Then for almost all x, t $\nu_{x,t} = \mu_{\rho(x,t)}$ for some $\rho(x,t) \in [0,1]$ and (3.11) yields

$$P\left(\left\{\int_0^1 \phi(x,0)\rho_0(x) + \int_0^\tau \int_0^1 \phi_t(x,t)\rho(x,t) + \phi_x(x,t)\rho(x,t)[1-\rho(x,t)]\right\}\right) = 1\,,$$

$$\rho_t + [\rho(1-\rho)]_x = 0, \quad \rho(x,0) = \rho_0(x) \quad \text{(weakly)}\,. \tag{3.20}$$

Thus the hydrodynamic equation associated to the asymmetric simple exclusion process is the Burgers equation. It is also proved that P is supported by the entropic solutions of (3.20) so that P is actually supported by a singleton. The picture emerging from this analysis can then be read on two levels. First it states that for each macroscopic space-time point (x,t) there is a density $\rho(x,t)$ and the collection of all such density values satisfy a hydrodynamic equation (which is the Burgers equation for the asymmetric exclusion). The second level I was referring to is that $\rho(x,t)$ is actually a parameter which specifies an equilibrium state in $\mathcal{G}_{\rm extr}$ which describes the local state of the system around the macroscopic point (x,t).

As mentioned the above picture has been established in several stochastic, interacting particle systems but its validity should in principle extend to deterministic evolutions as well, the most known example from where the above terminology is derived is the Boltzmann equation for which it has been shown that in the macroscopic (Grad-Boltzmann limit) the hydrodynamic equations are indeed the Euler equations, see [4].

4 – Gibbs measures and phase transitions

The ergodic problem of characterizing the set $\mathcal{G}_{\rm extr}$ is in general hard, also for stochastic systems. There is however an important class of models where the problem does not even arise, they are the systems with Glauber and Kawasaki dynamics, which are constructed with the requirement that all Gibbs measures are invariant.

Occurrence of singularities in the hydrodynamic equations require the introduction of additional properties, for instance the formation of shocks in the Burger equations involve the proof of an additional property, namely that the solution should be "entropic". Here we discuss another source of singularities which arise when the values of the order parameter (the parameter labelling the elements of $\mathcal{G}_{\rm extr}$, i.e. the density in particle systems or the magnetization density in spin systems) is not connected. Such a pathology is due to the occurrence of a phase transition. Let us go back to the case of Gibbs measures, recalling that a Gibbs measure assigns a probability proportional to $e^{-\beta H}$ to a configuration whose energy is H, β the inverse temperature. The dynamical problem of characterizing $\mathcal{G}_{\rm extr}$ becomes then the typical equilibrium statistical mechanics problem of finding the extremal Gibbs measure, a problem which has been solved in a variety of cases. Referring to the Ising model with Glauber dynamics, if β is large enough in $d \geq 2$ dimensions, $\mathcal{G}_{\rm extr}$ is made of two elements, $\mu_{\pm m_\beta}$, $m_\beta > 0$, $\mu_{\pm m_\beta}(\sigma(0)) = \pm m_\beta$, $\sigma(0)$ the spin at the origin.

If propagation of chaos holds, there will be for each t a set where $\nu_{x,t} = \mu_{m_\beta}$ while, in the complement $\nu_{x,t} = \mu_{-m_\beta}$. and the macroscopic equations become the geometric evolution of such sets. Clearly the mechanisms which rule the evolution depend upon the structure of the system at the interface, i.e. on sets of codimension 1 (if the evolution is regular) which from the point of view of the Young measure are irrelevant. A new approach is required and let us start from macroscopics.

5 – Phase coexistence, inputs from Geometric Measure theory

Thermodynamics says that the free energy excess in a body to create a bubble of the opposite phase (say the phase with magnetization m_β) in a regular region E of the domain $\Omega \subset \mathbb{R}^d$ (thus the magnetization density is $m(r) = m_\beta$ when $r \in E$ and $= -m_\beta$ when $r \in \Omega \setminus E$) is given by

$$I(m) = \int_{\partial E} \tau_\beta(n(r)) H^{d-1}(dr) \tag{5.1}$$

where $n(r)$ is the outward unit normal to ∂E at r; $\tau_\beta(n) = \tau_\beta(-n)$ is the surface tension of a flat surface with normal n; $H^{d-1}(dr)$ is the Hausdorff measure on ∂E.

Thus the cost of a bubble is determined by its geometry and the surface tension which are therefore the control parameters for phase coexistence. This immediately raises the question: where is the regularity assumption on E coming from? According to (5.1) the likelihood of a bubble depends on its cost $I(m)$ and the first problem is to characterize all regions E which can be approximated by regular ones keeping the cost uniformly bounded. These are the physically relevant bubbles, regular ones are only models to help intuition and simplify computations.

Geometric measure theory gives a complete answer to the question, the regions E which have finite cost are the sets of bounded variations, see for instance [7]. Such sets are pretty regular, one can define a perimeter measure on ∂E proving that modulo zero the surface is C^1-regular and a normal is well defined almost everywhere. Then a formula like (5.1) still holds.

The relaxation of an initial state with a bubble under a dynamics which preserves the total magnetization [it is physically conjectured that it] will lead to a state where the free energy is minimal under the given magnetization constraint. Such minimizers are the equilibrium states at the given magnetization and they are the solutions of the variational problem:

$$\inf \left\{ I(m), \fint_\Omega m = \alpha \right\}, \quad \alpha \in (-m_\beta, m_\beta) \tag{5.2}$$

the well known Wulff problem. Consider for instance perfect (Neumann) boundary conditions on $\partial\Omega$, namely when the functional (5.1) is replaced by

$$I^{\text{neum}}(m) = \int_{\partial E \setminus \partial\Omega} \tau_\beta(n(r)) H^{d-1}(dr)\,. \tag{5.3}$$

It is then known that in $d = 2$ there is $\alpha_c > 0$ so that for $|\alpha| > \alpha_c$ the minimizer is made by a bubble which is a quarter of a circle with center a vertex of Ω. For $|\alpha| < \alpha_c$ is a rectangle with three sides contained in $\partial\Omega$. In $d \geq 3$ it is not known if the same picture holds, it is known that for $\alpha = 0$ the minimizer is half of Ω and for α close to the extremes is again a quarter of circle, but the shape for intermediate values of α are not known, [17].

6 – Sharp interface limits, Gamma convergence

It is clear from the discussion in Section 5 that all the relevant physics is at the interface. The approach used to study thermodynamic limits is then completely inadequate as we need to identify the Young measure in sets of codimension one (in the limit) where the system is not in local equilibrium and we have again a problem of microstructures. To investigate the structure of the interface we need a blow up. Continuum theories approach the question by magnifying up to a mesoscopic scale, intermediate between macroscopic and microscopic, and defined in such a way that on such a scale the interface width has order 1. In the Ginzburg-Landau approximation, the thermodynamics of the system is completely described by an excess free energy functional of the form:

$$F_\Lambda(m) = \int_\Lambda W(m) + |Dm|^2, \quad W(m) = \frac{1}{4}(m^2 - m_\beta)^2 \tag{6.1}$$

(in general $W(m)$ is taken as a double well function whose minimum is 0). The function reflects the assumption that a penalty appears when either m deviates from the equilibrium values $\pm m_\beta$ or when m has spatial variations. Thus the minimizers are the homogeneous equilibria $m^{(\pm)} = \pm m_\beta$. A bubble like in the macroscopic theory where there is a sharp transition between $\pm m_\beta$ has here infinite cost due to the penalty term $|Dm|^2$. Thus, in the Ginzburg-Landau theory, interfaces are diffuse, they have a finite width which will turn out to be of the order of unity in the length units used to write (6.1).

Preliminary to the microanalysis of the interface we want compatibility with the macroscopic theory of Section 5, in particular we want to identify the surface tension in (6.1). The idea like in the hydrodynamic limits is that the macroscopic model describes the behavior of the mesoscopic one on large scales. Let us fix a macroscopic region Ω, for instance a cube of side 1 and center 0 (with perfect walls in the sense described in Section 5). We then consider the functional $F_{\varepsilon^{-1}\Omega}(m)$ with Neumann conditions, $(Dm \cdot n) = 0$ at the boundaries of $\varepsilon^{-1}\Omega$. A macroscopic bubble, i.e. a function $u = m_\beta$ in $E \subset \Omega$ and $= -m_\beta$ in $\Omega \setminus E$, is δ-approximated mesoscopically by functions $m \in L^1(\varepsilon^{-1}\Omega)$ such that $⨍\Omega|u(r) - m(\varepsilon r)| \le \delta$. Thus modulo δ, the cost of the bubble (per unit area) is given by

$$\inf\left\{\varepsilon^{d-1}F_{\varepsilon^{-1}\Omega}(m),\ ⨍_\Omega |u(r) - m(\varepsilon r)| \le \delta\right\} \tag{6.2}$$

hence the De Giorgi proposal to identify the macroscopic cost of the bubble with either one of the two quantities

$$\begin{aligned} I_<(u) &:= \lim_{\delta\to 0}\liminf_{\varepsilon\to 0}\inf\left\{\varepsilon^{d-1}F(m),\ ⨍_\Omega |u(r) - m(\varepsilon r)| \le \delta\right\} \\ I_>(u) &:= \lim_{\delta\to 0}\limsup_{\varepsilon\to 0}\inf\left\{\varepsilon^{d-1}F(m),\ ⨍_\Omega |u(r) - m(\varepsilon r)| \le \delta\right\}. \end{aligned} \tag{6.3}$$

By writing $v(r) = m(\varepsilon^{-1}r)$, $r \in \Omega$, $m \in L^1(\varepsilon^{-1}\Omega)$, $v \in L^1(\Omega)$ and

$$\varepsilon^{d-1} F_{\varepsilon^{-1}\Omega}(m) = \int_\Omega \varepsilon^{-1} W(v) + \varepsilon |Dv|^2 = \mathcal{F}_\varepsilon(v) \tag{6.4}$$

which is the functional studied by Modica, [11], Modica and Mortola, [12], and Luckhaus and Modica [10]. The above derivation clarifies the meaning of the small parameter $\varepsilon > 0$, it is the ratio between macroscopic and mesoscopic unit lengths; the sharp interface limit is the limit when the ratio vanish.

In the above references it is proved that $\mathcal{F}_\varepsilon$ Γ-converges to I (see for instance [5] for definitions and results), namely that

$$I_<(u) = I_>(u) = I(u) \tag{6.5}$$

with $I(u)$ as in (6.1) and $\tau_\beta(n) = F^{(1)}(\bar{m})$ independently of n, where $F^{(1)}$ is the $d = 1$ version of (6.1) and $\bar{m}(x) = m_\beta \tanh m_\beta x$ is the antisymmetric solution of the Euler-Lagrange equation for $F^{(1)}$, namely $m_{xx} = W'(m)$, with "boundary conditions" $\pm m_\beta$ at $\pm\infty$.

7 – Sharp interface limit and motion by curvature

If ∂E, $E := \{u = -m_\beta\}$, is regular, an optimizing sequence can be defined by setting (in mesoscopic units)

$$m^{(\varepsilon)}(r) = \bar{m}\big(d(r, \partial E)\big) \tag{7.1}$$

where $d(r, \partial E)$ is the signed distance of r from E, i.e. the distance from E if $r \notin E$ and minus the distance if $r \in E$. We thus have a candidate for the structure of the interface (at least in the present context) and we can then go back to dynamical problems. Dynamics in mesoscopic theories is usually defined as a gradient flow:

$$m_t = -C \frac{\delta F(m)}{\delta m} = C[\Delta m - W'(m)] \tag{7.2}$$

where C is a positive function which has the meaning of a mobility coefficient and that we take for simplicity equal to 1. Notice that by (7.2),

$$\frac{d}{dt} F(m) = -C \int \left(\frac{\delta F(m)}{\delta m} \right)^2 \leq 0 \tag{7.3}$$

thus, by construction, dynamics enjoys the correct property to make the free energy decrease, the decrease is strict unless m is a critical point of F.

The problem we want to discuss is about the behavior of (7.2) (taken in $\mathbb{R}^d$, $d>1$) with initial datum (7.1) in the limit as $\varepsilon \to 0$. Analogously to (6.4), it is convenient to go to macroscopic units defining $v^{(\varepsilon)}(r,t) = m(\varepsilon^{-1}r, \varepsilon^{-2}t)$. Then

$$v_t^{(\varepsilon)} = \Delta v^{(\varepsilon)} - \varepsilon^{-2} W'(v^{(\varepsilon)}), \quad v^{(\varepsilon)}(r,0) = \bar{m}\big(\varepsilon^{-1} d(r, \partial E)\big)\,. \tag{7.4}$$

The setup in (7.4) reminds of the Boltzmann equation in the Grad-Boltzmann limit, where an Hilbert expansion shows convergence to the Euler equation, [4]. Indeed De Mottoni and Schatzmann have actually carries out the analogy by proving under suitable assumptions of regularity that in the limit $\varepsilon \to 0$ there is a geometric motion $E(t)$, $E(0)=E$, characterized by the fact that any point of $\partial E(t)$ moves with velocity directed along the outward normal given by the mean curvature at that point (the signs are such that convex bodies shrink). Such a motion is well defined if E is regular at least for small positive times, but in $d>2$ there are examples where singularities may develop. The evolution can then be extended by using the notion of "viscosity solutions" and indeed it has been proved by several authors in several papers that if the viscosity solution has "no fattening" then the limit of (7.4) is actually given by the viscosity solution. By using the De Giorgi ideas of "barriers", Barles and Souganidis, [3], have proved that for systems where a comparison theorem holds, if there is convergence to motion by curvature in the classical case, then there is convergence to the viscosity solution if the latter has "no fattening". With this result it is sufficient to restrict to regular cases and the De Mottoni and Schatzmann work covers automatically also cases with singularities (but no fattening).

8 – A non local functional

With the ultimate goal of establishing a connection with microscopic systems of statistical mechanics, following the approach initially proposed by van der Waals and then pursued in the 70's first by Kac and then by Lebowitz and Penrose, we will consider here a variant of the Ginzburg-Landau functional. Let $m \in L^\infty(\Lambda, [-1,1]$ and

$$F_\Lambda(m) = \int_\Lambda W(m) + \frac{1}{4}\int_{\Lambda^2} J(r,r')[m(r)-m(r')]^2 \tag{8.1}$$

where $J(r,r') = J(0,r'-r) \ge 0$ is a smooth probability kernel supported in $|r-r'| \le 1$. $W(m) \ge 0$ is given by

$$W(m) = -\frac{m^2}{2} - \frac{\mathcal{S}(m)}{\beta} - C_\beta \tag{8.2}$$

$\mathcal{S}(m) = -\frac{1-m}{2}\log\{\frac{1-m}{2}\} - \frac{1+m}{2}\log\{\frac{1+m}{2}\}$ is the entropy with magnetization m (of a Bernoulli measure) and C_β is chosen so that $\min W(m) = 0$.

It has been proved, [1], [2], [3], that the analysis of Section 6 and 7 can be extended to the above functional. In particular the surface tension $\tau_\beta(n)$ which here depends on the unit vector n is given by $F^{(n)}(\bar{m})$ where $F^{(n)}(\bar{m})$ is the version of (8.1) on the line with J replaced by $J^{(n)}(x,y)$, where

$$J^{(n)}(x,y) = \int_{r\cdot n=0} J(0, n(y-x)+r)H^{d-1}(dr) \tag{8.3}$$

and $\bar{m}$ is the unique antisymmetric non zero solution of

$$\bar{m} = \tanh\{\beta J^{(n)} * \bar{m}\} := \tanh\{\beta \int J^{(n)}(x,y)\bar{m}(y)dy\}\,. \tag{8.4}$$

Defining the evolution by means of the equation

$$m_t = -m + \tanh\{\beta J * m\} \tag{8.5}$$

under the scaling used in Section 7 we obtain again in the limit motion by curvature, see [2] and [3]. In particular in $d = 2$ the velocity of a point is proportional to the curvature with a proportionality coefficient equal to $\mu[\tau_\beta + \tau_\beta'']$, where, representing n in terms of an angle θ with $\tau_\beta = \tau_\beta(\theta)$, then τ_β'' is the second derivative w.r.t. θ. The expression $[\tau_\beta + \tau_\beta'']$ is known as "the stiffness coefficient". $\mu = \mu(\theta)$ is a mobility coefficient, it is related to the speed of a travelling front under forcing by an external magnetic field, see [2] for details.

The next steps will be to relate the functional to Gibbs measures in Ising systems with Kac potentials and carry out the continuum limit. The program has been partially successful and it is still under investigation, but its description goes beyond the aims of this presentation and I rather refer to the literature, in particular to a book I am writing and which is almost completed, [16].

– Appendix A

For any positive integer n, partition $\mathbb{R}$ into the intervals $2^{-n}[j, j+1)$, $j \in \mathbb{Z}$. Call $I_x^{(n)}$ the interval which contains the point x. ϕ is called $I^{(n)}$-measurable if it is constant on each one of the intervals $I^{(n)}$.

Let $\nu_{x;k}^{(n)}$ be the measure on $\mathbb{R}$ such that for any interval $[a,b]$,

$$\nu_{x;k}^{(n)}(\{r \in [a,b]\}) = \frac{\big|\{y \in I_x^{(n)} : z_k(y) \in [a,b]\}\big|}{|I_x^{(n)}|}$$

and for any $f \in C_0(\mathbb{R})$ and any $I^{(n)}$-measurable function ϕ,

$$\nu_{x;k}^{(n)}(f) = ⨍_{I_x^{(n)}} f(z_k), \quad \int_0^1 \phi f(z_k) = \int_0^1 \phi \nu_{x;k}^{(n)}(f)\,.$$

By (2.3), for k large enough, $\nu^{(n)}_{x;k}(w(|r|) \le 2^n \int_0^1 w(|z_k|) \le c$, which implies that $\nu^{(n)}_{x;k}$ is a probability and that the set $\{\nu^{(n)}_{x;k}\}_{x\in\mathbb{N}_+}$ is tight, [15]. Then there is a subsequence $k^{(n)}_j$ and probabilities $\{\nu^{(n)}_x\}_{x\in[0,1]}$ so that $\{\nu^{(n)}_{x;k^{(n)}_j}\}$ converges weakly to $\nu^{(n)}_x$ for all $x \in [0,1]$, $\nu^{(n)}_x$ constant in each one of the intervals $I^{(n)}$. Thus, for any $I^{(n)}$-measurable function ϕ

$$\lim_{k^{(n)}_j\to\infty} \int_0^1 \phi f(z_{k^{(n)}_j}) = \int_0^1 \phi(x)\nu^{(n)}_x(f)\,.$$

We suppose inductively that for each n, $k^{(n+1)}_j$ is a convergent subsequence of $k^{(n)}_j$ and then have

$$\nu^{(n)}_x = ⨍_{I^{(n)}_x} \nu^{(n+1)}_y dy$$

which implies that for each $f \in C_0(\mathbb{R})$ the family of functions $M_n(x) = \nu^{(n)}_x(f)$, $x \in [0,1]$, is a martingale. Then, by Doob's martingale convergence theorem, [6], for any $f \in C_0(\mathbb{R})$, $\nu^{(n)}_x(f)$ converges as $n \to \infty$ for almost all x in $[0,1]$ to a limit $L_x(f)$. Let $\mathcal{D}$ be a countable dense subset in $C_0(\mathbb{R})$, then there is a subset I in $[0,1]$ of measure 1 where $L_x(f)$ is defined for all $f \in \mathcal{D}$ and by continuity L_x extends to a probability ν_x on $\mathbb{R}$ and for any x we have

$$\nu^{(n)}_x(f) = ⨍_{I^{(n)}_x} \nu_y(f)$$

and for any $I^{(n)}$-measurable function ϕ

$$\int_0^1 \phi(x)\nu^{(n)}_x(f) = \int_0^1 \phi(x)\nu_x(f)$$

hence, along the convergent subsequence,

$$\lim_{k_j\to\infty} \int_0^1 \phi f(z_{k_j}) = \int_0^1 \phi(x)\nu_x(f) \tag{A.1}$$

(A.1) holds for any n, any $I^{(n)}$-measurable function ϕ and any $f \in C_0(\mathbb{R})$. By continuity, it then holds for all $\phi \in L^1([0,1])$.

– **Appendix B**

Denote by ξ a pair $I, \{0,1\}^I$, where I is a finite subset of $\mathbb{Z}$, The collection of all ξ is denoted by

$$\Xi = \bigcup_{I \subset \mathbb{Z}, |I| < \infty} \{0,1\}^I \,. \tag{B.1}$$

Let $\xi \in \Xi$, I the interval associated to ξ and

$$\mathbf{1}_\xi(\eta) = \begin{cases} 1 & \text{if } \eta(x) = \xi(x), \text{ for all } x \in I \\ 0 & \text{otherwise}\,. \end{cases} \tag{B.2}$$

Denote by $I^{(n)}$ intervals in $[0,1] \times \mathbb{R}^+$ of the form $\{(x,t) : x \in 2^{-n}[j, j+1); t \in 2^{-n}[k, k+1), j, k \in \mathbb{N}\}$; call $I^{(n)}$-measurable a function of x, t constant on each one of the intervals $I^{(n)}$. Let then $\mathcal{X}$ be the collection of functions indexed by the pairs (ξ, n) so that an element $X \in \mathcal{X}$ is such that $X_{\xi,n}$ is a $I^{(n)}$-measurable function with values in $[0,1]$. $\mathcal{X}$ has then the structure of a product space with factors which are compact (under the natural topology), thus $\mathcal{X}$ is compact in the product topology.

To each element $\{\eta(x,t)\}$ of the exclusion process we can associate an element in $\mathcal{X}$ by setting

$$\{\eta(x,t)\} \to X_{\xi,n}(x,t) = \frac{\langle\langle \mathbf{1}_{I^{(n)}_{x,t}}, \mathbf{1}_\xi \rangle\rangle_N}{\langle\langle \mathbf{1}_{I^{(n)}_{x,t}}, 1 \rangle\rangle_N} \,. \tag{B.3}$$

Under the above map the probability $P^{(N)}$ induces a probability $Q^{(N)}$ on $\mathcal{X}$. By compactness there is a subsequence N_k such that $Q^{(N_k)}$ converges weakly on $\mathcal{X}$ to a limit probability Q. Thus

$$\begin{aligned} &\lim_{N_k \to \infty} P^{(N_k)}\Big(F[\dots, \langle\langle \phi_i, \mathbf{1}_{\xi_i} \rangle\rangle_N, \dots]\Big) \\ &\qquad = Q\left(F\left[\dots, \int_0^\infty \int_{x \in [0,1]} \phi_i(x,t) X_{\xi_i, n_i}(x,t), \dots\right]\right) \end{aligned} \tag{B.4}$$

where $F = F(r_1, \dots, r_m)$ is a bounded continuous function; ϕ_i, $i = 1, \dots, m$ are $I^{(n_i)}$-measurable functions and $\xi_i \in \Xi$, $i = 1, \dots, m$.

Call $\mathcal{X}^0$ the set of $X \in \mathcal{X}$ which are “additive”, “normalized” and “compatible”. Additivity means that if $\sum \xi_i = \xi$ then for all n, x and t,

$$\sum X_{\xi_i, n}(x,t) = X_{\xi,n}(x,t)\,. \tag{B.5}$$

Normalized means that if $\sum \xi_i = 1$ then

$$\sum X_{\xi_i,n}(x,t) = 1\,. \tag{B.6}$$

Finally compatibility means that for all ξ, n, x, t

$$⨍_{I^{(n)}_{(x,t)}} X_{\xi,n+1}(y,s) = X_{\xi,n}(x,t)\,. \tag{B.7}$$

By (B.4) it then follows that

$$P(\mathcal{X}^0) = 1\,. \tag{B.8}$$

On the other hand if $X \in \mathcal{X}^0$, for any n, x, t, $X_{\xi,n}(x,t)$ extends to an additive measure on the algebra of all cylinder sets in $\{0,1\}^{\mathbb{Z}}$. Then by the Caratheodory reconstruction theorem, there is a unique probability measure $\nu^{(n)}_{x,t}$ on $\{0,1\}^{\mathbb{Z}}$ such that

$$X_{\xi,n}(x,t) = \nu^{(n)}_{x,t}(\mathbf{1}_\xi)\,. \tag{B.9}$$

Moreover, by the martingale convergence theorem as in Appendix A, we then conclude that there is a probability $\nu_{x,t}$ such that

$$\nu^{(n)}_{x,t}(f) = ⨍_{I^{(n)}_{x,t}} \nu^{(n)}_{y,s}(f) \tag{B.10}$$

which proves (3.5) with P the law of $\{\nu_{x,t}\}$ under Q.

The proof that $P\big(\nu_{x,t} \in \mathcal{G}$, for a.a. $x,t\ \big) = 1$ follows from the following general properties. Referring to (3.9), we have

$$P^{(N)}\left(\sup_{s\le t} M_s^2\right) \le 4P^{(N)}\Big(M_t^2\Big) \tag{B11}$$

$$P^{(N)}\Big(M_t^2\Big) = \int_0^t P^{(N)}\Big(\{L_d g^2(\eta(\cdot,s),s) - 2g(\eta(\cdot,s),s)L_d g(\eta(\cdot,s),s)\}\Big)\,. \tag{B.12}$$

Finally if f_1 and f_2 are cylindrical functions which depend on $\eta(x)$ with $x \in I_1$ and, respectively, $x \in I_2$ and $\mathrm{dist}(I_1, I_2) > 1$, then

$$L_d f_1 f_2 = f_1 L_d f_2 + f_2 L_d f_1\,. \tag{B.13}$$

We then have by (3.10) with η_0 replaced by a cylindrical function f,

$$\langle\langle \phi, L_d f\rangle\rangle_N = -\frac{1}{N}\langle \phi, L_d f\rangle_{N,0} - \frac{1}{N} M_{\tau N}\,. \tag{B.14}$$

The first term on the r.h.s. vanishes in sup norm as $N \to \infty$. For the other one we write

$$\text{(B.15)} \quad P^{(N)}(M_{\tau N}^2) = \int_0^{\tau N} P^{(N)}\Big(\{L_d\langle\phi, f\rangle_{N,t}^2 - 2\langle\phi, f\rangle_{N,t} L_d\langle\phi, f\rangle_{N,t}\}\Big) \le c\tau N$$

having used (B.13). Thus $P^{(N)}(\frac{1}{N}|M_{\tau N}| \ge \delta) \to 0$ for any $\delta > 0$, proving that P is supported by stationary Young measures. Invariance by translations follows easily from the spatial averages involved in the definition of Young measures and Theorem 3.1 is proved.

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