

Homogenization of Lattice Systems

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These notes contain the material related to the three lectures that I have delivered at the Workshop 'Recent Advances in Homogenization' held at INdAM, Rome in the week 23–27 May 2005. The notes are thought just as a complement and reference for the single lectures, and not as a whole: I must warn that the chapters are unevenly written. Some are elaboration of articles that have already appeared, some have been completely written for the occasion. Minor details have not been fixed. As a consequence some notation may slightly vary from chapter to chapter.

1. A toy model: playing with spins

We start with the simplest non-trivial model of lattice systems; *i.e.*, when energies depend on functions that may take only two values. Of course, it is not restrictive to assume that those two values be 1 and -1 , and, taking some liberty, we may think of these lattices as spin systems. More precisely, we will consider energies depending on functions u defined on portions of N -dimensional lattices; *i.e.* $u : \varepsilon \mathbf{Z}^N \cap \Omega \rightarrow \{-1, 1\}$, where Ω is a sufficiently smooth open subset of \mathbf{R}^N .

1 A warm-up exercise: uncoupled energies

The ‘almost-trivial’ case is when the total energy of the system is simply obtained by the sum of the uncoupled energies of the single values:

$$E_\varepsilon(u) = \sum_i \varepsilon^N f(u_i).$$

where the sum runs on all $i \in \mathbf{Z}^N$ such that $\varepsilon i \in \Omega \cap \varepsilon \mathbf{Z}^N$. The normalization factor ε^N is necessary to have $E_\varepsilon(u)$ bounded and not infinitesimal as $\varepsilon \rightarrow 0$. We use the notation $u_i = u(\varepsilon i)$ if no other subscript is present.

Consider now a sequence of states u_ε that may vary with ε . Can we define a limit state u ? And correspondingly a limit energy? In this case the answer is affirmative: take any cube Q and define u as the function such that

$$\begin{aligned} \int_Q u \, dx &= \lim_{\varepsilon \rightarrow 0} \varepsilon^N (\#\{i \in \mathbf{Z}^N : \varepsilon i \in Q : u_\varepsilon(\varepsilon i) = 1\} - \#\{i \in \mathbf{Z}^N : \varepsilon i \in Q : u_\varepsilon(\varepsilon i) = -1\}) \\ &= \lim_{\varepsilon \rightarrow 0} \sum_{\varepsilon i \in Q} \varepsilon^N u_\varepsilon(\varepsilon i); \end{aligned}$$

that is, u is defined by the asymptotical statistical properties of u_ε . It is easily seen that, upon extracting a subsequence of ε , the function u is well defined (a short proof can be as follows: it is enough to take Q in a countable set of cubes; *e.g.*, those with rational vertices. Then, by a diagonal procedure, we may extract a sequence of ε such that the limit on the right-hand side above exists for all such Q . This is enough to define u by the equality above). Note that $-1 \leq u \leq 1$ and that (l being the side length of Q)

$$\int_Q u \, dx = \lim_{\varepsilon \rightarrow 0} \varepsilon^N (2\#\{i \in \mathbf{Z}^N : \varepsilon i \in Q : u_\varepsilon(\varepsilon i) = 1\} - \frac{1}{\varepsilon^N} l^N);$$

i.e.,

$$\lim_{\varepsilon \rightarrow 0} \varepsilon^N \#\{i \in \mathbf{Z}^N : \varepsilon i \in Q : u_\varepsilon(\varepsilon i) = 1\} = \frac{1}{2} \left(l^N + \int_Q u \, dx \right) = \frac{1}{2} \int_Q (1 + u) \, dx.$$

Correspondingly, the limit energy in the cube Q is given by

$$\begin{aligned} & \lim_{\varepsilon \rightarrow 0} \varepsilon^N \left(f(1) \#\{i \in \mathbf{Z}^N : \varepsilon i \in Q : u_\varepsilon(\varepsilon i) = 1\} + f(-1) \#\{i \in \mathbf{Z}^N : \varepsilon i \in Q : u_\varepsilon(\varepsilon i) = -1\} \right) \\ &= (f(1) - f(-1)) \lim_{\varepsilon \rightarrow 0} \varepsilon^N (\#\{i \in \mathbf{Z}^N : \varepsilon i \in Q : u_\varepsilon(\varepsilon i) = 1\} + f(-1)l^N) \\ &= (f(1) - f(-1)) \frac{1}{2} \int_Q (1 + u) dx + f(-1)l^N = \int_Q \left(f(-1) + \frac{1}{2}(u + 1)f(1) \right) dx. \end{aligned}$$

Note that the function $\psi(t) = (f(-1) + \frac{1}{2}(t + 1)f(1))$ is the affine function interpolating the values $f(\pm 1)$ in ± 1 . If the reference domain is not a cube, but an open set Ω such that our functions u_ε are defined on $\varepsilon \mathbf{Z}^N \cap \Omega$, then, summing up on the cubes contained in Ω we obtain that the limit energy corresponding to a state $u : \Omega \rightarrow [-1, 1]$ is

$$F(u) = \int_\Omega \psi(u) dx.$$

It will be useful to reinterpret part of what we have done above in terms of convergence of functions rather than statistics: if we identify each function $u_\varepsilon : \varepsilon \mathbf{Z}^N \cap \Omega \rightarrow \mathbf{R}$ with a piecewise-constant interpolation (we extend $u_\varepsilon(x) = u_\varepsilon(\varepsilon i)$ if $x \in \varepsilon i + \varepsilon(-\frac{1}{2}, \frac{1}{2})^N$) then the function u defined above is just the weak L^1 -limit of the sequence u_ε . In the case above we may define $F(u) = \lim_{\varepsilon \rightarrow 0} E_\varepsilon(u_\varepsilon)$ since the limit is independent of the sequence u_ε weakly converging to u .

Note that, after identifying each u_ε with a piecewise-affine function, the functionals E_ε can be read as integral functionals

$$E_\varepsilon(u_\varepsilon) = \int_\Omega f(u_\varepsilon) dx + o(1),$$

where the error $o(1)$ comes from the fact that a portion of the cubes $\varepsilon i + \varepsilon(-\frac{1}{2}, \frac{1}{2})^N$ may not be completely contained in Ω (we suppose $\partial\Omega$ sufficiently regular, in particular $|\partial\Omega| = 0$). The dependence on ε disappears from the form of the integral but remains in the domain of E_ε . Now, since $f(u_\varepsilon) = \psi(u_\varepsilon)$ and ψ is linear (so that, in particular, the integral functional F is continuous along weakly converging sequences) we have

$$\lim_{\varepsilon \rightarrow 0} E_\varepsilon(u_\varepsilon) = \lim_{\varepsilon \rightarrow 0} F(u_\varepsilon) = F(u).$$

2 Nearest-neighbour interactions

We now examine the case when

$$E_\varepsilon(u) = \frac{1}{2^N} \sum_{i,j} \varepsilon^N f(u_i, u_j),$$

and the sum is extended to all pairs of nearest neighbours; *i.e.* $|i - j| = 1$. The factor $\frac{1}{2^N}$ in front of the sum is due to the fact that each i has exactly 2^N nearest neighbours in \mathbf{Z}^N .

Upon rewriting

$$E_\varepsilon(u) = \frac{1}{2^N} \sum_{i,j} \varepsilon^N \frac{1}{2} (f(u_i, u_j) + f(u_j, u_i)) =: \frac{1}{2^N} \sum_{i,j} \varepsilon^N \tilde{f}(u_i, u_j),$$

we may suppose that f is symmetric: $f(u, v) = f(v, u)$. It is also not restrictive to suppose that $f(1, 1) = f(-1, -1)$. In fact, if we set

$$g(\pm 1, \pm 1) = f(\pm 1, \pm 1), \quad g(-1, 1) = g(1, -1) = \frac{1}{2}(f(1, 1) + f(-1, -1)),$$

we can rewrite

$$\begin{aligned} E_\varepsilon(u) &= \frac{1}{2^N} \sum_{i,j} \varepsilon^N (f(u_i, u_j) - g(u_i, u_j)) + \frac{1}{2^N} \sum_{i,j} \varepsilon^N g(u_i, u_j) \\ &= \frac{1}{2^N} \sum_{i,j} \varepsilon^N (f(u_i, u_j) - g(u_i, u_j)) \\ &\quad + \frac{1}{2^N} f(1, 1) \#\{(i, j) : u_i = u_j = 1\} + \frac{1}{2^N} f(-1, -1) \#\{(i, j) : u_i = u_j = -1\} \\ &\quad + \frac{1}{2^{N+1}} (f(1, 1) + f(-1, -1)) \#\{(i, j) : u_i = 1, u_j = -1\} \\ &= \frac{1}{2^N} \sum_{i,j} \varepsilon^N (f(u_i, u_j) - g(u_i, u_j)) + \frac{1}{2^N} \sum_i \varepsilon^N f(u_i, u_i). \end{aligned}$$

The last sum is an energy of the ‘almost-trivial’ form considered in the section above, that depends only on the ‘statistical’ properties of u . Hence we may just drop it, or study it separately as above.

The behaviour of our energy will be then just governed by the two values $f(1, 1) = f(-1, -1)$ and $f(1, -1) = f(-1, 1)$. Apart from the trivial case in which the two values are equal, we may always suppose that one of the two values is 1 and the other is -1 (this ‘renormalization’ amounts just to an affine change of the value of the energy). After these simplifications we are left with the two cases:

i) $f(u, v) = -uv$ (*ferromagnetic type energies*). In this case the minimization of E_ε will favour uniform states $u = v = 1$ or $u = v = -1$;

ii) $f(u, v) = uv$ (*anti-ferromagnetic type energies*). In this case the minimization of E_ε will favour oscillating states $u = -v$, alternating 1 and -1 .

We want to examine now the behaviour of the energy $E_\varepsilon(u_\varepsilon)$ as $\varepsilon \rightarrow 0$ along a sequence (u_ε) in the two cases.

The value of the limit of $E_\varepsilon(u_\varepsilon)$ will depend on the particular sequence, (u_ε) ; we first wish to provide a lower bound for this limit independent of this sequence. To this end for each u_ε we introduce an auxiliary function v_ε defined on a ‘dual lattice’: we set

$$\mathcal{Z} = \left\{ \frac{i+j}{2} : i, j \in \mathbf{Z}^N, |i-j| = 1 \right\},$$

and, given u_ε , we define

$$v_\varepsilon(\varepsilon k) = \frac{u_\varepsilon(\varepsilon i) + u_\varepsilon(\varepsilon j)}{2}, \quad \text{where } k = \frac{i+j}{2}, \quad i, j \in \mathbf{Z}^N, \quad |i-j| = 1.$$

Note that v_ε takes the three values

$$v_\varepsilon(\varepsilon k) = \begin{cases} -1 & \text{if } u_\varepsilon(\varepsilon i) = u_\varepsilon(\varepsilon j) = -1 \\ 0 & \text{if } u_\varepsilon(\varepsilon i) = -u_\varepsilon(\varepsilon j) \\ 1 & \text{if } u_\varepsilon(\varepsilon i) = u_\varepsilon(\varepsilon j) = 1. \end{cases}$$

As above we normalize the energy by multiplying by ε^N . We then have

$$E_\varepsilon(u_\varepsilon) = F_\varepsilon^\pm(v_\varepsilon) := \pm \frac{1}{2^{N-1}} \sum_k \varepsilon^N g(v_\varepsilon(\varepsilon k))$$

(the sign $-$ corresponding to the case (i), the sign $+$ to (ii)), where $g : \{-1, 0, 1\} \rightarrow \mathbf{R}$

$$g(v) = \begin{cases} 1 & \text{if } z = \pm 1, \\ -1 & \text{if } z = 0 \end{cases}$$

(the sum is performed over all $k \in \mathcal{Z}$ such that the corresponding i, j both satisfy $\varepsilon i, \varepsilon j \in \Omega$). Note that the factor 2 comes from the fact that each k corresponds to a pair (i, j) and the symmetric (j, i) , and that $\frac{1}{2^{N-1}}$ is the volume of the reference cube in the lattice \mathcal{Z} .

Note that if u_ε tends to u weakly then also the (piecewise-constant) extension of v_ε converges to the same u . The comparison energy $F_\varepsilon^\pm(v_\varepsilon)$ is almost an ‘almost-trivial’ energy as labeled in the previous section. The difference now is that v_ε may take three values, and correspondingly $g(v_\varepsilon(\varepsilon k))$ cannot be rewritten as $\psi(v_\varepsilon(\varepsilon k))$ with ψ linear. But for the time being we would like only to give a lower bound for the limit energy, and hence we would like to write

$$\pm g(v_\varepsilon(\varepsilon k)) \geq \psi^\pm(v_\varepsilon(\varepsilon k)),$$

where ψ^\pm is such that the corresponding integral is weakly lower semicontinuous; *i.e.*,

$$\int_\Omega \psi^\pm(u) dx \leq \liminf_{\varepsilon \rightarrow 0} \int_\Omega \psi^\pm(v_\varepsilon) dx$$

If this were the case then

$$\begin{aligned} \liminf_{\varepsilon \rightarrow 0} E_\varepsilon(u_\varepsilon) &\geq \liminf_{\varepsilon \rightarrow 0} \left(\pm \sum_k \frac{1}{2^{N-1}} \varepsilon^N g(v_\varepsilon(\varepsilon k)) \right) \geq \liminf_{\varepsilon \rightarrow 0} \sum_k \frac{1}{2^{N-1}} \varepsilon^N \psi^\pm(v_\varepsilon(\varepsilon k)) \\ &= \liminf_{\varepsilon \rightarrow 0} \int_\Omega \psi^\pm(v_\varepsilon) dx \geq \int_\Omega \psi^\pm(u) dx. \end{aligned}$$

We have then to invoke the theory of *lower semicontinuous integral functionals*. This, in particular, ensures that the integral $\int_\Omega \psi(v) dx$ is weakly lower semicontinuous if and only if $\psi : \mathbf{R} \rightarrow [-\infty, +\infty]$ is convex and lower semicontinuous. We then choose ψ^\pm as what is called the ‘convex and lower semicontinuous envelope’ of $\pm g$; *i.e.*, the greatest convex and lower semicontinuous function not greater than $\pm g$. We have

$$\psi^-(v) = \begin{cases} -1 & \text{if } |v| \leq 1 \\ +\infty & \text{otherwise,} \end{cases} \quad \psi^+(v) = \begin{cases} 2|v| - 1 & \text{if } |v| \leq 1 \\ +\infty & \text{otherwise.} \end{cases}$$

We then have the lower bounds: if u_ε tends to u weakly and $|u| \leq 1$ then

case (i) $\liminf_{\varepsilon \rightarrow 0} E_\varepsilon(u_\varepsilon) \geq -|\Omega|$ (independent of u);

case (ii) $\liminf_{\varepsilon \rightarrow 0} E_\varepsilon(u_\varepsilon) \geq \int_\Omega (2|u| - 1) dx$.

Are these estimates ‘optimal’? We have to be more precise: contrary to what happened when ψ was linear, in this case we cannot require that the \liminf is a limit and is independent of (u_ε) . In view of the application to minimum problems what we will need is that the lower bound we have obtained is ‘sharp’: we have to show that our lower estimate is not too ‘rough’ and check that its value can be achieved for a *particular* choice of u_ε weakly converging to u . It will suffice

to consider a (strongly) ‘dense’ class of target u : piecewise-constant ones (if we can do it for each of those then by approximation we can construct such a sequence for all u). We will show how to construct u_ε only when u is constant and Ω is a coordinate cube; the construction can be easily repeated for piecewise-constant u on each set where it is constant.

By symmetry we can choose $u = c \in [0, 1]$. Since the functions ψ^\pm are piecewise affine, we can use the results of the previous section: in case (i) we regard ψ^- as the affine interpolation of $-g$ on ± 1 ; in case (ii) ψ^+ as the affine interpolation of g on 0 and 1. The result in the previous sections says that the value

$$\int_{\Omega} \psi^\pm(u) dx = \lim_{\varepsilon \rightarrow 0} F^\pm(v_\varepsilon)$$

for every $v_\varepsilon \rightarrow u$ satisfying the constraint $v_\varepsilon \in \{-1, 1\}$ in the first case, $v_\varepsilon \in \{0, 1\}$ in the second. Can we recover the corresponding u_ε from such v_ε ? If v_ε are completely arbitrary in general not. Note in particular that in the first case, except for the trivial case v_ε identically equal to 1 or -1 , such a v_ε will *never* correspond to some u_ε : for any non-constant u_ε there will be some k such that $v_\varepsilon(\varepsilon k) = 0$. We have to choose u_ε such that these k are negligible. This is easily done:

(i) let $t = \frac{c+1}{2}$, let $\delta = \delta(\varepsilon)$ with $\varepsilon \ll \delta \ll 1$, and let

$$u_\varepsilon(\varepsilon i) = \begin{cases} 1 & \text{if } 0 < \varepsilon i_1 \leq t \text{ modulo } \delta \\ -1 & \text{if } t < \varepsilon i_1 \leq 1 \text{ modulo } \delta \end{cases}$$

(i_1 is the first component of $i \in \mathbf{Z}^N$). We then have

$$\lim_{\varepsilon \rightarrow 0} -\frac{1}{2^N} \sum_{i,j} \varepsilon^N u_\varepsilon(\varepsilon i) u_\varepsilon(\varepsilon j) = |\Omega| \left(-1 + \lim_{\varepsilon \rightarrow 0} 2 \frac{\varepsilon}{\delta} \right) = -|\Omega|;$$

(ii) let δ be as above and let

$$u_\varepsilon(\varepsilon i) = \begin{cases} 1 & \text{if } 0 < \varepsilon i_1 \leq c \text{ modulo } \delta \\ -1 & \text{if } c < \varepsilon i_1 \leq 1 \text{ modulo } \delta, \sum_j i_j \text{ even} \\ 1 & \text{if } c < \varepsilon i_1 \leq 1 \text{ modulo } \delta, \sum_j i_j \text{ odd.} \end{cases}$$

Reasoning as above we see that we have a vanishing contribution of the order (at most) $\frac{\varepsilon}{\delta}$, corresponding to the k where v_ε may take the value -1 , so that

$$\begin{aligned} \lim_{\varepsilon \rightarrow 0} \frac{1}{2^N} \sum_{i,j} \varepsilon^N u_\varepsilon(\varepsilon i) u_\varepsilon(\varepsilon j) &= \lim_{\varepsilon \rightarrow 0} (|\{v_\varepsilon = 1\}| - |\{v_\varepsilon = 0\}|) \\ &= c|\Omega| - (1-c)|\Omega| = \int_{\Omega} (2|u| - 1) dx. \end{aligned}$$

Note that, in this case, with some extra care, we can construct u_ε in such a way that there are no k where v_ε takes the value -1 , and for a piecewise-constant u in such a way that such k are all concentrated on the boundary of each set where u is constant.

What we have just proved is that the functionals F^\pm are the Γ -limits of the energies E_ε in the two cases. This notion of variational convergence corresponds to the asymptotic description of minimum problems, and states that minimum problems corresponding to the Γ -limit are ‘good approximations’ to those corresponding to the original sequence when $\varepsilon \rightarrow 0$.

3 An higher-order description: phase transitions

Consider the one-dimensional minimum problems (related to the case (i) above)

$$m_n = \min \left\{ - \sum_{i=1}^n u_i u_{i-1} : |u_i| = 1, \#\{i : u_i = 1\} = k \right\},$$

with $1 \leq k \leq n-1$ (we do not treat the trivial cases when the functions identically equal to 1 ($k = n$) or to -1 ($k = 0$) are admissible test functions for this problem). Then the two minimizers of this problem are given by

$$u_i = \begin{cases} 1 & \text{if } 0 \leq i \leq k-1 \\ -1 & \text{if } k \leq i \leq n, \end{cases} \quad u_i = \begin{cases} -1 & \text{if } 0 \leq i \leq n-k \\ 1 & \text{if } n-k+1 \leq i \leq n. \end{cases}$$

If we let $k = k_n$ depend on n in such a way that $k_n/n \rightarrow c$ as $n \rightarrow +\infty$, upon scaling $[0, n]$ to $[0, 1]$ by identifying $u(\varepsilon i) = u_i$ (where $(\varepsilon = 1/n)$), these minimizers approach the two functions

$$u(x) = \begin{cases} 1 & \text{if } 0 \leq x < c \\ -1 & \text{if } c \leq x \leq 1, \end{cases} \quad u(x) = \begin{cases} -1 & \text{if } 0 \leq x < 1-c \\ 1 & \text{if } 1-c \leq x \leq 1. \end{cases}$$

This example shows that for minimizers we may expect a more precise description than in the previous section; for example that for their limit u we still have $|u| = 1$ a.e., and u solves a minimum problem with fewer minimizers than the one described above.

In the general N -dimensional case, we consider (the notation of the energy follows the previous section taking the minus sign in the energy densities)

$$m_\varepsilon = \min \{ E_\varepsilon(u) : \sum_i \varepsilon^N u(\varepsilon i) = c_\varepsilon \},$$

where c_ε are such that these minima are not $+\infty$ (i.e., there are test functions for these problems, or equivalently $c_\varepsilon \#\{i \in \mathbf{Z}^N : \varepsilon i \in \Omega\} \in \mathbf{N}$) and $c_\varepsilon \rightarrow c$. The condition $\sum_i \varepsilon^N u(\varepsilon i) = c_\varepsilon$ prescribes the number of i such that $u(\varepsilon i) = \pm 1$.

The computation we showed above shows that the limit of these problems is the trivial problem

$$m^{(0)} = \min \left\{ F^-(u) : \int_\Omega u \, dx = c \right\} = -|\Omega|$$

(there is a little proof to do here: we have to show that if $\int u = c$ then we may construct the sequences u_ε above with $\sum \varepsilon^N u_\varepsilon(\varepsilon i) = c_\varepsilon$, but this is easily done). Since $F^-(u) = -|\Omega|$ is a constant when $|u| \leq 1$, the limit problem does not give much information on the form of minimizers.

The idea is then to look for finer properties of minimizers by considering a proper scaling of the energy, noting that if we consider constants r_ε and δ_ε then the minimizers of the problem above are the same as those of

$$m_\varepsilon^{(1)} = \min \left\{ \frac{E_\varepsilon(u) - r_\varepsilon}{\delta_\varepsilon} : \sum_i \varepsilon^N u(\varepsilon i) = c_\varepsilon \right\} = \frac{m_\varepsilon - r_\varepsilon}{\delta_\varepsilon}.$$

If we show that the new functionals

$$E_\varepsilon^{(1)}(u) = \frac{E_\varepsilon(u) - r_\varepsilon}{\delta_\varepsilon}$$

possess a Γ -limit $F^{(1)}$, so that the problems $m_\varepsilon^{(1)}$ converge to

$$m^{(1)} = \min \left\{ F^{(1)}(u) : \int_{\Omega} u \, dx = c \right\},$$

then we obtain that

$$\lim_{\varepsilon \rightarrow 0} \frac{m_\varepsilon - r_\varepsilon}{\delta_\varepsilon} = m^{(1)},$$

and the minimizers of m_ε (that are the same as those of $m_\varepsilon^{(1)}$) converge to those of $m^{(1)}$. Clearly, this information is meaningful only if $\delta_\varepsilon \rightarrow 0$.

In our case we have a ‘natural’ choice of r_ε by choosing

$$r_\varepsilon = -\frac{1}{2^N} \varepsilon^N \#\{\{i, j\} : \varepsilon i, \varepsilon j \in \Omega, |i - j| = 1\};$$

i.e., the number of pairs of nearest neighbours that intervene in the computation of the energy renormalized by the scaling factor $-\varepsilon^N$. This is nothing but $E_\varepsilon(1)$; *i.e.*, the energy of a configuration minimizing each interaction. Note that $r_\varepsilon \rightarrow -|\Omega|$.

We also choose $\delta_\varepsilon = \varepsilon$. In this way the energy is rewritten

$$E_\varepsilon^{(1)}(u) = \frac{1}{2^N} \sum_{i,j} \varepsilon^{N-1} (1 - u(\varepsilon i)u(\varepsilon j)).$$

Consider a term $\varepsilon^{N-1}(1 - u(\varepsilon i)u(\varepsilon j))$. If $u(\varepsilon i) = u(\varepsilon j)$ then the value is 0; otherwise it is equal to $2\varepsilon^{N-1}$. If $u(\varepsilon i)$ is extended as a constant on $\varepsilon(i + (-1/2, 1/2)^N)$ and likewise $u(\varepsilon j)$, then the value ε^{N-1} is exactly the $N - 1$ -dimensional measure of the common boundary between the two cubes. Hence, we may reinterpret $E_\varepsilon^{(1)}$ as an energy on the continuum that is not an integral energy, but a different type of energy depending on an interface. In fact, we may write

$$E_\varepsilon^{(1)}(u) = \frac{1}{2^{N-2}} (N - 1\text{-dimensional measure of } \partial\{u = 1\} \cap \Omega) + o(1)$$

(an additional factor 2 comes from the fact that to each (i, j) there corresponds the symmetric (j, i)). The remainder term $o(1)$ comes from the fact that close to the boundary of Ω , the $N - 1$ -dimensional measure of the common boundary between the two cubes internal to Ω may be less than ε^{N-1} .

A first piece of information that we obtain is that an estimate on $E_\varepsilon^{(1)}(u_\varepsilon)$ implies an estimate on the $N - 1$ -dimensional measure of ∂G_ε , where $G_\varepsilon = \{u_\varepsilon = 1\}$. These estimates in turn give a strong compactness result for the sets G_ε : upon passing to a subsequence their characteristic functions converge to a characteristic function of a limit set G ; *i.e.*, we have deduced the *strong* convergence of $u_\varepsilon (= -1 + 2\chi_{G_\varepsilon})$ to some u (related to some G).

Can we compute a limit energy in terms of u or E ? Fortunately, as for integral energies, a complete theory for functionals depending on boundaries of sets is also available: we may define energies of the form

$$F(G) = \int_{\partial^* G} \varphi(\nu_G) \, d\mathcal{H}^{N-1}, \quad (1)$$

where \mathcal{H}^{N-1} is the $N - 1$ -dimensional Hausdorff measure (that coincides with the usual notion of surface area for smooth manifolds), and $\partial^* G, \nu_G$ are the suitably defined boundary and normal to G (again, they coincide with the usual notions if ∂G is a smooth manifold). These energies are lower semicontinuous (with respect to the strong convergence of the characteristic functions of G ; precisely what we have!) if and only if φ is (the restriction to unit vectors of) a convex

function that is positively homogeneous of degree one. The value $F(G)$ can be regarded as a (possibly anisotropic) perimeter of the set G inside Ω . Indeed, in the case $\varphi = 1$ and G regular it coincides with the elementarily defined perimeter.

Now, we follow a sequence $u_\varepsilon \rightarrow u$, trying to give the best lower bound for $E_\varepsilon^{(1)}(u_\varepsilon)$ by writing

$$E_\varepsilon^{(1)}(u_\varepsilon) = \int_{\partial^* G_\varepsilon} \varphi(\nu_{G_\varepsilon}) d\mathcal{H}^{N-1} + o(1).$$

We must choose φ as large as we can. Now, note that the normal to ∂G_ε may just take the values $\pm e_i$; hence, φ must satisfy the only conditions to be convex, positively homogeneous of degree one, and

$$\varphi(\pm e_i) \leq \frac{1}{2^{N-2}} \text{ for all } i = 1, \dots, N.$$

The greatest function that satisfies all these conditions is

$$\varphi(\nu) = \frac{1}{2^{N-2}} \|\nu\|_1 = \frac{1}{2^{N-2}} \sum_{i=1}^N |\nu_i|.$$

We then have

$$\liminf_{\varepsilon \rightarrow 0} E_\varepsilon^{(1)}(u_\varepsilon) = \liminf_{\varepsilon \rightarrow 0} \frac{1}{2^{N-2}} \int_{\partial^* G_\varepsilon} \|\nu_{G_\varepsilon}\|_1 d\mathcal{H}^{N-1} \geq \frac{1}{2^{N-2}} \int_{\partial^* G} \|\nu_G\|_1 d\mathcal{H}^{N-1} =: F^{(1)}(u).$$

We may see that this inequality is sharp for all u of this form. Indeed by density it suffices to show this fact when G is a polyhedral set, and then, localizing our arguments, when the boundary of G is an hyperplane, or, equivalently

$$u(x) = \begin{cases} 1 & \text{if } \langle x, \bar{\nu} \rangle \geq 0 \\ -1 & \text{otherwise} \end{cases}$$

with $\bar{\nu}$ a fixed vector. In this case, it is easily seen that the functions u_ε defined in the same way; i.e.,

$$u_\varepsilon(\varepsilon i) = \begin{cases} 1 & \text{if } \langle i, \bar{\nu} \rangle \geq 0 \\ -1 & \text{otherwise,} \end{cases} \quad i \in \mathbf{Z}^N,$$

provide a sequence such that $E_\varepsilon^{(1)}(u_\varepsilon) \rightarrow F^{(1)}(u)$.

The argument of convergence of minimum problems outlined above then tells us that minimum points of m_ε converge to functions that can be written as $u = 2\chi_E - 1$, such that E minimize

$$m^{(1)} = \frac{1}{2^{N-2}} \min \left\{ \int_{\partial^* E} \|\nu_E\|_1 d\mathcal{H}^{N-1} : |E| = \frac{1}{2}(c + |\Omega|) \right\};$$

that is E is a set of minimal perimeter (in the sense of the energy above) subject to a constraint on its measure. This means that in order to minimize E_ε the values 1 and -1 will arrange in such a way as to minimize the 'interface between' the two regions. In other words, the two 'phases' 1 and -1 will not mix and will give rise to a sharp interface in the limit.

4 Anti-phase boundaries

We now consider case (ii), when the interaction energy favours the alternance of $+1$ and -1 . This case can be reduced to the previous one by using a different variable, setting

$$v(\varepsilon i) = (-1)^{i_1+i_2+\dots+i_N} u(\varepsilon i).$$

In the two-dimensional case $N = 2$, if we picture \mathbf{R}^2 as a black and white chessboard, with the points of the lattice $\varepsilon\mathbf{Z}^2$ in the centers of each square, then we can imagine that v has the same value as u on the white squares and it takes the value $-u$ on the black ones. In this way

$$E^+_\varepsilon(u) = \frac{1}{2^N} \sum_{i,j} \varepsilon^{N-1} u(\varepsilon i) u(\varepsilon j) = -\frac{1}{2^N} \sum_{i,j} \varepsilon^{N-1} v(\varepsilon i) v(\varepsilon j) = E^-_\varepsilon(v),$$

and the Γ -limit of the scaled energies

$$E^{(1)}_\varepsilon(v) = \frac{1}{2^N} \sum_{i,j} \varepsilon^{N-1} (1 - v(\varepsilon i) v(\varepsilon j)) = \frac{1}{2^N} \sum_{i,j} \varepsilon^{N-1} (1 + u(\varepsilon i) u(\varepsilon j))$$

Γ -converges to $F^{(1)}(v) = \frac{1}{2^{N-2}} \int_{\partial^* E} \|\nu_E\|_1 d\mathcal{H}^{N-1}$.

In terms of u this result can be read as follows: sequences of functions (u_ε) such that $E^+_\varepsilon(u_\varepsilon) = -|\Omega| + O(\varepsilon)$ will arrange in two regions where neighbouring values will alternate, but with a mismatch on the common boundary of these regions (anti-phase boundary). This mismatch may be forced on minimizers of some problems with boundary conditions. The simplest case is in dimension 1 when we consider the minimum problem ($\varepsilon = 1/n$)

$$m_n = \min \left\{ \sum_{i=1}^n u\left(\frac{i}{n}\right) u\left(\frac{i-1}{n}\right) : |u| = 1, u(0) = 1, u(1) = -1 \right\}.$$

If n is even then the minimizers are given by

$$u\left(\frac{i}{n}\right) = \begin{cases} (-1)^i & \text{if } 0 \leq i < i_0 \\ (-1)^{i+1} & \text{if } i_0 \leq i \leq n, \end{cases}$$

where i_0 is any number in $\{1, \dots, n\}$.

The anti phase boundary phenomenon is peculiar of a 'loose packed' lattice; *i.e.* a lattice that can be decomposed into two interpenetrating sublattices such that all the nearest neighbors of a spin on one sublattice belong to the other one. Thus an antiferromagnetic system can be decomposed into two ferromagnetic systems laying in two double interpenetrating lattices.

5 Hexagonal lattices

We consider the two-dimensional case $N = 2$ and in place of \mathbf{Z}^2 we take the 'hexagonal' lattice \mathcal{Z} , generated *e.g.* by the two vectors $(1, 0)$ and $(\frac{1}{2}, \frac{\sqrt{3}}{2})$. In this lattice each point possesses six nearest neighbours; *e.g.*, the nearest neighbours of 0 are $\pm(1, 0)$, $\pm(\frac{1}{2}, \frac{\sqrt{3}}{2})$, and $\pm(-\frac{1}{2}, \frac{\sqrt{3}}{2})$.

We then consider the energies

$$E^\pm_\varepsilon(u) = \pm \frac{1}{6} \sum_{i,j} \varepsilon^2 u(\varepsilon i) u(\varepsilon j),$$

where now the sum runs on all pairs $i, j \in \mathcal{Z}$ such that εi and εj belong to a fixed Ω .

We can extend each discrete uncton u to the piecewise-constant function that takes the same value on the rhombus with center εi and two sides parallel to the generators of the lattice and of length one. With this identification we can proceed in the computation of the Γ -limit.

It is not difficult to see that again the Γ -limit F^- of E^-_ε is finite only if $|u| \leq 1$ a.e. and on these functions its value is $-\frac{2}{\sqrt{3}}|\Omega|$ (the value $\frac{\sqrt{3}}{2}$ is simply the area of the unit rhombus,

by which we have to divide). We may also proceed further to show the appearance of phase transitions: after normalizing and dividing by ε , we obtain another Γ -limit of the form $F^{(1)}$ as in (1) with φ with hexagonal symmetries. We leave the details as an interesting exercise and we focus on the limit of E_ε^+ .

It is convenient now to introduce a new variable: for each triplet $(i, j, k) \in \mathcal{Z}^3$ identifying a minimal equilateral triangle; *i.e.*, such that each one of the three points is a nearest neighbour of the other two, we set

$$v(\varepsilon i, \varepsilon j, \varepsilon k) = \frac{1}{3}(u(\varepsilon i) + u(\varepsilon j) + u(\varepsilon k)).$$

Note that with this normalization, if u_ε converges weakly to u then v_ε (extended with the constant value $v_\varepsilon(\varepsilon i, \varepsilon j, \varepsilon k)$ in the triangle with vertices $\varepsilon i, \varepsilon j, \varepsilon k$) still converges to u . We have the following correspondence:

$$\begin{aligned} u(\varepsilon i) = u(\varepsilon j) = u(\varepsilon k) = \pm 1 &\implies v(\varepsilon i, \varepsilon j, \varepsilon k) = \pm 1, \\ u(\varepsilon i) = u(\varepsilon j) = 1, u(\varepsilon k) = -1 &\implies v(\varepsilon i, \varepsilon j, \varepsilon k) = \frac{1}{3}, \\ u(\varepsilon i) = u(\varepsilon j) = -1, u(\varepsilon k) = 1 &\implies v(\varepsilon i, \varepsilon j, \varepsilon k) = -\frac{1}{3}. \end{aligned}$$

We then set

$$f(v) = \begin{cases} \frac{3}{2} & \text{if } v = \pm 1 \\ -\frac{1}{2} & \text{if } v = \pm \frac{1}{3}, \end{cases}$$

so that

$$f(v(\varepsilon i, \varepsilon j, \varepsilon k)) = \frac{1}{2}(u(\varepsilon i)u(\varepsilon j) + u(\varepsilon j)u(\varepsilon k) + u(\varepsilon k)u(\varepsilon i)).$$

The factor two comes from the fact that each pair of such points belong to two different triangles. We can write

$$E_\varepsilon^+(u) = \frac{1}{6} \sum_{(i,j,k)} \varepsilon^2 f(v(\varepsilon i, \varepsilon j, \varepsilon k)) + o(1),$$

where the sum runs over all triangles with vertices $\varepsilon i, \varepsilon j, \varepsilon k$ contained in Ω . Again, the term $o(1)$ is an error due to the fact that some triangles may intersect the boundary of Ω .

We may now repeat the argument in the computation of F and show that the Γ -limit of E_ε^+ is

$$F(u) = \frac{2}{3\sqrt{3}} \int_{\Omega} \psi(u) dx,$$

where ψ is the convex envelope of f ; *i.e.*,

$$\psi(u) = \begin{cases} -\frac{1}{2} & \text{if } |u| \leq \frac{1}{3} \\ 3\left(|u| - \frac{1}{2}\right) & \text{if } \frac{1}{3} \leq |u| \leq 1. \end{cases}$$

Now, even if the ‘plus case’, the limit energy density presents a flat part. It is interesting to note however that the hexagonal geometry now does not ‘encourage’ phase transitions. We may easily exhibit a configuration converging to $\frac{1}{3}$ in one region and to $-\frac{1}{3}$ in another region of the plane and such that no interfacial energy appears between the two regions. This is best illustrated by Figure 1, where a microscopical pattern is shown (black dots represent the value 1 and white dots the value -1) such that above the dotted line each triangle has two ones and one minus one in the vertices (corresponding to the value $1/3$ and the energy $-1/2$) and conversely below the dotted line each triangle has two minus ones and one one in the vertices (corresponding to the value $-1/3$ and always to the energy $-1/2$).

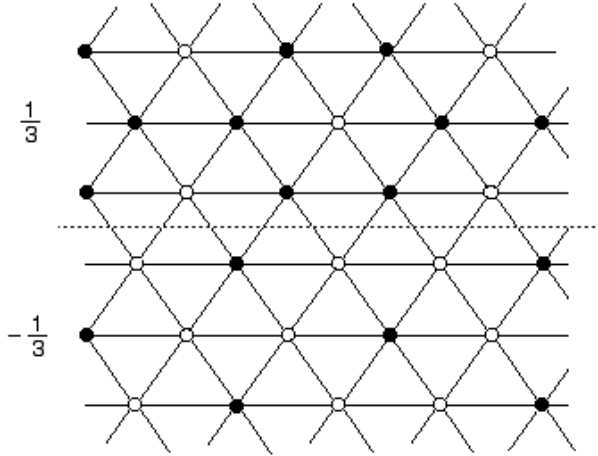


Figure 1: microscopical pattern for a transition with no interfacial energy

In this way each triangle has minimal energy, but, scaling this construction we will have a limit u on the continuum taking the value $1/3$ above the dotted line and $-1/3$ below. This construction can be repeated for all interfaces in the directions of the lattice, and then by approximation for all functions u with $|u| \leq 1/3$.

This lack of interfacial energy can be again described by studying the Γ -limit of the scaled energies

$$E_\varepsilon^{(1)}(v) = \frac{1}{6} \sum_{(i,j,k)} \varepsilon \left(f(v(\varepsilon i, \varepsilon j, \varepsilon k)) + \frac{1}{3} \right).$$

In the case of Ω a cube and v satisfying periodic conditions the Γ -limit of $E_\varepsilon^{(1)}$ is 0 on all $|u| \leq 1/3$ (by the construction above). If Ω is arbitrary then some contribution will appear from the lack of proper compatibility conditions between the geometry of the boundary and the construction made above.

6 Next-to-nearest neighbour interactions

We conclude this presentation with a brief study of the subsequent case (in order of complexity), when each point in a square lattice ‘interacts’ with its nearest and second-nearest neighbours. Again, the pattern that may appear depend on the ‘sign’ of the interactions that may favour or disfavour oscillating configurations, but also on the balance between first and second-neighbour interactions. We treat the two-dimensional setting only, in the case that we consider the most interesting.

We fix an open bounded set Ω in \mathbf{R}^2 with regular boundary. Our energy will be of the form

$$E_\varepsilon(u) = \frac{1}{4} c_1 \sum_{n.n.} \varepsilon^2 u_i u_j + \frac{1}{4} c_2 \sum_{n.n.n.} \varepsilon^2 u_i u_j,$$

where n.n. (nearest neighbours) entails that the sum is taken over all $i, j \in \mathbf{Z}^2$ such that $\varepsilon i, \varepsilon j \in \Omega$ and $|i - j| = 1$, while n.n.n. (next-to-nearest neighbours) are such that $|i - j| = \sqrt{2}$ (corresponding to the diagonals of the squares of the lattice).

In this case it is convenient to rewrite the energy taking into account the local interactions in a fashion similar to that used for the hexagonal lattice. Indeed we may rewrite

$$E_\varepsilon(u) = \frac{1}{4} \sum_{i,j,k,l} \varepsilon^2 \left(\frac{1}{2} c_1 (u_i u_j + u_j u_k + u_k u_l + u_l u_i) + c_2 (u_i u_k + u_j u_l) \right) + o(1)$$

where the sum is taken over all i, j, k, l vertices of a lattice square, ordered in such a way that $|i - j| = |j - k| = |k - l| = |l - i| = 1$ and $|i - k| = |j - l| = \sqrt{2}$. The factor $\frac{1}{2}$ comes from the fact that each pair of nearest neighbours belongs to two such lattice squares, and again the error $o(1)$ is due to the squares close to the boundary. Note that each cube is considered four times.

Note that indeed the sum above can be rewritten as parameterized on the centres of the cubes; *i.e.* on the points $m = \frac{1}{4}(i + j + k + l)$. We would like to introduce equivalent energies of a simpler form

$$F_\varepsilon(v) = \sum_m \varepsilon^2 f(v_m),$$

and

$$v_m = \frac{1}{4}(u_i + u_j + u_k + u_l).$$

The possible values of v are

$$\begin{aligned} u_i = u_j = u_k = u_l = 1 &\implies v_m = 1 \\ u_i = u_j = u_k = u_l = -1 &\implies v_m = -1 \\ u_i = u_j = u_k = 1, u_l = -1 &\implies v_m = \frac{1}{2} \\ u_i = u_j = u_k = -1, u_l = 1 &\implies v_m = -\frac{1}{2} \\ u_i = u_j = -1, u_k = u_l = 1 &\implies v_m = 0 \\ u_i = u_k = -1, u_j = u_l = 1 &\implies v_m = 0. \end{aligned}$$

The list comprises all different cases (upon cyclical permutation of the indices).

How to define f ? There is no ambiguity for $v = \pm 1$ and $v = \pm \frac{1}{2}$. In these cases

$$f(v_m) = \frac{1}{2} c_1 (u_i u_j + u_j u_k + u_k u_l + u_l u_i) + c_2 (u_i u_k + u_j u_l)$$

so that

$$f(v) = \begin{cases} 2c_1 + 2c_2 & \text{if } |v| = 1 \\ 0 & \text{if } |v| = \frac{1}{2}. \end{cases}$$

For $v = 0$ the definition must take into account the two values $-2c_2$, corresponding to the case $u_i = u_j = -1, u_k = u_l = 1$, and $-2c_1 + 2c_2$, corresponding to the case $u_i = u_k = -1, u_j = u_l = 1$. As we are interested in minimum energy configurations, the ‘natural’ definition for f is then

$$f(0) = \min\{-2c_2, -2c_1 + 2c_2\}.$$

This is a very simple case of a *homogenization formula* that gives the overall value of an averaged quantity in terms of a minimum problem among functions (in this case just two possible states) satisfying some average conditions (in this case, that their average be zero).

We have two cases, whether

$$-2c_2 \geq -2c_1 + 2c_2 \quad (\text{i.e., } 2c_2 \leq c_1)$$

or not. In the first case, when $f(0) = -2c_1 + 2c_2$, the minimum configuration is the same alternating state as that we encountered in the ‘plus case’ for nearest neighbours.

The case $f(0) = -2c_2$ is more interesting since the minimizers have less symmetries. We will consider this case only. We make the assumptions

$$0 < c_1 < 2c_2, \quad c_1 + 2c_2 > 0$$

(in particular, $f(0) = -2c_2 < 0$). In this case, the convex envelope of f is given by

$$\psi(v) = \begin{cases} 4c_2 \left(|v| - \frac{1}{2} \right) & \text{if } |v| \leq \frac{1}{2} \\ 4(c_1 + c_2) \left(|v| - \frac{1}{2} \right) & \text{if } \frac{1}{2} \leq |v| \leq 1, \end{cases}$$

and the Γ -limit can be again described by $\int_{\Omega} \psi(u) dx$ with the constraint that $|u| \leq 1$. The proof of this fact is the same as for nearest neighbours; the only care is in using the minimal configuration in the computation of $f(0)$ (that now corresponds to a layering of ones and minus ones).

The limit minimal state is now 0, as in the ‘plus case’ for nearest neighbours, where anti-phase boundaries appeared in the description of the second Γ -limit. In that computation, a simple change of sign in the variables allowed to use the computation for the ‘minus case’. Here, this is not possible since the minimal configuration have more symmetries.

Note that the locally minimal configurations u in \mathbf{Z}^2 (for $\varepsilon = 1$) are periodic with period two. Hence, it is natural to parameterize them after a translation in $2\mathbf{Z}^2$ to a reference cube. The four configurations we have after this translation may then be parameterized by four parameters, that is suggestive to take $\pm e_1$ and $\pm e_2$. We have the correspondence

$$\begin{aligned} u(0,0) = u(0,1) = -1, \quad u(1,0) = u(1,1) = 1 & \text{ corresponds to } e_1 \\ u(0,0) = u(1,0) = -1, \quad u(0,1) = u(1,1) = 1 & \text{ corresponds to } e_2 \\ u(0,0) = u(0,1) = 1, \quad u(1,0) = u(1,1) = -1 & \text{ corresponds to } -e_1 \\ u(0,0) = u(1,0) = 1, \quad u(0,1) = u(1,1) = -1 & \text{ corresponds to } -e_2. \end{aligned}$$

If we may neglect the effects of the boundary of Ω (for example, if Ω is a cube and we have periodic conditions for u), then we may describe the Γ -limit of the scaled functional

$$E_{\varepsilon}^{(1)}(u) = \frac{1}{4}c_1 \sum_{n.n.} \varepsilon u_i u_j + \frac{1}{4}c_2 \sum_{n.n.n.} \varepsilon (u_i u_j + 1)$$

in terms of a new four-dimensional parameter: for each u_{ε} we may define $w : 2\mathbf{Z}^2 \rightarrow \mathbf{R}^4$

$$w(\varepsilon i) = (u_i, u(\varepsilon(i + (1, 0))), u(\varepsilon(i + (1, 1))), u(\varepsilon(i + (0, 1)))).$$

If we follow a sequence (u_{ε}) with $\sup_{\varepsilon} E_{\varepsilon}^{(1)}(u_{\varepsilon}) < +\infty$ then we deduce that $u_{\varepsilon} \rightarrow 0$ and $w_{\varepsilon} \rightarrow w$, where w takes a.e. only the values $(-1, 1, 1, -1)$, $(-1, -1, 1, 1)$, $(1, -1, -1, 1)$ and $(1, 1, -1, -1)$, corresponding to $e_1, e_2, -e_1, -e_2$ above. In this case the surface energy depends also on the two states on both sides of the interface, and can be written as

$$F(w) = \int_{S(w)} \varphi(w^+, w^-, \nu_w) d\mathcal{H}^1,$$

where w^\pm are the traces of w on both sides of the jump set $S(w)$.

We do not describe the form of φ , but only give a picture of the ‘optimal transitions’ in Figure 2, where the microscopical transitions are shown between the states (from left to right) e_2 , e_1 , $-e_1$ and $-e_2$. The grey squares are those where the value of the interactions between the corners is not minimal. It must be noted that the transition between e_2 and $-e_2$ is less energetically favourable since it must use a ‘diffuse’ interface, while the transition between $-e_2$ and $-e_1$ with an interface at an angle of $\pi/4$ is more advantageous than that at $\pi/2$. Even though this does not immediately suggest the form of φ , it shows that it must be more complex than the surface energy in the nearest-neighbour case.

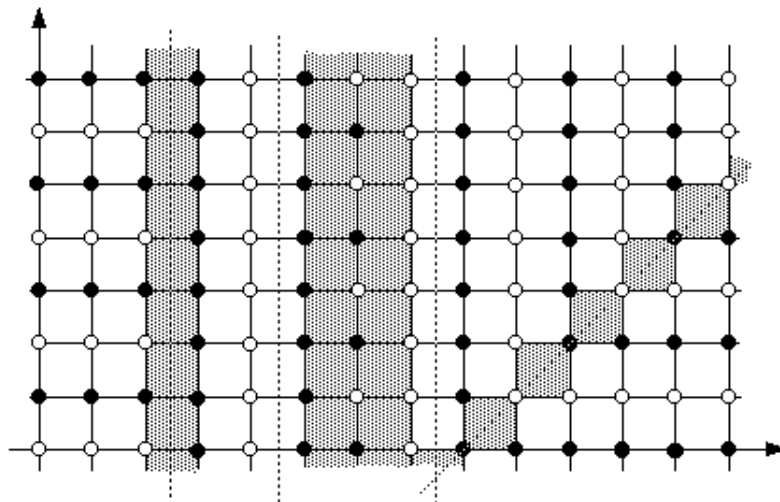


Figure 2: microscopical transitions between four different phases

7 Lessons to be learned

The simple interactions we have considered in this chapter allow us to highlight some aspects of the study of the passage from lattice systems to energies on the continuum, and to make some considerations on the techniques and notions that are needed to make this passage rigorous.

As for this second point we have seen how the limit of discrete states must be defined in terms of statistics and hence of weak limits. The oscillations and concentrations that from this weak convergence may come forbid in general to consider a strong notion of convergence of energies, but we may resort to Γ -convergence, that is sufficient to describe the asymptotic behaviour of minimum problems. Γ -convergence is linked to lower semicontinuity properties, and hence a good knowledge of lower semicontinuous energies will be required.

The simplest description we have encountered describes averaged properties of the energies through integral functionals. The way we compute these functionals is by using convexity properties and finding the right order parameters. When next-to-nearest neighbours are taken into account microscopical oscillations require some additional homogenization argument. We will see that when long-range interactions are taken into account more complex asymptotic homogenization formula will be needed. Higher-order descriptions may give rise to phase transition effects that are described by interfacial energies. In some cases these interfaces are anti-phase boundaries and are described by additional order parameters. The interfaces may be sharp, or diffuse and again must be described by suitable minimization processes.

2. Bounds on the effective behavior of linear networks

The derivation of bounds on the effective behavior of a mixture of two isotropic conductors in fixed volume fraction has a long history. It originates in the elementary so-called VOIGT & REUSS harmonic–arithmetic bounds on the possible conductivity tensors A , that is

$$\underline{a}(\theta)|\xi|^2 \leq \langle A\xi, \xi \rangle \leq \bar{a}(\theta)|\xi|^2, \xi \in \mathbb{R}^N$$

with

$$\frac{1}{\underline{a}(\theta)} := \frac{\theta}{\alpha} + \frac{1-\theta}{\beta}; \quad \bar{a}(\theta) := \theta\alpha + (1-\theta)\beta,$$

where we denote by α and β the conductivity of the core conductors and by θ the proportion of the α -conductor, and it culminates in the derivation by MURAT & TARTAR of optimal bounds for all conductivity tensors resulting from such mixtures: see [12]; see also the derivation of CHERKAEV & LURIE in the two-dimensional case [7]. The (two-dimensional) optimal bounds only constrain the eigenvalues λ_1, λ_2 of the macroscopic conductivity tensor A . The formula is

$$\begin{cases} \frac{1}{\lambda_1 - \alpha} + \frac{1}{\lambda_2 - \alpha} \leq \frac{1}{\bar{a}(\theta) - \alpha} + \frac{1}{\underline{a}(\theta) - \alpha} \\ \frac{1}{\beta - \lambda_1} + \frac{1}{\beta - \lambda_2} \leq \frac{1}{\beta - \bar{a}(\theta)} + \frac{1}{\beta - \underline{a}(\theta)}. \end{cases} \quad (1)$$

A great variety of constitutive behaviors has been subsequently analyzed resulting in a long list of bounds on various binary or multiphase mixtures of materials exhibiting those constitutive behaviors. Since most of the available mathematical methods used in such analyses derive from the mathematical notion of G- or H-convergence (see e.g. [9]), the problem of deriving those bounds has been assigned the generic name of G-closure problem in the mathematical literature. The interested reader is invited to consult the mammoth encyclopaedia [8] and references therein. But, in fact, two-phase isotropic conductivity is the only complete success of the available bounding methods as of yet.

In an apparently different direction, the derivation of continuum models from discrete lattice models has an even longer history. At the beginning of the XIXth century, CAUCHY deduced a first model for isotropic linear elasticity from a lattice of springs, his derivation constraining the POISSON's ratio ν to equal $\frac{1}{4}$. The model was later improved by MAXWELL and generalized to arbitrary $\nu \in (-1, \frac{1}{2})$. In solid state physics, it has become customary to introduce an atomic lattice and to postulate or argue in favor of an interatomic interaction potential as a means for deriving suitable macroscopic behaviors. In truth, the mathematical formalization of such an approach has been slow to emerge for a lack of appropriate mathematical tools.

Whenever inertia effects are neglected — an admittedly challengeable assumption — the passage from discrete models to a continuum may be conveniently framed in a variational (energetic) framework, that of Γ -convergence, first introduced by DE GIORGI. We do not recall the definition here but refer e.g. to [2] for a simple introduction to the topic, or to the compendium [4].

In that approach, the discrete energies associated to an energy minimizing configuration for the lattice in a given volume under well-suited boundary conditions on the boundary of that volume are shown to converge to the continuum energy associated to an energy minimizing configuration for the continuum model under those same boundary conditions. We refer to [1] and references therein.

In the present study, we attempt to investigate, on a decidedly over-simplistic model, the link between lattice mixing and macroscopic behavior. Specifically, we consider the simplest available model, that of a square two-dimensional lattice of resistors. If all resistors have the same resistivity α , then it is a simple matter to show (through e.g. Γ -convergence) that the corresponding continuum will be a linear isotropic conductor with conductivity α . We propose to examine the equivalent of the bounding problem evoked at the onset of this introduction, that is the lattice mixing of two resistivities α and β with given proportion θ of resistivity α . A first, and misguided, intuition would lead one to the conclusion that, since a square lattice with resistivity α gives rise to an isotropic conductor with conductivity α , the proposed mixture will give rise to a conductivity tensor which can be obtained as a mixture in volume fraction $\theta, 1 - \theta$ of α and β conductors. Thus, the resulting conductivity tensor should have eigenvalues that lie in the set defined by (1). Such is not the case and the resulting set of conductors is much larger (see Theorem 3.2 and the concluding remarks). In Fig. 1 we picture the two-dimensional sets of eigenvalues (λ_1, λ_2) corresponding to diagonal matrices in the two situations.

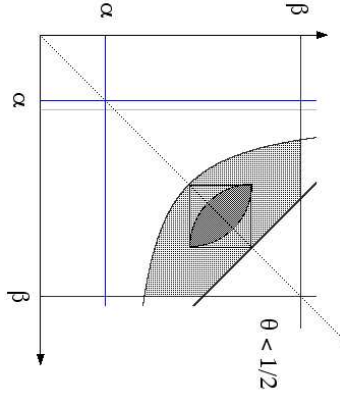


Figure 1: comparison of bounds

In truth, the problem seen as a mixture of continua, is more akin to that of a mixture of three conductors, two being isotropic with conductivities α and β , one being anisotropic with conductivity $\begin{pmatrix} \alpha & 0 \\ 0 & \beta \end{pmatrix}$ in a fixed basis of \mathbb{R}^2 . The volume fractions of each material $\theta_1, \theta_2, \theta_3$ with $\theta_1 + \theta_2 + \theta_3 = 1$ should be such that the total volume fraction of α is θ , i.e., $\theta_1 + \frac{1}{2}\theta_2 = \theta$.

In any case, in this paper we derive bounds on the set of macroscopic conductivities (Theorem 3.2, Proposition 4.1) and show those to be optimal in the case $\theta = \frac{1}{2}$ (see Theorem 5.1) and for all macroscopic conductivity tensors that are diagonal in the lattice basis (see Theorem 3.2). We conjecture in the concluding remarks that the obtained bounds are always optimal, although such optimality in the case $\theta \neq \frac{1}{2}$ has only been obtained for the ‘mid-matrix’ as explained in those remarks.

As a final note, our result could be interpreted as some weak challenge to the conceptual validity of bounds derived purely at the continuum level, provided of course that one trusts the discrete to continuum approach to be a reasonable one, at least as far as crystalline solids are concerned.

1 A G-closure problem

Let Ω be a bounded open subset of \mathbb{R}^2 with Lipschitz boundary. For every fixed $\varepsilon > 0$ and any open subset $U \subset \Omega$ we consider the quadratic discrete energy

$$F_\varepsilon(u, U) = \frac{1}{2} \sum_{i,j} c_{ij}^\varepsilon (u_i - u_j)^2 \quad (2)$$

defined on all functions $u : \varepsilon\mathbf{Z}^2 \cap \Omega \rightarrow \mathbb{R}$. The sum is performed on ‘nearest neighbours’; i.e., points $i, j \in \varepsilon\mathbf{Z}^2 \cap U$ such that $|i - j| = \varepsilon$, and we write $u_i = u(i)$. It is clearly not restrictive to suppose that $c_{ij}^\varepsilon = c_{ji}^\varepsilon$. It is often convenient to rewrite this energy as

$$F_\varepsilon(u, U) = \sum_i h_i^\varepsilon (u_{(i_1+1, i_2)} - u_{(i_1, i_2)})^2 + \sum_i v_i^\varepsilon (u_{(i_1, i_2+1)} - u_{(i_1, i_2)})^2, \quad (3)$$

where $h_i^\varepsilon = c_{i, i+e_1}^\varepsilon$, $v_i^\varepsilon = c_{i, i+e_2}^\varepsilon$, thus separating the ‘horizontal’ and ‘vertical’ interactions.

If the coefficients c_{ij}^ε are equibounded, thanks to general compactness results (see [13], [10], Propositions 2.6 and 2.15, [1], Theorems 3.2, 3.3), we can let $\varepsilon \rightarrow 0$ and obtain, upon passing to a subsequence (independent of U), a quadratic energy of the form

$$F_0(u, U) = \int_U \langle A(x) Du, Du \rangle dx \quad (4)$$

defined on $H^1(U)$ as a Γ -limit.

In this paper we face the problem of the description of all possible such F_0 when we suppose that $c_{ij}^\varepsilon \in \{\alpha, \beta\}$, where $0 < \alpha \leq \beta$ are two fixed positive numbers, and we fix the proportion of nearest neighbours such that $c_{ij}^\varepsilon = \alpha$ (and as a consequence of those such that $c_{ij}^\varepsilon = \beta$).

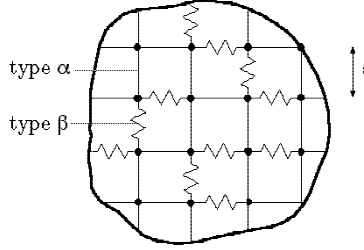


Figure 2: a square network

A particular case is when the coefficients c_{ij}^ε are obtained by scaling a fixed periodic function; i.e., there exists $N \in \mathbf{N}$ and periodic functions $h, v : \mathbf{Z}^2 \rightarrow \{\alpha, \beta\}$ periodic of period N in both arguments such that

$$h_i^\varepsilon = h\left(\frac{i}{\varepsilon}\right), \quad v_i^\varepsilon = v\left(\frac{i}{\varepsilon}\right). \quad (5)$$

In this case the matrix A is independent of x and is given by the *homogenization formula* ([1], Theorem 4.1):

$$\begin{aligned} \langle A\xi, \xi \rangle = & \frac{1}{N^2} \min \left\{ \sum_{i \in \{1, \dots, N\}^2} h_i (\xi_1 + \varphi(i_1 + 1, i_2) - \varphi(i_1, i_2))^2 \right. \\ & + \sum_{i \in \{1, \dots, N\}^2} v_i (\xi_2 + \varphi(i_1, i_2 + 1) - \varphi(i_1, i_2))^2 : \\ & \left. \varphi : \mathbf{Z}^2 \rightarrow \mathbb{R} \text{ } N\text{-periodic} \right\} \quad (6) \end{aligned}$$

Note that the particular cases c_{ij}^ε identically equal to α or β give $A = \alpha I$ and βI respectively.

If $\theta \in \mathbb{Q} \cap [0, 1]$ we then define $\mathcal{H}(\theta)$ as the set of matrices given by (6) and such that

$$\theta = \frac{1}{2N^2} (\#\{i \in \{1, \dots, N\}^2 : h_i = \alpha\} + \#\{i \in \{1, \dots, N\}^2 : v_i = \alpha\}); \quad (7)$$

i.e., the proportion of α -connections is θ (and hence that of β -connections is $1 - \theta$). The definition of $\mathcal{H}(\theta)$ is extended to $\theta \in [0, 1]$ by continuity.

If the coefficients are not periodic, we can describe the *local proportion* $\theta(x)$ of α -connections by

$$\theta(x) = \lim_{\rho \rightarrow 0} \lim_{\varepsilon \rightarrow 0} \frac{\#\{i \in \varepsilon \mathbf{Z}^2 \cap Q_\rho(x) : h_i^\varepsilon = \alpha\} + \#\{i \in \varepsilon \mathbf{Z}^2 \cap Q_\rho(x) : v_i^\varepsilon = \alpha\}}{2\#\{i \in \varepsilon \mathbf{Z}^2 \cap Q_\rho(x)\}}, \quad (8)$$

where $Q_\rho(x)$ is the coordinate cube centered at x and with side length ρ . Note that this quantity is well defined for $x \in \Omega \setminus N$, upon extraction of a subsequence in ε , where $|N| = 0$. Further, $\int_\Omega \theta dx$ represents the total proportion of α -connections.

Once such θ is defined the matrices A are characterized by a *localization principle* ([12], [5], [11]).

Proposition 1.1 $A(x) \in \mathcal{H}(\theta(x))$ for almost all $x \in \Omega$.

PROOF. We only sketch the main points of the proof. Let \bar{x} be a Lebesgue point for $\theta(x)$. Upon a translation argument we can suppose that $\bar{x} = 0$. For all open sets U the functional $\int_U \langle A(0)Du, Du \rangle dx$ is the Γ -limit of $\int_U \langle A(\rho x)Du, Du \rangle dx$ as $\rho \rightarrow 0$ since $A(\rho x)$ converges to $A(0)$ in L^1 on U . We can then infer that, for any fixed ξ ,

$$\langle A(0)\xi, \xi \rangle = \min \left\{ \int_{Q_1(0)} \langle A(\rho x)(\xi + D\varphi), (\xi + D\varphi) \rangle : \varphi \text{ 1-periodic} \right\} + o(1) \quad (9)$$

as $\rho \rightarrow 0$. We now remark that the passage from discrete to continuous is independent of the specific (well chosen) boundary condition, or still that the Γ -convergence result holds true as well if periodic boundary conditions are imposed on $\partial Q_{1/\rho}(0)$ (see [1], Theorem 3.12), which implies that

$$\begin{aligned} & \min \left\{ \int_{Q_1(0)} \langle A(\rho x)(\xi + D\varphi), (\xi + D\varphi) \rangle : \varphi \text{ 1-periodic} \right\} \\ &= \rho^{-2} \min \{ F_0(\xi + D\varphi, Q_\rho(0)) : \varphi \text{ } \rho\text{-periodic} \} \\ &= \lim_{\varepsilon \rightarrow 0} \rho^{-2} \min \{ F_\varepsilon(\xi + D\varphi, Q_\rho(0)) : \varphi \text{ } \rho\text{-periodic} \}. \end{aligned} \quad (10)$$

We may suppose that $N = \rho/\varepsilon \in \mathbf{N}$, so that the formula in the last limit is of the type (6) for some θ_ρ tending to $\theta(0)$ as $\rho \rightarrow 0$, and the proposition is proved.

The previous proposition reduces the problem of characterizing all $A(x)$ to that of studying the sets $\mathcal{H}(\theta)$ for fixed $\theta \in [0, 1]$, which is precisely the subject of the remainder of this work.

2 Trivial bounds

We denote by $\mathcal{H}(\theta_h, \theta_v)$ those matrices in $\mathcal{H}(\theta)$ with fixed volume fraction θ_h, θ_v of horizontal/vertical α -connections; i.e., for $\theta_h, \theta_v \in \mathbb{Q}$,

$$\theta_h = \frac{1}{N^2} \#\{i \in \{1, \dots, N\}^2 : h_i = \alpha\}, \quad (11)$$

$$\theta_v = \frac{1}{N^2} \#\{i \in \{1, \dots, N\}^2 : v_i = \alpha\}. \quad (12)$$

Note that

$$\theta_h + \theta_v = 2\theta, \quad (13)$$

so that we have

$$\begin{aligned} \mathcal{H}(\theta) &= \bigcup \{ \mathcal{H}(t, 2\theta - t) : 0 \leq t \leq 1, 0 \leq 2\theta - t \leq 1 \} \\ &= \begin{cases} \bigcup \{ \mathcal{H}(t, 2\theta - t) : 0 \leq t \leq 2\theta \} & \text{if } 0 \leq \theta \leq 1/2 \\ \bigcup \{ \mathcal{H}(t, 2\theta - t) : 1 - 2\theta \leq t \leq 1 \} & \text{if } 1/2 \leq \theta \leq 1. \end{cases} \end{aligned} \quad (14)$$

We define the harmonic and arithmetic means of α and β in proportion $s, 1 - s$ to be

$$\underline{a}(s) = \frac{\alpha\beta}{s\beta + (1-s)\alpha}, \quad \bar{a}(s) = s\alpha + (1-s)\beta,$$

respectively. Note that

$$\frac{1}{\underline{a}(\theta_h)} + \frac{1}{\underline{a}(\theta_v)} = \frac{2}{\underline{a}(\theta)}, \quad \bar{a}(\theta_h) + \bar{a}(\theta_v) = 2\bar{a}(\theta). \quad (15)$$

Let $A \in \mathcal{H}(\theta_h, \theta_v)$ be given by (6). By testing with $\varphi = 0$ in (6) we get

$$\langle A\xi, \xi \rangle \leq \frac{1}{N^2} \left(\sum_{i \in \{1, \dots, N\}^2} h_i \xi_1^2 + \sum_{i \in \{1, \dots, N\}^2} v_i \xi_2^2 \right) = \bar{a}(\theta_h) \xi_1^2 + \bar{a}(\theta_v) \xi_2^2. \quad (16)$$

Conversely, for all φ , the convexity of $(x, y) \rightarrow \frac{y^2}{x}$ for positive x 's yields

$$\begin{aligned} & \frac{1}{N^2} \left(\sum_{i \in \{1, \dots, N\}^2} h_i (\xi_1 + \varphi(i_1 + 1, i_2) - \varphi(i_1, i_2))^2 \right. \\ & \quad \left. + \sum_{i \in \{1, \dots, N\}^2} v_i (\xi_2 + \varphi(i_1, i_2 + 1) - \varphi(i_1, i_2))^2 \right) \\ &= \frac{1}{N^2} \sum_{i_2=1}^N \sum_{i_1=1}^N h_i (\xi_1 + \varphi(i_1 + 1, i_2) - \varphi(i_1, i_2))^2 \\ & \quad + \frac{1}{N^2} \sum_{i_1=1}^N \sum_{i_2=1}^N v_i (\xi_2 + \varphi(i_1, i_2 + 1) - \varphi(i_1, i_2))^2 \end{aligned} \quad (17)$$

$$\geq \frac{1}{N} \sum_{k=1}^N \underline{a}(\theta_h^k) \xi_1^2 + \frac{1}{N} \sum_{k=1}^N \underline{a}(\theta_v^k) \xi_2^2, \quad (18)$$

where

$$\theta_h^k = \frac{1}{N} \#\{i_1 : h_{(i_1, k)} = \alpha\}, \quad \theta_v^k = \frac{1}{N} \#\{i_2 : h_{(k, i_2)} = \alpha\}.$$

By the convexity of \underline{a} and the arbitrariness of φ we immediately obtain

$$\underline{a}(\theta_h) \xi_1^2 + \underline{a}(\theta_v) \xi_2^2 \leq \langle A\xi, \xi \rangle. \quad (19)$$

We obtain the ‘trivial’ estimates detailed in the following proposition.

Proposition 2.1 *If $A \in \mathcal{H}(\theta_h, \theta_v)$ then*

$$\underline{a}(\theta_h) \xi_1^2 + \underline{a}(\theta_v) \xi_2^2 \leq \langle A\xi, \xi \rangle \leq \bar{a}(\theta_h) \xi_1^2 + \bar{a}(\theta_v) \xi_2^2 \quad (20)$$

for all $\xi \in \mathbb{R}^2$.

3 Exact bounds for diagonal matrices

We denote by $\mathcal{H}_d(\theta)$, $\mathcal{H}_d(\theta_h, \theta_v)$ the set of diagonal matrices in $\mathcal{H}(\theta)$ and $\mathcal{H}(\theta_h, \theta_v)$, respectively.

The first observation is that for $A \in \mathcal{H}_d(\theta_h, \theta_v)$ the ‘trivial’ bounds are optimal. In particular we can obtain the ‘extremal’ matrices $\text{diag}(\underline{a}(\theta_h), \underline{a}(\theta_v))$ and $\text{diag}(\bar{a}(\theta_h), \bar{a}(\theta_v))$ that are obtained by placing all connections in series/parallel in both horizontal and vertical directions, a ‘microstructure’ which is not feasible in the continuous case.

Proposition 3.1 *We have*

$$\mathcal{H}_d(\theta_h, \theta_v) = \{\text{diag}(x, y) : \underline{a}(\theta_h) \leq x \leq \bar{a}(\theta_h), \underline{a}(\theta_v) \leq y \leq \bar{a}(\theta_v)\}.$$

PROOF. It suffices to prove that $\text{diag}(\underline{a}(\theta_h), \underline{a}(\theta_v)), \text{diag}(\bar{a}(\theta_h), \bar{a}(\theta_v)) \in \mathcal{H}_d(\theta_h, \theta_v)$, the construction for all other matrices following easily.

In order to obtain $\text{diag}(\underline{a}(\theta_h), \underline{a}(\theta_v))$, let $\theta_h = M_1/N$, and $\theta_v = M_2/N$. We then define (see Fig. 3)

$$h_{(i_1, i_2)} =: h_{i_1} = \begin{cases} \alpha & \text{if } 1 \leq i_1 \leq M_1 \\ \beta & \text{otherwise} \end{cases}, \quad (21)$$

$$v_{(i_1, i_2)} =: v_{i_2} = \begin{cases} \alpha & \text{if } 1 \leq i_2 \leq M_2 \\ \beta & \text{otherwise} \end{cases}. \quad (22)$$

It is easily seen that (19) is sharp for this choice of h_i, v_i . Indeed, if ζ and ψ are the one-dimensional minimizers for

$$\frac{1}{N} \sum_i h_i (\xi_1 + \varphi(i+1) - \varphi(i))^2 \quad (23)$$

and

$$\frac{1}{N} \sum_i v_i (\xi_2 + \varphi(i+1) - \varphi(i))^2 \quad (24)$$

among all N -periodic φ 's — for which the minimal values are respectively $\underline{a}(\theta_h)\xi_1^2$ and $\underline{a}(\theta_v)\xi_2^2$ — then $\zeta(i_1) + \psi(i_2)$ is a minimizer for (6) for the choice (21)–(22) for $h_{(i_1, i_2)}$ and $v_{(i_1, i_2)}$.

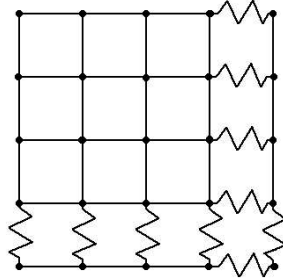


Figure 3: optimal network for harmonic means

Conversely, to obtain $\text{diag}(\bar{a}(\theta_h), \bar{a}(\theta_v))$ it suffices to choose

$$h_{(i_1, i_2)} =: h_{i_1} = \begin{cases} \alpha & \text{if } 1 \leq i_2 \leq M_1 \\ \beta & \text{otherwise} \end{cases},$$

$$v_{(i_1, i_2)} =: v_{i_2} = \begin{cases} \alpha & \text{if } 1 \leq i_1 \leq M_2 \\ \beta & \text{otherwise} \end{cases}$$

(see Fig. 4). In that case, $\varphi \equiv 0$ is a minimizer because 0 is a minimizer of the one-dimensional problems (23),(24).

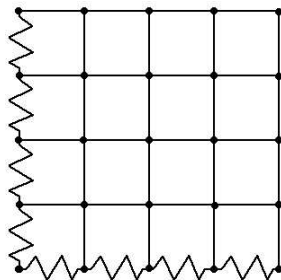


Figure 4: optimal network for arithmetic means

From Proposition 3.1 we immediately obtain the complete description of $\mathcal{H}_d(\theta)$.

Theorem 3.2 (exact bounds for diagonal matrices) *The set $\mathcal{H}_d(\theta)$ is composed of all matrices $\text{diag}(x, y)$ satisfying*

- (i) (case $0 \leq \theta \leq 1/2$) $\underline{a}(2\theta) \leq x, y \leq \beta$, $x + y \leq 2\bar{a}(\theta)$, $\frac{1}{y} + \frac{1}{x} \leq \frac{2}{\underline{a}(\theta)}$;
- (ii) (case $1/2 \leq \theta \leq 1$) $\alpha \leq x, y \leq \bar{a}(2\theta - 1)$, $x + y \leq 2\bar{a}(\theta)$, $\frac{1}{y} + \frac{1}{x} \leq \frac{2}{\underline{a}(\theta)}$.

Note that for $\theta = 1/2$ then the form of the bounds simplify since $\underline{a}(2\theta) = \alpha$ and $\bar{a}(2\theta - 1) = \beta$. The shape of the set $\mathcal{H}_d(\theta)$ in the three cases is pictured in Fig. 5.

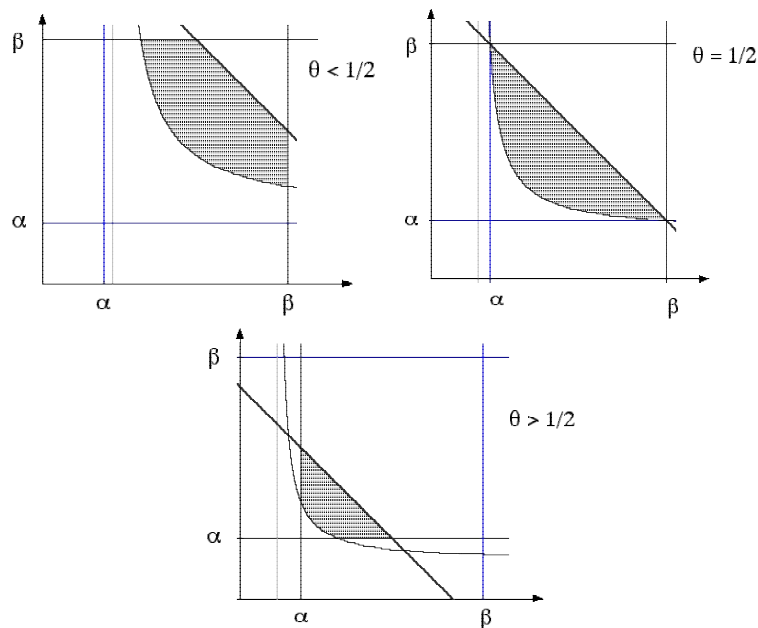


Figure 5: the sets $\mathcal{H}_d(\theta)$

PROOF. The proof is an immediate consequence of Proposition 3.1, taking into account (15) and (14).

4 An outer bound for non-diagonal matrices

Let $A = \begin{pmatrix} x & z \\ z & y \end{pmatrix} \in \mathcal{H}(\theta_h, \theta_v)$. From the ‘trivial’ bounds we obtain

$$\underline{a}(\theta_h)\xi_1^2 + \underline{a}(\theta_v)\xi_2^2 \leq \langle A\xi, \xi \rangle \leq \bar{a}(\theta_h)\xi_1^2 + \bar{a}(\theta_v)\xi_2^2 \quad (25)$$

for all $\xi \in \mathbb{R}^2$. By testing with the vectors $(1, 0)$ and $(0, 1)$ we get

$$\underline{a}(\theta_h) \leq x \leq \bar{a}(\theta_h), \quad \underline{a}(\theta_v) \leq y \leq \bar{a}(\theta_v), \quad (26)$$

i.e, $A_d = \begin{pmatrix} x & 0 \\ 0 & y \end{pmatrix} \in \mathcal{H}_d(\theta_h, \theta_v)$. That is, the projection of $\mathcal{H}(\theta_h, \theta_v)$ onto diagonal matrices is precisely $\mathcal{H}_d(\theta_h, \theta_v)$.

In general, we can obtain an estimate for the off-diagonal term z from (25) by optimizing the inequalities

$$(\underline{a}(\theta_h) - x)\xi_1^2 + (\underline{a}(\theta_v) - y)\xi_2^2 \leq 2z\xi_1\xi_2 \leq (\bar{a}(\theta_h) - x)\xi_1^2 + (\bar{a}(\theta_v) - y)\xi_2^2, \quad (27)$$

that gives

$$z^2 \leq \min\{(\bar{a}(\theta_h) - x)(\bar{a}(\theta_v) - y), (x - \underline{a}(\theta_h))(y - \underline{a}(\theta_v))\}. \quad (28)$$

We now fix $\theta \leq 1/2$ and maximize the range of values for z with respect to θ_h, θ_v with $\theta_h + \theta_v = 2\theta$ in the following two inequalities

$$z^2 \leq (\bar{a}(\theta_h) - x)(\bar{a}(\theta_v) - y) \quad (29)$$

$$z^2 \leq (x - \underline{a}(\theta_h))(y - \underline{a}(\theta_v)). \quad (30)$$

This computation will give us an analytic ‘outer bound’.

By symmetry we carry this computation for $x \leq y$ only.

Bound from arithmetic means. We choose $\bar{a}(\theta_h)$ as independent variable. The constraint that $A \in \mathcal{H}(\theta_h, \theta_v)$ becomes, in terms of $\bar{a}(\theta_h)$,

$$\begin{cases} \frac{\alpha\beta}{\alpha + \beta - \bar{a}(\theta_h)} \leq x \leq \bar{a}(\theta_h) \\ \frac{\alpha\beta}{\alpha + \beta - 2\bar{a}(\theta) + \bar{a}(\theta_h)} \leq y \leq 2\bar{a}(\theta) - \bar{a}(\theta_h) \end{cases}$$

that is

$$\begin{cases} x \leq \bar{a}(\theta_h) \leq \alpha + \beta - \frac{\alpha\beta}{x} \\ 2\bar{a}(\theta) - (\alpha + \beta) + \frac{\alpha\beta}{y} \leq \bar{a}(\theta_h) \leq 2\bar{a}(\theta) - y \end{cases}$$

Thus,

$$t_m(x, y) := \max\left\{x, 2\bar{a}(\theta) - (\alpha + \beta) + \frac{\alpha\beta}{y}\right\} \leq \bar{a}(\theta_h) \leq t_M(x, y) := \min\left\{2\bar{a}(\theta) - y, \alpha + \beta - \frac{\alpha\beta}{x}\right\}.$$

These two relations define three separate regions in $\mathcal{H}_d(\theta)$ bound by the non-intersecting curves

$$\begin{cases} x = 2\bar{a}(\theta) - (\alpha + \beta) + \frac{\alpha\beta}{y} \\ y = 2\bar{a}(\theta) - (\alpha + \beta) + \frac{\alpha\beta}{x}, \end{cases}$$

two hyperbolae passing respectively through the two upper and two lower corner points of $\mathcal{H}_d(\theta)$.

Recall the relation

$$\bar{a}(\theta_h) + \bar{a}(\theta_v) = 2\bar{a}(\theta) \quad (31)$$

and compute

$$\begin{aligned} f_a(x, y) &= \max\{(\bar{a}(\theta_h) - x)(\bar{a}(\theta_v) - y) : \text{diag}(x, y) \in \mathcal{H}(\theta_h, \theta_v)\} \\ &= \max\{(t - x)(2\bar{a}(\theta) - t - y) : t_m(x, y) \leq t \leq t_M(x, y)\}. \end{aligned} \quad (32)$$

That gives

$$f_a(x, y) = \begin{cases} \left(\bar{a}(\theta) - \frac{x+y}{2}\right)^2 & \text{if } x \geq 2(\bar{a}(\theta) - (\alpha + \beta)) + y + 2\frac{\alpha\beta}{y} \\ (\alpha + \beta - (\frac{\alpha\beta}{y} + y))((1 - 2\theta)(\beta - \alpha) + \frac{\alpha\beta}{y} - x) & \text{otherwise.} \end{cases} \quad (33)$$

The maximum in (33) is reached for

$$\bar{a}(\theta_h) = \begin{cases} \bar{a}(\theta) + \frac{x-y}{2} & \text{if } x \geq 2(\bar{a}(\theta) - (\alpha + \beta)) + y + 2\frac{\alpha\beta}{y} \\ 2\bar{a}(\theta) - (\alpha + \beta) + \frac{\alpha\beta}{y} & \text{otherwise.} \end{cases} \quad (34)$$

Bound from harmonic means. By choosing $\underline{a}(\theta_h)$ as independent variable, the constraint that $A \in \mathcal{H}(\theta_h, \theta_v)$ in terms of $\underline{a}(\theta_h)$ becomes

$$\begin{aligned} \underline{a}(\theta_h) &\leq x \leq \alpha + \beta - \frac{\alpha\beta}{\underline{a}(\theta_h)} \\ \frac{\underline{a}(\theta_h)\underline{a}(\theta_h)}{2\underline{a}(\theta_h) - \underline{a}(\theta)} &\leq y \leq \alpha + \beta + \frac{\alpha\beta}{\underline{a}(\theta_h)} - \frac{2\alpha\beta}{\underline{a}(\theta)}, \end{aligned}$$

that can be summarized in $t_m(x, y) \leq \underline{a}(\theta_h) \leq t_M(x, y)$, where

$$\begin{aligned} t_m(x, y) &= \max\left\{\frac{y\underline{a}(\theta)}{2y - \underline{a}(\theta)}, \frac{\alpha\beta}{\alpha + \beta - x}\right\}, \\ t_M(x, y) &= \min\left\{\frac{\alpha\beta\underline{a}(\theta)}{\underline{a}(\theta)(y - (\alpha + \beta)) + 2\alpha\beta}, x\right\}, \end{aligned}$$

Note that the regions defined by these relations are the same as those defined in the case of the arithmetic means.

We can then compute

$$f_h(x, y) := \max\left\{(x - t)\left(y - \frac{\underline{a}(\theta)t}{2t - \underline{a}(\theta)}\right) : t_m(x, y) \leq t \leq t_M(x, y)\right\}. \quad (35)$$

Recalling the relation

$$\frac{1}{\underline{a}(\theta_h)} + \frac{1}{\underline{a}(\theta_v)} = \frac{2}{\underline{a}(\theta)} = \frac{1}{\underline{a}(2\theta)} + \frac{1}{\beta}, \quad (36)$$

we then obtain

$$f_h(x, y) = \begin{cases} \frac{1}{4} \left(\underline{a}(\theta) - \sqrt{(2x - \underline{a}(\theta))(2y - \underline{a}(\theta))} \right)^2 & \text{if } 2\alpha\beta(\alpha\beta + \underline{a}(\theta)(y - (\alpha + \beta)))(2x - \underline{a}(\theta)) \leq \underline{a}(\theta)^2(\alpha + \beta)^2(y - x) \\ \frac{(\underline{a}(\theta)(x - \beta)(x - \alpha) + 2\alpha\beta(x - \underline{a}(\theta))(y - \alpha)(\beta - y))}{(y - (\alpha + \beta))(\underline{a}(\theta)(y - (\alpha + \beta)) + 2\alpha\beta)} & \text{otherwise.} \end{cases} \quad (37)$$

The maximum in (35) is reached for

$$\underline{a}(\theta_h) = \begin{cases} \frac{\underline{a}(\theta)}{2} \left(1 + \sqrt{\frac{2x - \underline{a}(\theta)}{2y - \underline{a}(\theta)}} \right) \\ \frac{\alpha\beta\underline{a}(\theta)}{\underline{a}(\theta)(y - (\alpha + \beta)) + 2\alpha\beta} \end{cases} \quad (38)$$

in the two cases respectively.

Proposition 4.1 (outer bound) *Let $A = \begin{pmatrix} x & z \\ z & y \end{pmatrix} \in \mathcal{H}(\theta)$ then we have*

$$z^2 \leq f_\theta(x, y) := \min\{f_a(x, y), f_h(x, y)\}. \quad (39)$$

PROOF. The proof follows immediately from the estimates above and from (28), since

$$\begin{aligned} & \max_{\theta_h, \theta_v} \min\{(\bar{a}(\theta_h) - x)(\bar{a}(\theta_v) - y), (x - \underline{a}(\theta_h))(y - \underline{a}(\theta_v))\} \\ & \leq \min\{\max_{\theta_h, \theta_v}\{(\bar{a}(\theta_h) - x)(\bar{a}(\theta_v) - y)\}, \max_{\theta_h, \theta_v}\{(x - \underline{a}(\theta_h))(y - \underline{a}(\theta_v))\}\} \\ & = \min\{f_a(x, y), f_h(x, y)\}. \end{aligned} \quad (40)$$

In the case where $\theta = 1/2$, it is easily deduced from the previous analysis that the expression for $f_{1/2}(x, y)$ in (39) is simply given by

$$f_{1/2}(x, y) = \begin{cases} \left(\frac{\alpha + \beta}{2} - \frac{x + y}{2} \right)^2 & \text{if } xy \geq \alpha\beta \\ \left(\frac{\alpha\beta}{\alpha + \beta} - \sqrt{\left(x - \frac{\alpha\beta}{\alpha + \beta}\right)\left(y - \frac{\alpha\beta}{\alpha + \beta}\right)} \right)^2 & \text{otherwise.} \end{cases}$$

5 Exact bounds for non-diagonal matrices (the case $\theta = 1/2$)

We prove that in the case $\theta = 1/2$ the outer bound given by Proposition 4.1 is optimal.

Theorem 5.1 (exact bounds) *The set $\mathcal{H}(1/2)$ is given by all matrices $A = \begin{pmatrix} x & z \\ z & y \end{pmatrix}$ such that*

$$\alpha \leq x, y \leq \beta, \quad x + y \leq \alpha + \beta, \quad \frac{1}{y} + \frac{1}{x} \leq \frac{1}{\alpha} + \frac{1}{\beta},$$

$$z^2 \leq \min \left\{ \left(\frac{\alpha + \beta}{2} - \frac{x + y}{2} \right)^2, \left(\frac{\alpha\beta}{\alpha + \beta} - \sqrt{\left(x - \frac{\alpha\beta}{\alpha + \beta} \right) \left(y - \frac{\alpha\beta}{\alpha + \beta} \right)} \right)^2 \right\}.$$

PROOF. Since, because of the equi-boundedness of the approximating sequences, Γ -convergence in the current setting is associated to a metrizable topology (see [4]), $\mathcal{H}(1/2)$ is closed under Γ -convergence. The proof will be achieved by layering on the continuum level. We first note that any solution (x, y, z) to the system $\begin{cases} z^2 = f_a(x, y) \\ z^2 = f_h(x, y) \end{cases}$ lives on the surface of equal determinant $xy - z^2 = \alpha\beta$; hence, we can divide the proof for A satisfying $xy - z^2 \geq \alpha\beta$ and $xy - z^2 \leq \alpha\beta$ for which the bounds for the off-diagonal term simply become $z^2 \leq f_a(x, y)$ and $z^2 \leq f_h(x, y)$, respectively.

The strategy is the following: given A compute the diagonal matrices A_1 and A_2 on the boundary of $\mathcal{H}_d(1/2)$ such that $\det A_i = \det A$; find η and ν such that if we layer A_1 and A_2 with volume fractions η and $(1 - \eta)$ in the direction ν we obtain A .

We first perform the proof for $\det A \geq \alpha\beta$ and check the bound $z^2 = f_a(x, y)$. The matrices $A_1 = \begin{pmatrix} s & 0 \\ 0 & t \end{pmatrix}$ and $A_2 = \begin{pmatrix} t & 0 \\ 0 & s \end{pmatrix}$ are characterized by the equations

$$st = xy - z^2 = xy - \left(\frac{\alpha + \beta}{2} - \frac{x + y}{2} \right)^2, \quad (41)$$

obtained by imposing the ‘extremality condition’ $z^2 = f_a(x, y)$ to the determinant constraint, and

$$s + t = \alpha + \beta, \quad (42)$$

given by the requirement that A_i belong to the boundary of $\mathcal{H}_d(1/2)$.

We layer A_1 and A_2 in proportions $\eta, 1 - \eta$ in direction $\nu = (C, S)$ and apply the layering formula in [12] (cf. Proposition 3). The resulting conductivity matrix X is given by

$$(X - A_1)^{-1} = \frac{1}{1 - \eta} \left((A_2 - A_1)^{-1} + \eta \frac{\nu \otimes \nu}{\langle A_1 \nu, \nu \rangle} \right),$$

that is

$$X = \begin{pmatrix} \frac{stC^2 + (\eta s + (1 - \eta)t)^2 S^2}{(\eta C^2 + (1 - \eta)S^2)t + (\eta S^2 + (1 - \eta)C^2)s} & - \frac{\eta(1 - \eta)(t - s)^2 CS}{(\eta C^2 + (1 - \eta)S^2)t + (\eta S^2 + (1 - \eta)C^2)s} \\ - \frac{\eta(1 - \eta)(t - s)^2 CS}{(\eta C^2 + (1 - \eta)S^2)t + (\eta S^2 + (1 - \eta)C^2)s} & \frac{stS^2 + (\eta s + (1 - \eta)t)^2 C^2}{(\eta C^2 + (1 - \eta)S^2)t + (\eta S^2 + (1 - \eta)C^2)s} \end{pmatrix}.$$

Since $\det A_1 = \det A_2$, Theorem 4 in [6] implies that $\det X = st$. This could also be checked directly with the expression above for X . It thus suffices to prove that we can find η, ν such that

$$\begin{cases} \frac{stC^2 + (\eta s + (1 - \eta)t)^2 S^2}{(\eta C^2 + (1 - \eta)S^2)t + (\eta S^2 + (1 - \eta)C^2)s} = x \\ \frac{stS^2 + (\eta s + (1 - \eta)t)^2 C^2}{(\eta C^2 + (1 - \eta)S^2)t + (\eta S^2 + (1 - \eta)C^2)s} = y \end{cases}$$

as z will thus automatically satisfy $z^2 = st - xy = f_a(x, y)$. This gives a homogeneous system in C^2 and S^2 , whose determinant must be zero; i.e.,

$$\begin{aligned} & (st - x(s + \eta(t - s)))(st - y(t - \eta(t - s))) \\ = & (t - \eta(t - s))(s + \eta(t - s))(t - \eta(t - s) - x)(s + \eta(t - s) - y). \end{aligned} \quad (43)$$

The proportion η is determined by requiring that the volume fractions related to A_1 and A_2 in proportions η and $1 - \eta$ must give the volume fractions θ_h, θ_v of A , determined by (34). This gives

$$\eta(\beta - s) + (1 - \eta)(\beta - t) = \frac{1}{2}((\beta - \alpha) + (y - x)). \quad (44)$$

By using (41), (42) and (44), we can easily verify (43).

The case $\det A \leq \alpha\beta$ can be proven likewise. In this case, the equal determinant condition (41) must be modified by substituting f_a with f_h , thus obtaining

$$st = xy - \left(\frac{\alpha\beta}{\alpha + \beta} - \sqrt{\left(x - \frac{\alpha\beta}{\alpha + \beta}\right)\left(y - \frac{\alpha\beta}{\alpha + \beta}\right)} \right)^2, \quad (45)$$

while (42) becomes

$$\frac{1}{s} + \frac{1}{t} = \frac{\alpha + \beta}{\alpha\beta}. \quad (46)$$

The proportion η is now determined by (38), which gives

$$\eta \frac{\alpha}{s}(\beta - s) + (1 - \eta) \frac{\beta}{t}(\beta - t) = \frac{\beta\sqrt{(\alpha + \beta)y - \alpha\beta} - \alpha\sqrt{(\alpha + \beta)x - \alpha\beta}}{\sqrt{(\alpha + \beta)y - \alpha\beta} + \sqrt{(\alpha + \beta)x - \alpha\beta}}. \quad (47)$$

By using (45)–(47), we can again verify (43).

6 Concluding remarks

The complete characterization of the set $\mathcal{H}(\theta)$ is missing at present. We conjecture that the outer bound, described in Section 4 (see Proposition 4.1) and found to be optimal in the case $\theta = 1/2$ (see Section 5 above), is optimal for all θ 's. As a first result in that direction, we briefly detail how to obtain the optimality of the outer bound for the ‘midmatrix’ with diagonal elements both equal to $\frac{1}{2}(\bar{a}(\theta) + \underline{a}(\theta))$. The corresponding outer bound yields $z = \pm \frac{1}{2}(\bar{a}(\theta) - \underline{a}(\theta))$, so that the two ‘midmatrices’ are

$$A_{\pm} = \begin{pmatrix} \frac{1}{2}(\bar{a}(\theta) + \underline{a}(\theta)) & \pm \frac{1}{2}(\bar{a}(\theta) - \underline{a}(\theta)) \\ \pm \frac{1}{2}(\bar{a}(\theta) - \underline{a}(\theta)) & \frac{1}{2}(\bar{a}(\theta) + \underline{a}(\theta)) \end{pmatrix}.$$

Note that the eigenvalues of A_{\pm} are $\underline{a}(\theta), \bar{a}(\theta)$ and the eigendirections $\pm \frac{\pi}{4}$.

The construction consists in layering the corresponding outer ‘midmatrix’ for $\theta = 1/2$, that is

$$B = \begin{pmatrix} \frac{1}{2}\left(\frac{\alpha + \beta}{2} + \frac{2\alpha\beta}{\alpha + \beta}\right) & \frac{1}{2}\left(\frac{\alpha + \beta}{2} - \frac{2\alpha\beta}{\alpha + \beta}\right) \\ \frac{1}{2}\left(\frac{\alpha + \beta}{2} - \frac{2\alpha\beta}{\alpha + \beta}\right) & \frac{1}{2}\left(\frac{\alpha + \beta}{2} + \frac{2\alpha\beta}{\alpha + \beta}\right) \end{pmatrix},$$

with αI (resp. βI) in the direction $\frac{\pi}{4}$ and with a volume fraction η such that $\eta^{\frac{1}{2}} + (1 - \eta) = \theta$ (resp. $\eta^{\frac{1}{2}} = \theta$). We skip the actual derivation.

Actually, as can be immediately checked by setting $x = y$ in Proposition 4.1, the outer matrices in $\mathcal{H}(\theta)$ such that $x = y$ have an off-diagonal element that grows linearly in x . Since layering A_{\pm} with the diagonal matrices $\underline{a}(\theta)I$ and $\bar{a}(\theta)I$ — extreme elements of $\mathcal{H}(\theta)$ in the plane $x = y$ of equal diagonal elements — in both directions $\pm\frac{\pi}{4}$ also yields a matrix with an off-diagonal element that grows linearly in $x = y$, we have also established the optimality of the outer bound for all matrices with equal diagonal elements. The computation for general outer matrices in $\mathcal{H}(\theta)$, $\theta \neq \frac{1}{2}$, with distinct diagonal elements remains open at this time.

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3. A weak membrane with randomly distributed defects

The discrete setting provides an easy framework where to model problems with some random choice. In this chapter we will study the description of a two-dimensional square network mixing two types of connections: ‘weak’ and ‘strong’ ones. The strong connections are simple quadratic ones, while the weak connections are ‘truncated quadratic potentials’ that are quadratic below some threshold, and constant above. We may imagine that this network model a two-dimensional membrane, and that the unknown function u represents the vertical displacement of the membrane. A ‘strong connection’ may be simply viewed as a linear spring between two neighboring nodes of the network. A ‘weak spring’ behaves in the same way as a ‘strong spring’ below the fracture threshold, at which it breaks, and the two neighboring nodes get disconnected. The distribution of weak springs can be viewed as a distribution of defects in an otherwise linear material. We will investigate the ‘typical’ overall behavior of such a model in the hypothesis that the defects be randomly distributed. To this end we will briefly give an overview of some percolation results, and preliminarily treat the case when only weak connections are present.

1 The weak membrane

We consider the energies

$$E_\varepsilon(u) = \frac{1}{2} \sum_{\alpha, \beta} \varepsilon^N f^\varepsilon \left(\frac{u(\alpha) - u(\beta)}{\varepsilon} \right)$$

where f^ε are truncated quadratic potentials:

$$f^\varepsilon(z) = \min \left\{ z^2, \frac{1}{\varepsilon} \right\}.$$

The sum is extended to all nearest neighbors. Note that if

$$\left| \frac{u(\alpha) - u(\beta)}{\varepsilon} \right|^2 \leq \frac{1}{\varepsilon}$$

for all α, β , then $F_\varepsilon(u)$ is just a discretization of the Dirichlet integral, while if for example u takes just two values, say u_0 and u_1 , then for ε small enough we have

$$f^\varepsilon \left(\frac{u(\alpha) - u(\beta)}{\varepsilon} \right) = \begin{cases} 0 & \text{if } u(\alpha) = u(\beta) \\ \frac{1}{\varepsilon} & \text{otherwise,} \end{cases}$$

so that, identifying each u with its piecewise-constant extension, we have

$$E_\varepsilon(u) = \varepsilon^{N-1} \# \{ \{\alpha, \beta\} : u(\alpha) \neq u(\beta) \} = \mathcal{H}^{N-1}(\partial\{u = u_0\}) + o(1),$$

where the $o(1)$ comes from some boundary corrections.

In general the Γ -limit will be finite on functions that may have a discontinuity set $S(u)$ of dimension $N - 1$ and such that this set is rectifiable, and that are otherwise approximately

differentiable outside this set. The space of such u is called the space of special functions of bounded variation $SBV(\Omega)$ and is defined as the space of all $u \in BV(\Omega)$ such that the distributional derivative of u can be split in a N -dimensional and a $N - 1$ -dimensional part. To be more precise, since we will not directly have a bound on BV norms, the u for which our limit energies will make sense are in $GSBV(\Omega)$ (*i.e.*, their truncations $(-T \vee u) \wedge T$ are in $SBV(\Omega)$ for all T).

On this space the Γ -limit of F_ε can be written as

$$F(u) = \int_{\Omega} |\nabla u|^2 dx + \int_{S(u)} \|\nu_u\|_1 d\mathcal{H}^{N-1}.$$

Note that if $u \in H^1(\Omega)$ then $F(u) = \int_{\Omega} |\nabla u|^2 dx$. Note moreover that in many problems we will have an a priori bound for the L^∞ norm of the solution, that in this way belongs to $SBV(\Omega)$.

2 A naive view to percolation theory

We want to compute a Γ -limit as in the previous section, of an energy where we randomly mix f^ε as above and simple quadratic interactions. To this end we have to introduce some notions of percolation theory for what is called the ‘bond percolation model’ (*i.e.*, when the random choice is thought to be performed on the connections. A different model, that can be treated similarly, is the *site percolation model*. In our intuition it would correspond to choosing weak and strong nodes – and to define a weak connection as a connection between two nodes of which at least one is a weak node).

We do not want to introduce the formal definition of a random variable, but just to look at the relevant elements of percolation theory that will allow us to describe the model of a weak membrane. From now on we will restrict to the two-dimensional case $N = 2$. We start by introducing the dual lattice

$$\mathcal{Z} = \left\{ \frac{\alpha + \beta}{2} : \alpha, \beta \in \mathbf{Z}^2, |\alpha - \beta| = 1 \right\}.$$

A choice of connections between nodes of \mathbf{Z}^2 is a function $\omega : \mathcal{Z} \rightarrow \{-1, 1\}$; 1 corresponds to a *strong connection*, and -1 to a *weak connection*. We identify each point $\gamma \in \mathcal{Z}$ with the segment $[\alpha, \beta]$ such that $\alpha, \beta \in \mathbf{Z}^2$ and $2\gamma = \alpha + \beta$. Given ω , we say that two points $\gamma, \gamma' \in \mathcal{Z}$ such that $\omega(\gamma) = \omega(\gamma')$ are connected if there exists a path in \mathcal{Z} (now identified as a set of segments) such that each element of this path γ'' is such that $\omega(\gamma'') = \omega(\gamma)$. Such a path is called a *weak channel* if $\omega(\gamma) = -1$ and a *strong channel* if $\omega(\gamma) = 1$. In this way, we subdivide \mathcal{Z} into ‘connected subsets’ where either $\omega(\gamma) = 1$ or -1 .

We now want to express the fact that

$$\omega(\gamma) = \begin{cases} 1 & \text{with probability } p \\ -1 & \text{with probability } 1 - p. \end{cases}$$

This can be done rigorously by introducing some ‘independent identically distributed’ random variables. This is not however the scope of our presentation. It suffices to describe the ‘almost-sure’ properties of such ω .

If $p < 1/2$ then it is ‘more probable’ to have some γ with $\omega(\gamma) = -1$; not only, it is not likely to have a large number of connected points with $\omega(\gamma) = 1$. This is expressed by the fact that there is one (necessarily unique) infinite connected component of $\{\omega = -1\}$. We call this set the *infinite weak cluster* (or simply weak cluster). Of course, the situation is symmetrical for $p > 1/2$, in which case we have an *infinite strong cluster*.

If two points γ and γ' belong to the weak cluster then there is at least one path L in the cluster (now we identify points with segments) joining γ and γ' . We denote by $|L|$ the length of this path. The *chemical distance* of γ and γ' is defined as

$$d^\omega(\gamma, \gamma') = \min |L|,$$

where the minimum is taken over all such paths L .

This distance is not isotropic (it suffices to think about the trivial case $p = 0$) and depends on ω . Nevertheless, its limit behavior as the points γ and γ' are scaled properly is well defined and independent of ω : we define

$$\varphi^p(\nu) = \liminf_{T \rightarrow +\infty} \inf \left\{ \frac{1}{|T|} d^\omega(\gamma, \gamma') : \gamma - \gamma' = T\nu \right\}.$$

This limit is finite and independent of ω for all ν , except for a set of ω with zero probability. Note that for $p = 1$ we have $\varphi^p(\nu) = \|\nu\|_1$.

The number $\varphi^p(\nu)$ describes the average distance on the weak cluster in the direction ν (and by symmetry also in the orthogonal direction). Its value cannot be decreased by using ‘small portions’ of strong connections: if $\delta > 0$ then there exists $T > 0$ and $c = c(\delta) \in (0, 1)$ such that if L is a path joining γ and $\gamma' = \gamma + T\nu$ and $|L| < (\varphi^p(\nu) - \delta)T$, then there are at least $c(\delta)T$ strong connections in the path L .

The weak cluster (and the strong cluster for $p > 1/2$) are ‘well distributed’. This can be expressed in the following way (*channel property*): there exist constants $c(p) > 0$ and $c_1(p) > 0$ such that a.s. for any δ , $0 < \delta \leq 1$ there is a large enough number $N_0 = N_0(\omega, \delta)$ such that for all $N > N_0$ and any square of size length δN contains at least $c(p)\delta N$ disjoint weak channels which connect opposite sides of the square. Moreover, the length of each such a channel does not exceed $c_1(p)\delta N$.

3 Randomly distributed defects

We fix the probability p of strong connections and choose a *realization* ω (naively, we toss a coin at each lattice connection) and, with this realization fixed, we consider the energy of the corresponding membrane

$$E_\varepsilon^\omega(u) = \frac{1}{2} \sum_{\alpha, \beta} \varepsilon^2 f_{\omega(\gamma)}^\varepsilon \left(\frac{u(\alpha) - u(\beta)}{\varepsilon} \right),$$

where

$$\gamma = \frac{\alpha + \beta}{2}, \quad f_1^\varepsilon(z) = z^2, \quad f_{-1}^\varepsilon(z) = f^\varepsilon(z),$$

with f^ε the weak membrane energy density defined above.

At the two extreme cases we have:

- $p = 0$ (zero probability of strong connections) then we almost surely are in the case of the weak membrane, and the Γ -limit is

$$F^0(u) = \int_\Omega |\nabla u|^2 dx + \int_{S(u)} \|\nu_u\|_1 d\mathcal{H}^{N-1}$$

defined on $SBV(\Omega)$;

• $p = 1$ (strong connections with probability one) then we almost surely are in the case of the ‘strong’ membrane, and the Γ -limit is simply

$$F^1(u) = \int_{\Omega} |\nabla u|^2 dx$$

on $H^1(\Omega)$.

We will show that

(1) the *percolation threshold* $p = 1/2$ separates two different regimes. Fracture may appear only below this threshold;

(2) below the percolation threshold the Γ -limit is of fracture type, and the surface interaction energy is described by the asymptotic chemical distance φ^p only, being independent of ω , and is given by

$$F^p(u) = \int_{\Omega} |\nabla u|^2 dx + \int_{S(u)} \varphi^p(\nu_u) d\mathcal{H}^{N-1}$$

defined on $SBV(\Omega)$. This means that fracture essentially occurs on the weak cluster, and that the energy density is simply obtained by minimizing the length of the fracture paths;

(3) above the percolation threshold the effect of the weak connections is negligible, and the overall behavior is simply described by the Dirichlet integral, independently of $p > 1/2$.

4 The supercritical case

We first treat the case $p > 1/2$. In this case we already have an upper bound since

$$E_{\varepsilon}^{\omega}(u) \leq E_{\varepsilon}^1(u) := \frac{1}{2} \sum_{\alpha, \beta} (u(\alpha) - u(\beta))^2 = \frac{1}{2} \sum_{\alpha, \beta} \varepsilon^2 \left(\frac{u(\alpha) - u(\beta)}{\varepsilon} \right)^2,$$

and the Γ -limit of the latter is the Dirichlet integral. We only have to prove the lower bound inequality.

To this end, we use an indirect argument: first, we use the coerciveness of the discrete energies for the weak membrane to deduce that we may suppose that the limit of a sequence such that $E_{\varepsilon}^{\omega}(u_{\varepsilon})$ is equi-bounded is indeed in $SBV(\Omega)$; subsequently, we use the percolation properties to show that the discontinuity set of the limit function u must be negligible and hence $u \in H^1(\Omega)$. The final equality then follows since on $H^1(\Omega)$ all limits coincide with the Dirichlet integral.

First step. We use the inequality $f_{\omega(\gamma)}^{\varepsilon} \geq f^{\varepsilon}$ to check that

$$E_{\varepsilon}^{\omega}(u) \geq E_{\varepsilon}^0(u) := \frac{1}{2} \sum_{\alpha, \beta} \varepsilon^2 f^{\varepsilon} \left(\frac{u(\alpha) - u(\beta)}{\varepsilon} \right).$$

Let $u_{\varepsilon} \rightarrow u$; we deduce that $\sup_{\varepsilon} E_{\varepsilon}^0(u_{\varepsilon})$ is equi-bounded and then that $u \in GSBV(\Omega)$. Moreover we have the lower bound

$$\liminf_{\varepsilon} E_{\varepsilon}^{\omega}(u_{\varepsilon}) \geq F^0(u).$$

Since $F^0 = F^1$ on $H^1(\Omega)$, it will suffice to prove that $u \in H^1(\Omega)$.

Second step. We now prove that $\mathcal{H}^1(S(u)) = 0$. This shows that $u \in H^1(\Omega)$ and concludes the proof. We will actually prove more: for any fixed any $c > 0$ the number of points in $S(u)$ such that $|u^+(x) - u^-(x)| \geq c$ is finite.

Take any N such points x_1, \dots, x_N . Let $\nu_i = \nu_u(x_i)$, and fix $\rho > 0$ such that the cubes $Q_{\rho}^{\nu_i}(x_i)$ of side length ρ , center x_i and one side orthogonal to ν_i have disjoint closures.

We now estimate the contribution to the total energy due to the interactions contained in $Q_\rho^{\nu_1}(x_1)$. Upon a translation we can suppose $x_1 = 0$. We may take ρ small enough so that it is not restrictive to suppose that $|u(x) - u(y)| \geq c/2$ if $x \in S_\rho^+$ and $y \in S_\rho^-$, where S_ρ^\pm are the two sides of $Q_\rho^{\nu_1}$ orthogonal to ν ; we may also suppose that $|u_\varepsilon(x) - u_\varepsilon(y)| \geq c/4$ for such x, y . We now use the channel property of the strong cluster (after scaling) to deduce that for ε small enough there are at least $c(p)\rho/\varepsilon$ disjoint strong channels C_j joining S_ρ^- and S_ρ^+ , of length at most $c_1\rho$. If x, y are points in S_ρ^- and S_ρ^+ belonging to the same strong channel, we can estimate

$$\begin{aligned} \frac{c}{4} &\leq |u_\varepsilon(x) - u_\varepsilon(y)| \leq \sum_{x', y'} \varepsilon \left| \frac{u_\varepsilon(x') - u_\varepsilon(y')}{\varepsilon} \right| \\ &\leq \sqrt{c_1\rho} \sqrt{\sum_{x', y'} \varepsilon \left| \frac{u_\varepsilon(x') - u_\varepsilon(y')}{\varepsilon} \right|^2}, \end{aligned}$$

where the sum is performed over ordered neighboring x', y' along the same strong channel, so that

$$\frac{c^2\varepsilon}{16c_1\rho} \leq \sum_{x', y'} \varepsilon^2 \left| \frac{u_\varepsilon(x') - u_\varepsilon(y')}{\varepsilon} \right|^2.$$

We sum up over all disjoint strong channels to obtain

$$\frac{c^2c(p)}{16c_1} \leq \sum_{C_j} \sum_{x', y'} \varepsilon^2 \left| \frac{u_\varepsilon(x') - u_\varepsilon(y')}{\varepsilon} \right|^2 \leq \frac{1}{2} \sum_{\alpha, \beta} \varepsilon^2 f_\omega^\varepsilon \left(\frac{u(\alpha) - u(\beta)}{\varepsilon} \right),$$

where the sum is performed over all pairs α, β in $Q_\rho^{\nu_1}$.

Since the $Q_\rho^{\nu_i}(x_i)$ are disjoint we can repeat the reasoning for all $i = 1, \dots, N$, and deduce the estimate

$$N \leq \frac{16c_1}{c^2c(p)} E_\varepsilon^\omega(u_\varepsilon)$$

on the number of such points, as desired.

5 The subcritical case

In the subcritical case we have to prove both an upper and a lower bound. Again, we can use a comparison argument with the weak-membrane energies to deduce that the limit of a sequence with equi-bounded energy is a function in $GSBV(\Omega)$.

We want to give a ‘local’ estimate on the limit energy. To this end, we define

$$E_\varepsilon^\omega(u, A) = \frac{1}{2} \sum_{\alpha, \beta \in A} \varepsilon^2 f_{\omega(\gamma)}^\varepsilon \left(\frac{u(\alpha) - u(\beta)}{\varepsilon} \right),$$

where we limit to interactions such that $\alpha, \beta \in A$.

Let $u_\varepsilon \rightarrow u$. We may suppose that $u \in L^\infty(\Omega)$, upon a truncation argument, and hence that $u \in SBV(\Omega)$. Fix $c > 0, \delta > 0$ and take $x \in S(u)$ such that $|u^+(x) - u^-(x)| \geq c$ and for all ρ small enough

$$\liminf_\varepsilon E_\varepsilon^\omega(u_\varepsilon, R_{\delta, \rho}^{\nu_u}(x)) \leq \rho(\varphi^p(\nu_u(x)) - 3\delta), \quad (1)$$

where $R_{\delta, \rho}^{\nu_u}(x)$ is the rectangle of center x , one side of length ρ orthogonal to ν and the other side of length $\delta\rho$. With fixed ρ we may suppose that $u_\varepsilon \rightarrow u$ on the two sides $S_\rho^\pm(x)$ of $R_{\delta, \rho}^{\nu_u}(x)$ that are orthogonal to $\nu_u(x)$.

We can give an estimate on the size of the set of indices γ such that the corresponding $\alpha, \beta \in R_{\delta, \rho}^{\nu_u(x)}(x)$, and

$$\omega(\gamma) = -1, \quad \left| \frac{u_\varepsilon(\alpha) - u_\varepsilon(\beta)}{\varepsilon} \right|^2 > \frac{1}{\varepsilon}.$$

If we denote by $I_\varepsilon(\rho)$ such set of indices, by (1) we have (upon passing to a subsequence of ε)

$$\#(I_\varepsilon(\rho)) \leq \frac{\rho}{\varepsilon} (\varphi^p(\nu_u(x)) - 2\delta)$$

for ρ small enough. In the complement of this set the interactions are quadratic (either because $\omega(\gamma) = 1$ or because the difference quotient is below the threshold $1/\sqrt{\varepsilon}$).

We then deduce that we may find $c(\delta)\frac{\rho}{\varepsilon}$ paths in the complement of $I_\varepsilon(\rho)$. In fact, upon scaling and setting $T = \frac{\rho}{\varepsilon}$, if this were not true then we could find a path L connecting two points γ, γ' with $\gamma - \gamma' = T\nu$ such that $|L| \leq (\varphi^p(\nu_u(x)) - \delta)T$ and with a percentage of strong connection less than $c(\delta)$.

At this point, we have a fixed percentage of paths where we can reason as in the supercritical case, to deduce in particular that for all $c > 0$

$$\mathcal{H}^1(\{x \in S(u) : |u^+(x) - u^-(x)| \geq c, (1) \text{ holds}\}) = 0,$$

and hence that for \mathcal{H}^1 -almost all $x \in S(u)$

$$\liminf_\varepsilon E_\varepsilon^\omega(u_\varepsilon, R_{\delta, \rho}^{\nu_u(x)}(x)) \geq \rho(\varphi^p(\nu_u(x)) - 3\delta). \quad (2)$$

By a covering argument of (compact sets of) $S(u)$ by rectangles $R_{\delta, \rho}^{\nu_u(x)}(x)$, (2) and the lower bound coming from the weak membrane (applied to the complement of such sets), for all $\sigma > 0$ we deduce that

$$\liminf_\varepsilon E_\varepsilon^\omega(u_\varepsilon) \geq \int_\Omega |\nabla u|^2 dx + \int_{S(u)} (\varphi^p(\nu_u(x)) - 3\delta) d\mathcal{H}^1 - \sigma,$$

and the lower bound by the arbitrariness of δ and σ .

It remains to check the upper bound. As usual we do not consider a general target function u , but limit our analysis to u in a ‘dense class’, the general case being obtained by approximation. In this case, we can consider u such that $S(u)$ is a finite union of segments, and $u \in C^1(\Omega \setminus \overline{S(u)}) \cap H^1(\Omega \setminus \overline{S(u)})$.

We only treat the case when $S(u) = (-1/2, 1/2) \times \{0\}$, since our argument is local and can be easily extended to all orientations of $S(u)$. We fix $\delta > 0$ consider the rectangle $\frac{1}{\varepsilon}([-1/2, 1/2] \times [0, \delta])$. We apply our percolation properties in a slightly different ‘dual’ way: we identify each point/segment $\gamma \in \mathcal{Z}$ with the orthogonal segment with the same middle point. This identification defines a ‘dual’ lattice \mathcal{Z}' , in which we may find a path L'_ε of weak connections (*i.e.*, still $\omega(\gamma) = -1$) joining the two opposite ‘vertical’ sides of $\frac{1}{\varepsilon}([-1/2, 1/2] \times (0, \delta))$ and with $|L'_\varepsilon| \leq (\varphi^p(e_2) + \delta)$.

The path L'_ε divides $\frac{1}{\varepsilon}([-1/2, 1/2] \times [0, \delta])$ in two connected components that we denote by R_ε^+ and R_ε^- (the latter the one containing $\frac{1}{\varepsilon}([-1/2, 1/2] \times \{0\})$). We then simply define:

$$u_\varepsilon(\alpha) = \begin{cases} u(\alpha_1, 0) & \text{if } \alpha/\varepsilon \in R_\varepsilon^- \\ u(\alpha) & \text{otherwise.} \end{cases}$$

Note that for ε small enough the set of $\gamma \in \varepsilon\mathbf{Z}^2$ such that

$$\left| \frac{u_\varepsilon(\alpha) - u_\varepsilon(\beta)}{\varepsilon} \right|^2 > \frac{1}{\varepsilon}$$

is contained in $\varepsilon L'_\varepsilon \cup (\{-1/2\} \times (0, \delta)) \cup (\{1/2\} \times (0, \delta))$, and hence we have

$$\limsup_\varepsilon E_\varepsilon^\omega(u_\varepsilon) \leq \int_\Omega |\nabla u|^2 dx + \mathcal{H}^1(S(u))\varphi^p(e_2) + 2\delta.$$

Now we may further extract a diagonal subsequence in δ and obtain a sequence, still denoted by (u_ε) , such that $u_\varepsilon \rightarrow u$ and

$$\limsup_\varepsilon E_\varepsilon^\omega(u_\varepsilon) \leq \int_\Omega |\nabla u|^2 dx + \mathcal{H}^1(S(u))\varphi^p(e_2) = \int_\Omega |\nabla u|^2 dx + \int_{S(u)} \varphi^p(\nu_u) d\mathcal{H}^1,$$

as desired.

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