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.* $u : \varepsilon\mathbf{Z}^N \cap \Omega \to \{-1, 1\}$, 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 $\varepsilon \to 0$. We use the notation $u_i = u(\varepsilon i)$ if no other subscript is present.

Consider now a sequence of states u_ε thay 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

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

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 $-1 \le u \le 1$ and that (l being the side length of Q)

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

i.e.,

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

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

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

Note that the function $\psi(t) = \big(f(-1) + \frac{1}{2}(t+1)f(1)\big)$ 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 $u:\Omega\to[-1,1]$ 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 $u_\varepsilon : \varepsilon\mathbf{Z}^N\cap\Omega\to\mathbf{R}$ 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 $F(u) = \lim_{\varepsilon\to 0} E_\varepsilon(u_\varepsilon)$ 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

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

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

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

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 $\varepsilon \to 0$ 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

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

and, given u_ε, we define

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

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 $g : \{-1, 0, 1\} \to \mathbf{R}$

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

(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 $\psi^\pm$ is such that the corresponding integral is weakly lower semicontinuous; *i.e.*,

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

If this were the case then

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

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 $\psi : \mathbf{R} \to [-\infty, +\infty]$ is convex and lower semicontinuous. We then choose $\psi^\pm$ 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

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

We then have the lower bounds: if u_ε tends to u weakly and $|u| \leq 1$ then
case (i) $\liminf_{\varepsilon\to 0} E_\varepsilon(u_\varepsilon) \geq -|\Omega|$ (independent of u);
case (ii) $\liminf_{\varepsilon\to 0} E_\varepsilon(u_\varepsilon) \geq \int_\Omega (2|u| - 1)\,dx$.

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 lim inf 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 in 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 $\psi^\pm$ 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

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

for every $v_\varepsilon \to u$ 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 $\varepsilon << \delta << 1$, and let

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

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

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

(ii) let δ be as above and let

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

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

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

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 $\varepsilon \to 0$.

3 An higher-order description: phase transitions

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

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

with $1 \le k \le n-1$ (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

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

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

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

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 $c_\varepsilon \to c$. 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

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

(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 $|u| \le 1$, 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

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

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

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

then we obtain that

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

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 $\delta_\varepsilon \to 0$.

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 $r_\varepsilon \to -|\Omega|$.

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

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

(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_ε $(= -1 + 2\chi_{G_\varepsilon})$ 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

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

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 $u_\varepsilon \to u$, 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

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

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

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

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

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

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

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

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

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

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

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 ($\varepsilon = 1/n$)

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

If n is even then the minimizers are given by

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

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 unction 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 $|u| \le 1$ 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:

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

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,

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

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 $-1/2$).

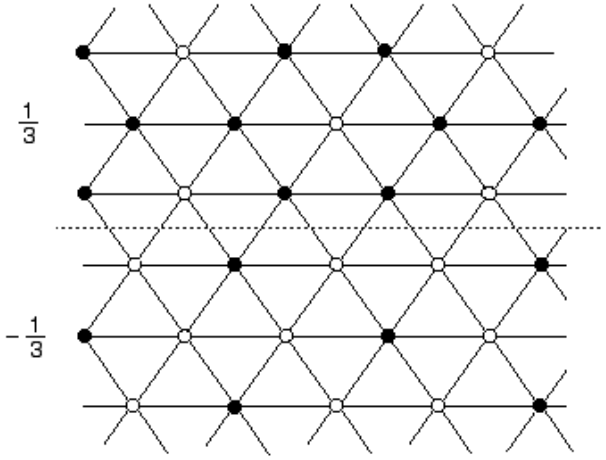

Figure 1: microscopical pattern for a transition with no interfacial energy

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

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

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

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

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

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

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

$$-2c_2 \geq -2c_1 + 2c_2 \qquad (i.e.,\ 2c_2 \leq c_1)$$

or not. In the first case, when $f(0) = -2c_1 + 2c_2$, the minimum configuration is the same alternating state as that we encoutered 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

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

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

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

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

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

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 $w : 2\mathbf{Z}^2 \to \mathbf{R}^4$

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

If we follow a sequence (u_ε) with $\sup_\varepsilon E_\varepsilon^{(1)}(u_\varepsilon) < +\infty$ then we deduce that $u_\varepsilon \to 0$ and $w_\varepsilon \to w$, 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.

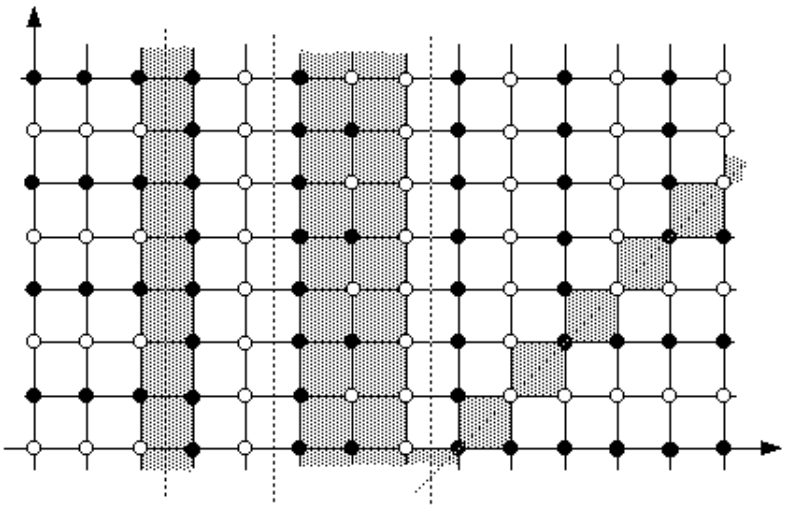

Figure 2: microscopical transitions between four different phases

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.