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Phase and anti-phase boundaries in binary discrete systems

Roberto Alicandro
DAEIMI - Università di Cassino
Via G. Di Biasio 43, 03043 Cassino (FR)
alicandr@unicas.it

I will present some results obtained in a joint work with Andrea Braides and Marco Cicalese [1], in which we provide a simple variational description of the overall properties of binary lattice systems; i.e., systems driven by energies defined on functions parameterized on a lattice and that may only take two values (which is not restrictive to suppose being the real numbers $+1$ and -1). These two values may have a physical interpretation as 'spins' or as parameterizing two types of atoms in a binary alloy.

Our main goal is to show how phase and anti-phase boundaries in binary lattice systems arise from minimization arguments, and can be conveniently described by computing some Γ-limits. To this end we will limit our analysis mainly to square lattices, and to nearest and next-to-nearest interactions, for which the energy densities of the limit surface energies can be explicitly and easily computed.

The simplest situation is when only nearest-neighbours are taken into account. If we denote by $u^i \in \{-1, 1\}$ the value taken by the function u at the point parameterized by the integer pair $i = (i_1, i_2)$ then, up to affine changes of variables that do not affect the overall behaviour of the system, the energy density between neighbouring u^i and u^j (i.e., with $|i - j| = 1$) can only be of one of the following two forms

$f_{\text{ferro}}(u^i, u^j) = -u^i u^j$ (ferromagnetic)
$f_{\text{anti}}(u^i, u^j) = u^i u^j$ (anti-ferromagnetic),

their labelling coming from the physical literature. Clearly, minimizing ferromagnetic energies favour uniform states $u^i \equiv 1$ and $u^i \equiv -1$, while anti-ferromagnetic energies favour neighbours with alternating signs.

A Γ-limit analysis of these energies can be performed by approximation with an energy on the continuum. To this end we fix a bounded open subset $\Omega \subset \mathbb{R}^N$ and consider the scaled energies

$$E_\varepsilon^{\text{ferro}}(u) = \sum_{\text{n.n.}} \varepsilon^N f_{\text{ferro}}(u^i, u^j), \qquad E_\varepsilon^{\text{anti}}(u) = \sum_{\text{n.n.}} \varepsilon^N f_{\text{anti}}(u^i, u^j), \tag{0.1}$$

where the sum is performed over nearest neighbours (n.n.) $i, j \in \mathbb{Z}^N$ such that $\varepsilon i, \varepsilon j \in \Omega$. In this way the array $\{u^i\}$ can be viewed as a function defined on $\Omega \cap \varepsilon\mathbb{Z}^N$. Upon identifying such functions with their piecewise-constant interpolations the energies $E_\varepsilon^{\text{ferro}}$, $E_\varepsilon^{\text{anti}}$ can be interpreted as defined on (a subset of) $L^1(\Omega)$, and can therefore undergo a process of Γ-limit in that framework.

The Γ-limit E_{ferro} of $E_\varepsilon^{\text{ferro}}$ is particularly simple, only giving the trivial constraint $|u| \le 1$, and the constant (minimum) value $-|\Omega|$ (corresponding to the uniform states) on all such functions. This summarizes the fact that a sequence (u_ε) can arbitrarily mix the uniform states -1 and 1 at a mesoscopic scale with a negligible variation from the value of the uniform states as $\varepsilon \to 0$. Note that the absolute minimum value at scale ε is precisely given by $c_\varepsilon = -\sum_{\text{n.n.}} \varepsilon^N$.

We can examine sequences that realize the minimum value with a sharper precision; i.e., such that

$$E_\varepsilon^{\text{ferro}}(u_\varepsilon) = c_\varepsilon + O(\varepsilon).$$

For such functions the limit states u will take the values ± 1 only, and the scaled Γ-limit will be an interfacial energy of the form

$$E_{\text{ferro}}^{(1)}(u) = \int_{S(u)} \|\nu\|_1 d\mathcal{H}^{N-1},$$

where $S(u)$ denotes the (essential) interface between the sets $\{u = 1\}$ and $\{u = -1\}$ and the interfacial energy density $\|\nu\|_1 = \sum_{i=1}^N |\nu_i|$ depending on the normal to $S(u)$ reflects the symmetries of the lattice.

In the anti-ferromagnetic case the first Γ-limit is itself not trivial, being given by the bulk energy

$$E_{\text{anti}}(u) = \int_\Omega (2|u| - 1)\, dx \qquad |u| \le 1 \text{ a.e.}$$

The form of the Γ-limit reflects that minimum values are given by the alternating state, whose average is 0 (the minimum point of $2|u| - 1$), and gives a quantitative estimate of the energy of a deviation from the minimal state. Note that the states not constantly equal to 0 or ± 1 are best approximated again by 'mixing' constant and alternating states at a mesoscopic level.

The analysis at higher order for anti-ferromagnetic energies is seemingly useless since the unique minimizer for E_{anti} is the constant 0. Nevertheless, the change of variables

$$v^i = (-1)^{i_1+i_2+\cdots+i_N} u^i \tag{0.2}$$

allows to repeat the analysis above, since

$$E_\varepsilon^{\text{ferro}}(v) = E_\varepsilon^{\text{anti}}(u).$$

The previous analysis can be read as follows: sequences (u_ε) with $E_\varepsilon^{\text{anti}}(u_\varepsilon) = c_\varepsilon + O(\varepsilon)$ in the limit as $\varepsilon \to 0$ determine a partition into two sets (corresponding to $\{v = 1\}$ and $\{v = -1\}$, where v is the limit of the corresponding v_ε) in which u_ε take the alternating states $u_0 := (-1)^{i_1+i_2+\cdots+i_N}$ and $u_1 = -u_0$. The interface $S(v)$ between these sets is an anti-phase boundary that is energetically described again by $E_{\text{ferro}}^{(1)}(v)$. Note that the appearance of anti-phase boundaries depends on the geometry of the lattice. Indeed we provide an example of an hexagonal lattice which does not exhibit such a phenomenon.

In the simple case above we have obtained the description of anti-phase boundaries by the simple change of parameter (0.2). This is no longer possible if longer-range interactions are taken into account, as in that case minimum states may possess less symmetries. To exemplify this fact, limiting our analysis to square lattices in dimension 2, we consider a next-to-nearest neighbour system, with energy

$$E_\varepsilon(u) = c_1 \sum_{n.n.} \varepsilon^2 u^i u^j + c_2 \sum_{n.n.n.} \varepsilon^2 u^i u^j,$$

where now n.n.n. (next-to-nearest neighbours) are those such that $|i-j| = \sqrt{2}$ (corresponding to the diagonals of the squares of the lattice).

The first order Γ-limit can be again computed for all c_1, c_2 giving a non-trivial bulk energy. We are interested in the case

$$0 < 2c_2 < c_1, \tag{0.3}$$

that is the one bringing new features to the problem. In this case alternating next-to-nearest neighbours give the minimal energy. This implies that

1) again the minimum of the bulk energy is obtained by $u = 0$;

2) locally minimizing configurations can be viewed as 2-periodic functions on the lattice taking alternatingly values 1 and -1 on rows or on columns. It is suggestive to identify this four possible states as follows: with e_1 in the case $u^i = -(-1)^{i_1}$ (I.e., when the value 1 is taken on even columns), with e_2 if $u^i = -(-1)^{i_2}$ (i.e., when the value 1 is taken on even rows), and with $-e_1$, $-e_2$ in the cases with exchanged signs.

Note that these are not all the states corresponding to $u = 0$, the alternating function $u^i = -(-1)^{i_1+i_2}$ having this same average. This choice entails a homogenization process. We have chosen condition (0.3) precisely to avoid the alternating situation already considered.

With this description of the new limit parameter $v \in \{\pm e_1, \pm e_2\}$ we can prove a Γ-limit result for the scaled energies, showing that, up to a boundary layer term, the limit behaviour is now described by an energy of the form

$$F^{(1)}(v) = \int_{S(v)} \varphi(v^+, v^-, \nu) d\mathcal{H}^1.$$

Again this formula describes a limit partition into sets $\{v = \pm e_j\}$, of which $S(v)$ describes the interfaces. The energy density now not only depends on the normal ν to $S(v)$, but also on the traces $v^\pm$ on both sides of $S(v)$. The form of φ can be explicitly computed, and also takes into account, beside the anisotropy of the lattice, that at a discrete level the interface can be 'sharp' (i.e. concentrated on one cell) or 'diffuse' (i.e. concentrated on more cells).

Eventually, I would also like to give a brief description of a model considered in a work in progress in collaboration with Marco Cicalese. Here we restrict to the 2-D case and consider energies of the form

$$E_\varepsilon(u) = -\sum_{\text{n.n.}} \varepsilon^2(u^i, u^j),$$

where u take values in the unit sphere S^1 and $(\cdot,\cdot)$ denotes the scalar product. We show that a proper scaling of these energies has the same asymptotic behaviour of the complex Ginzburg-Landau functional, thus giving rise to 'topological type' phase transitions.

REFERENCES

1. R. Alicandro, A. Braides and M. Cicalese, *Networks and Heterogeneous Media*, vol. 1, 2006, 85–107.