1
Introduction

The object of the analysis presented in this book is discrete systems with a large number of nodes, whose overall behavior is driven by what can be considered a surface energy. Many of these systems have some origin or analogy in models in science and technology. It is not our intention to attempt here an impossible list and description of the many problems leading to such models. We only describe a few paradigmatic examples in order to highlight the width of the field of applications. A first clarifying example is variational models in computer vision such as the one by Blake and Zisserman (1987). There, the unknown, representing the output picture, is a real-valued function defined on pixels, whose ensemble can be regarded as a portion of a lattice. Pairs of pixels on which the difference of the values of this function exceeds some threshold are regarded as separated by an interface. This model has a counterpart in the continuum variational approach to image processing by Mumford and Shah (1989). Among the many other examples, we may single out another key model coming from atomic physics with similar features. This regards atomistic pair potentials such as the Lennard–Jones potential. Even though the overall behavior of systems energetically driven by such potentials is extremely complex, such types of energies can be analyzed close to absolute minima (physically, at zero temperature), showing a phenomenon of *crystallization*; that is, ground states tend to arrange on a regular lattice. Even this expected property of minimizers is a very subtle issue and can be formalized as the stability under finite perturbations of the arrangement of atoms in a lattice. It has been proved to hold only in dimension two and for a limited class of interatomic potentials (Theil, 2006). If crystallization holds, then the energies can again be parameterized on an underlying lattice. A possible continuum approximation gives rise to theories of brittle fracture (Braides et al., 2006; Friedrich and Schmidt, 2014), where the main unknown is the crack site, whose atomistic interpretation can be again given in terms of neighboring nodes with large relative displacements.

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In variational theories for data science, data are sometimes regarded as randomly distributed objects and are often labeled by parameters on which interfacial energies are used in order to separate families of similar data (García Trillos and Slepčev, 2016), which is a typical problem of machine learning. Such energies are then thought as defined on some type of random lattices. Also spin systems are a classical issue in statistical mechanics, and often the energies driving their behavior are defined on a regular lattice, with a random dependence that can be interpreted as a property of the interactions. Many of the energies just mentioned can be studied within a multiscale perspective, deriving a number of large-scale behaviors depending on the energy level of the system (Blanc et al., 2005; E and Ming, 2007; Le Bris and Lions, 2005).

Early analyses of variational problems involving nonconvex functionals defined on lattices were mainly carried on from the perspective of numerical analysis in order to implement finite-difference or finite-element schemes. As examples we refer to the discretization of the Ambrosio and Tortorelli (1990) functional in computer vision (Bellettini and Coscia, 1994), or the analysis of the Blake–Zisserman model (Chambolle, 1995). A systematic analysis of classes of discrete energies was performed with different techniques and scopes almost at the same time in a number of papers such as the ones by Blanc et al. (2002), Braides and Gelli (2002), E and Ming (2007), and Friesecke and Theil (2002). The first purely variational analysis of surface energies alone was later carried out by Caffarelli and de la Llave (2005), and shortly after by Alicandro et al. (2006), followed by a number of applications and results. In some cases, as in computer vision theories or brittle fracture, these results involve at the same time an interface energy and some bulk energy; nevertheless, in such analyses the surface part can be studied separately and, conversely, results involving bulk and surface energies can be specialized and refined for purely superficial energies. Moreover, note that in order to describe interfacial energies it is not restrictive to assume that discrete systems are defined only on functions taking a finite number of values; for fracture, for example, this amounts to considering interfaces at a scale where the displacement is approximately constant on the two sides of the crack, which can be justified by a blow-up argument.

In view of these considerations, the object of our analysis is energies whose domain is functions defined on a lattice $\mathcal{L}$ in $\mathbb{R}^d$, or a portion of that lattice, and taking values in a finite set Y. The abundance of techniques and results obtained directly for such types of energies, or for problems where these energies are part of the description, has stimulated the need of a systematization both for a unitary formal structure and in order to highlight in a clear way completely novel directions both applied and theoretical, such as links with discrete dynamical systems and graph theory. The book is intended to be a proposal for the

formalization of a common language both within the rich and various subject of variational methods, and toward quite different lines of research, which are essentially discrete. The choice of focusing on discrete interfacial energies is due to the ease of expressing in their terms problems that are intrinsically discrete and not only a discretization of a continuous analog, and at the same time to the generality of the methods and results, which can be exported to problems with other scalings and physical interpretations.

The simplest lattice functions are *spin functions*, where the set of values Y has cardinality two, and is usually taken to be $\{-1, 1\}$. Note that here and after we borrow some terminology from the physical literature – "spin" is one of such terms – but we highlight that we claim no direct application to physical theories, the terminology serving just as a suggestion for the writer and hopefully to the reader. The prototypical energies defined on spin functions depend on *pair interactions*; that is, the overall energy is the sum of the energy between pairs of nodes. Analytically, if we denote by u_i the value of a function u at a node i in $\mathcal{L}$, the energy is a sum of terms depending only on u_i and u_j. A class of energy densities is those minimized when $u_i = u_j$, which are called *ferromagnetic*, here using a terminology borrowed from statistical mechanics. In this case, we may suppose that the energy between two points is proportional to $(u_i - u_j)^2$. A typical spin energy is of the form

$$E(u) = \sum_{i,j} a_{ij}(u_i - u_j)^2. \tag{1.1}$$

Note that in statistical mechanics energies usually take the form $-\sum_{ij} a_{ij}u_iu_j$, which is equivalent to the one just shown since the two expressions only differ by constants independent of u and only depending on the set of nodes that are taken into account. Other analytical expressions can be equivalently used, such as $\sum_{ij} a_{ij}|u_i - u_j|$.

The overall properties of such an energy can be studied using a *discrete-to-continuum* approach. We introduce a small parameter ε, and consider a portion of the scaled lattice $\varepsilon\mathcal{L}$ contained in a fixed bounded Lipschitz open subset Ω of $\mathbb{R}^d$. In this way we allow the number of nodes under analysis to diverge as $\varepsilon \to 0$. Correspondingly, we consider energies

$$E_\varepsilon(u) = \sum_{i,j} \varepsilon^{d-1} a^\varepsilon_{ij}(u_i - u_j)^2, \tag{1.2}$$

where now u is a spin function defined on $\Omega \cap \varepsilon\mathcal{L}$ and $u_i = u(\varepsilon i)$. Accordingly, the sum is taken for i, j such that $\varepsilon i, \varepsilon j \in \Omega \cap \varepsilon\mathcal{L}$. Such functions u can be identified with their piecewise-constant interpolations on the Voronoi cells of the lattice, so that the domain of E_ε can be seen as a subset of $L^\infty(\Omega)$, and

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the behavior of minimum problems related to E_ε can be stated in terms of a continuum approximation defined in a Lebesgue space. Discrete-to-continuum limits in this spirit have been analyzed in many contexts both in terms of pointwise expansions (e.g. Blanc et al., 2005), numerical approximations (e.g. E and Ming, 2007), and variational limits (e.g. Braides and Gelli, 2002). The scaling ε^{d-1} (*surface scaling*) highlights that we expect the relevant limit contribution as $\varepsilon \to 0$ to be described by a surface energy. This is in accord with the constraint that $u \in \{-1, 1\}$, which allows us to identify u with the set $\{u = 1\}$. Note that in (1.2) we include a dependence of the coefficients a_{ij}^ε on the parameter ε in order to allow for the maximal freedom on the modeling assumptions of our energies.

Under a positiveness assumption on a_{ij}^ε, energies $E_\varepsilon(u^\varepsilon)$ along a sequence of lattice spin functions u^ε can be interpreted as interfacial energies taking into account the interactions through the boundary of the sets $\{u^\varepsilon = 1\}$, after introducing a continuum interpolation of the discrete spin functions. The requirement that such sets converge to a set A defines the *discrete-to-continuum convergence of lattice functions* u^ε to A. The problem of the computation of the Γ-*limit* of energies E_ε can then be set within the framework of such interfacial energies (perimeter energies), which have the form

$$F(A) = \int_{\partial^* A} \varphi(x, \nu) d\mathcal{H}^{d-1}, \tag{1.3}$$

where A is a set of finite perimeter representing the continuum counterpart of $\{u = 1\}$; $\partial^* A$ denotes its reduced boundary, whose normal at $\mathcal{H}^{d-1}$-almost every point is denoted by ν; and $\mathcal{H}^{d-1}$ denotes the $d-1$-dimensional (surface) Hausdorff measure. In this way a limit set of finite perimeter and a continuum energy are obtained from a family of discrete energies defined on scaled copies of a lattice, as the scaling parameter tends to 0. The limit energies capture the behavior of the discrete ones in the sense of the convergence of minimum problems: the solutions of minimum problems at a discrete level can be seen as discretizations of an effective continuum problem. Typically, such minimum problems are *minimal-cut problems* for discrete interactions, which are approximated by minimal-perimeter problems on the continuum. In particular, we can consider minimum problems in the whole space, in which case the minimizers are the so-called *Wulff shapes*.

Wulff shapes are connected to classical problems of Statistical Mechanics regarding the collective behavior of microscopic spin systems when the number of configurations diverges, and to the analysis of some crystallization problems involving the asymptotic behavior as N diverges of ensembles of N points in $\mathbb{R}^d$ whose location is such that some energy is minimized involving the

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distances between points. The minimal configurations tend to arrange as a portion of a lattice whose overall shape is a Wulff shape for some surface energy. Even though closely related to our analysis, we do not examine in detail the connections with such interesting problems.

Back to the description of our discrete-to-continuum approach, once an analytic framework has been established, the focus is on conditions that allow one to prove existence of a Γ-limit and characterize the resulting perimeter functional. A first class of energies that can be analyzed elementarily is *homogeneous ferromagnetic energies* defined on Bravais lattices, of the form

$$E_\varepsilon(u) = \sum_{i,j} \varepsilon^{d-1} \alpha_{i-j} (u_i - u_j)^2; \tag{1.4}$$

that is, when the interaction coefficients are independent of ε and are homogeneous, in the sense that $a_{ij}^\varepsilon = \alpha_{i-j}$. We may assume that the indices are taken in $\mathbb{Z}^d$ since all Bravais lattices can be identified with that lattice, up to a change of variables. We may regroup the interactions as

$$E_\varepsilon(u) = \sum_k \sum_i \varepsilon^{d-1} \alpha_k (u_{i+k} - u_i)^2 \tag{1.5}$$

and study separately the terms $\sum_i \varepsilon^{d-1} \alpha_k (u_{i+k} - u_i)^2$ at fixed k. Usually, the Γ-limit of a sum is not the sum of a Γ-limit, but in this case a *superposition principle* holds due to the fact that a recovery sequence for a planar interface is simply its discretization, independently of k. The outcome is that in this case φ is x-independent and is given by

$$\varphi(\nu) = 4 \sum_{k \in \mathbb{Z}^d} \alpha_k |\langle \nu, k \rangle|, \tag{1.6}$$

the factor 4 coming from the fact that $(u_i - u_j)^2 \in \{0, 4\}$. This superposition property can be interpreted as an interfacial version of a *Cauchy–Born rule*, which states that macroscopic energies correspond to a regular arrangement of discrete values. This property is often crucial for computational and modeling reasons and is often analyzed in problems in continuum mechanics (Friesecke and Theil, 2002; E and Ming, 2007; Schmidt, 2008).

In order to obtain the convergence just mentioned, two conditions are necessary:

(i) (*coerciveness on nearest neighbors*) $\alpha_k > 0$ if $\|k\| = 1$;
(ii) (*decay of the coefficients*) $\sum_k \alpha_k \|k\| < +\infty$.

Condition (i) allows one to estimate the perimeter of the interpolated sets $\{u = 1\}$ by the energy $E_\varepsilon(u)$ and thus guarantees compactness of families of

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functions with equibounded energies. Condition (ii) guarantees that indeed the limit energy is finite only on sets of finite perimeter.

The next level in complexity is periodic systems on $\mathbb{Z}^d$; that is, when the coefficients a_{ij} in (1.2) are still ε-independent, but are periodic of some integer period K; that is,

$$a_{ij} = a_{kl} \text{ if } i = k \text{ and } j = l \text{ modulo } K, \tag{1.7}$$

the case $K = 1$ reducing to that of homogeneous coefficients. This is a first case of *homogenization*, in which the Γ-limit exists and the limit energy density φ_{hom} is homogeneous, that is, x-independent. The main issue here is the characterization of φ_{hom}, which can be achieved in various ways. We present a characterization through an *asymptotic homogenization formula*, which turns out to be flexible to treat systems with other geometrical assumptions. If the range of interactions is R, then this formula is

$$\varphi_{\text{hom}}(\nu) = \lim_{T\to+\infty} \frac{1}{T^{d-1}} \min \Big\{ \sum_{i,j\in Q_T^\nu} a_{ij}(u_i - u_j)^2 \colon\ u \colon \mathbb{Z}^d \cap Q_T^\nu \to \{-1,+1\},\\ u_i = 1 \text{ if and only if } \langle i, \nu\rangle \geq 0 \text{ in } Q_T^\nu \setminus Q_{T-2R}^\nu, \Big\},$$

where Q_t^ν denotes a cube of side length t centered in 0 and one face orthogonal to ν. Note that, while analog formulas are valid for the homogenization of continuum energies, here the nonlocal character of discrete energies must be taken into account in the definition of boundary values, which are imposed in a "cubic annulus" close to the boundary. This is a technical point that is often present when defining boundary values for discrete systems, and is slightly more complex if the range of the interaction is infinite. We present two different techniques to obtain such a formula. The first one is based on the Fonseca and Müller (1992) *blow-up method* adapted to lattice problems, and the second one follows De Giorgi's *localization method*. Both methods are relatively self-contained, up to general measure-theoretical arguments, and do not need further functional notions beside the ones related to perimeter functionals. Other arguments that can be used in this context are Caffarelli and de la Llave's (2005) *plane-like minimizer* arguments, or extensions to convex one-homogeneous functionals as by Ambrosio and Braides (1990b) in the continuum and by Chambolle and Kreutz (2023) for lattice energies, the latter requiring bulk-scale homogenization techniques.

The blow-up technique is useful to provide lower bounds along a discrete-to-continuum converging sequence of functions and is based on the idea of interpreting functionals as measures. The key point is then to describe the relevant density of a limit measure concentrated on the perimeter of the limit set

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in terms of φ_{hom}. Note that, for discrete problems such as the one just presented, the measures to study are

$$\mu_\varepsilon = \sum_i \Big(\sum_j \varepsilon^{d-1} a_{ij} (u_i - u_j)^2 \Big) \delta_{\varepsilon i}. \tag{1.8}$$

The coefficient of the Dirac delta at εi describes the interaction of such points with the remaining points of the lattice. It is therefore a nonlocal quantity, even though its nonlocality is vanishing with ε. This method allows one to clearly separate the estimate of a lower bound and the construction of recovery sequences for the upper bound, which are directly obtained from the homogenization formula and the density of polyhedral sets. An essential technical point in both computations is the use of *discrete coarea arguments* that are used to match boundary data with asymptotically negligible energetic expense cost.

It is worth noting the flexibility of the blow-up method, which is not limited to Bravais-lattice energies or periodic coefficients. In particular, coupling it with a *projection method*, we may use it to derive homogenization theorems for *aperiodic lattices* obtained by projection from higher-dimensional Bravais lattices on incommensurate lower-dimensional linear spaces, such as *quasicrystals* or *Penrose lattices*. This is a genuinely discrete setting with only a partial counterpart on the continuum. Such lattices are not periodic but they retain some *quasiperiodicity* properties: for a relatively dense set of translations, lattices superpose up to well-separated isolated points whose presence does not invalidate the proof of the asymptotic homogenization formula. A simpler setting, corresponding to the case when the projection is on a commensurate lower-dimensional linear space gives rise to a theory of homogenized surface energies on *thin objects*. Even though this has a counterpart in the continuum, the nonlocal nature of discrete energies gives rise to new phenomenon such as a nonadditive dependence of the thin-film thickness, and is closer to a rigorous treatment of atom deposition theories.

Another issue particularly suited to a lattice formulation is that of a *random dependence* on the interactions for systems of independently distributed coefficients, which again can be studied using the blow-up technique. The existence, and deterministic nature, of the homogenization formula in this case is an almost sure property of the system and is closely connected to *percolation theory* (Kesten, 1982; Grimmett, 1999). For systems with coercive and bounded interactions this can be interpreted as a *first-passage percolation* formula (Boivin, 1990). We also can study some *percolation-threshold variational phenomena* depending on some probability parameter. One such case is obtained by considering a system whose interaction coefficients take a positive finite value with probability $p \in [0,1]$ and the value $+\infty$ with probability $1 - p$. In the

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latter case the coefficients define what we call *rigid bonds*; for such a bond, having finite energy amounts to requiring that the corresponding pair u_i and u_j have the same value. The corresponding homogenization formula is linked to asymptotic metric properties on the cluster of points with no rigid bonds. In the two-dimensional setting this cluster is almost surely infinite if and only if $p > 1/2$, which is the case when φ_{hom} is finite, and it only depends on p. Its form is related to the so-called *chemical distance* of the system (Garet and Marchand, 2007). Another case in which a variational percolation phenomena occurs is that of the so-called *dilute systems*, whose coefficients mix a positive value with probability p and the value 0 (*weak bonds*) with probability $1 - p$. In this case, in two dimensions the cluster of points with weak bonds is infinite for $p > 1/2$, which is the case when φ_{hom} is identically 0, while otherwise φ_{hom} is given by a first-passage percolation formula only depending on p, which holds also in this case (Wouts, 2009; Cerf and Théret, 2011). In these types of results, percolation techniques are used to describe the geometry of the infinite clusters of coercive interactions, when they exist, proving the existence of "lattice-like" subsets, which are sufficient in order to carry on the discrete-to-continuum process.

De Giorgi's localization method allows one to obtain general compactness and integral-representation results under minimal conditions. In the context of ferromagnetic energies E_ε of the form (1.2) it allows one to prove that, upon extraction of subsequences, the discrete-to-continuum limit of every such family exists and is a possibly inhomogeneous perimeter energy of the form (1.3). The localization method consists in introducing a set variable U and considering localized functionals

$$E_\varepsilon(u, U) = \sum_{\varepsilon i, \varepsilon j \in U \cap \varepsilon \mathcal{L}} \varepsilon^{d-1} a_{ij}^\varepsilon (u_i - u_j)^2, \tag{1.9}$$

and studying their behavior both as functionals of the function u and of the set U. By proving abstract properties on the dependence on U we obtain the Γ-convergence to a measure, which then can be represented as an integral. The extension of this method to lattice energies, which are nonlocal by definition, requires some care, since, for example, the functionals in (1.9) are not subadditive in the set variable, contrary to their continuum counterpart. In order for this procedure to work, besides coerciveness assumptions we have to require a uniform decay condition, without which easy examples show that the Γ-limit may fail to be represented by a surface energy.

The generality and flexibility of the localization method allow one to abandon Bravais lattices, spin functions, and pair interactions and guarantee the extension to very general environments and energies. The domain of the energies

can be any infinite discrete set with a minimal distance between its points and no balls with a large diameter in its complement; we call such a set $\mathcal{L}$ an *admissible lattice*. The functions we consider are defined on portions of scaled copies of $\mathcal{L}$ with values in a discrete set Y. If $Y = \{-1, 1\}$, we recover spin systems, but we can also consider, for example, *ternary systems* by choosing $Y = \{-1, 0, 1\}$ or $Y = \{e_1, e_2, e_3\} \subset \mathbb{R}^3$. The energies can take into account *many-body interactions* or also interactions between all possible sites. To that end we may rewrite energies as

$$E_\varepsilon(u) = \sum_{\varepsilon i \in \Omega \cap \varepsilon \mathcal{L}} \varepsilon^{d-1} \phi_i^\varepsilon(\{u_{i+j}\}_j), \tag{1.10}$$

where the function ϕ_i^ε takes into account interactions involving the site i; for example, in the case of ferromagnetic interactions,

$$\phi_i^\varepsilon(\{z_k\}_k) = \sum_k a_{i\,i+k}^\varepsilon (z_k - z_0)^2. \tag{1.11}$$

If the functions ϕ_i^ε satisfy suitable coerciveness and growth conditions, which reduce to the abovementioned conditions on a_{ij}^ε for ferromagnetic interactions, then the Γ-limit exists up to subsequences and can be represented as a functional defined on *partitions of sets of finite perimeter* parameterized by a subset Y_0 of Y, and represented as a sum of integrals on the boundary of the elements of the partition. Note that the notions of nearest-neighbor and of discrete-to-continuum convergence must be suitably modified, which can be done using *Voronoi tessellations*. The compactness result can be applied, for example, to ensure that mixtures of two (or more) types of bonds can be represented on the continuum by a perimeter functional, the property of whose integrand can be then described by computing suitable *energy bounds*. This is a fundamental step in the field of *Optimal Design* of networks.

The range of applications of the compactness theorem makes it necessary to allow for the greatest generality, as the geometry of the lattice and the parameters involved are concerned. This is the case both when dealing with pair interactions in random environments that can be described by admissible lattices and when the assumption of positiveness of ferromagnetic interactions is removed, allowing for a multiplicity of ground states, whose overall behavior can be described by partitions. As for random sets, a notion of *stochastic lattices* can be given, which are almost surely admissible lattices and on which we can define random energies

$$E_\varepsilon^\omega(u) = \sum_{\varepsilon i, \varepsilon j \in U \cap \varepsilon \mathcal{L}^\omega} \varepsilon^{d-1} a_{ij}^\omega (u_i - u_j)^2, \tag{1.12}$$

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with coefficients depending on the distance between sites of the lattices. In (1.12) we highlight the dependence on ω, the realization of a suitable random variable. Under conditions of *stationarity* and *ergodicity* the Γ-limit is almost surely deterministic and described by an asymptotic homogenization formula that is the stochastic version of the asymptotic homogenization formula. A key ingredient in the proof of the validity of such a formula is a *subadditivity theorem for discrete stochastic processes*. We note that the hypothesis of admissibility of the lattice can sometimes be removed; for example, for *Poisson random sets*, for which compactness properties are achieved by using Percolation techniques (more precisely, a lemma on *polyominos* covering of Voronoi cells). Note that for the simplest nearest-neighbor energies on scaled Poisson random sets the isotropy of the Poisson process guarantees the isotropy of the limit energy; that is, almost surely we have Γ-convergence to a multiple of the Euclidean perimeter, in contrast with the crystallinity of short-range homogenization in Bravais lattices.

We note that the general compactness theorem sometimes must be integrated with other techniques in order to better describe the limit behavior of the system. One example is that of systems with many parameters Y of which only a subset Y_0 participate in the limit description. In this case the effect of the variables $Y \setminus Y_0$ is minimized out in the computation of the interfacial energy φ_{hom} given by the compactness theorem. If we want to better keep track of those parameters, we introduce their *measure of concentration* at the interface. This can be done, for example, for ternary systems giving rise to *surfactants*. Such systems can be parameterized on $\{-1, 0, 1\}$, and their ground states are only the constant states -1 and 1. The effect of the 0-phase can be described by adding to φ_{hom} a dependence on the density of a measure μ describing the limit amount of that phase on the interface

$$\int_{\partial^* A} \varphi_{\text{hom}}\Big(\frac{d\mu}{d\mathcal{H}^{d-1} \llcorner \partial^* A}, \nu\Big) d\mathcal{H}^{d-1}. \tag{1.13}$$

This energy density can be explicitly computed, for example, for the *Blume–Emery–Griffiths model* for surfactants. Similarly, a correction to the description by simple interfaces, but more for reasons of a geometric origin, is needed for systems with *high-contrast energies*. Models with such types of energies in the continuum case are used in applications, for example, to the study of the flow in a naturally fractured reservoir (Arbogast et al., 1990). In this case, coerciveness conditions are satisfied on one or more admissible sublattices (*perforated domains*) to each of which the compactness theorem can be applied. The remaining connections may give rise to an additional *interaction term* of bulk type describing the separate effect of the lower-coerciveness interactions between

the higher-coerciveness sublattices (*double-porosity energies*). Another type of correction can be necessary if the uniform-decay assumption on the interactions is relaxed, in which case an additional term of *nonlocal type* may appear besides the surface energy of the form

$$\int_{\partial^* A} \varphi_{\hom}(\nu) d\mathcal{H}^{d-1} + \int_{A\times(\Omega\setminus A)} K(x,y)\, d\mu(x,y), \tag{1.14}$$

such as a *nonlocal perimeter* or an *Ohta–Kawasaky type* functional. Another case, in which the methods of the compactness theorem can be applied after an initial modeling analysis, is that of systems describing (*chiral*) *molecules*. In the simplest case these systems can be described by homogenous ferromagnetic interactions where the sites of the relevant parameter (say, where $u_i = 1$) must be arranged as unions of sets of given shape (molecules). The analysis of the possible minimal configurations of such ensembles gives then a way to obtain a set of parameters that play the role of the set Y_0 in the compactness theorem, and obtain a description in terms of partitions into sets of finite perimeter.

The complexity of the compactness theorem is also justified by its application to *frustrated systems*; that is, to spin systems of pair interactions mixing positive and negative coefficients where there is no ground state that minimizes separately all pair interactions. As a consequence, such systems cannot by reduced to a ferromagnetic system and often possess many periodic ground states. If this is the case, the ground states themselves parameterize the set Y_0 of the compactness theorem, up to a *coarse-graining process* at the level of a period, considering Y as all possible arrays of values in such a period. This allows one to describe the behavior of the system again as an interfacial energy on partitions of sets of finite perimeter, which describe different microscopic *patterns*, or *modulated phases* within the same pattern. Note that the number of the limit parameters can be arbitrarily high even though the system we start with only takes the two values -1 and 1 into account. Note also that not all systems can be asymptotically described in this way: some present some degeneracies due to the possibility of having interfaces with zero energy between variants of ground states, and some others present a *total frustration* with an infinite family of periodic and nonperiodic ground states.

In the terminology of *Graph Theory*, the graphs with vertices and edges corresponding to the systems we have just described are essentially *sparse*; that is, the number of (relevant) edges is much lower than the total number of possible connections. More precisely, the assumptions of the compactness theorem are stated in terms of a decay condition, which implies that the relevant connections are of *equibounded range*. This assumption can be relaxed by a *coarse-graining* approach if the connections give a locally strongly dense graph;

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that is, a graph where all connections are considered at a scale much larger than that of the lattice dimensions but still infinitesimal as $\varepsilon \to 0$. If this assumption is relaxed, we may have sparse systems with *diffuse interfaces*; that is, whose behavior is determined by the presence of many interfaces that give an overall bulk energy in the limit. These interfaces also are at the basis of the behavior of *dense graphs*; that is, for which the number of edges is of the same order as the total number of possible connections. In this case the geometry of the set of vertices is irrelevant, and we may parameterize the graph as a discrete subset of $[0,1]$. The theory of *graphons* (Lovász, 2012; Janson, 2013) in Combinatorics allows us then to study the Γ-limit with respect to the weak* L^∞-convergence of the interpolations, which is of the form

$$F(u) = \int_{[0,1]^2} W(x,y)(u(x) - u(y))^2 \, dx \, dy, \tag{1.15}$$

where u now takes values in $[-1,1]$ and W is a symmetric positive function, the limit graphon of the dense graphs. Even though the resulting energy is of bulk type, the parameter u is interpreted as a limit density of sets and W describes the overall effect of the diffuse interfaces of such sets.

For general discrete systems, as remarked at the beginning of this chapter, the surface-energy description must be placed in a proper multiscale framework, together with effects related to other types of scaling. Note that, even when only energetic contributions are taken into account in a static picture described by a Γ-limit process, the same type of functionals can be considered with different scaling depending on the energy level. For the same quadratic energies we may have, for example,

(i) (*bulk scaling*) $\sum_{ij} \varepsilon^d a_{ij}^\varepsilon |u_i - u_j|^2$ giving integral energies $\int f(x,u(x))\,dx$;
(ii) (*surface scaling*) $\sum_{ij} \varepsilon^{d-1} a_{ij}^\varepsilon |u_i - u_j|^2$ giving surface energies as described in the preceding presentation;
(iii) (*vortex scaling*) $\sum_{ij} \varepsilon^{d-2} |\log \varepsilon|^{-1} a_{ij}^\varepsilon |u_i - u_j|^2$ giving *vortex energies* defined on point singularities;
(iv) (*gradient scaling*) $\sum_{ij} \varepsilon^{d-2} a_{ij}^\varepsilon |u_i - u_j|^2$ giving integral energies depending on gradients $\int f(x, \nabla u(x))\,dx$, and so on.

Such effects, and others, may be present at the same time. For some of them, methods corresponding to those described for surface energies have been developed and used. In general, the different scalings can be analyzed in a multiscale setting, in which the single scaling is a part of a whole (see e.g. Braides and Truskinovsky, 2008).

The unitary description of a subject with such a complexity and number of methods, results, and applications necessarily requires one to make some

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choice between the possible approaches. In this book we have chosen one that to us seems open enough to enclose the most standpoints and directions of research.

Bibliographical Notes to the Introduction

The Introduction focuses on problems for lattice systems with an emphasis on the surface energies discussed in this book from the standpoint of the direct approach to the Calculus of Variations. For an account of atomistic-to-continuum methods for Computational Materials Science we refer to the review articles by Blanc et al. (2007) and Le Bris and Lions (2005). Computational problems for which details of interfacial interactions are important to obtain a coupling between continuum discretization procedures and atomistic fine-mesh analysis are quasicontinuum models (see e.g. Tadmor et al., 1996; Blanc et al., 2005; Ortner and Süli, 2008). Multiscale Γ-convergence issues in the passage discrete-to-continuum are also dealt with in Section 11 of the handbook by Braides (2006) and are related to the concepts of Γ-development (see Anzellotti et al., 1994) or Γ-expansion (see Braides and Truskinovsky, 2008).

The discrete-to-continuum description of surface energies is also connected to a problem of crystallization, where now this is interpreted as the analysis of the asymptotic arrangement as N diverges of ensembles of N points in $\mathbb{R}^d$ whose location is such that some energy is minimized involving the distances between points. The points tend to arrange in a configuration close to a portion of a lattice, whose asymptotic shape is driven by the boundary interactions, which is then connected to a perimeter energy on that lattice. Again, the analysis of such asymptotic behavior has been carried out only in various simplified settings (see e.g. Heitmann and Radin, 1980; Radin, 1981; E and Li, 2009; Theil, 2011; Blanc and Lewin, 2015; De Luca and Friesecke, 2017).

Another classical problem in Statistical Mechanics connected to the emergence of macroscopic Wulff shapes is the analysis of the collective behavior of microscopic spin systems when the number of configurations diverges. In that context, a different point of view is usually taken and instead of minimizers, whose role is mainly relevant when, in the terminology the temperature is "close to zero," the object of the analysis is "typical configurations"; that is, sets of configurations with high probability according to a properly defined probability measure (see Dembo and Zeitouni, 1998 and the references therein and Cerf, 2006).

Interfacial problems are connected with problems defined on curves and related to metric properties of graphs. This is evident in dimension 2 where

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interfaces are one-dimensional objects, and the analogy can be further pushed to higher dimension (see e.g. Braides and Piatnitski, 2013). This analysis can be applied to problems on graphs from the standpoint of Hamilton–Jacobi equations (see e.g. Achdou et al., 2013; Imbert et al., 2013; Lions and Souganidis, 2020; Ishii and Kumagai, 2021), traffic flow (Garavello and Piccoli, 2006), or Aubry–Mather Theory (Siconolfi and Sorrentino, 2021).

Lattice systems can be seen as a particular case of nonlocal energies, and in particular as discretizations of double-integral energies such as in peridynamics (Macek and Silling, 2007; Silling and Lehoucq, 2010). In that perspective the discrete-to-continuum process is connected to what is called the limit of peridynamics "when the horizon goes to zero" (Bellido et al., 2015). We also mention the connection with repulsive-attractive interaction energies (e.g. Carrillo et al., 2014).

Reference texts for theory of graphons are Lovász (2012) and Janson (2013). For complex graphs of a fractal form, a different standpoint could be to consider a multiscale approach, for which we refer to Heida et al. (2020).

Dynamical problems on lattices can be framed in a variational setting using modern techniques of gradient-flow type as in the book of Ambrosio et al. (2008). Their analysis is related to issues in the study of motion in heterogenous media, which is a very wide and largely unexplored territory. For some results on evolutions of interfaces in planar lattices we refer to the recent book by Braides and Solci (2021).