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# Hexagonal lattices with three-point interactions

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ABSTRACT

We characterize the macroscopic effective behavior of hexagonal lattices with nonpolynomial growth, two-body interactions as well as angular interactions. The results apply to the mechanical behavior of atomic sheets, such as graphenes, with Lennard-Jones repulsive two-atomic energy and angular energy.
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RÉSUMÉ

Nous considérons des réseaux hexagonaux dont l'énergie résulte d'interactions à deux points à croissance non nécessairement polynomiale et d'interactions angulaires. Nous en donnons l'énergie macroscopique équivalente. Notre résultat s'applique, en particulier, aux réseaux atomiques tels que les graphènes, pour lesquels nous autorisons une énergie répulsive de Lennard-Jones et une énergie angulaire.
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## 1. Introduction

We consider a two-dimensional hexagonal atomic network with two- and three-point interactions. Such a network can be used to model the mechanical behavior of a graphene sheet with nearest neighbor atom to atom interaction on the one hand, and torques resulting from three-point interactions on the other hand. We are interested in deriving an equivalent continuum mechanics model for the deformations of the sheet by means of a homogenization procedure when the rest lengths of the bonds go to 0, using Γ-convergence techniques, since we work with an energy minimization formulation. The electronic properties of graphene are out of the scope of this article.

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There is a comprehensive body of work on the homogenization of discrete networks, see for instance [1,2,4,6,7,18], mostly in the context of two-point interactions, either short or long range, with polynomial growth energies. Our previous work on hexagonal networks was also concerned with only two-point, nearest neighbor interactions with polynomial growth, see [13,14]. There are relatively few works dealing with three-point interactions, let us mention [3,8,10,15,17] in this direction, or nonpolynomial growth, see [4,18], which do not seem to apply to our problem. We emphasize the fact that the angles that matter in a hexagonal network are not angles between vectors of a Bravais lattice. Moreover, some of the angles span several cells.

The two-point interactions we consider are composed of two terms, an elastic term as in [14], and a Lennard-Jones type term. The Lennard-Jones type energy is a phenomenological term which is supposed to model quantum repulsion between neighboring atoms. Since it tends to $+\infty$ when the distance between two bonded atoms goes to 0, its presence precludes any polynomial growth assumption. The addition of an elastic term is compatible with physical behavior around the ground state, but not necessarily elsewhere. We however add it for coercivity reasons, as is classically done in most of the above-mentioned works.

The three-point interactions correspond to the fact that the three chemical bonds radiating from any given atom in a graphene sheet have a preferred pairwise angle of $\frac{2\pi}{3}$. Deviations from this angle thus result in torques relative to the angle vertex, caused by the deformations of triangles of atoms. Energy densities corresponding to such torques can be found in the material science literature. They penalize deviations from the preferred angle, see, *e.g.*, [19].

In the same spirit as [6] and many other works in the literature, we rewrite the problem as a sequence of problems in the calculus of variations, indexed by a parameter representing the interatomic distance. We replace the discrete displacements of the atoms in the sheet by continuous piecewise affine functions defined on a domain, which makes it easy to talk about convergence in a Sobolev space setting. As opposed to [14], it is not possible to replace the discrete energies by continuous energies at the onset, because of the three-point interactions which have a slightly nonlocal effect. We therefore use an entirely different approach, following the work of Alicandro–Cicalese, [2], taking in addition advantage of a simplified slicing technique introduced in [12].

We show that the discrete energy minimizers for the energy with Dirichlet boundary conditions weakly converge in a Sobolev space to minimizers of a limit continuous energy, see Proposition 16 and Corollary 18, when the parameter goes to 0. We also identify the limit energy density via a homogenization formula, see Proposition 17.

## 2. Setting of the problem

In our previous article [14], we considered graphene sheets of arbitrary shape and devoted a lot of effort to properly defining boundary conditions. In order to avoid such technicalities, we consider here a much simpler setup, which we presently introduce. A sheet is a discrete two-dimensional structure that deforms in three-dimensional Euclidean space. We choose an orthonormal basis $(e_1, e_2, e_3)$ of $\mathbb{R}^3$. The scalar product and norm in $\mathbb{R}^3$ are respectively denoted by $\cdot$ and $|\ |$.

The basic hexagonal lattice in $\mathbb{R}^2$ is spanned by the three vectors

$$s_1 = \sqrt{3}e_1, \quad s_2 = \frac{\sqrt{3}}{2}e_1 + \frac{3}{2}e_2 \quad \text{and} \quad p = \frac{1}{3}(s_1 + s_2).$$

In the description we use, the lattice is comprised of two types of nodes: The type-1 nodes, which occupy points $is_1 + js_2$ with $(i, j) \in \mathbb{Z}^2$, and the type-2 nodes, which occupy points $is_1 + js_2 + p$, again with $(i, j) \in \mathbb{Z}^2$, see Fig. 1. Associated with this set of nodes are two Delaunay triangulations. The main Delaunay triangulation we use is depicted in Fig. 2, its edges are the solid lines and the dashed lines. The alternate one, which we will use less, is depicted in Fig. 3.

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