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Mathematical Problems in Mechanics/Calculus of Variations

Homogenization of hexagonal lattices

Homogénéisation d'un réseau hexagonal

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ABSTRACT

We characterize the macroscopic effective behavior of a graphene sheet modeled by a hexagonal lattice of elastic bars, using Γ-convergence.

RÉSUMÉ

Nous identifions le comportement macroscopique d'une feuille de graphène modélisée par un réseau hexagonal de barres élastiques. Nous utilisons pour cela les techniques de la Γ-convergence.

Version française abrégée

Nous considérons une feuille de graphène modélisée par un réseau hexagonal de barres élastiques, voir [3]. Nous cherchons à en caractériser le comportement mécanique macroscopique. Il s'agit d'un réseau complexe et à notre connaissance, les travaux récents sur le passage à la limite discret vers continu, voir [1,2], ne s'appliquent pas.

Le principe de notre analyse consiste à associer aux inconnues discrètes d'une part des fonctions affines par morceaux décrivant le comportement des atomes qui sont situés sur les sommets d'une triangulation, et d'autre part, des fonctions constantes par morceaux permettant de prendre en compte les atomes restants. L'énergie (1) du système discret se réécrit sous la forme (2), qui permet d'utiliser les techniques du calcul des variations et de l'homogénéisation. Il ne s'agit toutefois pas d'un problème d'homogénéisation classique, car il fait intervenir deux champs indépendants, des densités qui s'annulent sur la moitié des triangles et des énergies valant $+\infty$ en dehors d'espaces de dimension finie.

Nous effectuons une analyse de Γ-convergence quand la longueur des barres tend vers 0. L'énergie limite obtenue prend la forme d'une énergie élastique non linéaire membranaire, voir Proposition 3.3 de la version anglaise, dont la densité homogénéisée est donnée par les formules (4) et (6). Pour la démonstration, nous adaptons certains arguments de l'homogénéisation périodique [7,8], au contexte du passage du discret au continu. En particulier, nous introduisons une version discrète de la méthode de slicing de De Giorgi. La densité homogénéisée satisfait le principe d'indifférence matérielle. Les rotations d'angle multiple entier de $\frac{\pi}{3}$ appartiennent à son groupe de symétrie matérielle.

Pour conclure, nous faisons quelques remarques sur la règle de Cauchy–Born dans le contexte du modèle de feuille de graphène considéré ici. Nous montrons qu'une feuille de graphène n'obéit pas à cette règle au niveau discret. Cependant, le modèle limite satisfait une version affaiblie de la règle de Cauchy–Born.

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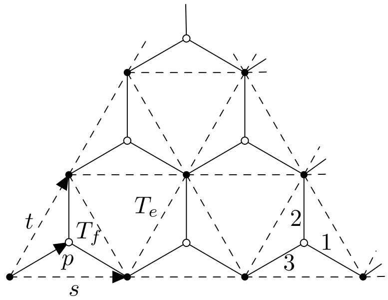

Fig. 1. •: type 1 nodes, ◦: type 2 nodes, bar types shown on rightmost triangle.

1. Introduction

We consider a graphene sheet modeled by a hexagonal network of elastic bars, see [3]. 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 bars go to 0, using Γ-convergence techniques in order to obtain rigorous convergence results. There is a comprehensive body of work on the homogenization of discrete networks, see for instance [1,2]. However, to our knowledge, the present problem remained to be solved.

Let us describe the reference configuration of the sheet. Let (e_1, e_2) be an orthonormal basis in $\mathbb{R}^2$, and $s = \sqrt{3}e_1$, $t = \sqrt{3}(\frac{1}{2}e_1 + \frac{\sqrt{3}}{2}e_2)$ and $p = \frac{1}{3}(s+t)$. In our description, the network is comprised of two types of nodes, the type 1 nodes that sit at points $is + jt$ with $(i, j) \in \mathbb{Z}^2$, and the type 2 nodes that sit at points $is + jt + p$ again with $(i, j) \in \mathbb{Z}^2$, see Fig. 1. The actual graphene sheet is a scaled version of the basic hexagonal network by a small factor ε, furthermore cropped to fit inside a given open set ω of $\mathbb{R}^2$. Thus, when at rest, the nodes are located at $\varepsilon(is + jt)$ or $\varepsilon(is + jt + p)$ depending on their type and for those integers i and j that are such that the corresponding points fall within ω. This description using two types of nodes is consistent with the standard description of complex lattices, which are superpositions of a finite number of shifted simple Bravais lattices, see [4,5].

For simplicity, we will ignore external forces. It is fairly straightforward to add corresponding terms in the energy. We impose a boundary condition of place on part of $\partial\omega$.

The internal energy of the sheet is assumed to only derive from elastic bars that join type 1 nodes to their nearest neighboring type 2 nodes. There are thus three types of bars: type 1 bars parallel to s–p, type 2 bars parallel to t–p, and type 3 bars parallel to p. Under loading and/or boundary conditions, the sheet deforms in $\mathbb{R}^3$ and stores an elastic energy that is assumed to be of the form

$$E^\varepsilon = \sum_{\text{all bars}} k\big((\text{deformed bar length}) - \varepsilon\big)^2, \tag{1}$$

where k is a stiffness coefficient. This specific form is not crucial for the later convergence result, but we keep it to fix ideas.

Deformed bar lengths are computed using the relative displacements of nodes. The deformation of type α nodes is given by a function $\chi_\alpha^\varepsilon : \mathbb{Z}^2 \to \mathbb{R}^3$, which is actually only defined on the subset of $\mathbb{Z}^2$ corresponding to nodes in ω. A typical deformed bar length thus assumes the form $|\chi_1^\epsilon(i, j) - \chi_2^\epsilon(i', j')|$ where $|\cdot|$ denotes the Euclidean norm in $\mathbb{R}^3$ and the integer pairs (i, j) and (i', j') are related to one another in a way that is simple to work out depending on the type of the bar. The deformed configuration of the sheet minimizes the total energy among all possible configurations.

2. Continuous formulation

In order to derive a limit continuous model, we replace the discrete unknowns χ_α^ε by continuous counterparts while keeping the same energy, see [1–3]. First, we define a piecewise affine function φ^ε by declaring that $\varphi^\varepsilon(\varepsilon(is+jt)) = \chi_1^\varepsilon(i, j)$. Since type 1 nodes are located at the vertices of a triangulation $\mathcal{T}^\varepsilon$, this determines φ^ε. Type 2 nodes are taken into account via a piecewise constant deviation vector defined by $\gamma^\varepsilon(x) = \chi_2^\varepsilon(i, j) - \chi_1^\varepsilon(i, j)$ in the triangles that contain a type 2 node, which we call full triangles, and $\gamma^\varepsilon(x) = 0$ in those that do not contain a type 2 node, which we call empty triangles. It is then a simple matter to express the deformed lengths ℓ_1, ℓ_2 and ℓ_3 of each type of bar with these new unknowns as

$$\ell_1 = \left|\varepsilon\partial_s\varphi^\varepsilon(x) - \gamma^\varepsilon(x)\right|, \qquad \ell_2 = \left|\varepsilon\partial_t\varphi^\varepsilon(x) - \gamma^\varepsilon(x)\right| \quad \text{and} \quad \ell_3 = \left|\gamma^\varepsilon(x)\right|,$$

where $\partial_s\varphi = D\varphi(s)$, $\partial_t\varphi = D\varphi(t)$ are the directional derivatives in directions s and t, and x is any point in a full triangle containing these particular three bars. This asymmetric treatment of nodes and bars of different types is in a sense artificial from the point of view of mechanics. It is however, as already noticed before, in keeping with the standard description of complex lattices.

Let $Y = T_f \cup T_e$ be the parallelogram obtained from the reference full triangle T_f whose vertices are $(0, 0)$, $(1, 0)$ and $(0, 1)$ in the oblique coordinate system based on s and t, and the reference empty triangle T_e whose vertices are $(1, 0)$,

$(1, 1)$ and $(0, 1)$, and $\mathcal{L}$ be the $\mathbb{Z}$-lattice generated by s and t. From now on, all computations will be performed in this oblique coordinate system. Let $L(\mathbb{R}^2; \mathbb{R}^3)$ be the space of linear mappings from $\mathbb{R}^2$ into $\mathbb{R}^3$. Because all the intervening quantities are piecewise constant, we can rewrite the elastic energy as an integral $E^\varepsilon = I^\varepsilon(\varphi^\varepsilon, \gamma^\varepsilon)$ where

$$I^\varepsilon(\psi, \delta) = \int_\omega W^\varepsilon\big(\varepsilon^{-1}x, D\psi(x), \delta(x)\big)\,\mathrm{d}x, \tag{2}$$

and $W^\varepsilon : \mathbb{R}^2 \times L(\mathbb{R}^2; \mathbb{R}^3) \times \mathbb{R}^3 \to \mathbb{R}$ is defined by

$$W^\varepsilon(y, g, \tau) = \begin{cases} 2k[(|g(s) - \varepsilon^{-1}\tau| - 1)^2 + (|g(t) - \varepsilon^{-1}\tau| - 1)^2 + (\varepsilon^{-1}|\tau| - 1)^2] & \text{if } y \in T_f + \mathcal{L}, \\ 0 & \text{if } y \in T_e + \mathcal{L}. \end{cases}$$

We denote by $A(\varepsilon)$ (resp. $C(\varepsilon)$) the space of functions that are piecewise affine continuous (resp. piecewise constant and zero in empty triangles) on $\mathcal{T}^\varepsilon$ and satisfy the boundary condition of place. We extend the sheet energy functional to the space $H = L^2(\omega; \mathbb{R}^3) \times L^2(\omega; \mathbb{R}^3)$ by letting $I^\varepsilon(\psi, \delta) = +\infty$ whenever $\psi \notin A(\varepsilon)$ or $\delta \notin C(\varepsilon)$.

It is clear that we have rephrased the equilibrium of the sheet as a problem in the calculus of variations: Find $(\varphi^\varepsilon, \gamma^\varepsilon) \in H$ such that

$$I^\varepsilon\big(\varphi^\varepsilon, \gamma^\varepsilon\big) = \inf_{(\psi,\delta)\in H} I^\varepsilon(\psi, \delta). \tag{3}$$

Our objective now is to let $\varepsilon \to 0$ and find a limit problem that describes the asymptotic behavior of the continuous sheet deformation φ^ε and deviation vector γ^ε. This is a periodic nonlinear variational homogenization problem, see [7,8], with several differences compared with the classical case: the energy functionals are $+\infty$ outside of finite-dimensional subspaces of H that depend on ε and the densities are not coercive on the unit cell Y.

3. Gamma-limit of the energies

For our purposes here, we are interested in computing $(\Gamma\text{-}\lim_{\varepsilon\to 0} I^\varepsilon)$ in the strong topology of H. It should be noted that the specific form of the energy used earlier plays no role in the ensuing analysis, and the Γ-convergence result holds true for more general energies, defined for instance on $W^{1,p}(\omega; \mathbb{R}^3)$ with $p < +\infty$. We start with an a priori bound. Let $H^1_\Gamma(\omega; \mathbb{R}^3)$ denote the space of H^1 deformations that satisfy the boundary condition of place.

Proposition 3.1. *For all $(\psi, \delta) \in H$ and given any sequence $(\psi^\varepsilon, \delta^\varepsilon) \to (\psi, \delta)$ in H such that $I^\varepsilon(\psi^\varepsilon, \delta^\varepsilon) \leqslant M$ for some M independent of ε, there exists C independent of ε such that*

$$\big\|\psi^\varepsilon\big\|_{H^1(\omega;\mathbb{R}^3)} \leqslant C \quad \text{and} \quad \big\|\delta^\varepsilon\big\|_{L^2(\omega;\mathbb{R}^3)} \to 0.$$

Consequently, for any Γ-convergent subsequence, we have $(\Gamma\text{-}\lim_{\varepsilon\to 0} I^\varepsilon)(\psi, \delta) = +\infty$ if $\psi \notin H^1_\Gamma(\omega; \mathbb{R}^3)$ or $\delta \neq 0$.

Note that, even though W^ε vanishes on empty triangles, the fact that $(\psi^\varepsilon, \delta^\varepsilon)$ belongs to $A(\varepsilon) \times C(\varepsilon)$ enables us to recover uniform coercivity.

Let us now introduce the function

$$W_0(y, g) = \inf_{\tau\in\mathbb{R}^3} W^\varepsilon(y, g, \tau), \tag{4}$$

which is defined on $\mathbb{R}^2 \times L(\mathbb{R}^2; \mathbb{R}^3)$, no longer depends on ε and vanishes for $y \in T_e + \mathcal{L}$, and the functional

$$I^\varepsilon_0(\psi) = \int_\omega W_0\big(\varepsilon^{-1}x, D\psi(x)\big)\,\mathrm{d}x \quad \text{if } \psi \in A(\varepsilon), \qquad I^\varepsilon_0(\psi) = +\infty \quad \text{if } \psi \in L^2\big(\omega; \mathbb{R}^3\big) \setminus A(\varepsilon). \tag{5}$$

The following proposition gives the connection between the functionals I^ε and I^ε_0.

Proposition 3.2. *For any Γ-convergent subsequence, we have, for all $\psi \in H^1_\Gamma(\omega; \mathbb{R}^3)$,*

$$\Big(\Gamma\text{-}\lim_{\varepsilon\to 0} I^\varepsilon\Big)(\psi, 0) = \Big(\Gamma\text{-}\lim_{\varepsilon\to 0} I^\varepsilon_0\Big)(\psi).$$

We define a homogenized energy density on $L(\mathbb{R}^2; \mathbb{R}^3)$ by

$$W_{\text{hom}}(g) = \inf_{k\in\mathbb{N}} \left\{ \frac{1}{k^2} \left(\inf_{\theta\in A(kY)} \int_{kY} W_0\big(y, g + D\theta(y)\big)\,\mathrm{d}y \right) \right\}, \tag{6}$$

where $A(kY)$ denotes the set of piecewise affine functions on the mesh defined on kY that vanish on $\partial(kY)$.

Proposition 3.3. *For any Γ-convergent subsequence, we have, for all $\psi \in H^1_\Gamma(\omega;\mathbb{R}^3)$,*

$$\Big(\Gamma\text{-}\lim_{\varepsilon\to 0} I_0^\varepsilon\Big)(\psi) = \int_\omega W_{\mathrm{hom}}\big(D\psi(x)\big)\,\mathrm{d}x.$$

The proof of Proposition 3.3 takes arguments from [7,8], adapted to the discrete to continuous context. In particular, it uses a discrete version of De Giorgi's slicing method. The uniqueness of the Γ-limit and the compactness of functional sequences with respect to Γ-convergence imply that the whole sequence Γ converges to the above limit. In addition, the bounds given in Proposition 3.1 show that the usual De Giorgi argument applies, *i.e.*, the limit points of the sequence of minimizers in the weak topology of H^1 minimize the Γ-limit functional. We have thus obtained an asymptotic description of the mechanical behavior of the graphene sheet.

It is easy to see that the homogenized energy density is frame-indifferent and that its material symmetry group contains all rotations of angle an integer multiple of $\frac{\pi}{3}$, see also [9]. Finally, the homogenized density vanishes on deformations that compress the sheet, which is normal behavior for a membrane model, see Section 4.

4. Remarks on the Cauchy–Born rule

The Cauchy–Born rule postulates that if a homogeneous deformation is imposed on the boundary of a monoatomic crystal, all the atoms move according to the same homogeneous deformation, see [4,6]. In the case of a graphene sheet as modeled here, the Cauchy–Born rule fails. Indeed, assume that g is a linear mapping from $\mathbb{R}^2$ to $\mathbb{R}^3$ such that the radius of the circumcircle to the triangle $g(\varepsilon T_f)$ is strictly less than ε. Then, there are two points on the normal to $g(\varepsilon T_f)$ passing through its circumcenter that are at distance ε from the three vertices. Choosing τ corresponding to one of these points yields $W^\varepsilon(y,g,\tau)=0$, whereas $W^\varepsilon(y,g,g(\varepsilon p))>0$ for such a g. This corresponds to an energy-minimizing, out-of-plane and nonhomogeneous deformation of type 2 nodes. Even if deformations are restricted to the plane, it is possible to fold a hexagonal network on itself with zero energy, whereas a homogeneous compression has a strictly positive energy cost.

If we look now at the limit problem, then by the abstract properties of Γ-convergence, we know that the homogenized density W_{hom} is quasiconvex, that is to say

$$\int_\omega W_{\mathrm{hom}}\big(g + D\theta(x)\big)\,\mathrm{d}x \geqslant \int_\omega W_{\mathrm{hom}}(g)\,\mathrm{d}x$$

for all $g \in L(\mathbb{R}^2;\mathbb{R}^3)$ and θ Lipschitz vanishing on the boundary of ω. Hence, the homogeneous deformation $\phi(x)=g(x)$ in ω is an energy minimizer for the boundary condition $\phi(x)=g(x)$ on $\partial\omega$. This is an expression of the Cauchy–Born rule in terms of energy minimization. Hence, it can be argued that a slightly weaker version of the Cauchy–Born rule is recovered in the homogenization limit, in the sense that homogeneous deformations minimize the limit energy for homogeneous boundary data, but that they may not be the only minimizers.

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