

# Continuum Limit and Homogenization of Stochastic and Periodic Discrete Systems – Fracture in Composite Materials

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The limiting behaviour of a one-dimensional discrete system is studied by means of  $\Gamma$ -convergence. We consider a toy model of a chain of atoms. The interaction potentials are of Lennard-Jones type and periodically or stochastically distributed. The energy of the system is considered in the discrete to continuum limit, i.e. as the number of atoms tends to infinity. During that limit, a homogenization process takes place. The limiting functional is discussed, especially with regard to fracture. Secondly, we consider a rescaled version of the problem, which yields a limiting energy of Griffith's type consisting of a quadratic integral term and a jump contribution. The periodic case can be found in [8], the stochastic case in [6, 7].

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This article summarizes some recent results on a one-dimensional model for composite elastic materials that allows for brittle fracture. The heterogeneities are assumed to be periodically and stochastically distributed, respectively. We are interested in the discrete to continuum limit as the number  $n$  of atoms tends to infinity, which leads to a homogenized continuous model. The analytical method of choice is  $\Gamma$ -convergence.

The  $\Gamma$ -limits described below extend related results in [1, 9, 10] and are based also on methods developed in [2–4]. Further, ergodic theorems of Birkhoff, Tempel'man and Akcoglu & Krengel are used in the stochastic setting.

**Atomistic model problem.** We consider a one-dimensional chain of  $n + 1$  atoms in the continuous interval  $[0, 1]$ , with lattice spacing  $\lambda_n = \frac{1}{n}$  and reference positions  $x_n^i := i\lambda_n$ , cf. Fig. 1. We suppose nearest neighbour interactions and impose Dirichlet boundary conditions  $u(0) = 0$  and  $u(1) = \ell$ , for some given  $\ell > 0$ . The zero-order limit (see below) is also worked out for finite range interaction, see [6], but we will restrict ourselves here to the case of nearest neighbour interactions.

The stochastically distributed interaction potentials  $J$  are defined by  $J(\omega, i, \cdot) := \tilde{J}(\tau_i\omega, \cdot)$ , with a probability space  $(\Omega, \mathcal{F}, \mathbb{P})$  and an additive, stationary, ergodic group action  $(\tau_i)_{i \in \mathbb{Z}}$ . In our model, we allow for continuous probability densities in the distribution of the potential, which is one of the differences to the related work [5]. The periodic case is included in this setting, [8].

We regard the deformation  $u_n : \lambda_n\mathbb{Z} \cap [0, 1] \rightarrow \mathbb{R}$  as an affine interpolation in the space  $\mathcal{A}_n(0, 1) := \left\{ u \in C([0, 1]) : u \text{ is affine on } (i, i+1)\lambda_n, i \in \mathbb{Z} \right\}$ . Then, the energy of the chain is  $H_n^\ell : \Omega \times L^1(0, 1) \rightarrow (-\infty, +\infty]$ , given by

$$H_n^\ell(\omega, u) := \begin{cases} \sum_{i=0}^{n-1} \lambda_n J\left(\omega, i, \frac{u^{i+1} - u^i}{\lambda_n}\right) & \text{if } u \in \mathcal{A}_n(0, 1) \text{ and } u(0) = 0, u(1) = \ell, \\ +\infty & \text{otherwise.} \end{cases}$$

**Lennard-Jones potentials.** The potentials  $\tilde{J}(\omega, \cdot)$  in our model are of Lennard-Jones type, which is a large class of potentials including the classical Lennard-Jones potential  $J_{LJ}$ , given by

$$J_{LJ}(\omega, z) = \epsilon(\omega) \left[ \left(\frac{\delta(\omega)}{z}\right)^{12} - 2 \left(\frac{\delta(\omega)}{z}\right)^6 \right], \quad \epsilon(\omega), \delta(\omega) > 0,$$

with minimizer  $\delta(\omega)$  and minimum  $-\epsilon(\omega)$ , see Fig. 2. Using these non-convex potentials allows for fracture in the limiting system. There exists a large number of previous work on fracture mechanics. For further references see, e.g., [8].

The non-convexity of the Lennard-Jones potential and its blowup at the origin yield several difficulties in the proofs. To handle the latter problem, we appeal to a suitable approximation argument, see [6] for details.

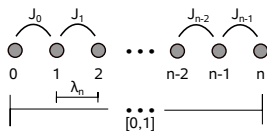
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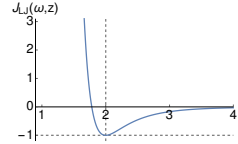
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**Fig. 1** Chain of  $n + 1$  atoms in the continuous interval  $[0, 1]$ , with lattice spacing  $\lambda_n = \frac{1}{n}$  and nearest neighbour interactions  $J_i$ .



**Fig. 2**  $J_{LJ}(\omega, \cdot)$  with  $\delta(\omega) = 2$  and  $-\epsilon(\omega) = J_{LJ}(\omega, \delta(\omega)) = -1$ .

**$\Gamma$ -Limit of the Energy.** We can now consider the  $\Gamma$ -limit of the energy functional defined above. The integrand is given by an asymptotic homogenization formula, which turns out to be independent of the stochastic parameter.

**Theorem 0.1** For  $\ell > 0$ , there exists a set  $\Omega' \subset \Omega$ ,  $\mathbb{P}(\Omega') = 1$ , such that for all  $\omega \in \Omega'$  the  $\Gamma$ -limit of the energy  $H_n^\ell$  w.r.t. the  $L^1(0, 1)$ -topology is  $H^\ell : L^1(0, 1) \rightarrow (-\infty, +\infty]$ , given by

$$H^\ell(u) = \begin{cases} \int_0^1 J_{\text{hom}}(u'(x)) \, dx & \text{if } u \in BV^\ell(0, 1), D^s u \geq 0 \text{ on } [0, 1], \\ +\infty & \text{otherwise,} \end{cases}$$

with the asymptotic homogenization formula  $J_{\text{hom}}(z) = \lim_{N \rightarrow \infty} \frac{1}{N} \inf \left\{ \sum_{i=0}^{N-1} J(\omega, i, z^i), z^i \in \mathbb{R}, \sum_{i=0}^{N-1} z^i = Nz \right\}$ . In the periodic case, the limit reduces to the cell formula  $J_{\text{hom}}(z) = \min \left\{ \frac{1}{M} \sum_{i=0}^{M-1} J_i^{**}(z^i), z^i \in \mathbb{R}, \sum_{i=0}^{M-1} z^i = Mz \right\}$ , where  $M \in \mathbb{N}$  is the periodicity length and  $J^{**}$  is the lower semicontinuous and convex envelope of  $J$ .

Moreover, the minimum values of  $H_n^\ell$  and  $H^\ell$  satisfy  $\lim_{n \rightarrow \infty} \inf_u H_n^\ell(\omega, u) = \min_u H^\ell(u) = J_{\text{hom}}(\ell)$ .

**Rescaled Energy and  $\Gamma$ -Limit.** The  $\Gamma$ -limit  $H^\ell$  above allows for jumps, as expected. However, the jumps do not cost any energy, which is not reasonable from a physical point of view. The reason for this is a tacitly assumed separation of scales between the bulk and surface energy contributions. Therefore, inspired by [4, 10, 11], we rescale our model by  $v^i := \left( u^i - \sum_{k=0}^{i-1} \lambda_n \delta(\tau_k \omega) \right) / \sqrt{\lambda_n}$ . Further, we consider  $\ell_n \rightarrow \mathbb{E}[\delta]$  (expectation value of  $\delta(\omega)$ ), rescaled boundary data  $\eta_n = \left( \ell_n - \sum_{i=0}^{n-1} \lambda_n \delta(\tau_i \omega) \right) / \sqrt{\lambda_n} \rightarrow \eta$ , and the rescaled version  $E_n^{\eta_n} : \Omega \times L^1(0, 1) \rightarrow (-\infty, +\infty]$  of the energy,

$$E_n^{\eta_n}(\omega, v) = \begin{cases} \sum_{i=0}^{n-1} \left( J \left( \omega, i, \frac{v^{i+1} - v^i}{\sqrt{\lambda_n}} + \delta(\tau_i \omega) \right) - J(\omega, i, \delta(\tau_i \omega)) \right) & \text{if } v \in \mathcal{A}_n(0, 1), v^0 = 0, v^n = \eta_n, \\ +\infty & \text{otherwise.} \end{cases}$$

The limiting energy now is like a Griffith model of fracture mechanics with an elastic energy and a surface term for cracks.

**Theorem 0.2** For  $\eta_n \rightarrow \eta$ , there exists a set  $\Omega' \subset \Omega$ ,  $\mathbb{P}(\Omega') = 1$ , such that for all  $\omega \in \Omega'$  the  $\Gamma$ -limit w.r.t. the  $L^1(0, 1)$ -topology of this energy is  $E^\eta : L^1(0, 1) \rightarrow (-\infty, +\infty]$ , given by

$$E^\eta(v) = \begin{cases} \underline{\alpha} \int_0^1 |v'(x)|^2 \, dx + \beta \#S_v & \text{if } v \in SBV^\eta(0, 1), v' \in L^2(0, 1), \#S_v < +\infty, [v] \geq 0 \text{ in } [0, 1], \\ +\infty & \text{otherwise,} \end{cases}$$

where  $\underline{\alpha} := (\mathbb{E}[\alpha^{-1}])^{-1}$  with  $\alpha(\omega) := \frac{1}{2} \frac{\partial^2 \tilde{J}(\omega, z)}{\partial z^2} \Big|_{z=\delta(\omega)}$ , and  $\beta = \inf \{ -\tilde{J}(\omega, \delta(\omega)), \omega \in \Omega \}$ . In the periodic case, this

reduces to  $\underline{\alpha} = \left( \frac{1}{M} \sum_{i=0}^{M-1} \alpha_i^{-1} \right)^{-1}$  and  $\beta = \min_{0 \leq i \leq M-1} \{ -J_i(\delta_i) \}$  with periodicity length  $M \in \mathbb{N}$ .

Moreover, for  $\eta > 0$  it holds true that  $\lim_{n \rightarrow \infty} \inf_v E_n^{\eta_n}(\omega, v) = \min_v E^\eta(v) = \min \{ \underline{\alpha} \eta^2, \beta \}$ .

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