Multiscale problems in dislocation theory

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HERIOT WATT UNIVERSITY

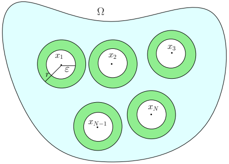
PART II

Upscaling of dislocation energies

Energy scaling: close vs far from dislocations

$$E_{n,\varepsilon}(\beta,\mu) = \frac{1}{2}\int_{\Omega_\varepsilon(\mu)} \mathcal{C}\beta : \beta \, dx, \quad \mathrm{Curl}\beta = \mu = \frac{1}{n}\sum_{i=1}^{n} b_i \delta_{x_i}$$

$$= \underbrace{E^{\mathrm{self}}_{n,\varepsilon}(\beta,\mu)}_{\text{“close" energy}} + \underbrace{E^{\mathrm{far}}_{n,\varepsilon}(\beta,\mu)}_{\text{“far" energy}}$$



- Close to dislocations (self)

  $$E^{\mathrm{self}}_{n,\varepsilon}(\beta,\mu) \simeq \frac{1}{n}\varepsilon^2 |\log\varepsilon|$$

- Far from dislocations

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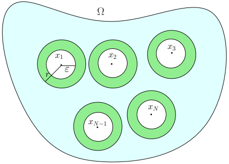

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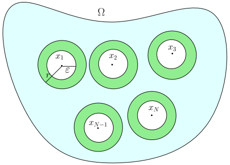

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Note: We are assuming separation of dislocations: $\varepsilon \ll \rho_\varepsilon \ll 1$

(No separation: De Luca, Garroni, Ponsiglione, Ginster)

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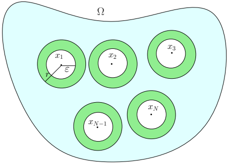

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Note: Nonlinear energies same scalings

(Müller, Scardia, Zeppieri, Lauteri, Luckhaus, Palombaro, Garroni, Marziani, Scala, Ginster)

Critical energy scaling

$$\widetilde{E}_\varepsilon(\beta,\mu) = \frac{1}{\varepsilon^2}\int_{\Omega_\varepsilon(\mu)} \frac{1}{2}\mathcal{C}\beta : \beta\, dx$$

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Result (Garroni-Leoni-Ponsiglione; Müller-Scardia-Zeppieri; De Luca; Ginster etc.)

$$\widetilde{E}_\varepsilon \longrightarrow \int_\Omega \frac{1}{2}\mathcal{C}\beta : \beta dx + \int_\Omega \varphi\left(\frac{d\mu}{d|\mu|}\right) d|\mu|, \quad \mathrm{Curl}\beta = \mu$$

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- φ relaxation of the minimal self-energy of a single dislocation

$$\psi(\hat{b}) = \lim_{\varepsilon\to 0}\frac{1}{|\log\varepsilon|}\min\left\{\int_{B_{\rho_\varepsilon}\setminus B_\varepsilon} \tfrac{1}{2}\mathcal{C}\eta : \eta dx : \eta \in L^2(B_{\rho_\varepsilon}\setminus B_\varepsilon), \right.$$
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- φ 1-homogeneous $\Rightarrow$ concentration possible

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$$\|\beta_j^{\text{skw}}\|^2_{L^2} \leq C \left(\|\beta_j^{\text{sym}}\|^2_{L^2} + |\mathrm{Curl}\beta_j|^2(\Omega) \right)$$

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- Not true that $\mathrm{Curl}\beta_j = \mu_j$! But almost true, up to modifying β_j inside $B_{\varepsilon_j}(x_i^j)$.
- Nonlinear case: Use generalised Rigidity (Müller-Scardia-Zeppieri)

$$\|\beta_j - R_j\|_{L^2}^2 \leq C \left(\|\text{dist}(\beta_j, SO(2))\|_{L^2}^2 + |\mathrm{Curl}\beta_j|^2(\Omega) \right)$$

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- Idea of lower bound

Critical energy scaling

$$\widetilde{E}_\varepsilon(\beta,\mu) = \frac{1}{\varepsilon^2|\log\varepsilon|^2}\int_{\Omega_\varepsilon(\mu)} \frac{1}{2}\mathcal{C}\beta : \beta\, dx$$

$$\mathrm{Curl}\beta = 0 \quad \text{in } \Omega_\varepsilon(\mu), \qquad \int_{\partial B_\varepsilon(x_i)} \beta\tau ds = b_i, \qquad |b_i| = \varepsilon$$

- Idea of compactness (well-separated!) $\widetilde{E}_{\varepsilon_j}(\beta_j,\mu_j) \leq C$.
- Bound for the measures (μ_j): $\dfrac{\mu_j}{\varepsilon_j|\log\varepsilon_j|} \rightharpoonup \mu$ ☺
- Bound for the strains (β_j): $\dfrac{\beta_j}{\varepsilon_j|\log\varepsilon_j|} \rightharpoonup \beta$ ☺
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$$\to \frac{1}{2}\int_\Omega \mathcal{C}\beta : \beta\, dx$$

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$$\ge \frac{1}{|\log\varepsilon_j|}\sum_{i=1}^{|\log\varepsilon|}\left(\frac{1}{|\log\varepsilon_j|}\int_{B_{\rho_{\varepsilon_j}}\setminus B_{\varepsilon_j}} \frac{1}{2}\mathcal{C}\left(\frac{\beta_j}{\varepsilon_j}\right) : \left(\frac{\beta_j}{\varepsilon_j}\right) dx\right)$$

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$$\ge \frac{1}{|\log\varepsilon_j|}\sum_{i=1}^{|\log\varepsilon|}\psi(\hat{b}_i) \text{ + relaxation}$$

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Result (Garroni-Leoni-Ponsiglione; Müller-Scardia-Zeppieri; De Luca; Ginster etc.)

$$\widetilde{E}_\varepsilon \longrightarrow \int_\Omega \frac{1}{2}\mathcal{C}\beta : \beta dx + \int_\Omega \varphi\left(\frac{d\mu}{d|\mu|}\right) d|\mu|, \quad \mathrm{Curl}\beta = \mu$$

- Strain-gradient plasticity model
- φ relaxation of the minimal self-energy of a single dislocation

$$\psi(\hat{b}) = \lim_{\varepsilon\to 0} \frac{1}{|\log\varepsilon|} \min\left\{ \int_{B_{\rho_\varepsilon}\setminus B_\varepsilon} \tfrac{1}{2}\mathcal{C}\eta : \eta dx : \eta \in L^2(B_{\rho_\varepsilon} \setminus B_\varepsilon), \right.$$
$$\left. \mathrm{Curl}\eta = 0 \text{ in } B_{\rho_\varepsilon} \setminus B_\varepsilon, \int_{\partial B_\varepsilon} \eta\tau ds = \hat{b} \right\}$$

- φ 1-homogeneous $\quad\Rightarrow\quad$ concentration possible

Focus on interactions

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$$E_n(\mu) = \min_\beta \int_{\Omega_{\varepsilon_n}} \frac{1}{2}\mathcal{C}\beta : \beta dx, \quad \mu = \frac{1}{n}\sum_{i=1}^{n} b_i \delta_{x_i}, \ \boxed{b_i = e_1, |x_i - x_j| \gg \varepsilon_n}$$

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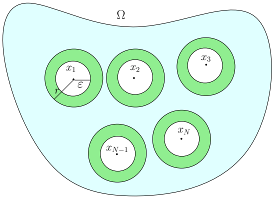
$$= \underbrace{E_n^{\text{self}}(\mu)}_{\text{“close'' energy}} + \underbrace{E_n^{\text{far}}(\mu)}_{\text{“far'' energy}}$$



- Close to dislocations (self)

$$E_n^{\text{self}}(\mu) \simeq \frac{1}{n}|\log \varepsilon_n|$$

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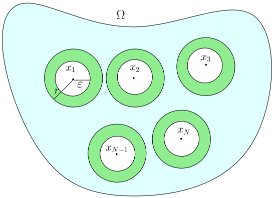

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Extract “Interaction contribution" (Cermelli-Leoni)

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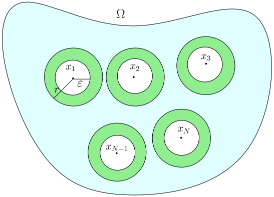

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Similar spirit: Fanzon-Palombaro-Ponsiglione

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The minimiser β_n solves the Euler-Lagrange equations

$$\begin{cases} \operatorname{div} \mathcal{C}\beta_n = 0 & \text{in } \Omega_{\varepsilon_n} \\ \mathcal{C}\beta_n \nu = 0 & \text{on } \partial\Omega_{\varepsilon_n} \\ \int_{\partial B_{\varepsilon_n}(x_i)} \beta_n \tau ds = \frac{e_1}{n}, \quad i = 1, \ldots, n \end{cases}$$

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$$+ \underbrace{\frac{1}{2}\int_{\Omega_{\varepsilon_n}} \mathcal{C}\nabla v_n : \nabla v_n dx + \frac{1}{2n}\sum_{i=1}^n \int_{\Omega_{\varepsilon_n}} \mathcal{C}K^n_{x_i} : \nabla v_n dx}_{=:\min_v I_n^{\mu,\Omega}(v)}$$

Focus on interactions

$$I_n(\mu) = E_n(\mu) - E_n^{\text{self}}(\mu)$$
$$(!) \simeq \underbrace{\frac{1}{2n^2} \sum_{i,j \neq i} \int_\Omega \mathcal{C} K_{x_i} : K_{x_j}\, dx}_{\text{Interaction energy}} + \underbrace{\min_v I_n^{\mu,\Omega}(v)}_{\text{Boundary contribution}}$$

* Helmholtz decomposition of the optimal strain: $\beta_\mu = \frac{1}{n} \sum_i K_{x_i}^n + \nabla v_n$

Focus on interactions

$$
\begin{aligned}
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\end{aligned}
$$

* Helmholtz decomposition of the optimal strain: $\beta_\mu = \frac{1}{n}\sum_i K_{x_i}^n + \nabla v_n$
* K_{x_i} is the standard incompatible field for a single dislocation at x_i in $\mathbb{R}^2$

$$
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\end{cases}
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Focus on interactions

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$$\simeq \frac{1}{2n^2}\sum_{i,j\neq i} V_\Omega(x_i,x_j) + \min_v I_n^{\mu,\Omega}(v)$$

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* $V_\Omega(x_i,x_j) := \displaystyle\int_\Omega \mathcal{C}K_{x_i}(x) : K_{x_j}(x)\,dx \rightsquigarrow$ pairwise interaction potential
* $|V_\Omega(x_i,x_j)| \sim -\log|x_i - x_j|$ for x_i close to x_j (e.g. vortices, Coulomb gases)

Focus on interactions

$$I_n(\mu) \simeq \frac{1}{2n^2} \sum_{i,j \neq i} V_\Omega(x_i, x_j) + \min_v I_n^{\mu,\Omega}(v)$$

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I_n Γ-converges to I as $n \to \infty$, where

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- Upscaling result: from individual dislocations to a continuum dislocation density μ
- Two energy contributions: Interaction energy + boundary effects (interaction of dislocations with the boundary)

Idea of recovery sequence

Let μ with $I(\mu) < \infty$.

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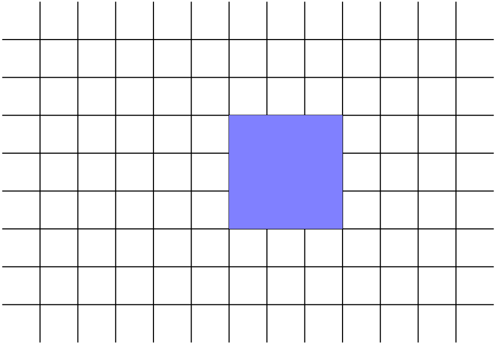

Tessellate Ω with squares $\tilde{Q}_k^h$ of side $3h$

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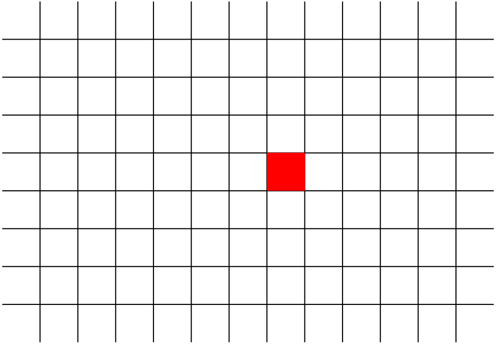

Replace μ in $\tilde{Q}_k^h$ with $\frac{\mu(\tilde{Q}_k^h)}{h^2}\chi_{Q_k^h}$

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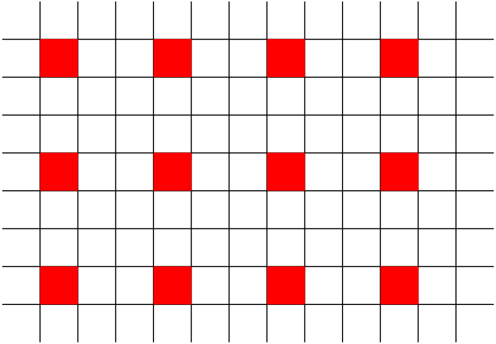

$$\mu \rightsquigarrow \mu^h := \sum_k \frac{\mu(\tilde{Q}_k^h)}{h^2} \chi_{Q_k^h}$$

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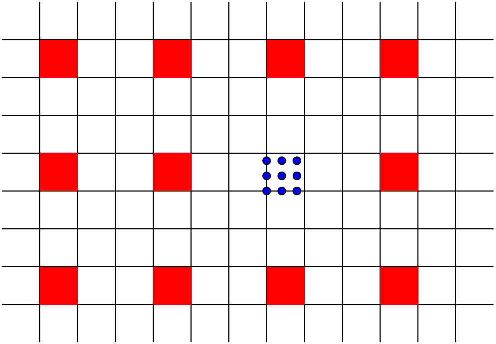

Replace μ^h in Q_k^h with $n\mu^h(Q_k^h)$ equi-distributed Diracs $\rightsquigarrow$ μ_n

Similar dislocation interaction energies

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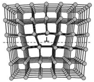
$$I_n(x) = \frac{1}{n^2} \sum_{i, j \neq i} V(x_i - x_j), \quad x_i \in \mathbb{R}^2,$$

with the singular interaction potential (in $\mathbb{R}^2$, no boundary effect)

$$V(x) = -\log|x| + \frac{x_1^2}{|x|^2}$$



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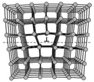

- Heuristically V is the limit of V_Ω (from previous energy) for $\Omega \to \mathbb{R}^2$
  $V(x-y) = c(\mu,\lambda)V_\Omega(x,y) + g_\Omega(x,y), \quad g_\Omega \in C^2$
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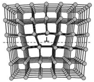

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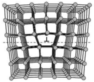

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- Geers-Peerlings-Peletier-Scardia, ARMA 2014 - 1d case (vertical walls)

Positive and negative dislocations

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$$I_n(x) = \frac{1}{n^2} \sum_{i,j=1}^{n} b_i b_j V(x_i - x_j), \quad x_i \in \mathbb{R}^2, \quad \boxed{b_i = \pm 1}$$

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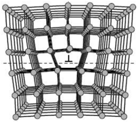

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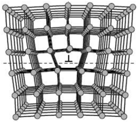

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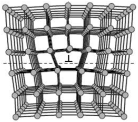

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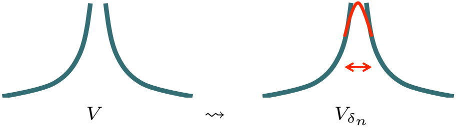

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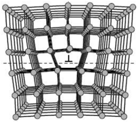

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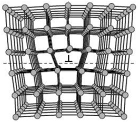

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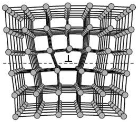

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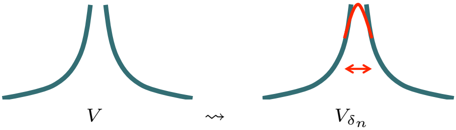

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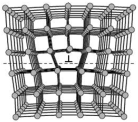

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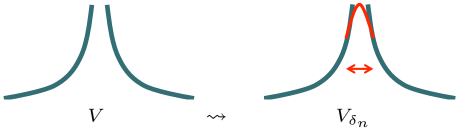

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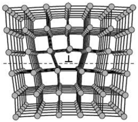

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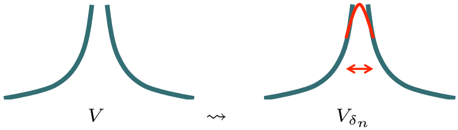

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For smaller δ_n ($\delta_n \lesssim e^{-n}$) upscaling unclear (Patrick van Meurs)