Multiscale models of metal plasticity
Lecture III: Dilute dislocations and the line tension model

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Sixth Summer School in Analysis and Applied Mathematics

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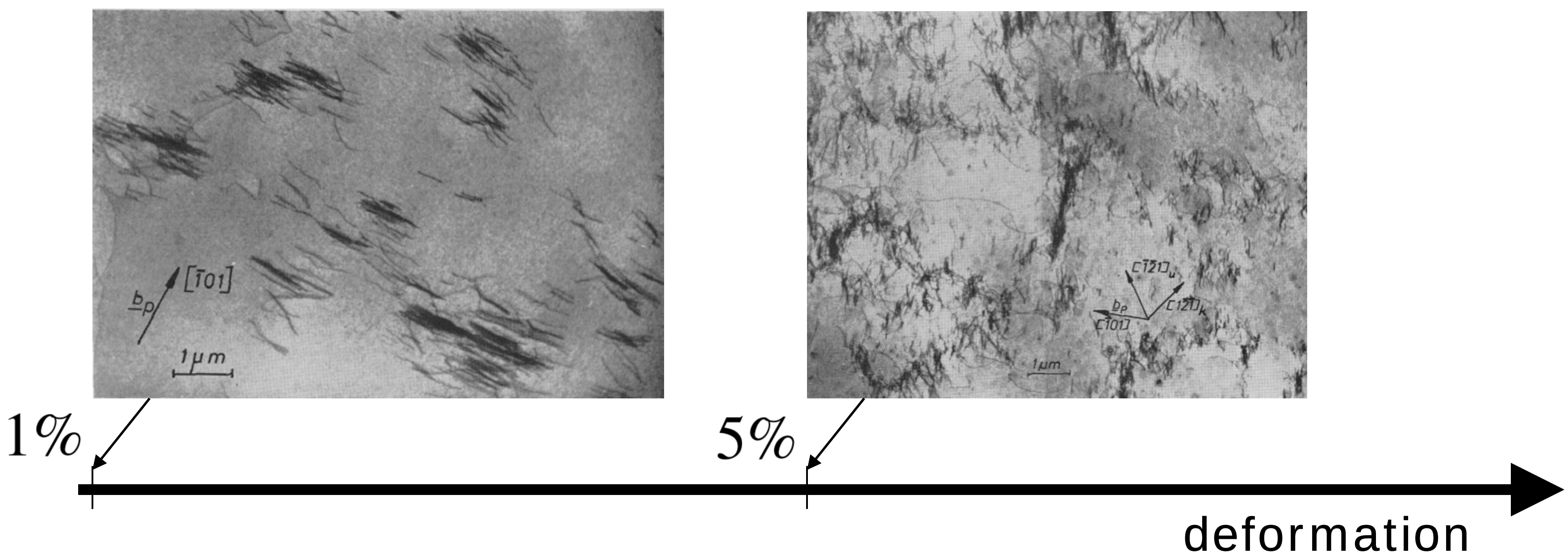
Outline of Lecture #3

- Beyond formal linear-elastic dislocation theory
- The dilute limit: Γ-convergence



Dislocations in
copper single crystal

H. Mughrabi, *Phil. Mag*. **23** (1971) 869

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Recall: The Micro-to-Macro transition

- Let $\bar{\boldsymbol{\beta}}^e \equiv \bar{\boldsymbol{\beta}} - \bar{\boldsymbol{\beta}}^p \equiv$ macroscopic elastic distortion. Then:

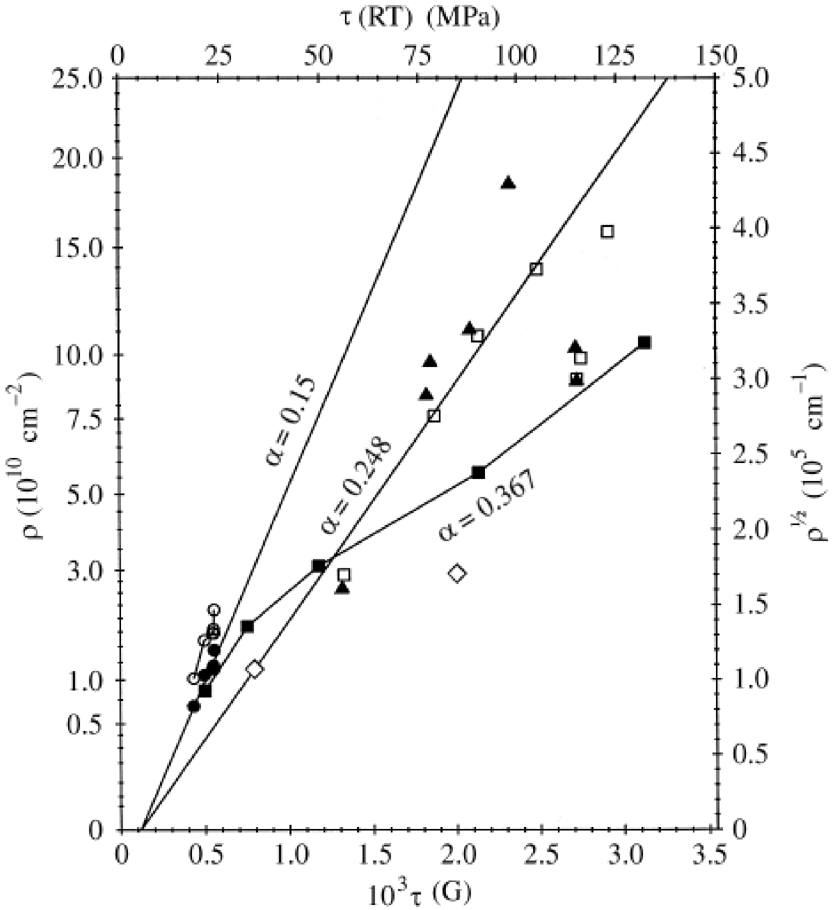
$$E = \frac{V}{2} c_{ijkl} \bar{\beta}^e_{ij} \bar{\beta}^e_{kl} + \int_\Omega \frac{1}{2} c_{ijkl} (\beta^*_{ij} - \beta^p_{ij})(\beta^*_{kl} - \beta^p_{kl}) dV + E^{\text{core}}$$

- Strain-energy density: $\bar{W} \equiv E/V$. Then $\boxed{\bar{W} = \bar{W}^e + \bar{W}^p}$,

$$\begin{aligned}
\bar{W}^e &= \bar{W}^e(\bar{\boldsymbol{\beta}}^e) = \frac{1}{2} c_{ijkl} \bar{\beta}^e_{ij} \bar{\beta}^e_{kl} \quad \equiv \text{elastic energy density} \\
\bar{W}^p &= \bar{W}^p[\boldsymbol{\beta}^p] = \bar{W}^p[\boldsymbol{\alpha}] \\
&= \frac{1}{V} \left\{ \int_\Omega \frac{1}{2} c_{ijkl} (\beta^*_{ij} - \beta^p_{ij})(\beta^*_{kl} - \beta^p_{kl}) dV + E^{\text{core}} \right\} \\
&\equiv \text{stored energy density, } \underline{\text{independent of } \bar{\boldsymbol{\beta}}}
\end{aligned}$$

- $\bar{W}^p$ cannot be expressed in closed form for general distributions of disocations $\Rightarrow$ Need to *model* $\bar{W}^p$ at the macroscopic level.

The dilute limit – Line tension

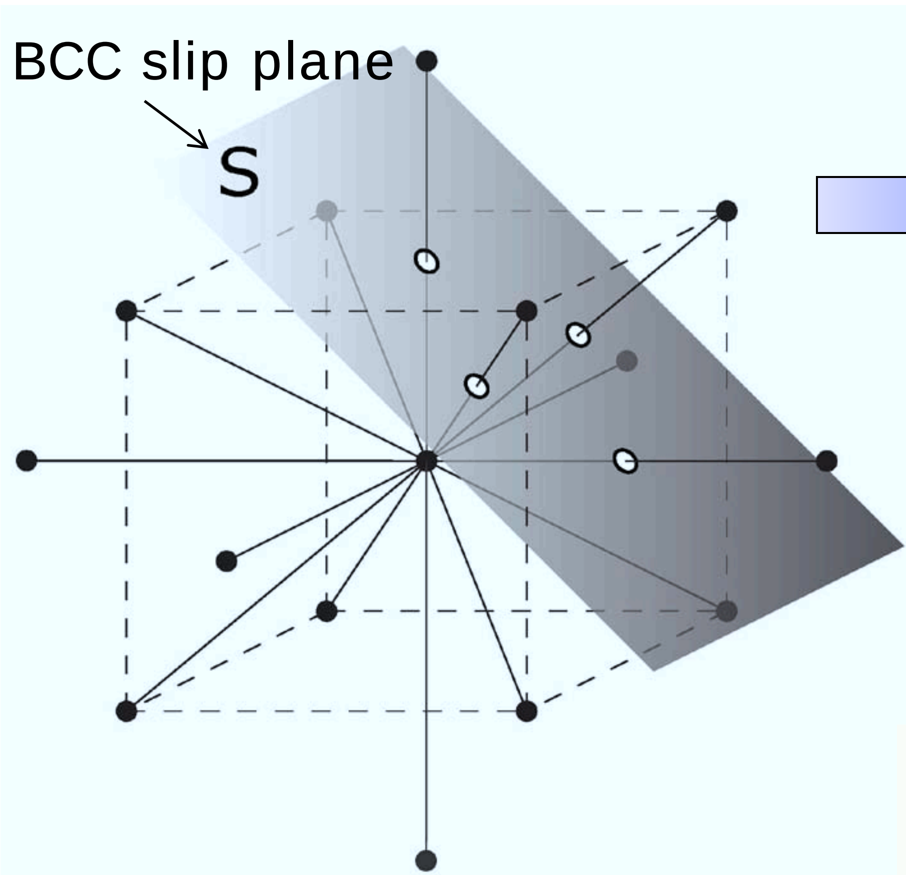


- Initial dislocation density ~ 10^{10} cm^{-2}
- Saturation dislocation density ~ 25 x 10^{10} cm^{-2}
- Initial mean distance between dislocations ~ 100 nm (278 lattice constants)
- Mean distance between dislocations at saturation ~ 20 nm (56 lattice constants)
- Investigate ***dilute limit***!

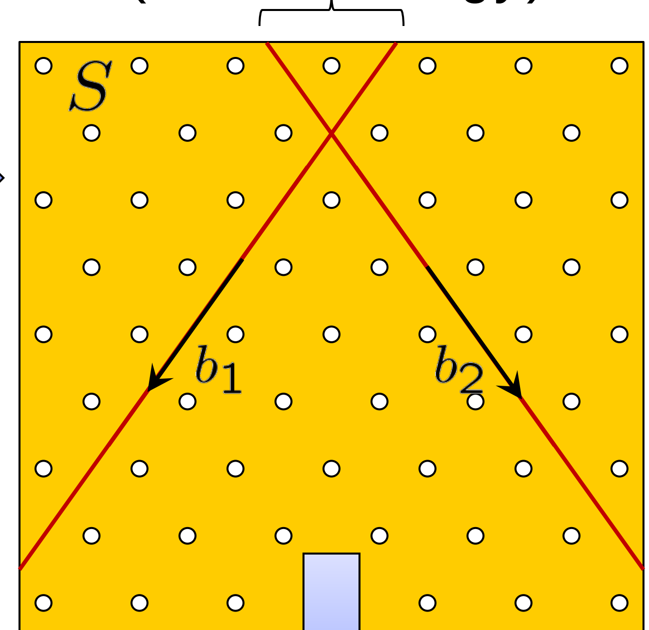
Total dislocation density *vs.* applied stress in single-crystal and polycrystalline copper in the deformation range of $\varepsilon \leq 0.4$

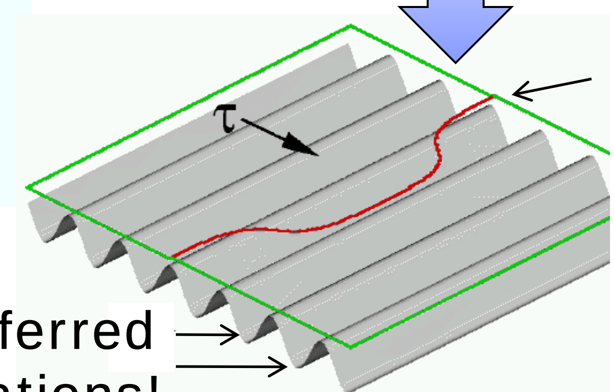
D. Breuer, P. Klimanek and W. Pantleon, *J. Appl. Cryst*., **33** (2000) 1284-1294.

The dilute limit – Discrete dislocations



screw segments
(lowest energy)





screw segments

Peierls potential

preferred locations!

- Wish to account for Peierls potential: ***Discrete dislocations***!

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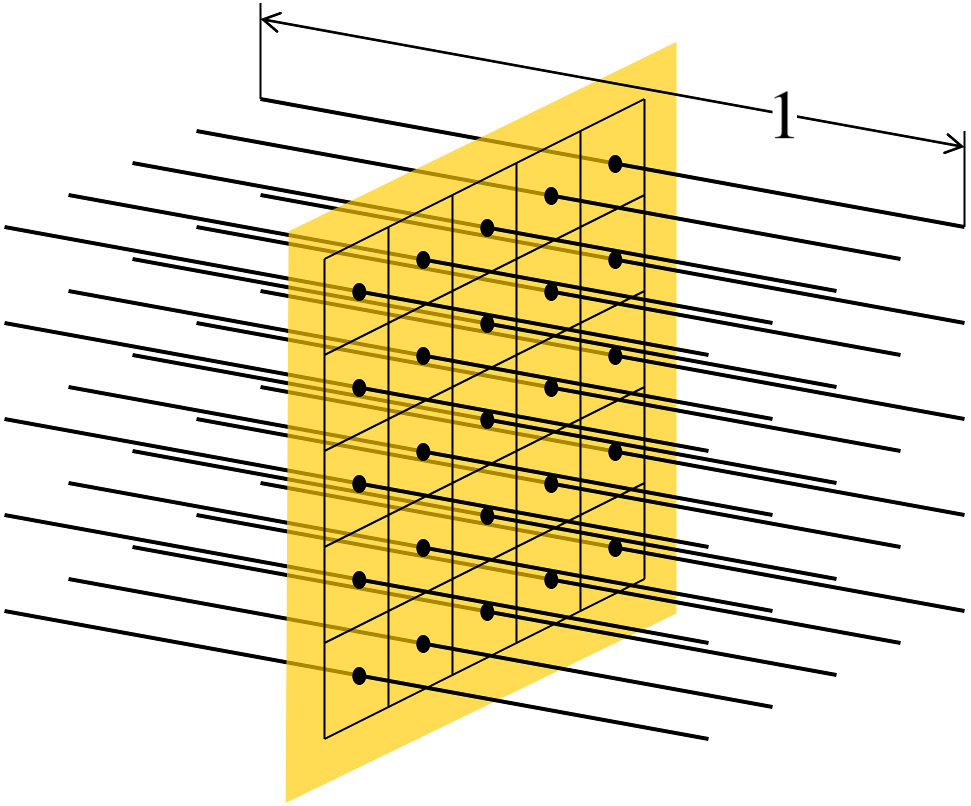
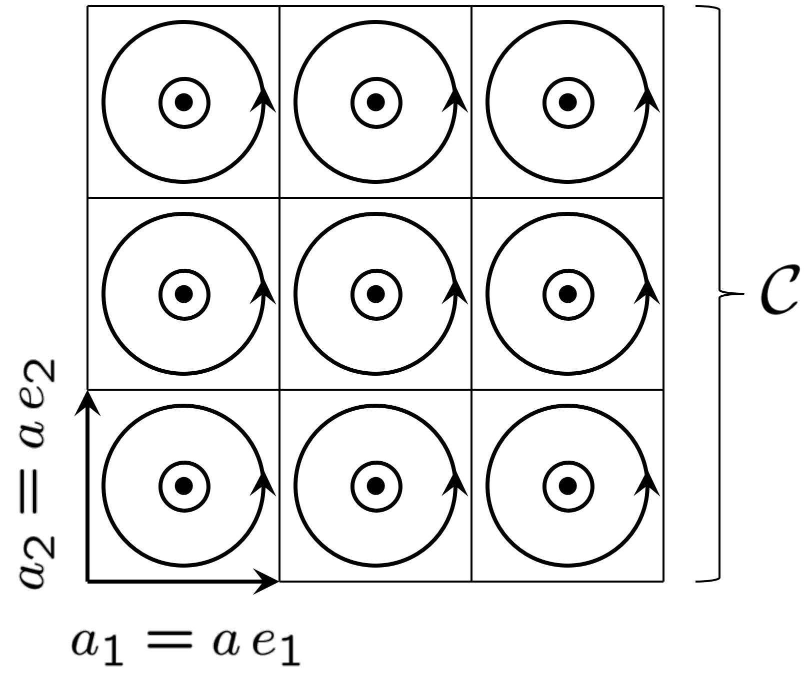
Discrete dislocations – Square lattice



Screw-dislocation bundle



Square lattice complex

- Discrete dislocations (2-forms over $\mathcal{C}$):

$$\mathcal{D}^2(C;\mathbb{R}) \equiv \{\alpha = \sum_{r\in a\mathbb{Z}^2} b_r \delta_r,\ b_r \in \mathbb{R}\}$$

- Coboundary operator (div): $d\alpha = \sum_{r\in a\mathbb{Z}^2} b_r$

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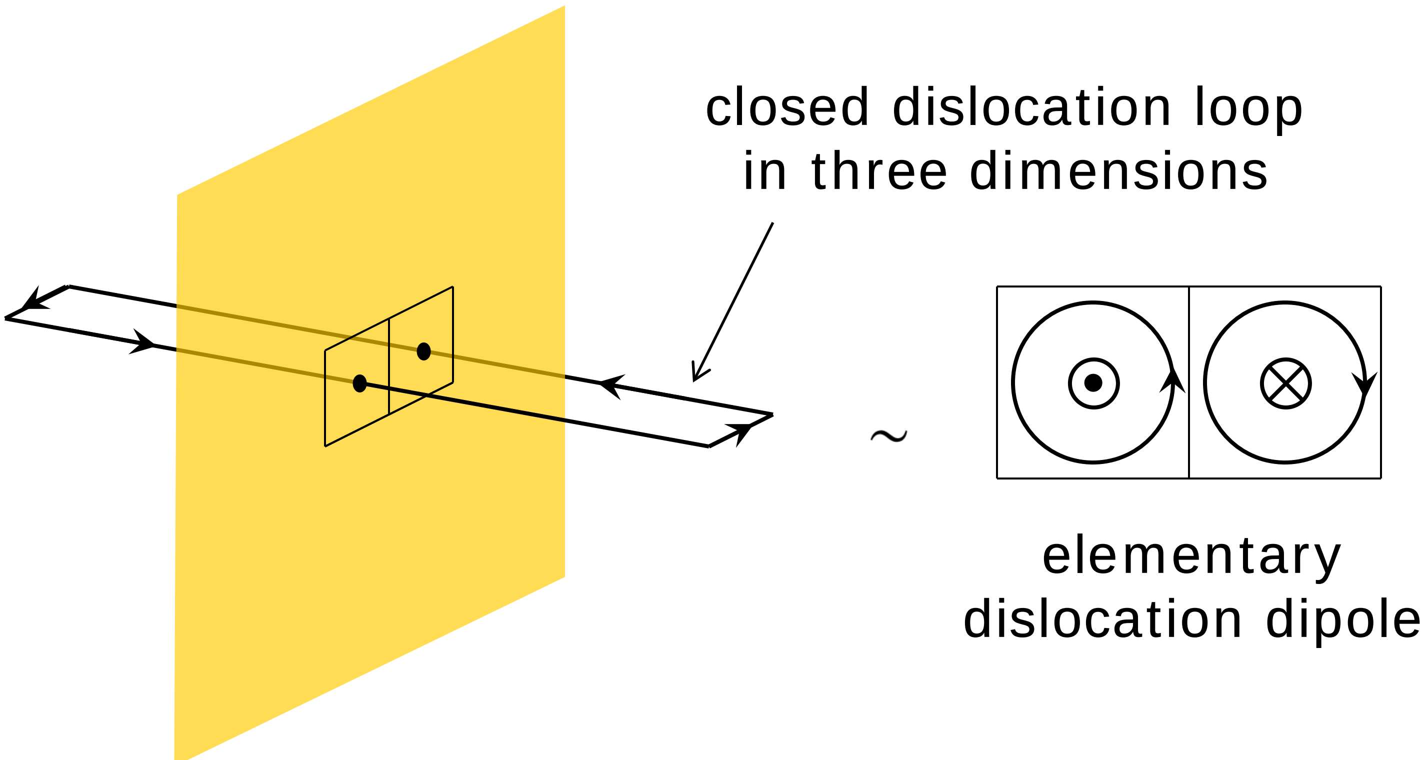
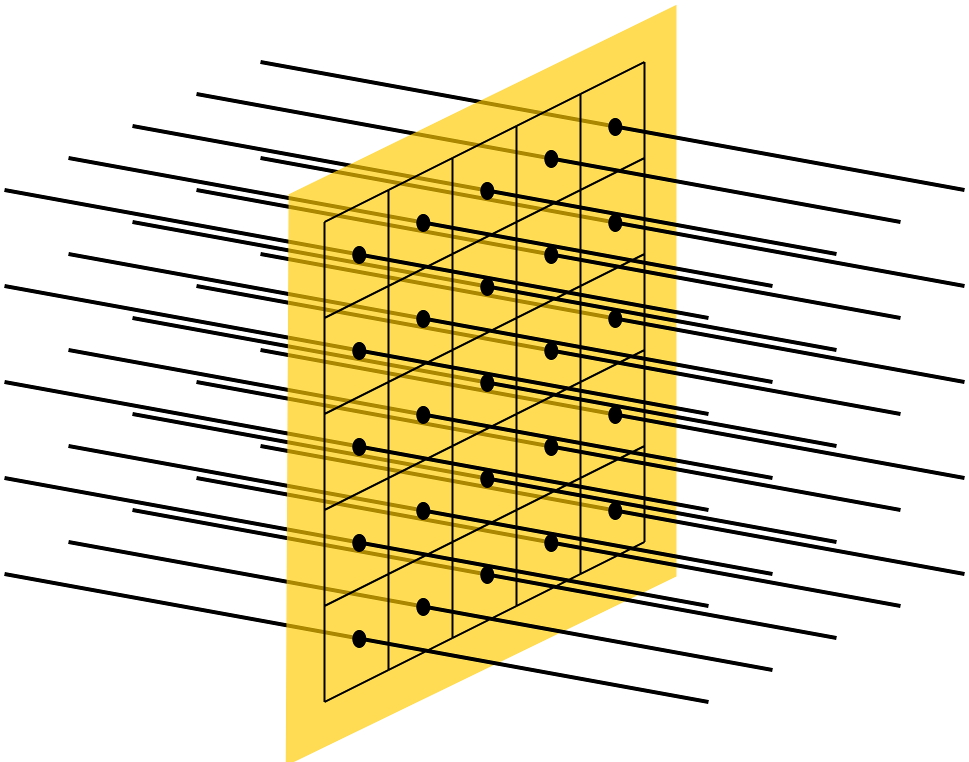
Discrete dislocations – Square lattice



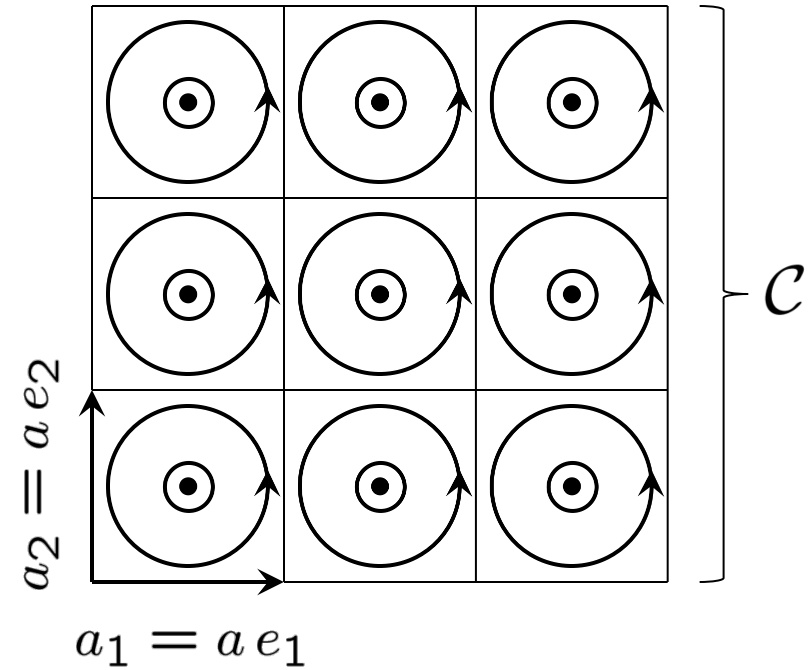
- Dislocation dipole: $d\alpha = \sum_{r \in a\mathbb{Z}^2} b_r = b - b = 0$
- If $d\alpha = 0 \Rightarrow \alpha$ linear combination of elementary dipoles
- Discrete Helmholtz decomposition theorem!

M.P. Ariza and M. Ortiz, *ARMA*, **178** (2005) 149–226.

Discrete dislocations – Square lattice



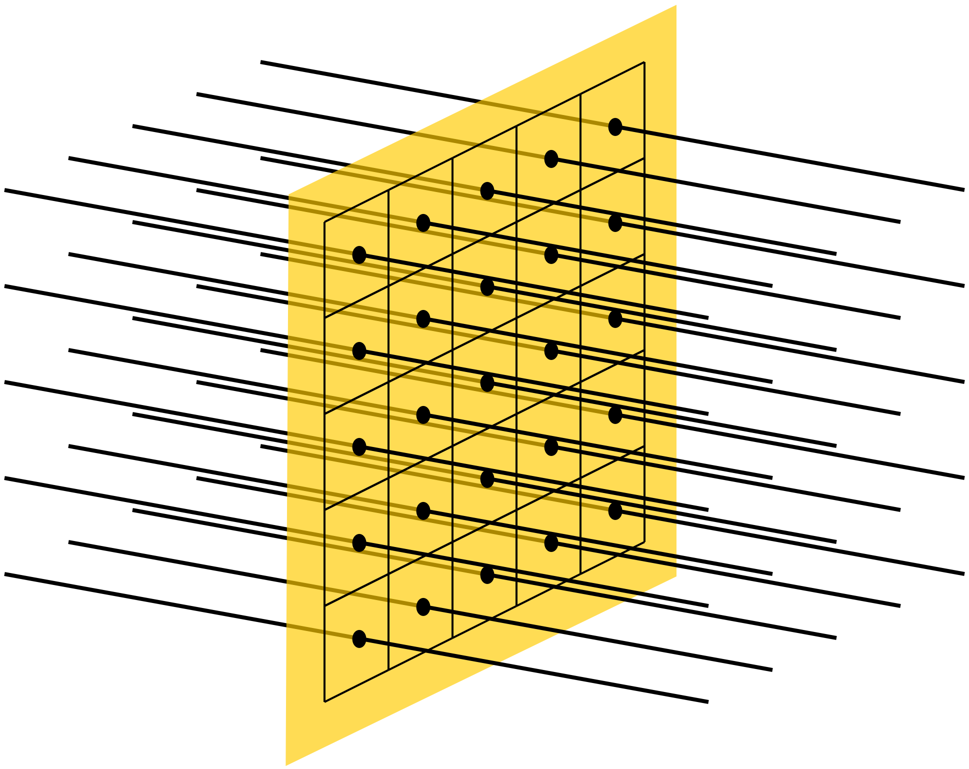
Screw-dislocation bundle



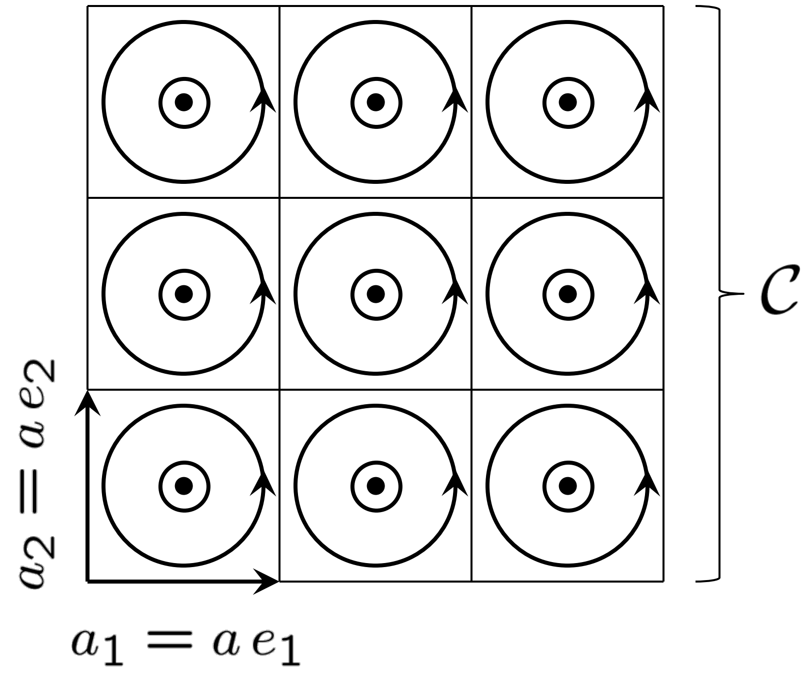
Square lattice complex

- Fourier representation: $\hat{\alpha}(k) = \sum_{r \in a\mathbb{Z}^2} b_r \mathrm{e}^{-ik\cdot r}$
- Brillouin zone of square lattice: $B \equiv [-\pi/a, \pi/a]^2$
- $\alpha \in \mathcal{D}^2(C; \mathbb{R}) \Leftrightarrow \hat{\alpha}$ is B-periodic

Discrete dislocations – Square lattice



Screw-dislocation bundle



Square lattice complex

- Inner product: $\alpha' = \sum_{r \in a\mathbb{Z}^2} b'_r \delta_r$, $\alpha'' = \sum_{r \in a\mathbb{Z}^2} b''_r \delta_r$,

$$\langle \alpha', \alpha'' \rangle = \sum_{r \in a\mathbb{Z}^2} b'_r b''_r = \fint_B \hat{\alpha}'(k) \hat{\alpha}''^*(k)\, dk$$

- NB: None of the usual metrizations of $\mathcal{M}(\Omega)$!

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Discrete dislocations – Square lattice

- Stored energy, Fourier: For $\alpha = \sum_{r\in a\mathbb{Z}^2} b_r\delta_r$,

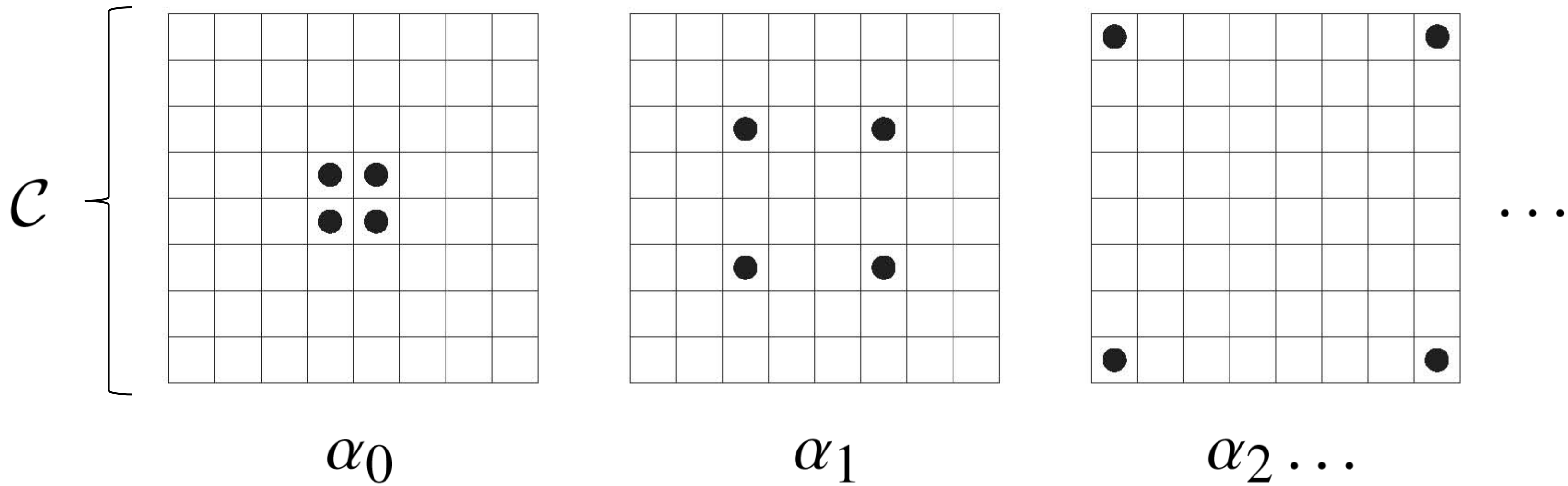
$$E(\alpha) = \begin{cases} \frac{1}{(2\pi)^2}\int_B \frac{1}{2}\Gamma(k)|\hat{\alpha}(k)|^2\, dk, & \text{if } b_r \in b\mathbb{Z},\ d\alpha = 0, \\ +\infty, & \text{otherwise.} \end{cases}$$

- Properties of kernel Γ: B-periodic, $\Gamma(k) \sim |k|^{-2}$, $k \to 0$.
- Long wavelength (continuum) limit: $\Gamma_0(k) = \lim_{\epsilon\to 0} \epsilon^2\Gamma(\epsilon k)$
- Homogeneity: $\Gamma_0(\lambda k) = \lambda^{-2}\Gamma_0(k)$
- Example: N-N interactions, $\mu \equiv$ shear modulus,

$$\Gamma(k) = \frac{\mu/2}{\sin^2\frac{k_1 a}{2} + \sin^2\frac{k_2 a}{2}}, \qquad \Gamma_0(k) = \frac{2\mu}{a^2}\frac{1}{|k|^2}.$$

M.P. Ariza and M. Ortiz, *ARMA*, **178** (2005) 149–226.

Square lattice – The dilute limit (I)

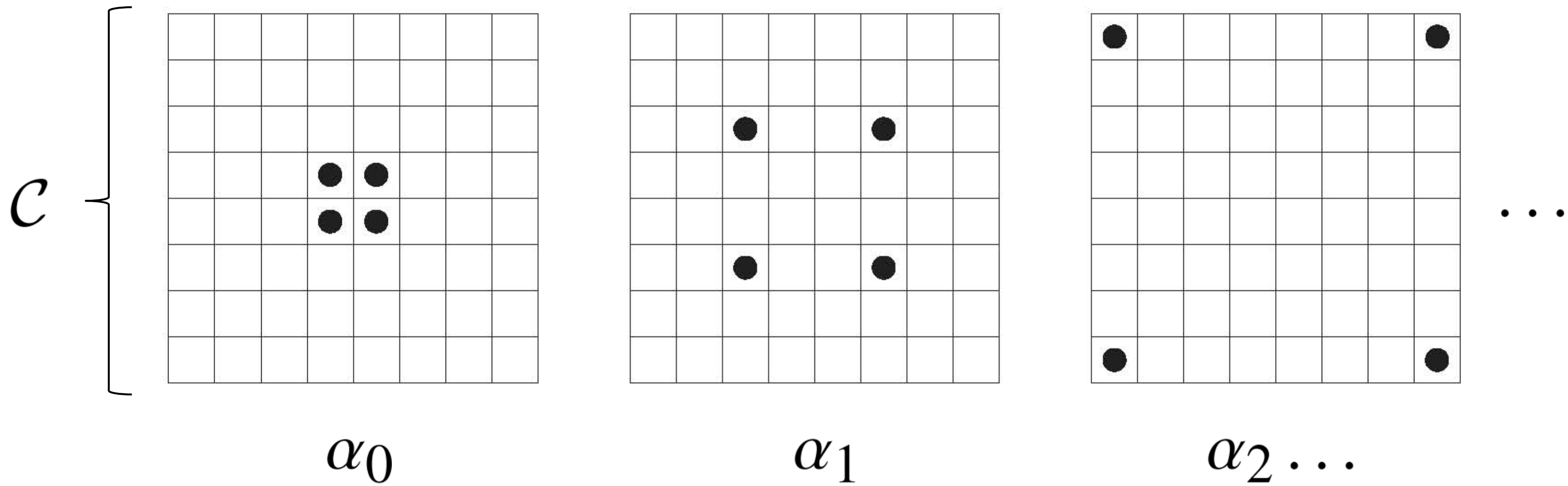


Sequence of increasingly ***dilute*** quadrupoles

- Fourier representation: $\hat{\alpha}_h(k) = \hat{\alpha}_0(\epsilon_h k), \quad \epsilon_h = 2^{-h},$
- Stored energy: For $\alpha_0 = \sum_{r \in a\mathbb{Z}^2} b_r \delta_r, \; b_r \in b\mathbb{Z}, \; d\alpha_0 = 0,$

$$E(\alpha_h) \equiv E_h(\alpha_0) = \frac{1}{(2\pi)^2} \int_{B/\epsilon_h} \frac{1}{2} \epsilon_h^2 \Gamma(\epsilon_h k) |\hat{\alpha}_0(k)|^2 \, dk$$

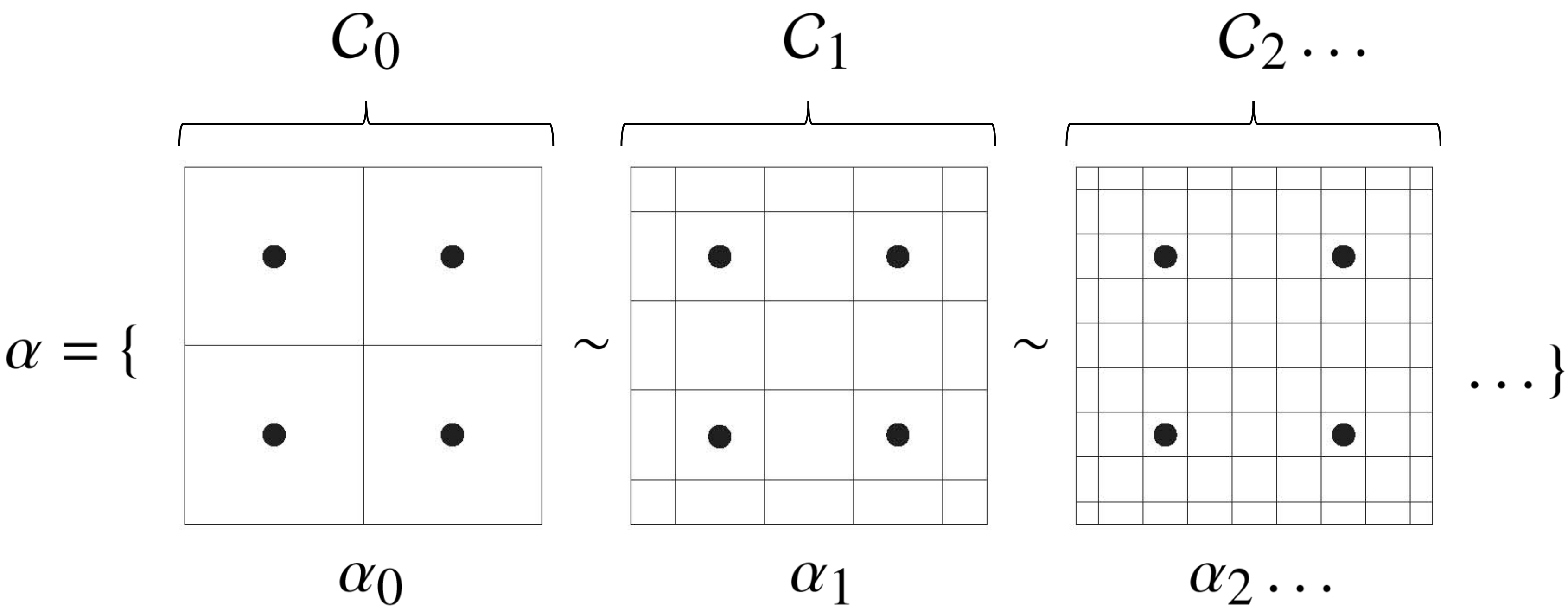
Square lattice – The dilute limit (I)



Sequence of increasingly ***dilute*** quadrupoles

- Fourier representation: $\hat{\alpha}_h(k) = \hat{\alpha}_0(\epsilon_h k), \;\; \epsilon_h = 2^{-h},$
- Weak limit: $\langle \alpha_h, \varphi \rangle \to 0, \; \forall \varphi \in \mathcal{D}^2(C, \mathbb{R}) \Rightarrow \alpha_h \rightharpoonup 0!$
- All dislocations 'go off' to infinity in the limit...

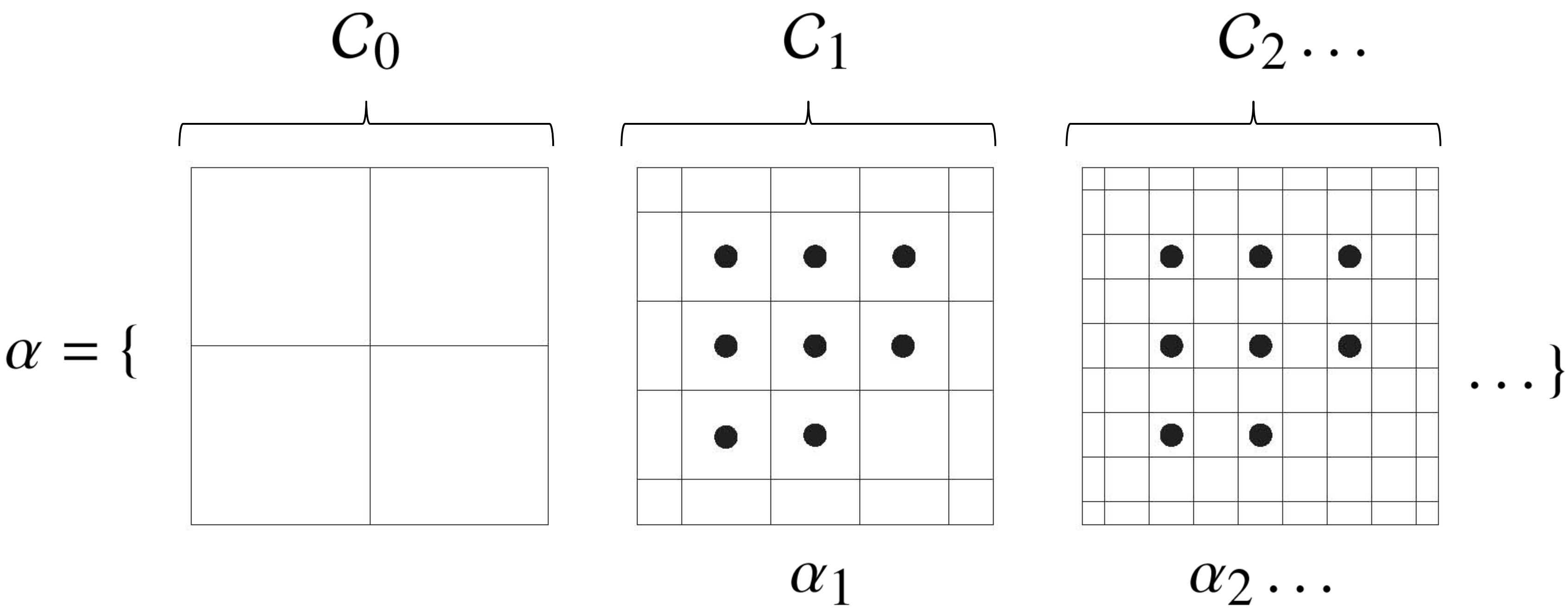
Square lattice – The dilute limit (II)



Sequence of increasingly ***dilute*** quadrupoles

- Lattice refinement $\Rightarrow C_h$, $a_h = \epsilon_h a$, $\epsilon_h = 2^{-h}$, $h \in \mathbb{N}$
- Difficulty: α_h's 'live' in different spaces $\mathcal{D}^2(C_h;\mathbb{R})$

Square lattice – The dilute limit (II)

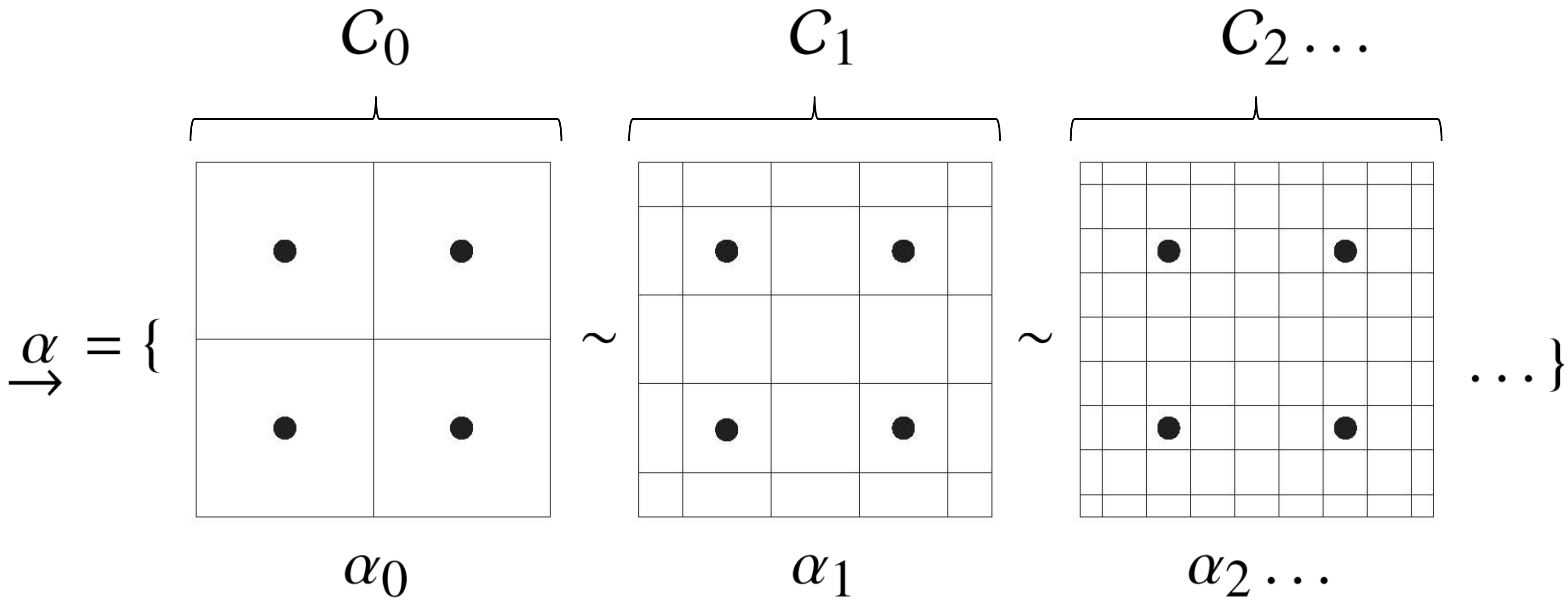


- Example:

  $\alpha_1 \in \mathcal{D}^2(C_1;\mathbb{R})$ also 'lives' in $\mathcal{D}^2(C_2;\mathbb{R})$ but not in $\mathcal{D}^2(C_0;\mathbb{R})$

- Inclusions: $\mathcal{D}^2(C_0;\mathbb{R}) \subset \mathcal{D}^2(C_1;\mathbb{R}) \subset \mathcal{D}^2(C_2;\mathbb{R}) \ldots$

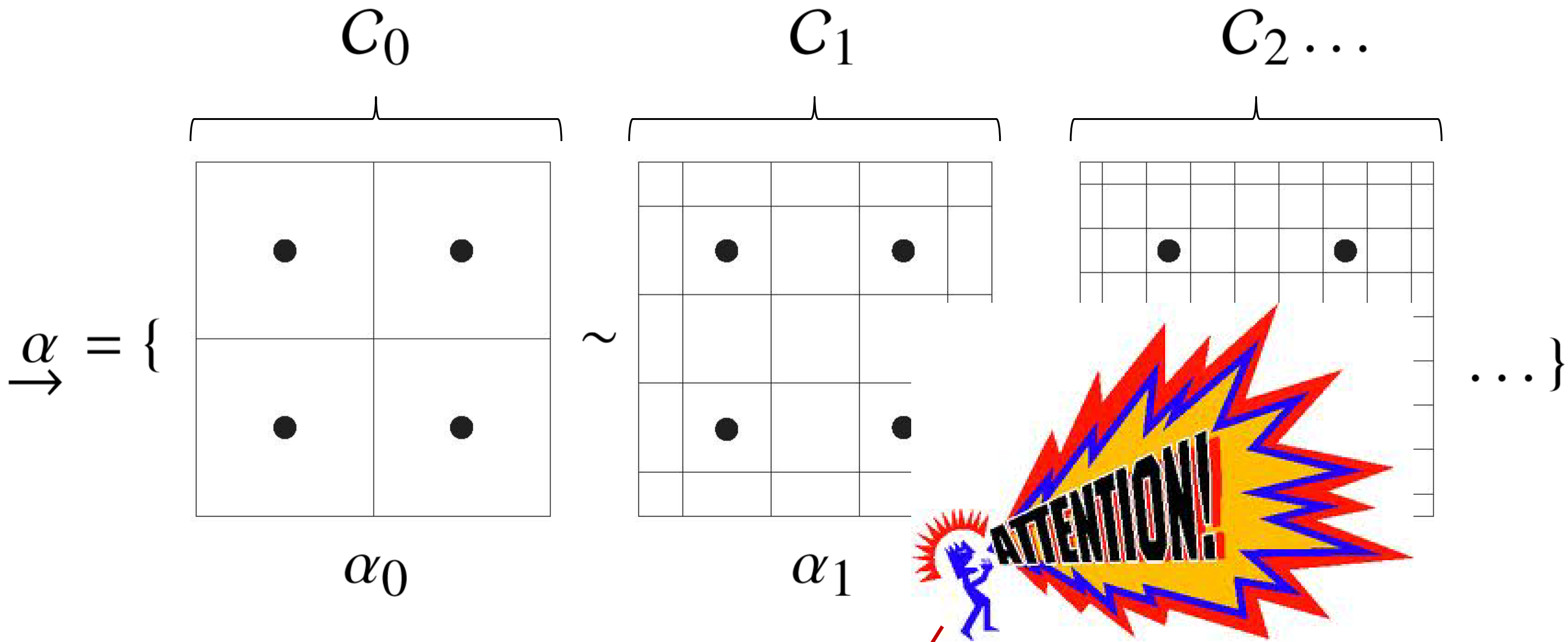
Square lattice – Dilute dislocations



- Identify: $\alpha_i \sim \alpha_j$ if $\sum_{r_i \in a_i\mathbb{Z}} b_{r_i}\delta_{r_i} = \sum_{r_j \in a_j\mathbb{Z}} b_{r_j}\delta_{r_j}$ or $\hat{\alpha}_i = \hat{\alpha}_j$
- Direct limit: $\underrightarrow{\mathcal{D}}^2(C;\mathbb{R}) \equiv \left(\prod_{h\in\mathbb{N}} \mathcal{D}^2(C_h;\mathbb{R})\right) / \sim$
- Inner product: $\langle \underrightarrow{\alpha}', \underrightarrow{\alpha}'' \rangle = \langle \alpha'_h, \alpha''_h \rangle$ if $\alpha'_h \in \underrightarrow{\alpha}'$, $\alpha''_h \in \underrightarrow{\alpha}''$
- Coboundary operator: $\underrightarrow{d}\,\underrightarrow{\alpha} = d_h \alpha_h$

J.R. Munkres, *Elements of Algebraic Topology*, Perseus (1984)

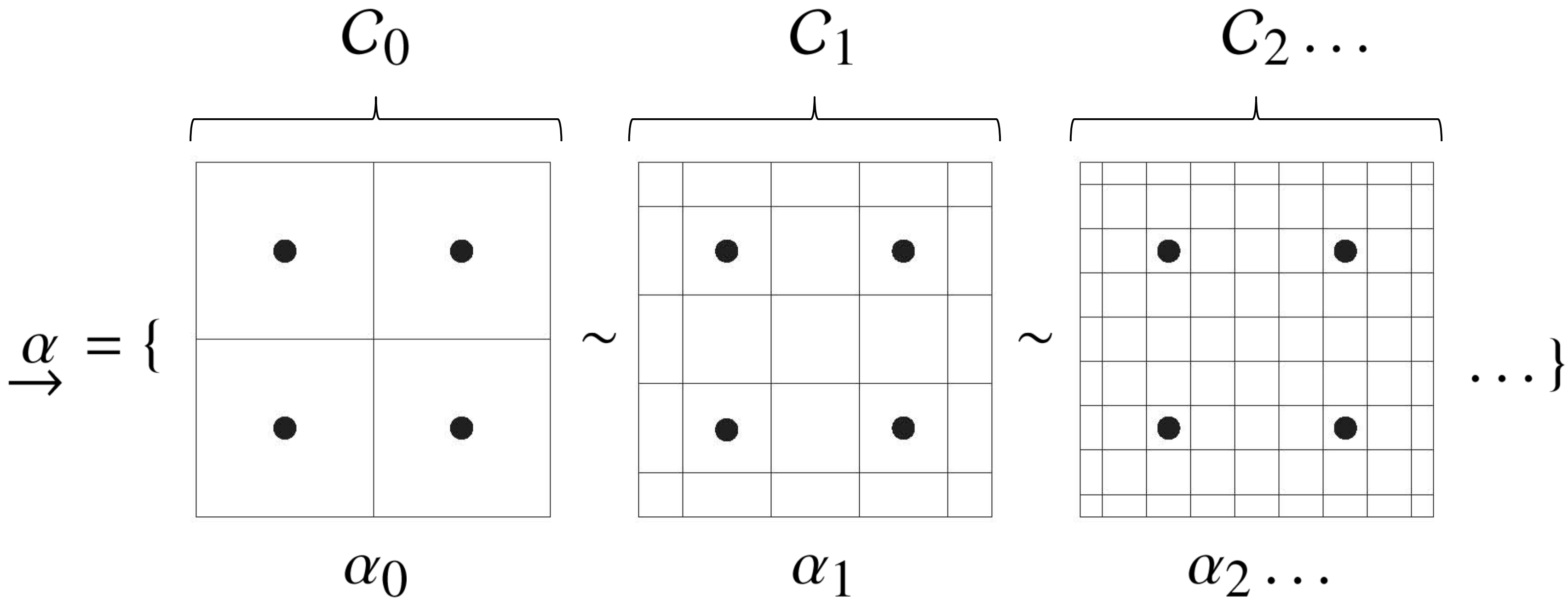
Square lattice – Dilute dislocations



- Dilute dislocation space: $X = \{\underset{\rightarrow}{\alpha} \in \underset{\rightarrow}{\mathcal{D}}^2(C;\mathbb{R}),\ \|\underset{\rightarrow}{\alpha}\| < +\infty\}$
- Equivalenty: $X = \{\underset{\rightarrow}{\alpha} = \sum_{r \in a\mathbb{Q}^2} b_r \delta_r,\ \|\underset{\rightarrow}{\alpha}\| < +\infty\}$
- Inner product: $\langle \underset{\rightarrow}{\alpha}', \underset{\rightarrow}{\alpha}'' \rangle = \sum_{r \in a\mathbb{Q}^2} b_r' b_r''$
- Coboundary operator: $\underset{\rightarrow}{d}\,\underset{\rightarrow}{\alpha} = \sum_{r \in a\mathbb{Q}^2} b_r$

J.R. Munkres, *Elements of Algebraic Topology*, Perseus (1984)

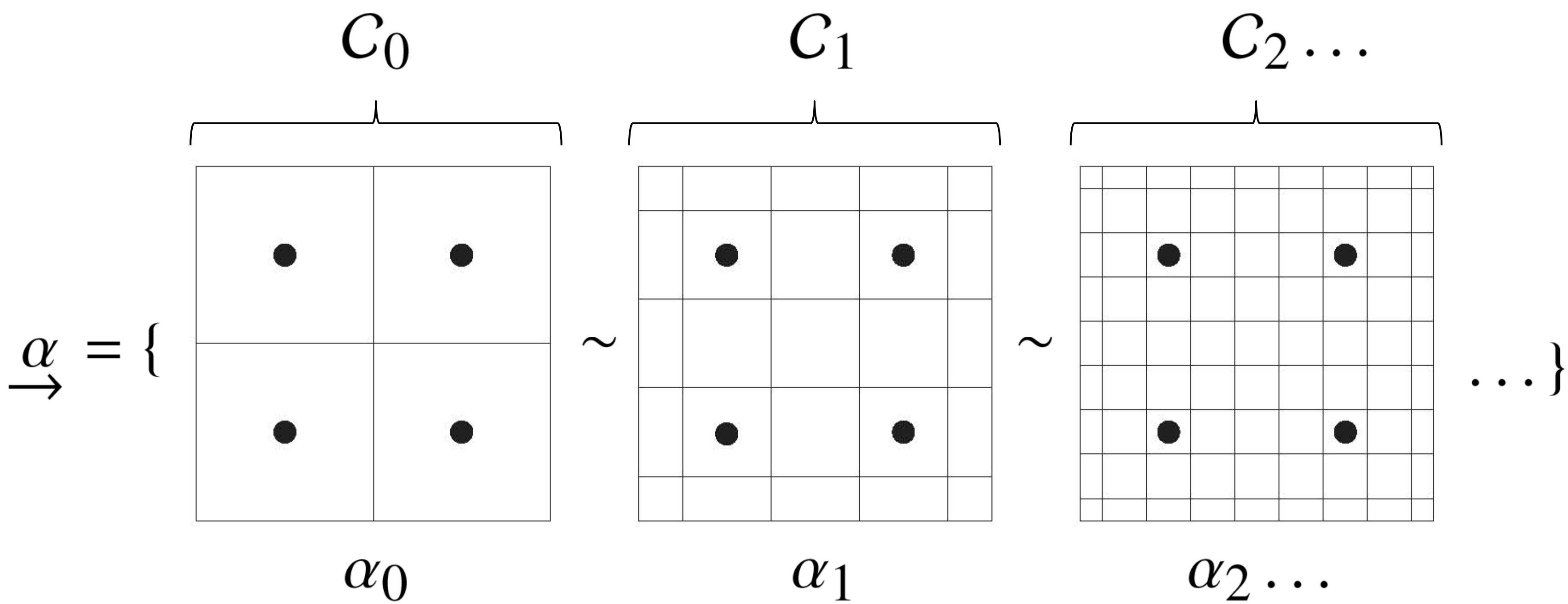
Square lattice – Dilute dislocations



- Dilute dislocation space: $X = \{\underrightarrow{\alpha} \in \underrightarrow{\mathcal{D}}^2(C;\mathbb{R}),\ \|\underrightarrow{\alpha}\| < +\infty\}$
- Equivalenty: $X = \{\hat{\alpha}_h : \mathbb{R}^2 \to \mathbb{C},\ B/\epsilon_h\text{-periodic},\ h \in \mathbb{N}\}$
- Inner product: $\langle \underrightarrow{\alpha}', \underrightarrow{\alpha}'' \rangle = \fint_{B/\epsilon_h} \hat{\alpha}'_h(k)\hat{\alpha}''^{*}_h(k)\, dk$
- Coboundary operator: $\underrightarrow{d}\,\underrightarrow{\alpha} = \hat{\alpha}_h(0)$

J.R. Munkres, *Elements of Algebraic Topology*, Perseus (1984)

Square lattice – Dilute dislocations



- Enumerate $\mathbb{Q}^2$: $X \sim l^2(\mathbb{Z};\mathbb{R})$, separable Hilbert space
- Bounded sets in X are sequentially compact in the weak topology $\Rightarrow$ compactness!
- Contrast to Ponsiglione (2008): $X = \{\alpha = \sum_{r\in\mathbb{R}^2} b_r\delta_r\}$

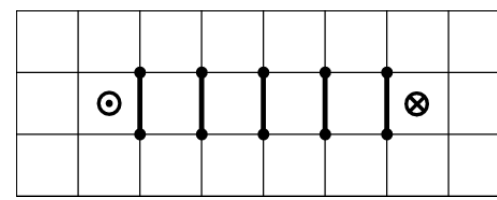
M. Ponsiglione, *SIAM J. Math. Anal*. **39** (2008) 449-469

Square lattice – Dilute limit

- Stored energy: For $\underset{\rightarrow}{\alpha} = \sum_{r \in a\mathbb{Q}^2} b_r \delta_r \in X$,

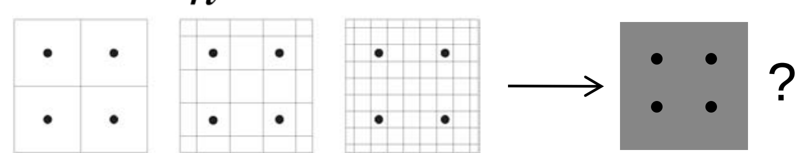
$$E_h(\underset{\rightarrow}{\alpha}) = \begin{cases} \frac{1}{(2\pi)^2} \int_{B/\epsilon_h} \frac{1}{2} \epsilon_h^2 \Gamma(\epsilon_h k) |\hat{\alpha}(k)|^2 \, dk, & \text{if } \sum_{r \in a\mathbb{Q}^2} b_r = 0, \\ & \text{and } b_r \in b\mathbb{Z}, \\ +\infty, & \text{otherwise.} \end{cases}$$

- Dislocation dipole: $E_h \sim \frac{\mu b^2}{2\pi} \log \epsilon_h^{-1}$



- Scaled energy: $F_h(\underset{\rightarrow}{\alpha}) = \frac{1}{1 + \log \epsilon_h^{-1}} E_h(\underset{\rightarrow}{\alpha})$

- Question: $\Gamma\text{-}\lim_{h \to \infty} F_h$?



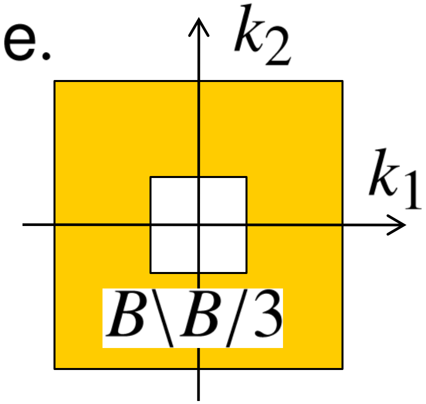
Square lattice – Dilute limit

- Limiting energy: For $\underset{\rightarrow}{\alpha} = \sum_{r\in a\mathbb{Q}^2} b_r \delta_r \in X$,

$$F(\underset{\rightarrow}{\alpha}) = \begin{cases} K\|\underset{\rightarrow}{\alpha}\|^2 = K\sum_{r\in a\mathbb{Q}^2} b_r^2, & \text{if } \sum_{r\in a\mathbb{Q}^2} b_r = 0, \\ & \text{and } b_r \in b\mathbb{Z}, \\ +\infty, & \text{otherwise.} \end{cases}$$

where: $K = \dfrac{1}{\log(3)} \dfrac{a^2}{(2\pi)^2} \displaystyle\int_{B\setminus B/3} \frac{1}{2}\Gamma_0(k)\,dk$

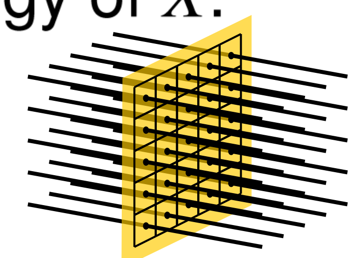
$\equiv$ prelogarithmic energy factor



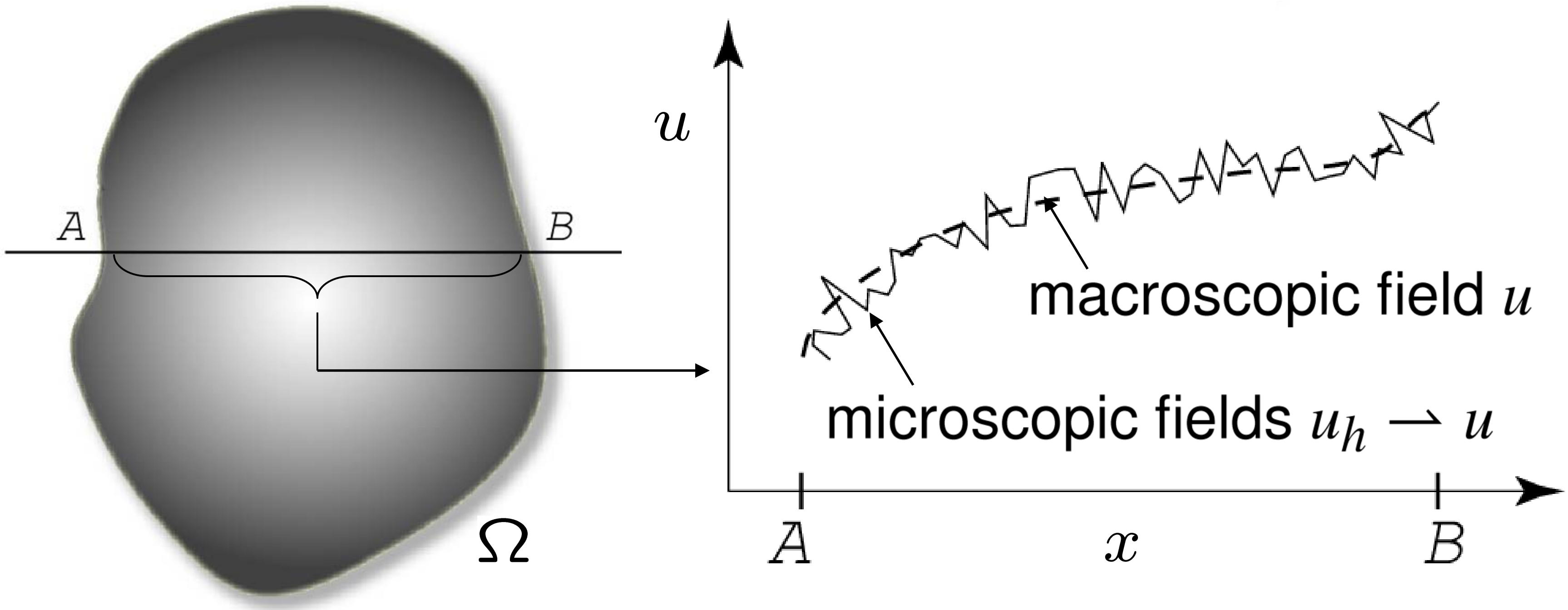
Theorem $\Gamma\text{-}\lim_{h\to\infty} F_h = F$ in the weak topology of X.

- Interpretation: i) $|b_r| > b$ penalized by F.

ii) No long-range interation $\to$ Line tension!.



Review of Γ-convergence



Definition Let X be a first-countable topological space, $F_h, F : X \to \bar{\mathbb{R}}$. Then, F_h Γ-converges to F if:

i) $\forall u \in X$ and $u_h \to u$ in X: $F(u) \leq \liminf_{h\to\infty} F_h(u_h)$.

ii) $\forall u \in X$, $\exists u_h$ in X s. t.: $\lim_{h\to\infty} F_h(u_h) = F(u)$.

G. dal Maso, *An Introduction to Γ Convergence*, Birkhäuser, 1993

Review of Γ-convergence

Definition Let X be a first-countable topological space. A function $F : X \to \bar{\mathbb{R}}$ is *lower-semicontinuous* iff $F(u) \leq \liminf_{h\to\infty} F(u_h)$ for every sequence $u_h \to u$ in X.

Definition A sequence $F_h : X \to \bar{\mathbb{R}}$ is equicoercive iff there exists a lower semicontinuous coercive function $\Psi : X \to \bar{\mathbb{R}}$ s. t. $F_h \geq \Psi$ on X for every $h \in \mathbb{N}$.

Theorem Suppose that F_h is equicoercive and Γ-converges to a function F with a unique minimum u_0 in X. Let u_h be a sequence of ϵ_h-minimizers of F_h. Then u_h converges to u_0 and $F_h(u_h)$ converges to $F(u_0)$.

G. dal Maso, *An Introduction to Γ Convergence*, Birkhäuser, 1993

Review of Γ-convergence

Theorem Let X be a completely regular topological space, $F_h : X \to [0, +\infty]$ equicoercive and $F : X \to [0, +\infty]$ lower-semicontinuous. Then, F_h Γ-converges to F iff $\inf_X(F + G) = lim_{h\to\infty} \inf_X(F_h + G)$ for every continuous $G : X \to [0, +\infty)$.

- G may be regarded as a *forcing* of the system
- Then, F is the Γ limit of F_h if it delivers the exact macroscopic response, i. e., $inf_X(F+G) = \lim_{h\to\infty}(F_h+G)$, *for all forcings of the system*.
- F and F_h are *macroscopically indistinguishable* in limit.

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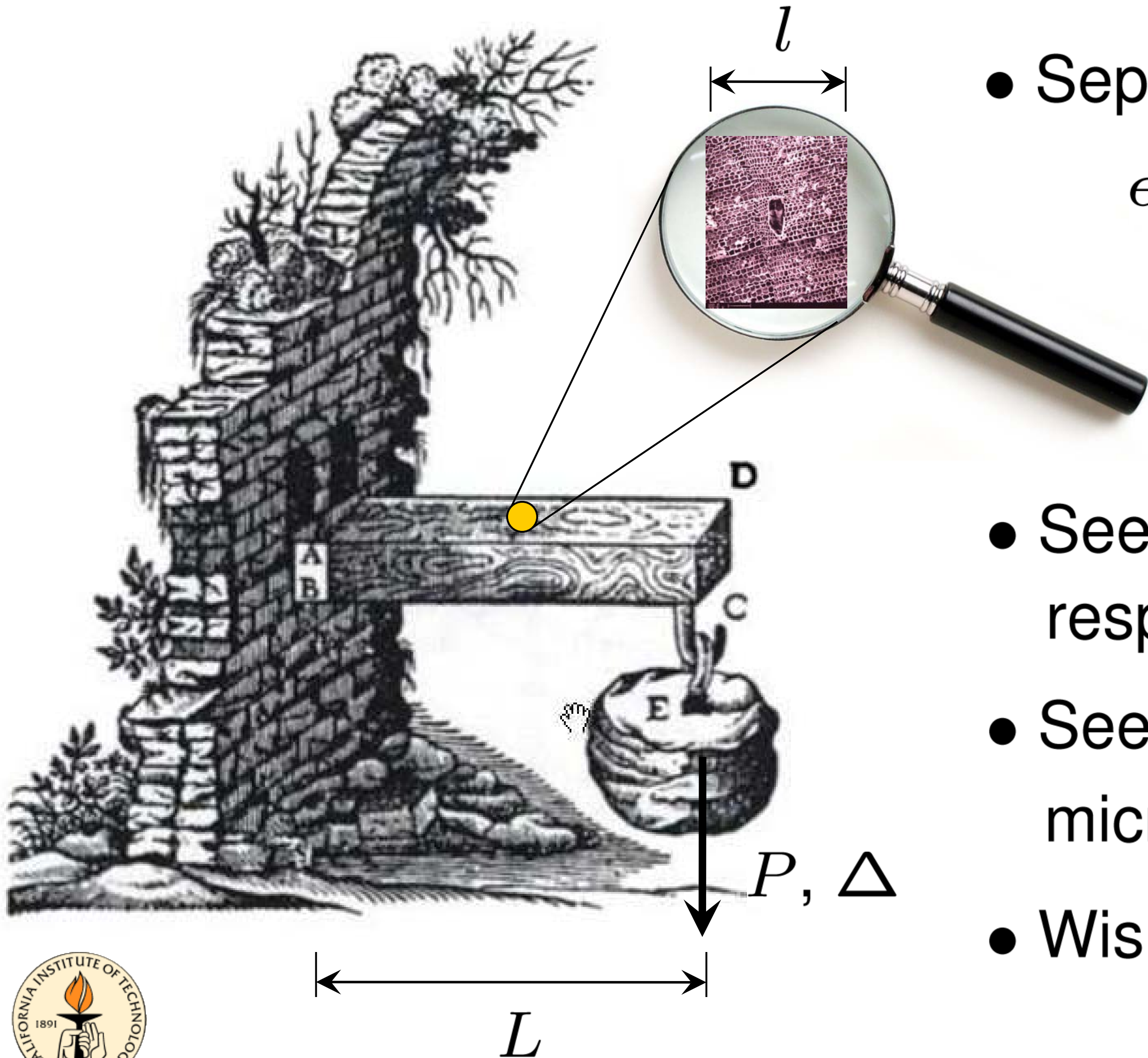
Γ-convergence - Homogeneization



- Separation of scales:

$$\epsilon = l/L \to 0$$

- Seek macroscopic response P-Δ
- Seek to eliminate microscopic scale
- Wish return option...

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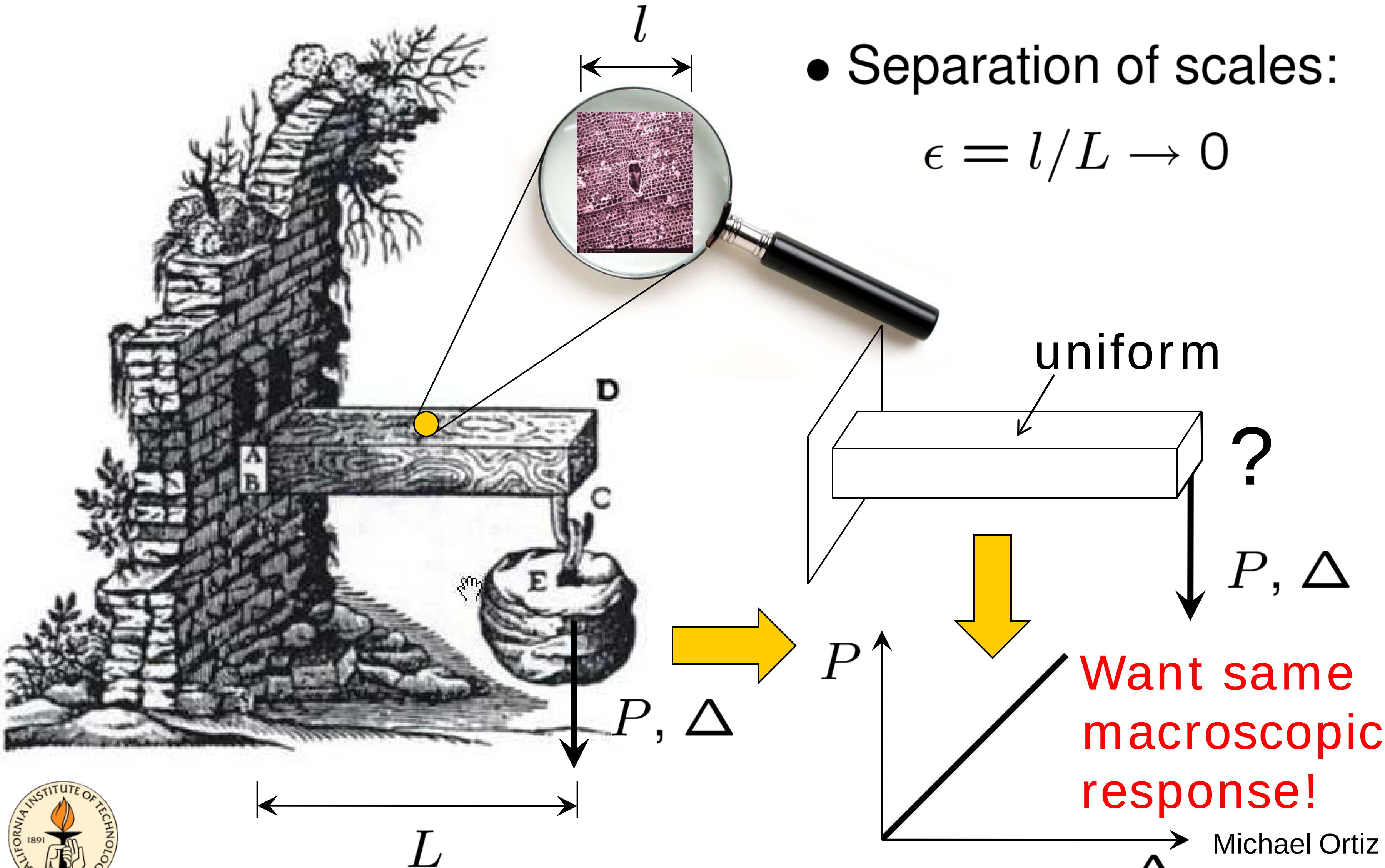
Γ-convergence - Homogeneization

- Separation of scales:

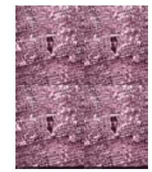
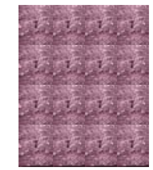
$$\epsilon = l/L \to 0$$



Γ-convergence - Homogeneization

- Equicoercive functionals $F_\epsilon : X \to [0, +\infty]$, e. g.:

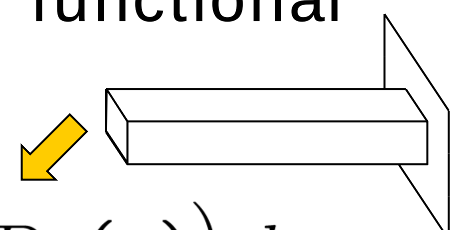
$$F_\epsilon(u) = \int_\Omega W\Big(\frac{x}{\epsilon}, Du(x)\Big)\, dx \to \text{inf!}$$

- Separation-of-scales limit: $\epsilon \to 0$: , ,  $\dots$

- $\Gamma - \lim\limits_{\epsilon \to 0} F_\epsilon = F_0$ (*wlsc*) iff, for all $f \in X^*$ (loadings),

$$\underbrace{\inf_{u \in X} \Big(F_\epsilon(u) + \langle f, u\rangle\Big)}_{\text{minimum energies of sequence of functionals}} \longrightarrow \underbrace{\inf_{u \in X} \Big(F_0(u) + \langle f, u\rangle\Big)}_{\text{minimum energy of limiting functional}}$$

- Example: Homogeneization limit,



$$W_0(\xi) = \inf_{W^{1,1}_{\text{per}}(P)} \frac{1}{|P|} \int_P W\Big(x, \xi + Dv(x)\Big)\, dx$$

Square lattice – Dilute limit

- Sequence: For $\underset{\rightarrow}{\alpha} = \sum_{r\in a\mathbb{Q}^2} b_r\delta_r \in X$, $F_h(\underset{\rightarrow}{\alpha}) =$

$$\begin{cases} \frac{1}{1+\log\epsilon_h^{-1}}\frac{1}{(2\pi)^2}\int_{B/\epsilon_h}\frac{1}{2}\epsilon_h^2\Gamma(\epsilon_h k)|\hat{\alpha}(k)|^2\,dk, & \text{if } \sum_{r\in a\mathbb{Q}^2} b_r = 0, \\ & \text{and } b_r \in b\mathbb{Z}, \\ +\infty, & \text{otherwise.} \end{cases}$$

- Limiting energy: For $\underset{\rightarrow}{\alpha} = \sum_{r\in a\mathbb{Q}^2} b_r\delta_r \in X$,

$$F(\underset{\rightarrow}{\alpha}) = \begin{cases} K\|\underset{\rightarrow}{\alpha}\|^2 = K\sum_{r\in a\mathbb{Q}^2} b_r^2, & \text{if } \sum_{r\in a\mathbb{Q}^2} b_r = 0, \\ & \text{and } b_r \in b\mathbb{Z}, \\ +\infty, & \text{otherwise.} \end{cases}$$

where: $K = \frac{1}{\log(3)}\frac{a^2}{(2\pi)^2}\int_{B\setminus B/3}\frac{1}{2}\Gamma_0(k)\,dk$

Theorem $\Gamma\text{-}\lim_{h\to\infty} F_h = F$ in the weak topology of X.

Square lattice – Dilute limit (1 of 4)

Sketch of proof. i) Separate the singularity at the origin,

$$F_h(\alpha) = \frac{1}{1+\log\epsilon_h^{-1}} \frac{1}{(2\pi)^2} \int_{B/\epsilon_h} \frac{1}{2}\Gamma_0(k)|\hat{\alpha}(k)|^2\,dk$$
$$+\frac{1}{1+\log\epsilon_h^{-1}} \frac{1}{(2\pi)^2} \int_{B/\epsilon_h} \frac{1}{2}(\epsilon_h^2\Gamma(\epsilon_h k) - \Gamma_0(k))|\hat{\alpha}(k)|^2\,dk$$

Assume $\Gamma - \Gamma_0$ integrable, $\alpha \in X$, $b_r \in b\mathbb{Z}^2$,

$$\left|\frac{1}{(2\pi)^2}\int_{B/\epsilon_h} \frac{1}{2}(\epsilon_h^2\Gamma(\epsilon_h k) - \Gamma_0(k))|\hat{\alpha}(k)|^2\,dk\right| \leq$$
$$\|\hat{\alpha}\|^2_{L^\infty}\frac{1}{(2\pi)^2}\int_B |\Gamma(k) - \Gamma_0(k)|\,dk < +\infty,$$

second term drops out in the limit.

Square lattice – Dilute limit (2 of 4)

Lemma. $B = [-\pi/a, \pi/a]^2$, $\epsilon_h = 2^{-h}$, $f_h, g : \mathbb{R}^2 \to \mathbb{R}$ *s. t.:*

i) f_h B/ϵ_n*-periodic for some* $n \in \mathbb{N}$.

ii) $|k|^{-2} f_h \in L^1(B/\epsilon_n)$ *for all* $h \in \mathbb{N}$.

iii) The sequence $\fint_{B/\epsilon_n} f_h(k)\, dk$ *converges.*

iv) g *homogeneous of degree* -2.

v) $|k|^2 g(k) \in L^\infty(\mathbb{R}^2)$. *vi)* $|k|^3 |\nabla g(k)| \in L^\infty(\mathbb{R}^2)$.

Then: $$\lim_{h\to\infty} \frac{1}{1 + \log \epsilon_h^{-1}} \frac{1}{(2\pi)^2} \int_{B/\epsilon_h} f_h(k) g(k)\, dk =$$

$$\frac{1}{\log(3)} \left(\frac{1}{(2\pi)^2} \int_{B\setminus B/3} g(k)\, dk \right) \left(\fint_{B/\epsilon_n} f_h(k)\, dk \right)$$

Square lattice – Dilute limit (3 of 4)

By estimate and lemma, $\lim_{h\to\infty} F_h(\alpha) =$

$$\lim_{h\to\infty} \frac{1}{1+\log\epsilon_h^{-1}} \frac{1}{(2\pi)^2} \int_{B/\epsilon_h} \frac{1}{2}\Gamma_0(k)|\hat{\alpha}(k)|^2\, dk = F(\alpha),$$

i. e., the constant sequence is a recovery sequence.

ii) Let $\alpha_h \rightharpoonup \alpha$. Assume $\epsilon_h^2\Gamma(\epsilon_h k) \geq \Gamma_0(k)$. Then,

$$\lim_{h\to\infty} (F_h(\alpha_h) - F(\alpha)) \geq$$

$$\lim_{h\to\infty} \frac{1}{1+\log\epsilon_h^{-1}} \frac{1}{(2\pi)^2} \int_{B/\epsilon_h} \frac{1}{2}\Gamma_0(k)(|\hat{\alpha}_h(k)|^2 - |\hat{\alpha}(k)|^2)\, dk$$

Square lattice – Dilute limit (4 of 4)

Identity:

$$|\hat{\alpha}_h(k)|^2 - |\hat{\alpha}(k)|^2 = |\hat{\alpha}_h(k) - \hat{\alpha}(k)|^2 + \hat{\alpha}^*(k)(\hat{\alpha}_h(k) - \hat{\alpha}(k)).$$

By lemma and weak convergence,

$$\lim_{h\to\infty} \frac{1}{1+\log \epsilon_h^{-1}} \frac{1}{(2\pi)^2} \int_{B/\epsilon_h} \frac{1}{2}\Gamma_0(k)\hat{\alpha}^*(k)(\hat{\alpha}_h(k)-\hat{\alpha}(k))\, dk = 0.$$

Assume $\epsilon_h^2\Gamma(\epsilon_h k) \geq \Gamma_0(k)$, $\Gamma_0(k) \geq 0$. Then,

$$\lim_{h\to\infty} (F_h(\alpha_h) - F(\alpha)) \geq$$

$$\lim_{h\to\infty} \frac{1}{1+\log \epsilon_h^{-1}} \frac{1}{(2\pi)^2} \int_{B/\epsilon_h} \frac{1}{2}\Gamma_0(k)|\hat{\alpha}_h(k) - \hat{\alpha}(k)|^2\, dk \geq 0.$$

q. e. d.

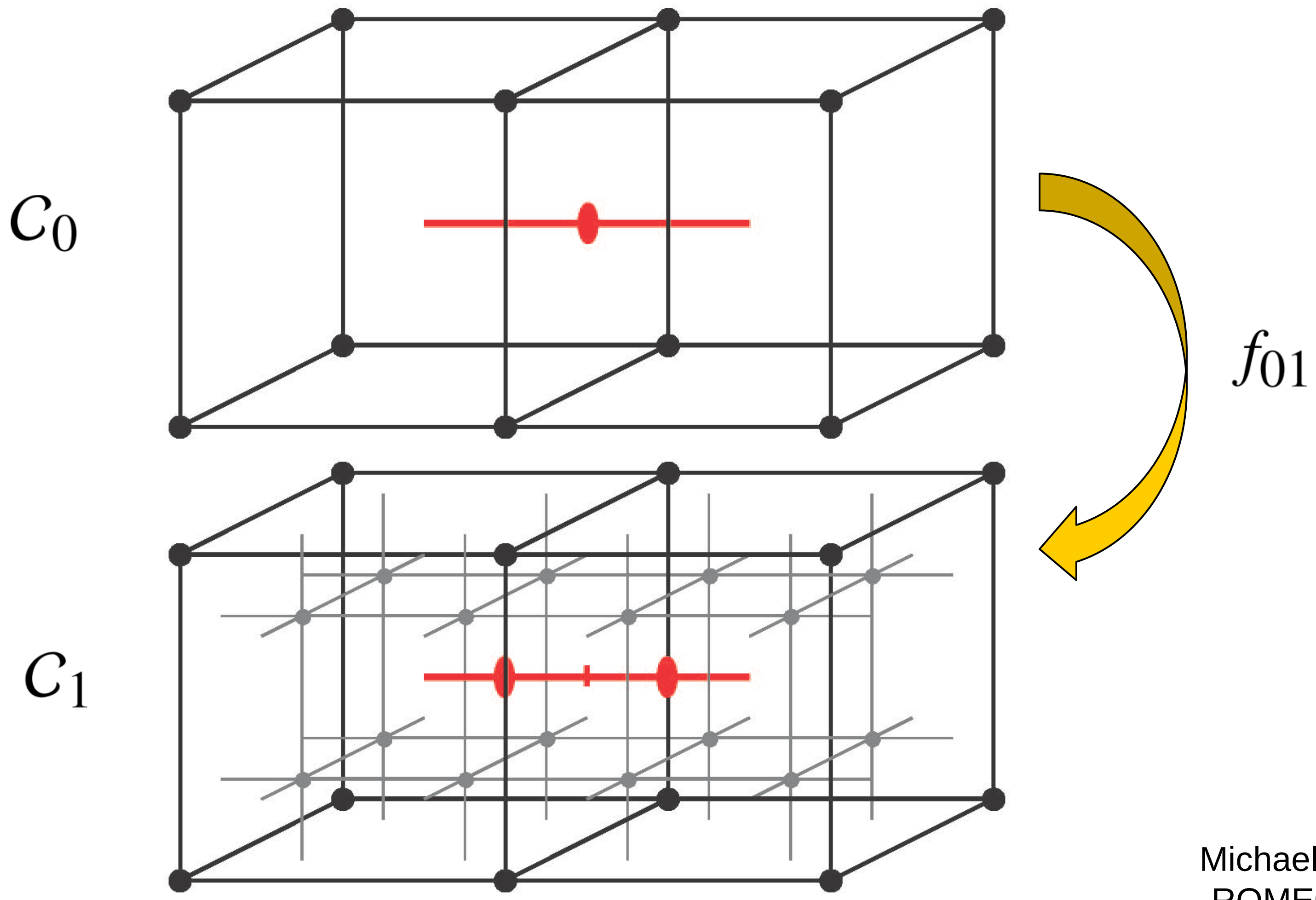
The dilute limit – General case

Definition. A *direct system* $\{G_\alpha, f_{\alpha\beta}\}$ of abelian groups and homomorphisms, corresponding to the directed set J, is and indexed family $\{G_\alpha\}_{\alpha\in J}$ of abelian groups, and a family of homomorphisms $f_{\alpha\beta} : G_\alpha \to G_\beta$, defined for every pair of indices $\alpha \leq \beta$, such that: i) $f_{\alpha\alpha} : G_\alpha \to G_\alpha$ is the identity; ii) If $\alpha \leq \beta$ and $\beta \leq \gamma$, then $f_{\beta\gamma} \circ f_{\alpha\beta} = f_{\alpha\gamma}$.

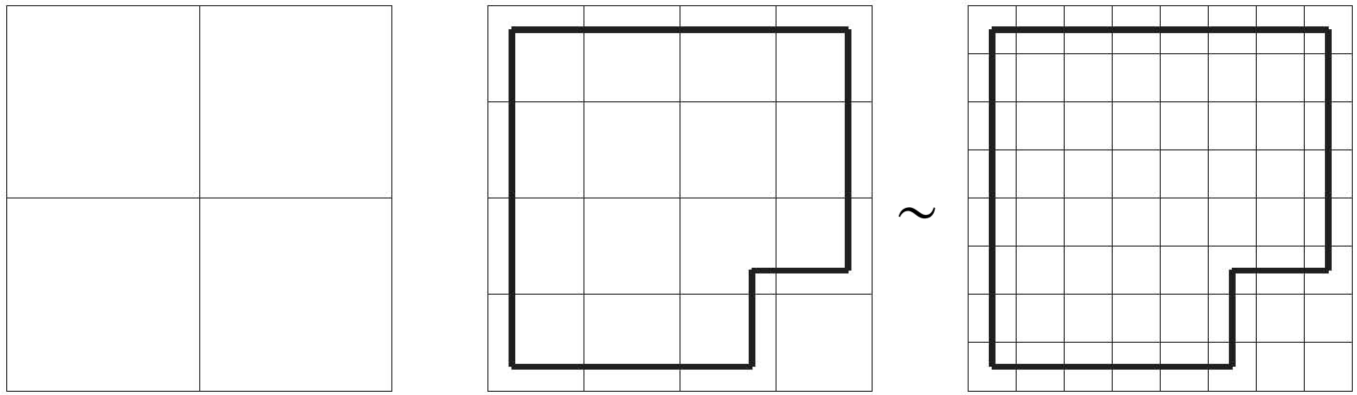
Definition. The *direct limit* direct limit of the direct system $\{G_\alpha, f_{\alpha\beta}\}$ is $\varinjlim_{\alpha\in J} G_\alpha = \sqcup_{\alpha\in J} G_\alpha / \sim$, where $g_\alpha \sim g_\beta$ iff $f_{\alpha\gamma}(g_\alpha) = f_{\beta\gamma}(g_\beta)$ for some upper bound γ of α and β.

The dilute limit – General case

- 3D dilute dislocations: $X \equiv \varinjlim_{h\in\mathbb{N}} \mathcal{D}^2(C_h, \mathbb{R}^3)$

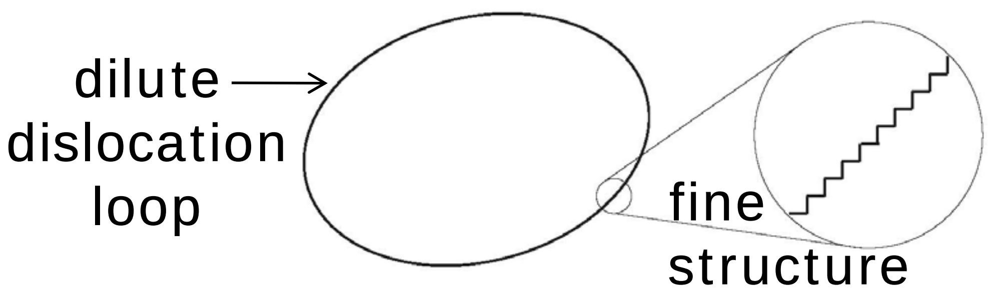


The dilute limit – General case



Direct system of dislocation lattices defined by refinement and sequence of increasingly ***dilute*** dislocation loops

- Dilute dislocations: Direct limit!



- Limiting energy:

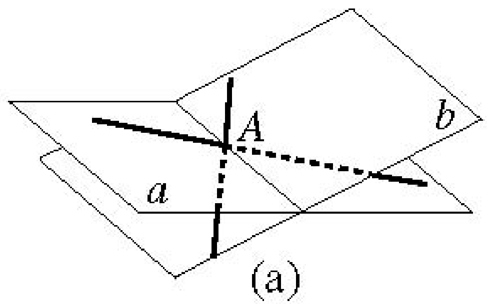
$$\Gamma\text{-}\lim_{h\to\infty} F_h(\underset{\rightarrow}{\alpha}) = \langle K\underset{\rightarrow}{\alpha}, \underset{\rightarrow}{\alpha}\rangle$$

$K \equiv$ Prelog. energy tensor

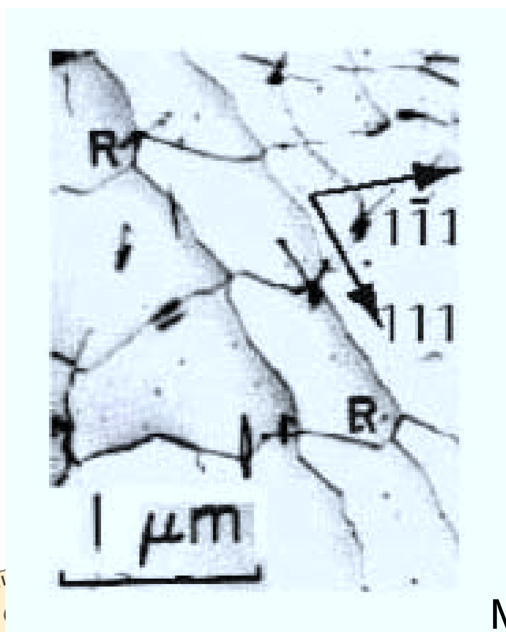
- No long-range interactions in the limit: Line-tension!

M.P. Ariza and M. Ortiz (preprint)

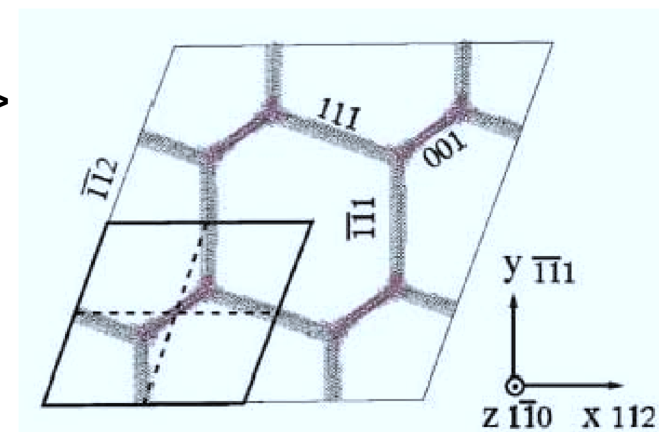
Line tension – Dislocation junctions



a) Dislocation lines on planes *a and b* collide at *A.*
b) Junction bounded by two 3-nodes *B and C is formed.*



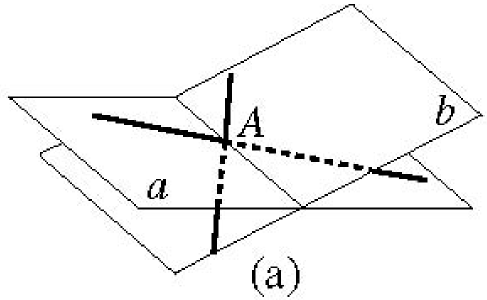
Network of ½<111> screw dislocations forming <001> screw junctions



Atomistic simulations of Bulatov and Cai (2002)

M.P. Ariza and M. Ortiz (preprint)
V.V. Bulatov and W. Cai, *PRL*, **89** (2002) 115501.
H. Matsui and H. Kimura, *Mater. Sci. Eng*., **24** (1976) 247 .

Line tension – Dislocation junctions



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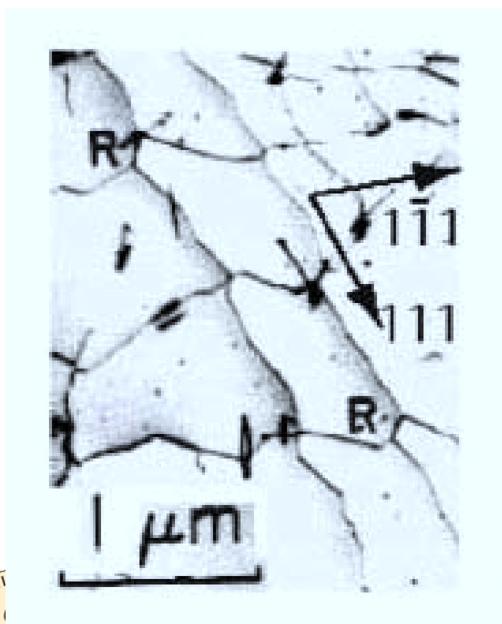

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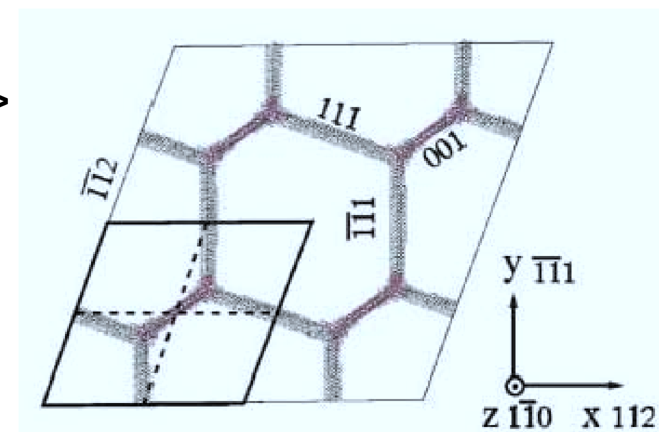

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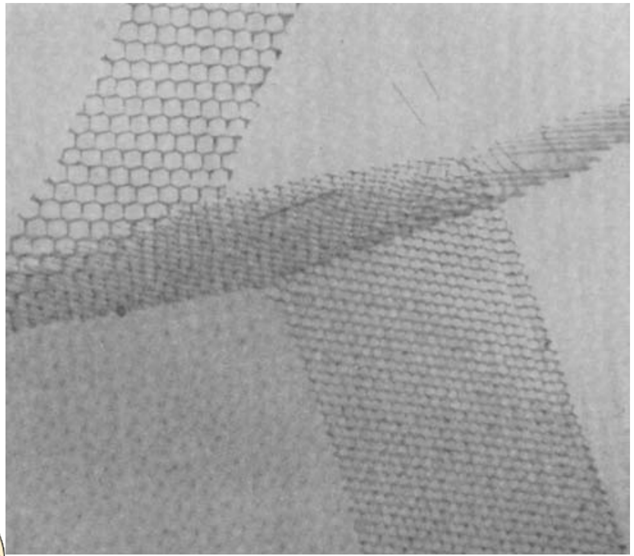
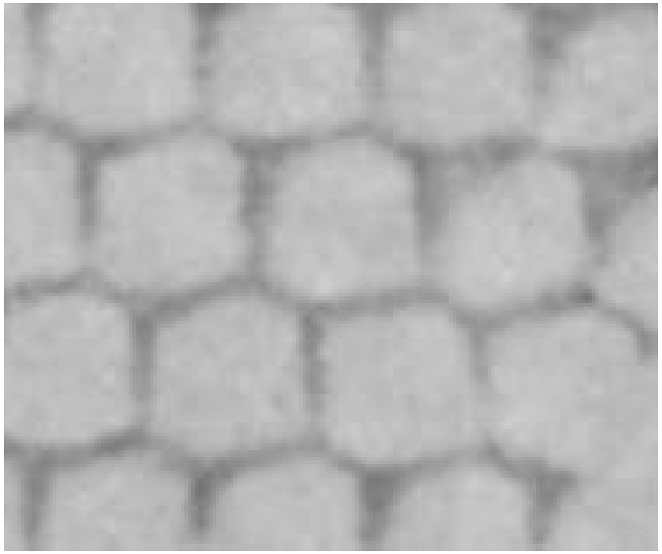
Summary – Outlook

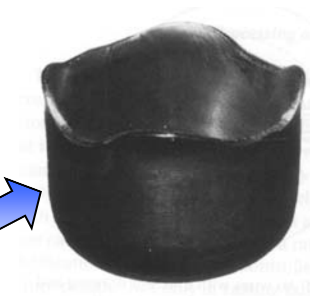
- The stored energy of a crystal reduces to line tension in the dilute limit
- In this limit, long-range interactions between dislocation segments are lost
- Beyond energy? Kinetics?



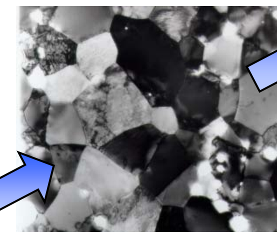


Metal plasticity − Multiscale analysis

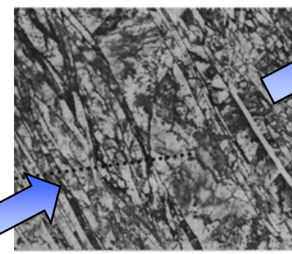
Objective: Derive *ansatz*-free, physics-based, predictive models of macroscopic behavior



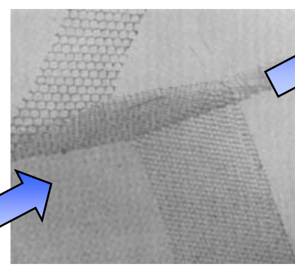
Engineering applications



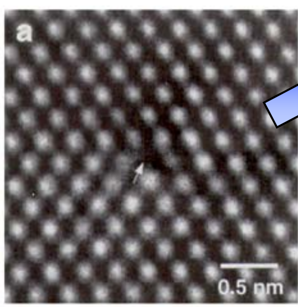
Polycrystals



Subgrain structures ← **Lecture #4**: Subgrain dislocation structures



Dislocation dynamics ← **Lecture #3**: Dislocation kinetics, the forest-hardening model



Lattice defects, EoS ← **Lecture #2**: Dislocation energies, the line-tension approximation

time: ns, μs, ms

length: nm, μm, mm