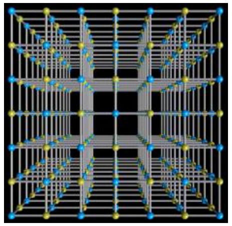
Coarse Graining of Electric Field Interactions with Materials



Prashant Kumar Jha
Ph.D., CMU
prashant.j16o@gmail.com

Adviser
Dr. Kaushik Dayal

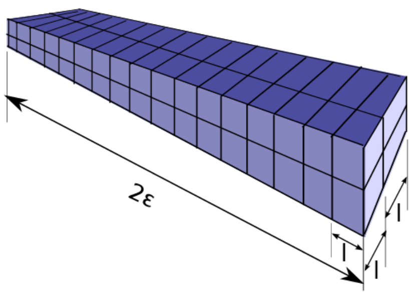
Funded by
Army Research Office

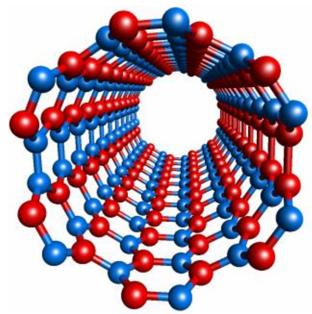
Research Talk
University of Minnesota, Minneapolis

*Figure : http://www.themolecularuniverse.com/mile/mile1.htm

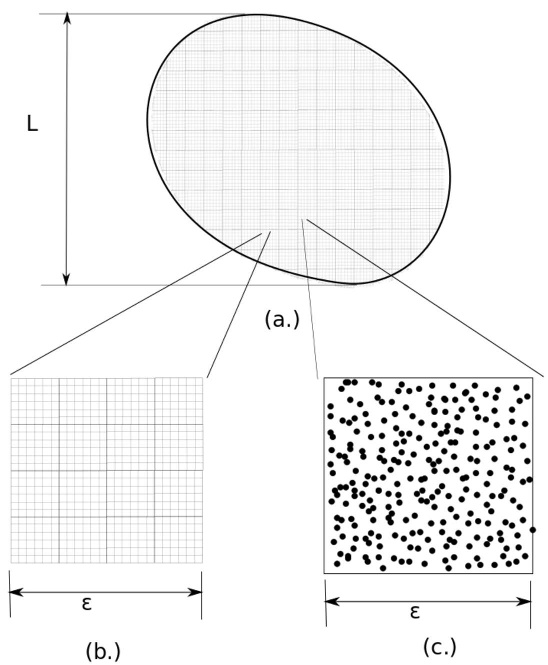
Goal

1. Electrostatics in nanostructures

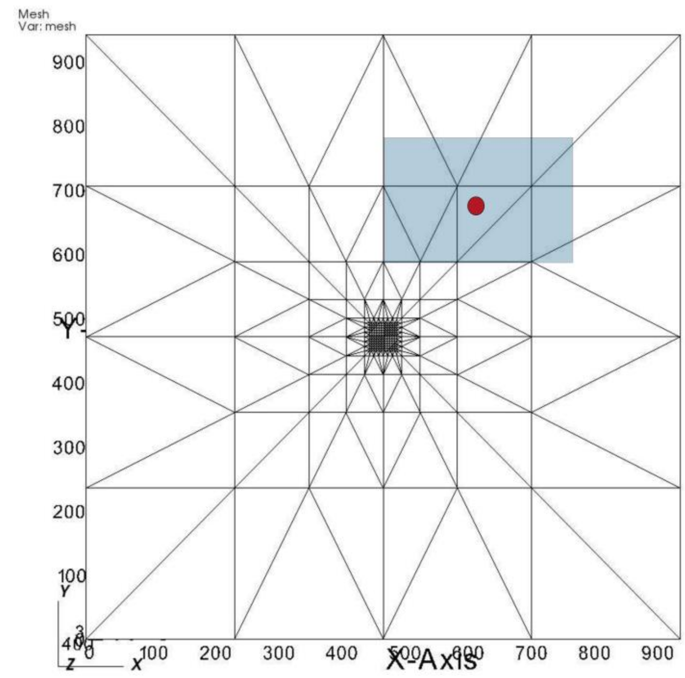




2. Electrostatics in random media



3. Multiscale method for ionic solids at finite temperature



Nanotube Image - http://nano-bio.ehu.es/areas/nanostructures-and-nanotubes

Motivation

- Electrostatics interaction
  - Storage devices
  - Ferroelectric RAM
  - Piezoelectric sensors
- Finite temperature
  - Thermal fluctuations of atoms
  - Coupling of deformation, electric field with temperature

(a) Hard drive

(b) Ferroelectric RAM

(c) Piezoelectric sensor

(a) http://phys.org/news/2009-10-hard_1.html
(b) http://abdulmoeez55.blogspot.com/2015/12/ferroelectric-ram.html
(c) http://www.meas-spec.com/product/piezo/MiniSense_100NM.aspx

Long range interactions

$$\text{Energy density at X} = \int_Y G(X,Y) f(Y) dY$$

Field at X due to charge/dipole at Y

Charge/dipole at Y

Expansion of kernel G for charge distribution

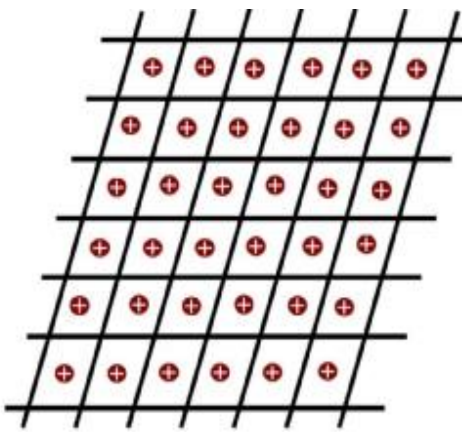
$$\frac{1}{|\boldsymbol{x} - (\boldsymbol{y} + \boldsymbol{y}_0)|} = \frac{1}{|\boldsymbol{x} - \boldsymbol{y}_0|} + \left[\frac{\partial}{\partial \boldsymbol{z}} \frac{1}{|\boldsymbol{z}|}\right]_{\boldsymbol{z}=\boldsymbol{x}-\boldsymbol{y}_0} \cdot \boldsymbol{y} + \left[\frac{\partial^2}{\partial \boldsymbol{z}^2} \frac{1}{|\boldsymbol{z}|}\right]_{\boldsymbol{z}=\boldsymbol{x}-\boldsymbol{y}_0} : \boldsymbol{y} \otimes \boldsymbol{y} + \ldots$$

Long range interactions…

$$\text{Energy density at X} = \int_Y G(X,Y)f(Y)dY$$

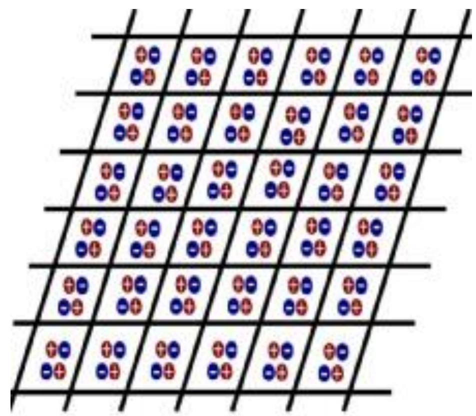
Field at X due to charge/dipole at Y

Charge/dipole at Y



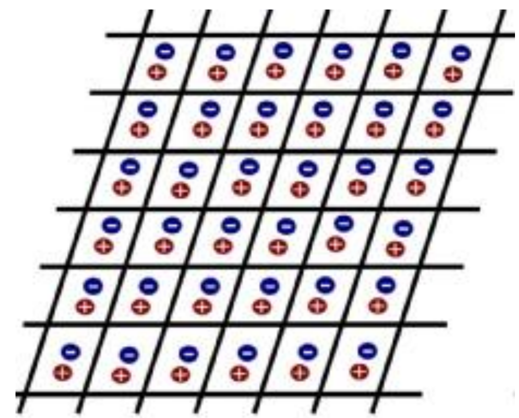
Charge distribution

$$W \approx \sum_{r=1}^{\infty} 1/r \times r^2 = \sum_{r=1}^{\infty} r$$



Quadrupole distribution

$$W \approx \sum_{r=1}^{\infty} 1/r^5 \times r^2 = \sum_{r=1}^{\infty} 1/r^3$$



Dipole distribution

$$W \approx \sum_{r=1}^{\infty} 1/r^3 \times r^2 = \sum_{r=1}^{\infty} 1/r$$

Figure: Marhsall and Dayal 2013

Long range interactions…

Linear Elasticity → $$W(\boldsymbol{x}) = \frac{1}{2}\boldsymbol{\epsilon}(\boldsymbol{x}) \cdot \mathbb{C}\boldsymbol{\epsilon}(\boldsymbol{x})$$

Electrostatics → $$W(\boldsymbol{x}) = \boldsymbol{\nabla}\phi(\boldsymbol{x}) \cdot \boldsymbol{\nabla}\phi(\boldsymbol{x})$$

$$\boldsymbol{\nabla} \cdot \boldsymbol{\nabla}\phi = \boldsymbol{\nabla} \cdot \boldsymbol{p}$$

Energy density depends on polarization field over whole material domain

Long range interactions...

$$\mathrm{E} = V(\boldsymbol{q}) + \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{n}\frac{Q_i Q_j}{|\boldsymbol{q}_i - \boldsymbol{q}_j|}$$

Continuum limit of electrostatic energy

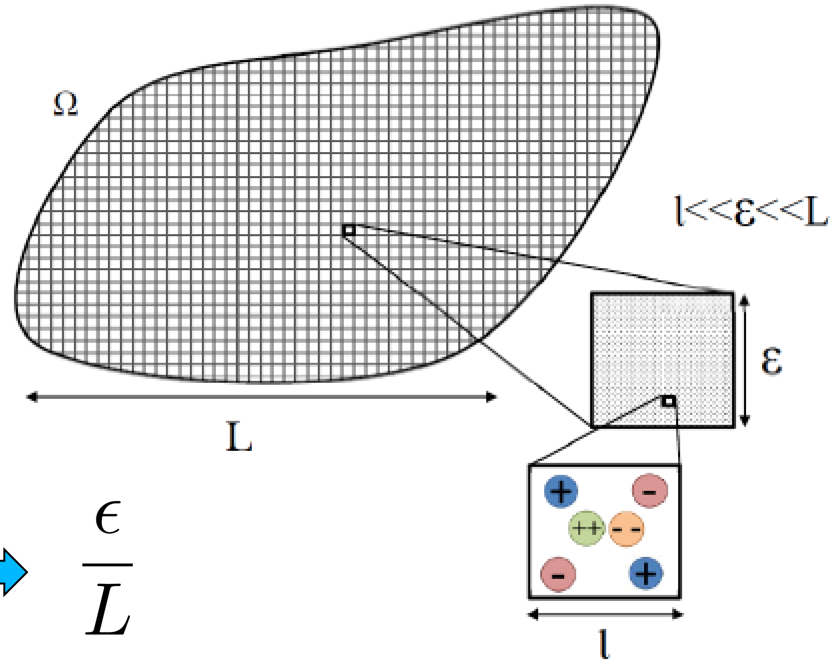
$$\mathrm{E} = V(\boldsymbol{q}) + \frac{1}{2}\int_{\mathbb{R}^3} |\boldsymbol{\nabla}\phi|^2$$

$$\nabla^2\phi = \boldsymbol{\nabla}\cdot\boldsymbol{p} \quad \in \mathbb{R}^3, \boldsymbol{p} = \mathbf{0} \quad \in \mathbb{R}^3 - \Omega$$

$\boldsymbol{p}$: polarization field in a material

Length scales

- Continuum Length scale : L
- Size of material point : ϵ
- Atomic spacing : l



Macroscopic field vary at the scale → $\dfrac{\epsilon}{L}$

Interested in limit

- **Continuum mechanics** → $\epsilon << L$

  Fields vary at fine scale compared to size of material

- **Continuum limit approximations** → $l << \epsilon$

  Atomic spacing is fine compared to scale at which fields vary

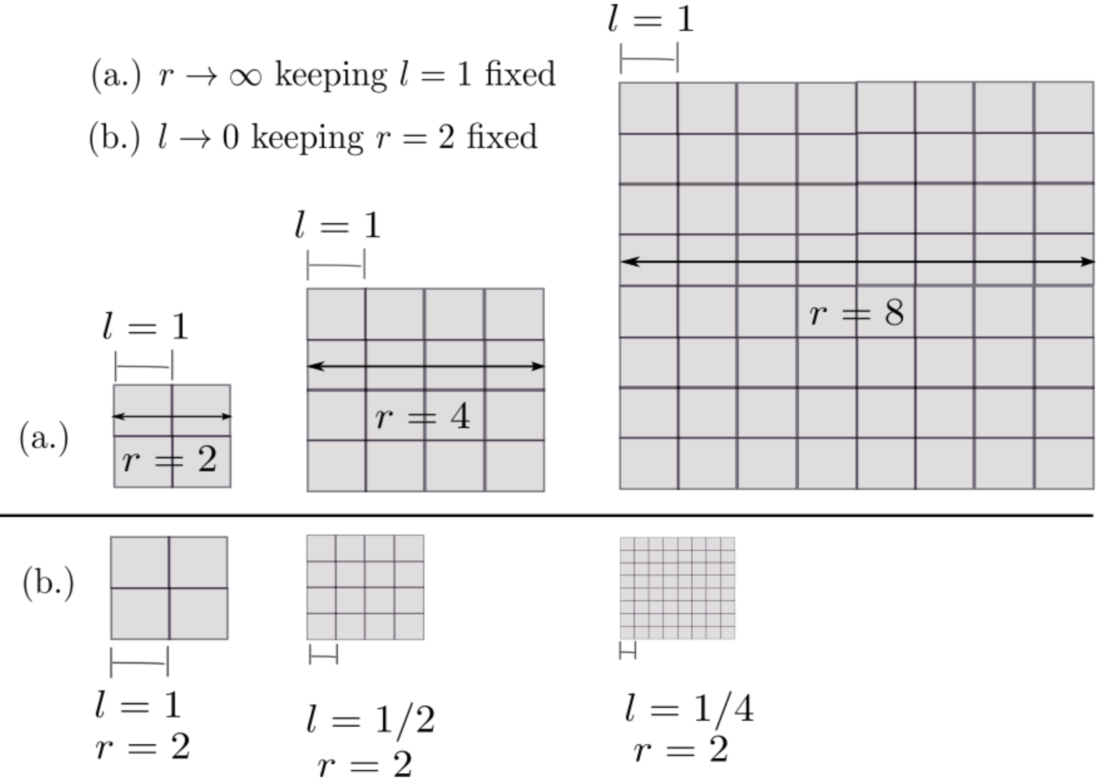
Figure: Marhsall and Dayal 2013

Continuum limit

$$E_{limit} = \lim_{r\to\infty}\left\{\frac{1}{vol(B_r(\mathbf{0}))}\sum_{i,j}\Phi(\boldsymbol{x}_i - \boldsymbol{x}_j)\right\}$$

Average energy of atoms in Sphere $B_r(0)$

Two equivalent approach



Scaled potential

$$\Phi_l(\boldsymbol{x}) = \Phi\left(\frac{\boldsymbol{x}}{l}\right)$$

Continuum limit...

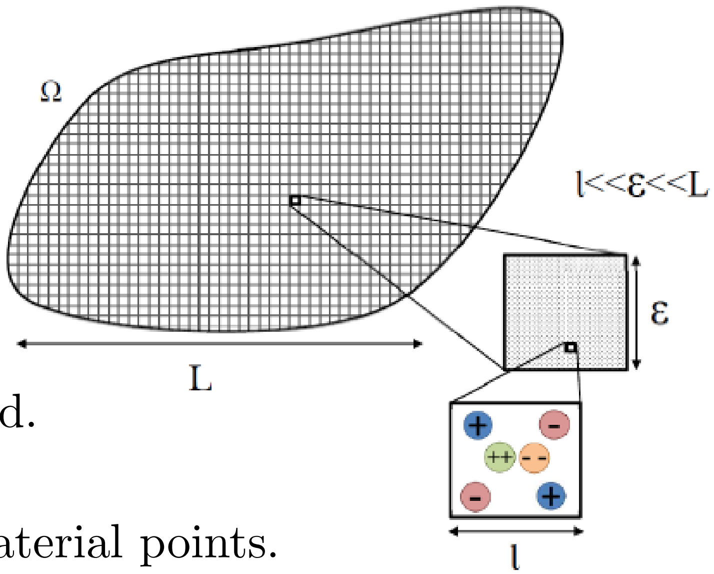
Energy of domain

$$E(\Omega) \approx vol(\Omega) \times E_{limit}$$

Accuracy increases as

$\dfrac{diam(\Omega)}{l}$ **increases**

Electrostatics energy: Periodic media



In Marshall and Dayal [1], the periodic media is considered.

- Ω material domain, $\Omega_\epsilon = \Omega \cap (\epsilon\mathbb{Z})^3$ be discrete set of material points.
- Let $B_\epsilon(\boldsymbol{x}) \subset \mathbb{R}^3$ be the sphere of radius ϵ, at material point $\boldsymbol{x} \in \Omega$.
- Let $\rho : \Omega \times \mathbb{R}^3 \to \mathbb{R}$ be a charge density field. It satisfies following

$$\rho(\boldsymbol{x}, \boldsymbol{y} + \boldsymbol{z}) = \rho(\boldsymbol{x}, \boldsymbol{y}) \qquad \forall \boldsymbol{y} \in [0,1]^3, \boldsymbol{z} \in \mathbb{Z}^3$$

- Let ρ_l be associated to atomic length scale l. We assume

$$\rho_l(\boldsymbol{x}, \boldsymbol{y}, \omega) = \rho(\boldsymbol{x}, \frac{\boldsymbol{y}}{l}, \omega)$$

Figure: Marhsall and Dayal 2013

Scaling on charge density field: Periodic media

Electrostatics energy

- $$E = \sum_{\substack{\boldsymbol{x}\in\Omega_\epsilon \\ \boldsymbol{x}'\in\Omega_\epsilon}} \int_{\substack{\boldsymbol{z}\in B_\epsilon(\boldsymbol{x}), \\ \boldsymbol{z}'\in B_\epsilon(\boldsymbol{x}')}} \frac{\rho_l(\boldsymbol{x},\boldsymbol{z})\rho_l(\boldsymbol{x}',\boldsymbol{z}')}{|\boldsymbol{x}+\boldsymbol{z}-\boldsymbol{x}'-\boldsymbol{z}'|} dV_{\boldsymbol{z}} dV_{\boldsymbol{z}'}$$
$$= E_{local} + E_{nonlocal}$$

- $$E_{local} = \sum_{\boldsymbol{x}\in\Omega_\epsilon} \epsilon^3 \left(l^2 \int_{\substack{\boldsymbol{z}\in U, \\ \boldsymbol{z}'\in B_\epsilon/l(\boldsymbol{x})}} \frac{\rho(\boldsymbol{x},\boldsymbol{z})\rho(\boldsymbol{x},\boldsymbol{z}')}{|\boldsymbol{z}-\boldsymbol{z}'|} dV_{\boldsymbol{z}} dV_{\boldsymbol{z}'} \right) \rightarrow \rho_l(\boldsymbol{x},\boldsymbol{y}) = \frac{\rho(\boldsymbol{x},\boldsymbol{y}/l)}{l}$$

Energy of one unit cell due to charge distribution in material point x

Continuum limit and two scale homogenization

- *The general theory of homogenization* by Tartar 2010.
- *Homogenization and two-scale convergence* by Allaire 1992.
- *Modeling materials: Continuum, atomistic, and multiscale techniques* by Tadmor and Miller 2011.
- *On the Cauchy-Born rule* by Ericksen 2008.
- *The elastic dielectric* by Toupin 1956.
- *Internal variables and fine-scale oscillations in micromagnetics* by James and Muller 1994.
- *Micromagnetics of very thin films* by Gioia and James 1997.
- *From molecular models to continuum mechanics* by Blanc, Le Bris, and Lions 2002.

Homogenization with random fields

- In Blanc, Le Bris, and Lions 2007, they consider the homogenization of short range atomic forces for random media.

- In Blanc, Lions, Legoll, and Patz 2010, homogenization in one-d is considered. The thermal fluctuations are modeled as random field. Other related works are: Blanc, Le Bris, and Lions 2007.

- Chapter 7 of Jikov, Kozlov, and Oleinik 1994 gives brief introduction to stationarity and ergodicity and considers the homogenization of Poissons equation with random coefficient.

$$\nabla \cdot (a(x/\epsilon)\nabla u(x)) = f(x)$$

- In chapter 3 of Bensoussan, Lions, and Papanicolaou, stochastic homogenization of Poissons equation and diffusion equation is considered.

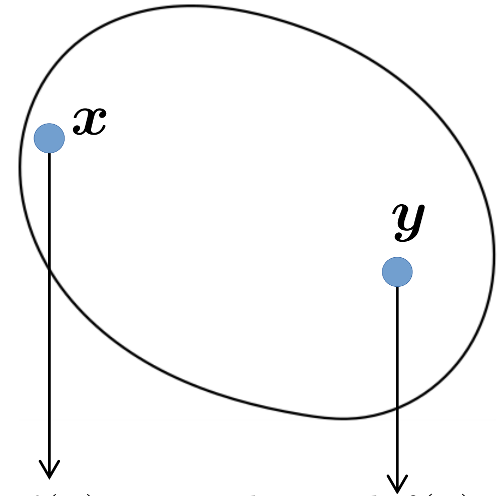
- A book "Random heterogeneous materials" by Salvatore 2002 is another reference on materials with randomness.

Stationary and Ergodic random field

Stationarity

- $f : \Omega \times D \to \mathbb{R}$
- $\mathbb{E}[f(\boldsymbol{x}, \cdot)] = \int f(\boldsymbol{x}, \omega) d\mu(\omega)$ is independent of $\boldsymbol{x}$

Similar to periodic media
average over unit cell is independent of unit cell



observed $f(\boldsymbol{x})$ $= \int f(\boldsymbol{x}, \omega) d\mu(\omega)$

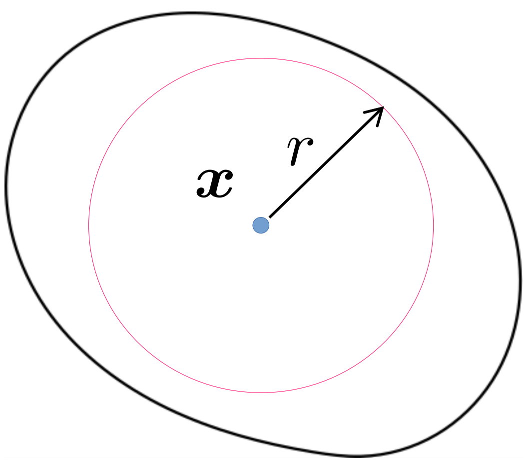
observed $f(\boldsymbol{y})$ $= \int f(\boldsymbol{y}, \omega) d\mu(\omega)$

Ergodicity

- $$\int_{\omega \in D} f(\boldsymbol{x}, \omega) d\mu(\omega) = \lim_{r \to \infty} \frac{1}{\mathrm{vol}(B_r(\boldsymbol{x}))} \int_{\boldsymbol{y} \in B_r(\boldsymbol{x})} f(\boldsymbol{y}, \omega) dV_{\boldsymbol{x}}$$

Spatial average

$$= \frac{1}{c} \lim_{l \to 0} \int_{\boldsymbol{y} \in B_1(\boldsymbol{x})} f(\boldsymbol{y}/l, \omega) d\mu(\omega)$$



Dynamical system

We follow Jikov, Kozlov, and Oleinik 1994 as a reference for probability theory.

- Stationary random fields are described using linear transformation on D.

- Family of $(T_{\boldsymbol{x}})_{\boldsymbol{x}\in\mathbb{R}^3}$ are called dynamical system with 3-dimensional time if
  - $T_{\boldsymbol{x}+\boldsymbol{y}} = T_{\boldsymbol{x}}T_{\boldsymbol{y}}$
  - $\mu(T_{\boldsymbol{x}}A) = \mu(A)$
  - If $\psi : D \to \mathbb{R}$ is measureable then $f : \mathbb{R}^3 \times D \to \mathbb{R}$ as defined below is also measureable

$$f(\boldsymbol{x}, \omega) = \psi(T_{\boldsymbol{x}}\omega)$$

- If $f : \mathbb{R}^3 \times D \to \mathbb{R}$ is stationary then $\exists(T_{\boldsymbol{x}})$ and $\bar{f} : D \to \mathbb{R}$ such that

$$f(\boldsymbol{x}, \omega) = \bar{f}(T_{\boldsymbol{x}}\omega)$$

- Dynamical system T is ergodic if

$$(\forall \boldsymbol{y} \in \mathbb{R}^3)\ \psi(T_{\boldsymbol{y}}\omega) = \psi(\omega) \Rightarrow \psi(\omega) = \text{constant}$$

Fix any $\omega_0 \in D$, then for all $\omega \in D$ there exists $\boldsymbol{x} \in \mathbb{R}^3$ such that

$$\omega = T_{\boldsymbol{x}}\omega_0$$

Examples

Periodic field

Let $D = [0,1]^3$. Let $T_{\boldsymbol{z}}$ be defined as

$$T_{\boldsymbol{z}}\omega = \boldsymbol{z} + \omega \; (mod \; 1) \qquad \forall \omega \in D$$

If $\rho : \mathbb{R}^3 \times D \to \mathbb{R}$ is stationary with $\bar{\rho}$ given by $\rho(\boldsymbol{z}, \omega) = \bar{\rho}(T_{\boldsymbol{z}}\omega)$, then

$$\rho(\boldsymbol{y} + \boldsymbol{z}, \omega) = \bar{\rho}(T_{\boldsymbol{y}+\boldsymbol{z}}\omega) = \bar{\rho}(T_{\boldsymbol{y}}\omega) = \rho(\boldsymbol{y}, \omega) \qquad \forall \boldsymbol{y} \in \mathbb{R}^3, \boldsymbol{z} \in \mathbb{Z}^3$$

Quasiperiodic field

Let $D = [0,1]^3$. Let M be 3×3 matrix. Let $T_{\boldsymbol{z}}$ be defined as

$$T_{\boldsymbol{z}}\omega = M\boldsymbol{z} + \omega \; (mod \; 1) \qquad \forall \omega \in D$$

Birkhoff Ergodic theorem

Let $f : \Omega \times \mathbb{R}^3 \times D \to \mathbb{R}$ is in $L^p[\Omega, L^1_{loc}(\mathbb{R}^3)]$ for a.e. $\omega \in D$.

We define the mean value $M[f(\boldsymbol{x}, \omega)]$ of f in $\mathbb{R}^3$

$$M[f(\boldsymbol{x}, \omega)] := \lim_{r \to \infty} \frac{1}{|B_r(\boldsymbol{0})|} \int_{B_r(\boldsymbol{0})} f(\boldsymbol{x}, \boldsymbol{y}, \omega) d\boldsymbol{y}, \quad \text{a.e. } \boldsymbol{x}$$

Theorem 1 *Let $\psi : \Omega \times D \to \mathbb{R} \in L^p[\Omega, L^\alpha(D)]$, $p, \alpha \geq 1$. Then for almost all $\omega \in D$, and for almost all $\boldsymbol{x} \in \Omega$, the realization $\psi(\boldsymbol{x}, T_{\boldsymbol{y}}\omega)$, as a function of $\boldsymbol{x} \in \Omega$ and $\boldsymbol{y} \in \mathbb{R}^3$, has a mean value $M[\psi(\boldsymbol{x}, T\omega)]$ defined as below*

$$M[\psi(\boldsymbol{x}, T\omega)] = \lim_{r \to \infty} \frac{1}{|B_1(\boldsymbol{0})|} \int_{B_1(\boldsymbol{0})} \psi(\boldsymbol{x}, T_{\boldsymbol{y}}\omega) d\boldsymbol{y}$$

Further, $M[\psi(\boldsymbol{x}, T\omega)]$, as a random process in $\Omega \times D$, is invariant and satisfies following relation

$$\mathbb{E}[\psi(\boldsymbol{x}, \cdot)] = \int_D \psi(\boldsymbol{x}, \omega) d\mu(\omega) = \int_D M[\psi(\boldsymbol{x}, T\omega)] d\mu(\omega) \qquad \forall \boldsymbol{x}$$

If T is ergodic dynamical system, then we have

$$M[\psi(\boldsymbol{x}, T\omega)] = \mathbb{E}[\psi(\boldsymbol{x}, \cdot)] \quad \textit{a.e. } \boldsymbol{x} \textit{ a.e. } \omega$$

(1) Chapter 7, Theorem 7.2 Jikov, Kozlov, and Oleinik 1994 . (2) Linear Operators by Dunford and Schwartz.

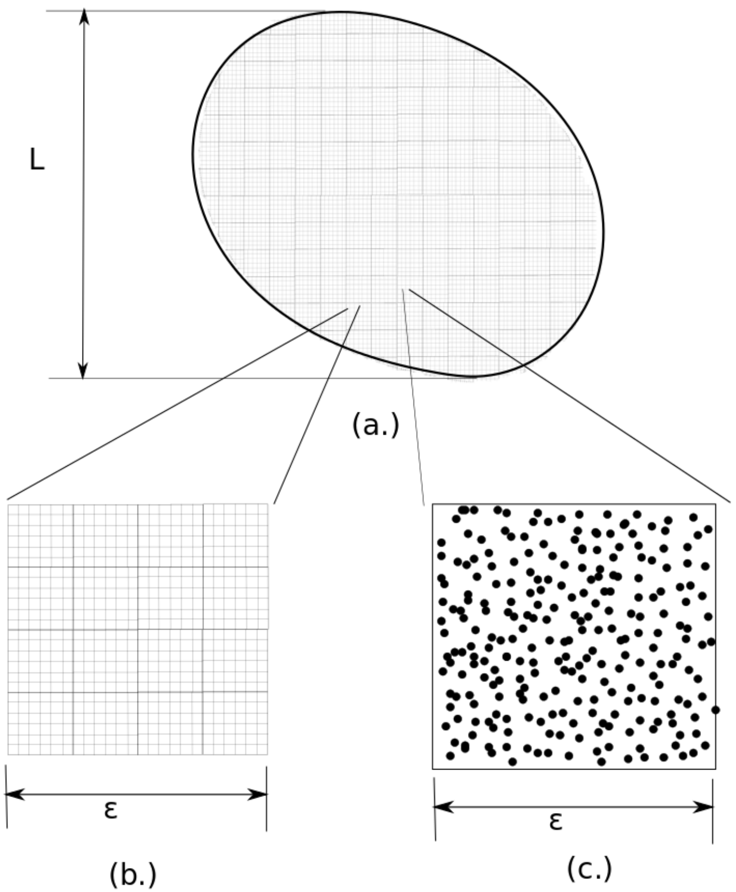
Random media: Charge density field

- Ω material domain, $\Omega_\epsilon = \Omega \cap (\epsilon\mathbb{Z})^3$ be discrete set of material points.
- Let $B_\epsilon(\boldsymbol{x}) \subset \mathbb{R}^3$ be the sphere of radius ϵ.
- Let $\rho : \Omega \times \mathbb{R}^3 \times D \to \mathbb{R}$ be a random process.
- Assumption:

(1) electric potential $\phi : \Omega \times \mathbb{R}^3 \to \mathbb{R}$ is well defined where

$$\phi(\boldsymbol{x}, \boldsymbol{z}, \omega) := \frac{4\pi}{3} \int_{\mathbb{R}^3} \frac{\rho(\boldsymbol{x}, \boldsymbol{z}', \omega)}{|\boldsymbol{z} - \boldsymbol{z}'|} dV_{\boldsymbol{z}'}$$

(2) ρ is ergodic and stationary.



- $\{T_{\boldsymbol{x}} : \boldsymbol{x} \in \mathbb{R}^3\}$ is ergodic dynamical system and $\bar{\rho} : \Omega \times D \to \mathbb{R}$ is another random process such that

$$\rho(\boldsymbol{x}, \boldsymbol{z}, \omega) = \bar{\rho}(\boldsymbol{x}, T_{\boldsymbol{z}}\omega) \; \forall \boldsymbol{z} \in \mathbb{R}^3, \omega \in D$$

Random media: Electrostatic energy

- Let ρ_l be associated to atomic length scale l. We assume

$$\rho_l(\boldsymbol{x}, \boldsymbol{y}, \omega) = \rho(\boldsymbol{x}, \frac{\boldsymbol{y}}{l}, \omega) = \bar{\rho}(\boldsymbol{x}, T_{\boldsymbol{y}/l}\omega)$$

- $$E(\omega) = \sum_{\substack{\boldsymbol{x}\in\Omega_\epsilon \\ \boldsymbol{x}'\in\Omega_\epsilon}} \int_{\substack{\boldsymbol{z}\in B_\epsilon(\boldsymbol{x}), \\ \boldsymbol{z}'\in B_\epsilon(\boldsymbol{x}')}} \frac{\rho_l(\boldsymbol{x}, \boldsymbol{z}, \omega)\rho_l(\boldsymbol{x}', \boldsymbol{z}', \omega)}{|\boldsymbol{x}+\boldsymbol{z}-\boldsymbol{x}'-\boldsymbol{z}'|} dV_{\boldsymbol{z}} dV_{\boldsymbol{z}'} = E_{local} + E_{nonlocal}$$

- $$E_{local} = \sum_{\boldsymbol{x}\in\Omega_\epsilon} \int_{\boldsymbol{z},\boldsymbol{z}'\in B_\epsilon(\boldsymbol{x})} \frac{\rho_l(\boldsymbol{x}, \boldsymbol{z}, \omega)\rho_l(\boldsymbol{x}, \boldsymbol{z}', \omega)}{|\boldsymbol{z}-\boldsymbol{z}'|} dV_{\boldsymbol{z}} dV_{\boldsymbol{z}'}$$

- $$E_{nonlocal} = \sum_{\substack{\boldsymbol{x},\boldsymbol{x}'\in\Omega_\epsilon, \\ \boldsymbol{x}\neq\boldsymbol{x}'}} \int_{\substack{\boldsymbol{z}\in B_\epsilon(\boldsymbol{x}), \\ \boldsymbol{z}'\in B_\epsilon(\boldsymbol{x}')}} \frac{\rho_l(\boldsymbol{x}, \boldsymbol{z}, \omega)\rho_l(\boldsymbol{x}', \boldsymbol{z}', \omega)}{|\boldsymbol{x}+\boldsymbol{z}-\boldsymbol{x}'-\boldsymbol{z}'|} dV_{\boldsymbol{z}} dV_{\boldsymbol{z}'}$$

Random media: Local energy

$$E_{local} = \sum_{\boldsymbol{x}\in\Omega_\epsilon} \int_{\boldsymbol{z},\boldsymbol{z}'\in B_\epsilon(\boldsymbol{x})} \frac{\rho_l(\boldsymbol{x},\boldsymbol{z},\omega)\rho_l(\boldsymbol{x},\boldsymbol{z}',\omega)}{|\boldsymbol{z}-\boldsymbol{z}'|} dV_{\boldsymbol{z}} dV_{\boldsymbol{z}'}$$

Change in variable $\boldsymbol{y} = \boldsymbol{z}/l$ and $\rho_l(\boldsymbol{x},\boldsymbol{y},\omega) = \rho(\boldsymbol{x},\boldsymbol{y}/l,\omega)$

$$= \sum_{\boldsymbol{x}\in\Omega_\epsilon} \int_{\boldsymbol{z},\boldsymbol{z}'\in B_{\epsilon/l}(\boldsymbol{x})} l^5 \frac{\rho(\boldsymbol{x},\boldsymbol{z},\omega)\rho(\boldsymbol{x},\boldsymbol{z}',\omega)}{|\boldsymbol{z}-\boldsymbol{z}'|} dV_{\boldsymbol{z}} dV_{\boldsymbol{z}'}$$

$$= \sum_{\boldsymbol{x}\in\Omega_\epsilon} \frac{|B_{\epsilon/l}(\boldsymbol{x})|}{|B_{\epsilon/l}(\boldsymbol{x})|} l^5 \int_{\boldsymbol{z}\in B_{\epsilon/l}(\boldsymbol{x})} \rho(\boldsymbol{x},\boldsymbol{z},\omega) \left(\int_{\boldsymbol{z}'\in B_{\epsilon/l}(\boldsymbol{x})} \frac{\rho(\boldsymbol{x},\boldsymbol{z}',\omega)}{|\boldsymbol{z}-\boldsymbol{z}'|} dV_{\boldsymbol{z}'} \right) dV_{\boldsymbol{z}}$$

$$\frac{3}{4\pi}\phi(\boldsymbol{x},\boldsymbol{z},\omega)$$

$$= \sum_{\boldsymbol{x}\in\Omega_\epsilon} \frac{|B_{\epsilon/l}(\boldsymbol{x})|}{|B_{\epsilon/l}(\boldsymbol{x})|} l^5 \int_{\boldsymbol{z}\in B_{\epsilon/l}(\boldsymbol{x})} \rho(\boldsymbol{x},\boldsymbol{z},\omega) \left(\int_{\boldsymbol{z}'\in \mathbb{R}^3} \frac{\rho(\boldsymbol{x},\boldsymbol{z}',\omega)}{|\boldsymbol{z}-\boldsymbol{z}'|} dV_{\boldsymbol{z}'} \right) dV_{\boldsymbol{z}} \rightarrow I_1$$

$$- \sum_{\boldsymbol{x}\in\Omega_\epsilon} \frac{|B_{\epsilon/l}(\boldsymbol{x})|}{|B_{\epsilon/l}(\boldsymbol{x})|} l^5 \int_{\boldsymbol{z}\in B_{\epsilon/l}(\boldsymbol{x})} \rho(\boldsymbol{x},\boldsymbol{z},\omega) \left(\int_{\boldsymbol{z}'\in \mathbb{R}^3 - B_{\epsilon/l}(\boldsymbol{x})} \frac{\rho(\boldsymbol{x},\boldsymbol{z}',\omega)}{|\boldsymbol{z}-\boldsymbol{z}'|} dV_{\boldsymbol{z}'} \right) dV_{\boldsymbol{z}} \rightarrow I_2$$

Random media: Local energy...

$\phi(\boldsymbol{x}, \boldsymbol{y}, \omega)$ is ergodic and stationary, .i.e. there exists $\bar{\phi}$ such that

$$\phi(\boldsymbol{x}, \boldsymbol{z}, \omega) = \bar{\phi}(\boldsymbol{x}, T_{\boldsymbol{z}}\omega)$$

We prove this as follows: define $\bar{\phi}(\boldsymbol{x}, \omega) := \phi(\boldsymbol{x}, \boldsymbol{0}, \omega)$. Using change in variable in definition of ϕ, we get

$$\boldsymbol{y} = \boldsymbol{z}' - \boldsymbol{z}$$

$$\begin{aligned}
\phi(\boldsymbol{z}, \boldsymbol{z}, \omega) &= \int_{\mathbb{R}^3} \frac{\rho(\boldsymbol{x}, \boldsymbol{z}', \omega)}{|\boldsymbol{z}' - \boldsymbol{z}|} dV_{\boldsymbol{z}'} \\
&= \frac{4\pi}{3} \int_{\mathbb{R}^3} \frac{\rho(\boldsymbol{x}, \boldsymbol{y} + \boldsymbol{z}, \omega)}{|\boldsymbol{y}|} dV_{\boldsymbol{y}} \\
&= \frac{4\pi}{3} \int_{\mathbb{R}^3} \frac{\rho(\boldsymbol{x}, \boldsymbol{y}, T_{\boldsymbol{z}}\omega)}{|\boldsymbol{y}|} dV_{\boldsymbol{y}} \\
&= \phi(\boldsymbol{x}, \boldsymbol{0}, T_{\boldsymbol{z}}\omega) \\
&= \bar{\phi}(\boldsymbol{x}, T_{\boldsymbol{z}}\omega)
\end{aligned}$$

where we have used the group property of T, $T_{\boldsymbol{x}+\boldsymbol{y}} = T_{\boldsymbol{x}} T_{\boldsymbol{y}}$, as follwos

$$\rho(\boldsymbol{x}, \boldsymbol{y} + \boldsymbol{z}, \omega) = \rho(\boldsymbol{x}, T_{\boldsymbol{y}+\boldsymbol{z}}\omega) = \rho(\boldsymbol{x}, T_{\boldsymbol{y}}(T_{\boldsymbol{z}}\omega)) = \rho(\boldsymbol{x}, \boldsymbol{y}, T_{\boldsymbol{z}}\omega)$$

Random media: Local energy...

Using Ergodicity theorem, we get

$$\lim_{\epsilon/l\to\infty} \frac{1}{|B_{\epsilon/l}(\boldsymbol{x})|}\int_{\boldsymbol{z}\in B_{\epsilon/l}(\boldsymbol{x})} \rho(\boldsymbol{x},\boldsymbol{z},\omega)\phi(\boldsymbol{x},\boldsymbol{z},\omega)dV_{\boldsymbol{z}}$$
$$= \mathbb{E}\left[\bar{\rho}(\boldsymbol{x},\cdot)\bar{\phi}(\boldsymbol{x},\cdot)\right]$$
$$= \int_{\omega\in D} \bar{\rho}(\boldsymbol{x},\omega)\bar{\phi}(\boldsymbol{x},\omega)d\mu(\omega)$$

Writing I_1 here

$$I_1 = \sum_{\boldsymbol{x}\in\Omega_\epsilon} \epsilon^3 \left[l^2 \left\{ \frac{1}{|B_{\epsilon/l}(\boldsymbol{x})|}\int_{\boldsymbol{z}\in B_{\epsilon/l}(\boldsymbol{x})} \rho(\boldsymbol{x},\boldsymbol{z},\omega)\phi(\boldsymbol{x},\boldsymbol{z},\omega)dV_{\boldsymbol{z}} \right\}\right]$$

- Riemann sum:

$$\int_\Omega f(\boldsymbol{x})dV_{\boldsymbol{x}} = \lim_{\epsilon/L\to 0}\sum_{\Omega_\epsilon}\epsilon^3 f(\boldsymbol{x})$$

- Term inside curly bracket is bounded

Therefore, the scaled charge density must satisfy following scaling

$$\rho_l(\boldsymbol{x},\boldsymbol{y},\omega) = \frac{\rho(\boldsymbol{x},\boldsymbol{y}/l,\omega)}{l} \quad \longrightarrow \quad I_1 = \int_\Omega \mathbb{E}[\bar{\rho}(\boldsymbol{x},\cdot)\bar{\phi}(\boldsymbol{x},\cdot)]dV_{\boldsymbol{x}}$$

Random media: Local energy...

$$E_{local} = \int_D \left[\int_{\boldsymbol{x}\in\Omega} \left(\int_{\mathbb{R}^3} \frac{\rho(\boldsymbol{x},\mathbf{0},\omega)\rho(\boldsymbol{x},\boldsymbol{z}',\omega)}{|\mathbf{0}-\boldsymbol{z}'|} dV_{\boldsymbol{z}'} \right) dV_{\boldsymbol{x}} \right] d\mu(\omega)$$

$$= \mathbb{E}\left[\text{realization of local energy corresponding to event } \omega\right]$$

Random media: Non-local energy

After change of variable and dividing and multiplying $\mathrm{vol}(B_{\epsilon/l}(\boldsymbol{x}))\,\mathrm{vol}(B_{\epsilon/l}(\boldsymbol{x}'))$

$$E_{nonlocal} = \left(\frac{4\pi}{3}\right)^2 \sum_{\substack{\boldsymbol{x},\boldsymbol{x}'\in\Omega_\epsilon,\\ \boldsymbol{x}\neq\boldsymbol{x}'}} \epsilon^6 \left(\frac{1}{l^2} \frac{1}{|B_{\epsilon/l}(\boldsymbol{x})|} \frac{1}{|B_{\epsilon/l}(\boldsymbol{x}')|} \int_{\substack{\boldsymbol{z}\in B_{\epsilon/l}(\boldsymbol{x}),\\ \boldsymbol{z}'\in B_{\epsilon/l}(\boldsymbol{x}')}} \frac{\rho(\boldsymbol{x},\boldsymbol{z},\omega)\rho(\boldsymbol{x}',\boldsymbol{z}',\omega)}{|\boldsymbol{x}+l\boldsymbol{z}-\boldsymbol{x}'-l\boldsymbol{z}'|} dV_{\boldsymbol{z}} dV_{\boldsymbol{z}'} \right)$$

Taylor's series expansion

$$\frac{1}{|\boldsymbol{x}+l\boldsymbol{z}-\boldsymbol{x}'-l\boldsymbol{z}'|} = \frac{1}{|\boldsymbol{x}-\boldsymbol{x}'|} + \left[\frac{\partial}{\partial \boldsymbol{y}}\frac{1}{|\boldsymbol{y}|}\right]_{\boldsymbol{y}=\boldsymbol{x}-\boldsymbol{x}'} l\cdot(\boldsymbol{z}-\boldsymbol{z}') + \left[\frac{\partial^2}{\partial \boldsymbol{y}^2}\frac{1}{|\boldsymbol{y}|}\right]_{\boldsymbol{y}=\boldsymbol{x}-\boldsymbol{x}'} l^2 : (\boldsymbol{z}-\boldsymbol{z}')\otimes(\boldsymbol{z}-\boldsymbol{z}') + O(l^3)$$

Second order term

Zeroth order term

$$\frac{1}{l^2}\left\{\frac{1}{|B_{\epsilon/l}(\boldsymbol{x})|}\int_{\boldsymbol{z}\in B_{\epsilon/l}(\boldsymbol{x})} \rho(\boldsymbol{x},\boldsymbol{z},\omega)dV_{\boldsymbol{z}}\right\} \times \left\{\frac{1}{|B_{\epsilon/l}(\boldsymbol{x}')|}\int_{\boldsymbol{z}'\in B_{\epsilon/l}(\boldsymbol{x}')} \rho(\boldsymbol{x}',\boldsymbol{z}',\omega)dV_{\boldsymbol{z}'}\right\}$$

Go to infinity, unless term in bracket is zero

Charge neutrality condition

$$\lim_{\epsilon/l\to\infty} \frac{1}{|B_{\epsilon/l}(\boldsymbol{x})|}\int_{\boldsymbol{z}\in B_{\epsilon/l}(\boldsymbol{x})} \rho(\boldsymbol{x},\boldsymbol{z},\omega)dV_{\boldsymbol{z}} = 0 \quad \forall \boldsymbol{x}\in\Omega$$

↓ By Ergodic theorem

$$\mathbb{E}[\rho(\boldsymbol{x},\boldsymbol{y},)] = 0 \quad \forall \boldsymbol{x}\in\Omega, \boldsymbol{y}\in\mathbb{R}^3$$

Random media: Non-local energy...

$$E_{nonlocal}$$

$$= \sum_{\substack{\boldsymbol{x},\boldsymbol{x}'\in\Omega_\epsilon,\\ \boldsymbol{x}\neq\boldsymbol{x}'}} \epsilon^6 \mathbb{K}(\boldsymbol{x}-\boldsymbol{x}') : \left\{ \frac{1}{|B_{\epsilon/l}(\boldsymbol{x})|} \int_{\boldsymbol{z}\in B_{\epsilon/l}(\boldsymbol{x})} \rho(\boldsymbol{x},\boldsymbol{z},\omega)\boldsymbol{z} dV_{\boldsymbol{z}} \right\} \otimes \left\{ \frac{1}{|B_{\epsilon/l}(\boldsymbol{x}')|} \int_{\boldsymbol{z}'\in B_{\epsilon/l}(\boldsymbol{x}')} \rho(\boldsymbol{x}',\boldsymbol{z}',\omega)\boldsymbol{z}' dV_{\boldsymbol{z}'} \right\}$$

$$= \int_{\substack{\boldsymbol{x},\boldsymbol{x}'\in\Omega,\\ \boldsymbol{x}\neq\boldsymbol{x}'}} \mathbb{K}(\boldsymbol{x}-\boldsymbol{x}') : \boldsymbol{p}(\boldsymbol{x},\omega) \otimes \boldsymbol{p}(\boldsymbol{x}',\omega) dV_{\boldsymbol{x}} d_{\boldsymbol{x}'}$$

where, $\boldsymbol{p}(\boldsymbol{x},\omega)$ is a polarization within the material point. It is defined as

$$\boldsymbol{p}(\boldsymbol{x},\omega) = \lim_{r\to\infty} \frac{c}{|B_r(\boldsymbol{x})|} \int_{\boldsymbol{z}\in B_r(\boldsymbol{x})} \rho(\boldsymbol{x},\boldsymbol{z},\omega)\boldsymbol{z} dV_{\boldsymbol{z}}$$

Dipole field kernel $\mathbb{K}(\boldsymbol{x})$ is defined as follows

$$\mathbb{K}(\boldsymbol{x}) := -\frac{1}{4\pi |\boldsymbol{x}|^3} \left\{ \boldsymbol{I} - 3\frac{\boldsymbol{x}}{|\boldsymbol{x}|} \otimes \frac{\boldsymbol{x}}{|\boldsymbol{x}|} \right\},\ \boldsymbol{x} \in \mathbb{R}^3$$

Random media: Non-local energy...

$E_{nonlocal}$ energy is invariant of $\omega \in D$. This will follow if we could show $\boldsymbol{p}$ to be invariant. Using change in variable $\boldsymbol{y} = \boldsymbol{z} - \boldsymbol{z}$, we get

$$\begin{aligned}
\boldsymbol{p}(\boldsymbol{x}, \omega) &= \lim_{r \to \infty} \frac{c}{|B_r(\boldsymbol{x})|} \int_{\boldsymbol{z} \in B_r(\boldsymbol{x})} \rho(\boldsymbol{x}, \boldsymbol{z}, \omega) \boldsymbol{z} dV_{\boldsymbol{z}} \\
&= \lim_{r \to \infty} \frac{c}{|B_r(\boldsymbol{x})|} \int_{\boldsymbol{y} \in B_r(\boldsymbol{x}) - \boldsymbol{a}} \rho(\boldsymbol{x}, \boldsymbol{y} + \boldsymbol{a}, \omega)(\boldsymbol{y} + \boldsymbol{a}) dV_{\boldsymbol{y}} \\
&= \lim_{r \to \infty} \frac{c}{|B_r(\boldsymbol{x})|} \int_{\boldsymbol{y} \in B_r(\boldsymbol{x}) - \boldsymbol{a}} \bar{\rho}(\boldsymbol{x}, T_{\boldsymbol{y}+\boldsymbol{a}} \omega) \boldsymbol{y} dV_{\boldsymbol{y}} \\
&+ \left[\lim_{r \to \infty} \frac{c}{|B_r(\boldsymbol{x})|} \int_{\boldsymbol{y} \in B_r(\boldsymbol{x}) - \boldsymbol{a}} \bar{\rho}(\boldsymbol{x}, T_{\boldsymbol{y}+\boldsymbol{a}} \omega) dV_{\boldsymbol{y}} \right] \boldsymbol{a} \\
&= \lim_{r \to \infty} \frac{c}{|B_r(\boldsymbol{x})|} \int_{\boldsymbol{y} \in B_r(\boldsymbol{x}) - \boldsymbol{a}} \rho(\boldsymbol{x}, \boldsymbol{y}, T_{\boldsymbol{a}} \omega) \boldsymbol{y} dV_{\boldsymbol{y}} \\
&+ \left[\mathbb{E}[\bar{\rho}(\boldsymbol{x}, \cdot)] \right] \boldsymbol{a} \\
&= \boldsymbol{p}(\boldsymbol{x}, T_{\boldsymbol{a}} \omega)
\end{aligned}$$

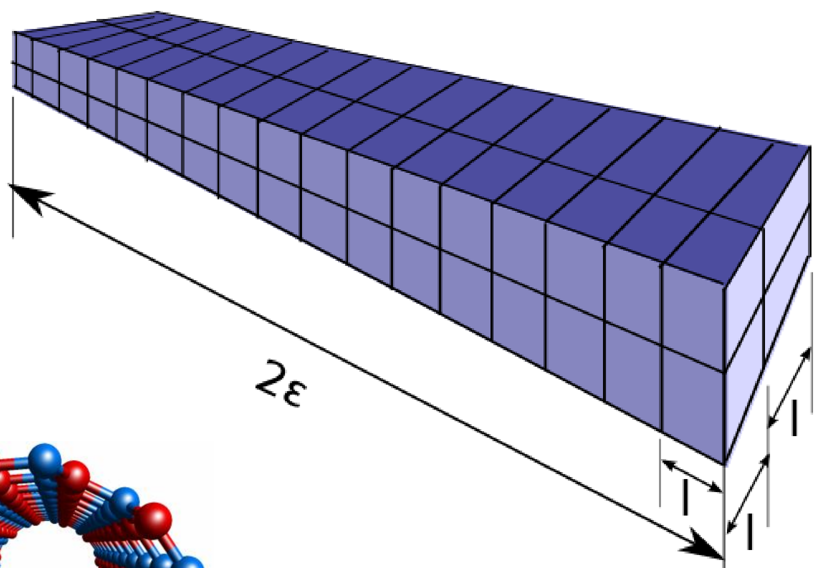
Since T is ergodic dynamical system and by definition of ergodicity of dynamical system, any invariant function will be a constant function. Hence $\boldsymbol{p}$ is a constant function wrt ω. Therefore $E_{nonlocal}$ energy is constant wrt ω.

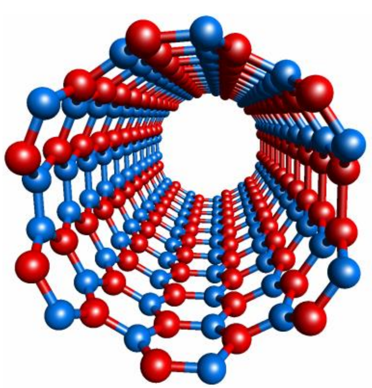
Random media: Discussion

- Local energy in the limit is expectation of local energy $e_{local}(\omega)$. Where $e_{local}(\omega)$ is the local energy corresponding to configuration ω.
- In case of nonlocal energy, we find that the energy is due to dipole-dipole interaction. We also find that the dipole field is constant with respect to the ω. As a result nonlocal energy is also constant wrt ω.
- We explain this as follows: the randomness of charge density field is at the scale of l. Whereas the nonlocal energy is due to interaction of material points which are at the scale ϵ. In the limit $\epsilon/l \to \infty$, we do not see the effect of randomness on the limiting energy.
- We further note that in case of nonlinear interaction, it is in general not necessary that small scale perturbation die out in the large scale interaction. However, in our case we are dealing with linear coulombic interaction.

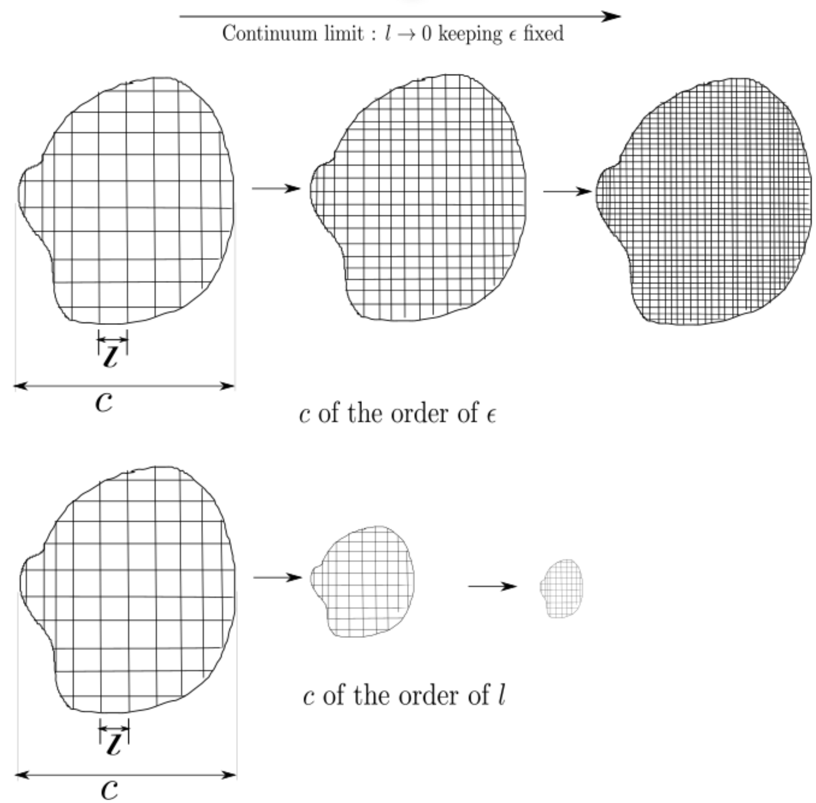
Nanostructures

- Cross-section is of few atomic thickness
- Long in axial direction
- Translational, and/or rotational symmetry





Nanostructure and macroscopically thick structures in a continuum limit



Nanotube Image: http://nano-bio.ehu.es/areas/nanostructures-and-nanotubes

Objective nanorod

- Let $\Omega \subset \mathbb{R}$ be one-d material domain and $\Omega_\epsilon = \Omega \cap \epsilon\mathbb{Z}$ be discret set of material points.

- Let $M_\epsilon(x)$ be the atomistic domain associated to $x \in \Omega_\epsilon$.

$$M_\epsilon(x) := x\boldsymbol{e}_1 + \bigcup_{i=-N_{\epsilon,l}}^{N_{\epsilon,l}} g_l^i([0,l]^3) \qquad \text{where} N_{\epsilon,l} = \lfloor \frac{\epsilon}{2l} \rfloor$$

- $(g_l^i)_{|i| \leq N_{\epsilon,l}}$ is the group operation defined as

$$g_l^i(\boldsymbol{y}) = \boldsymbol{Q}^i(x)\boldsymbol{y} + il\lambda(x)\boldsymbol{e}_1$$

- where $\boldsymbol{Q}(x)$ is the rotation tensor with axis $\boldsymbol{e}_1$. It rotates the vector in plain $(\boldsymbol{e}_2, \boldsymbol{e}_3)$ by an angle $\theta_o(x)$. Therefore, the rotation $\boldsymbol{Q}$ depends on material point.

- $\lambda(x)$ is the stretch as a function of x.

- The microstructure depend on material point due to two parameters $\theta_0(x)$ and $\lambda(x)$.

- Corresponding to each material point, we have objective structure. In Section 3.4 James 2006, more broad class of structures including structures with pure torsion, pure bending, and combination of bending and torsion is forulated.

Nanostructures: Charge density field

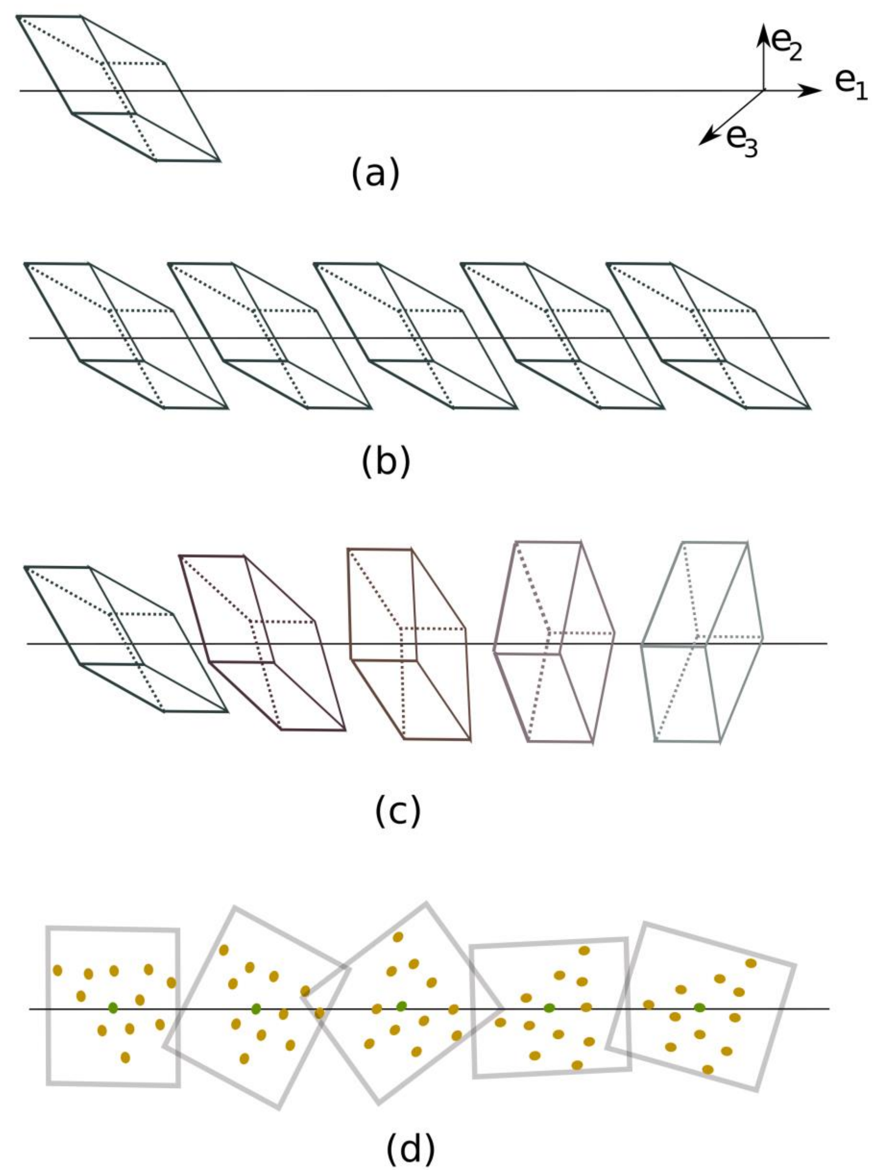
Let $\rho(x, \boldsymbol{y})$ be the charge density field which depends on $x \in \Omega$ and $\boldsymbol{y} \in [0,1]^3$

We assume that it satisfies the symmetry of structure, i.e.

$$\rho(x, \boldsymbol{Q}^k(x)\boldsymbol{y} + k\lambda(x)\boldsymbol{e}_1) = \rho(x, \boldsymbol{y}) \qquad \forall k \in \mathbb{Z}$$

Let scaled charge density field is defined as

$$\rho_l(x, \boldsymbol{y}) = \rho(x, \boldsymbol{y}/l)$$



Nanostructures: Result

- ρ_l must have following scaling to ensure that local energy does not trivially go to zero.

$$\rho_l(x, \boldsymbol{y}) = \frac{\rho(x, \boldsymbol{y}/l)}{l^2}$$

- $$E = \int_{x \in \Omega} E_{local}(x) dl_x + \int_{\substack{x, x' \in \Omega, \\ x \neq x'}} E_{nonlocal}(x, x') dl_x dl_{x'}$$

- $$E_{local}(x) = \lim_{N \to \infty} \int_{\substack{\boldsymbol{u} \in x\boldsymbol{e}_1 + \bigcup_{i=0}^{N}(g_1^i([0,1]^3)), \\ \boldsymbol{u}' \in x\boldsymbol{e}_1 + [0,1]^3}} \frac{\rho(x, \boldsymbol{u})\rho(x, \boldsymbol{u}')}{|\boldsymbol{u} - \boldsymbol{u}'|} dV_{\boldsymbol{u}} dV_{\boldsymbol{u}'}$$

Interaction energy due to charges within material point.

- $$E_{nonlocal}(x, x') = \frac{q(x)q(x')}{|x\boldsymbol{e}_1 - x'\boldsymbol{e}_1|} = 0$$

If net charge in unit cell is zero.

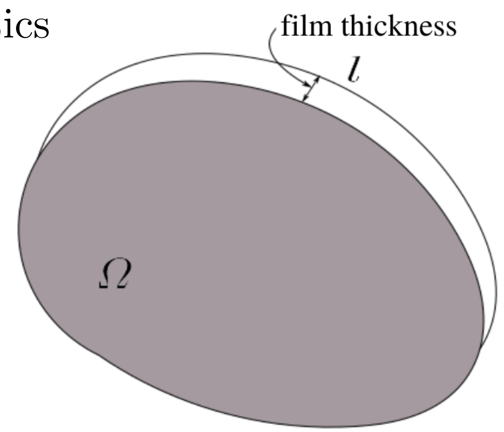
- $$\text{net charge } q(x) := \int_{\boldsymbol{u} \in x\boldsymbol{e}_1 + [0,1]^3} \tilde{\rho}(x, \boldsymbol{u}) dV_{\boldsymbol{u}} = 0$$

No long range interaction

Nanostructures: Discussion

- In Gioia and James 1997, they consider the thin film limit of magnetostatics energy

$$E = \frac{1}{2}\int_{\mathbb{R}^3} \boldsymbol{\nabla}_p \phi(\boldsymbol{y}) \cdot \boldsymbol{\nabla}_p \phi(\boldsymbol{y}) + \frac{1}{l^2}\phi_{,3}(\boldsymbol{y})\phi_{,3}(\boldsymbol{y}) d\boldsymbol{y}$$



- The limiting energy does not have long-range interaction.

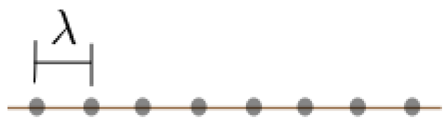
- Similar calculations for two dimensional nanofilm shows that the limiting energy does not have long range interaction.

- This has to with the scaling we obtain for the scaled charge density field and $1/r^3$ type singularity of dipole field kernel.

Nanostructures/thin films behave differently

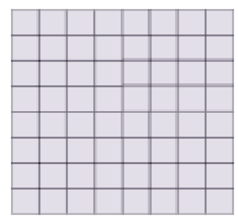
Field at $\boldsymbol{x}$ due to dipole $\boldsymbol{d}$ at origin is $\boldsymbol{K}(\boldsymbol{x})\boldsymbol{d}$ → $\boldsymbol{K}(\boldsymbol{x}) = -\frac{1}{4\pi\,|\boldsymbol{x}|^3}\left\{\boldsymbol{I} - 3\frac{\boldsymbol{x}}{|\boldsymbol{x}|}\otimes\frac{\boldsymbol{x}}{|\boldsymbol{x}|}\right\}$

Estimate of dipole energy for 1-D, 2-D and 3-D materials



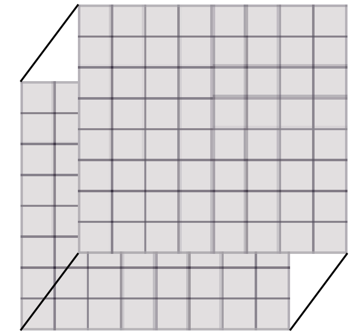
$$W = \sum_{r=1}^{\infty}\frac{1}{r^3}\times 1 = \sum_{r=1}^{\infty}\frac{1}{r^3}$$

At distance r
net dipole is 1



$$W = \sum_{r=1}^{\infty}\frac{1}{r^3}\times r = \sum_{r=1}^{\infty}\frac{1}{r^2}$$

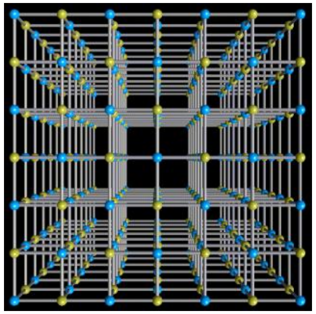
Along the circumference of
circle of r, net dipole is 2*pi*r



$$W = \sum_{r=1}^{\infty}\frac{1}{r^3}\times r^2 = \sum_{r=1}^{\infty}\frac{1}{r}$$

At the surface of sphere of
radius r, net dipole is 4*pi*r*r

Dipole field kernel decays fast for 1-D and 2-D materials



Thank you!