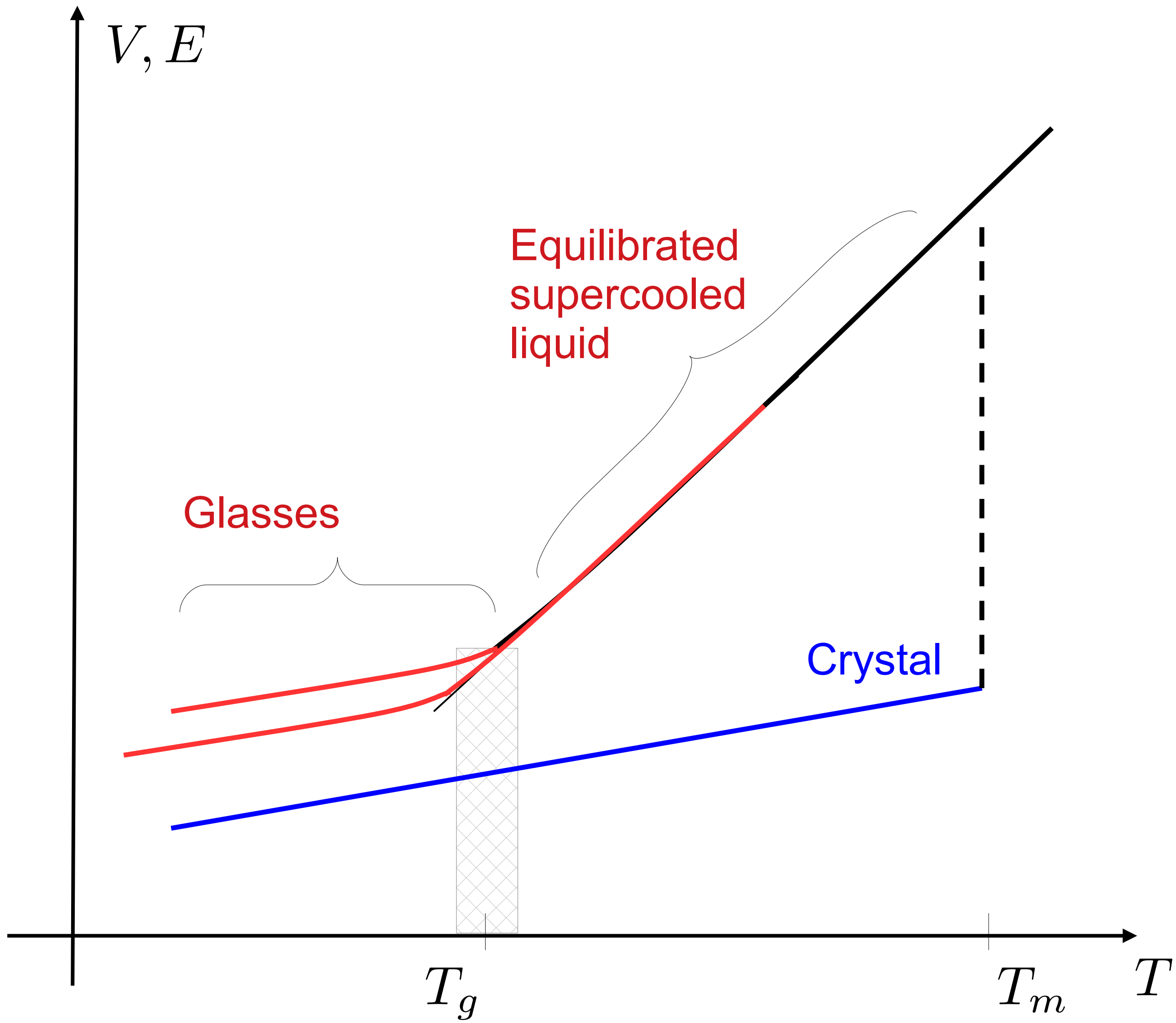
Origin and consequences of long-range stress correlations in glasses

Anaël Lemaître

The glass transition



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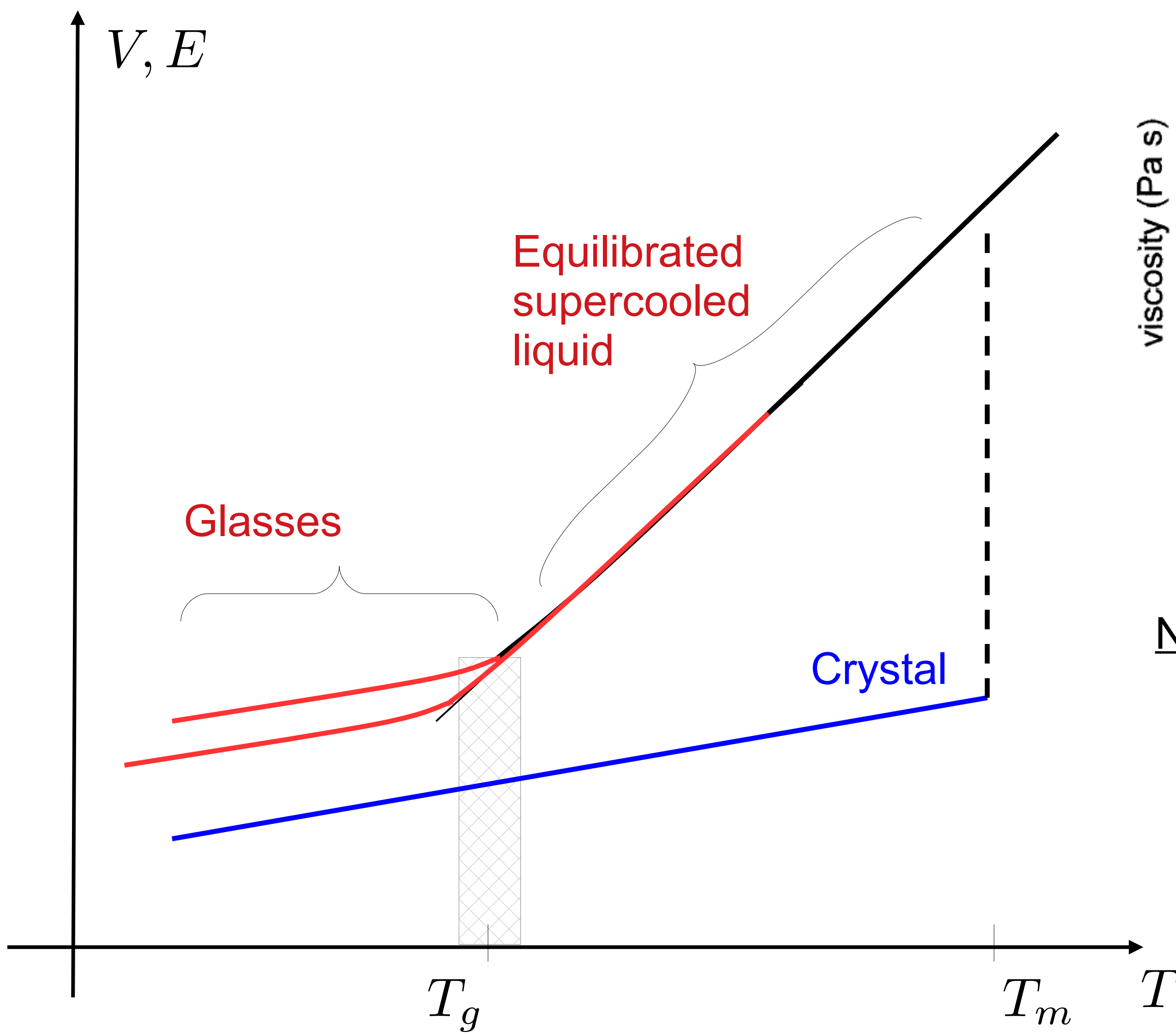
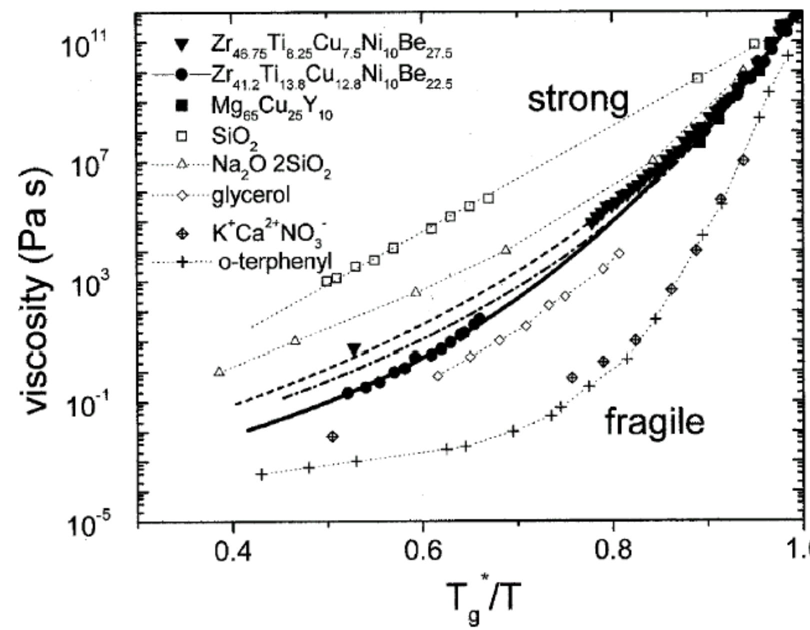
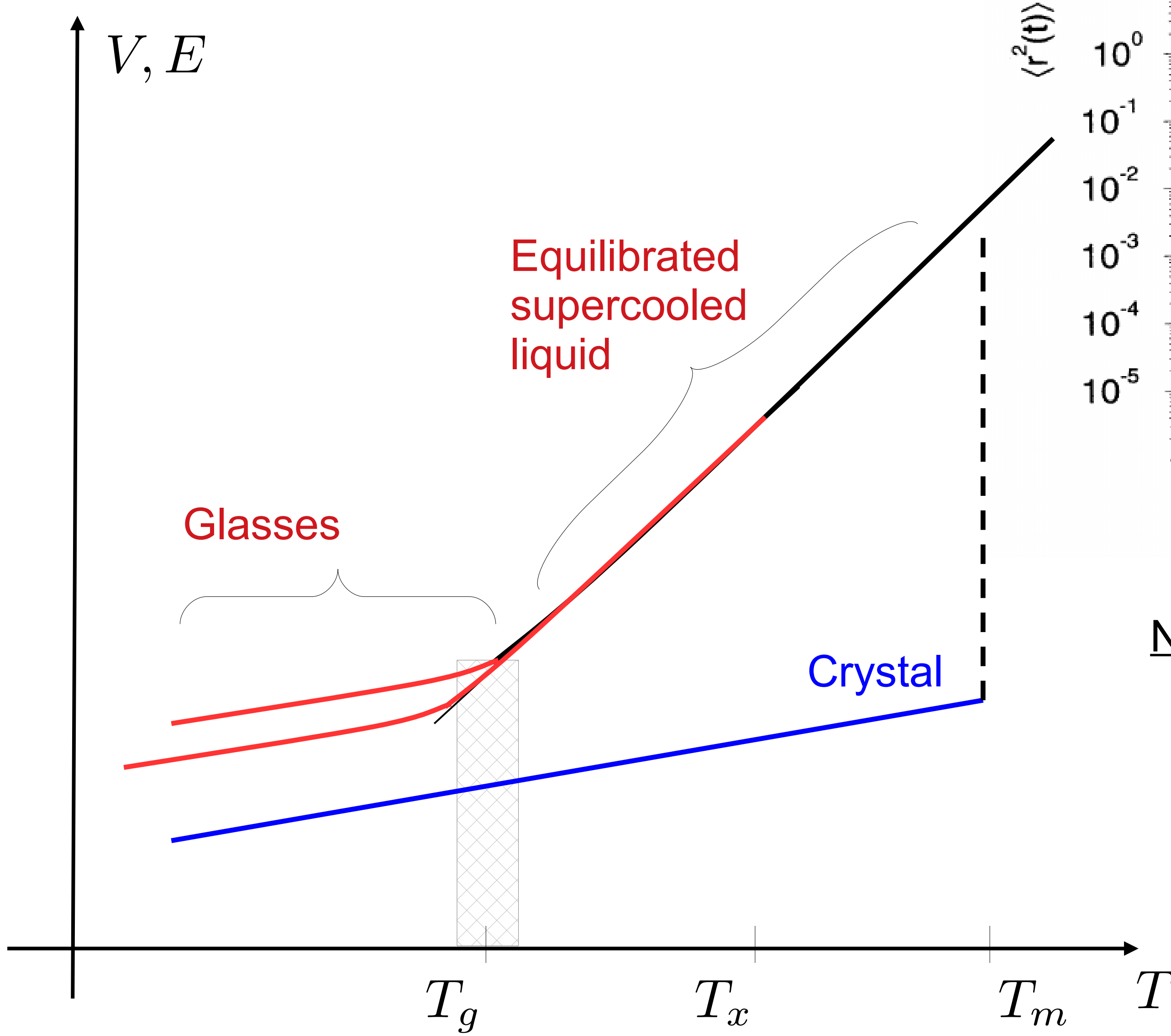


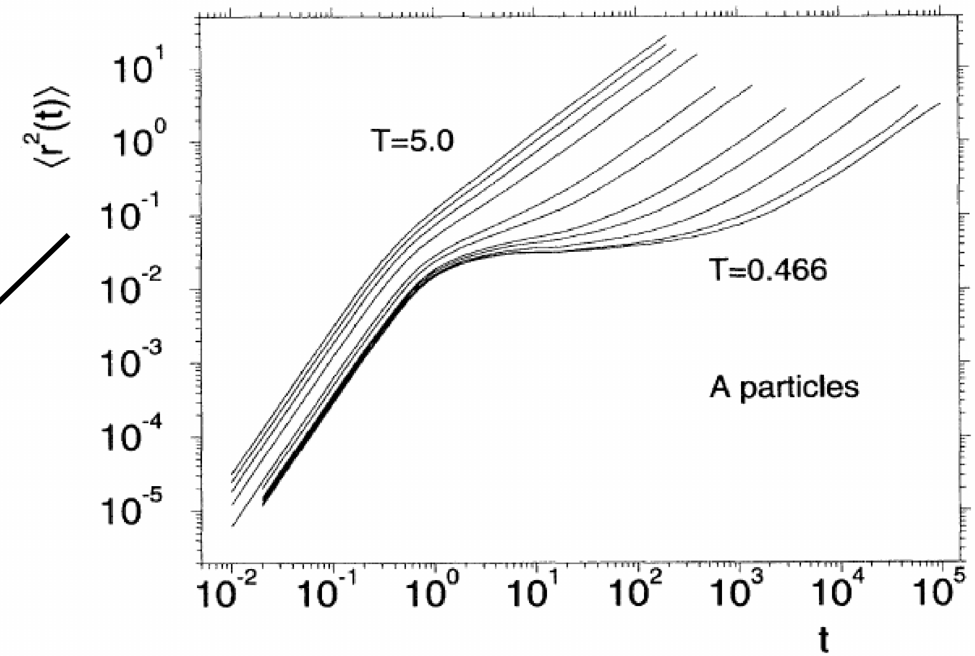


<u>Noticeable SL properties:</u>

- non-Arrhenius behaviour (fragility)

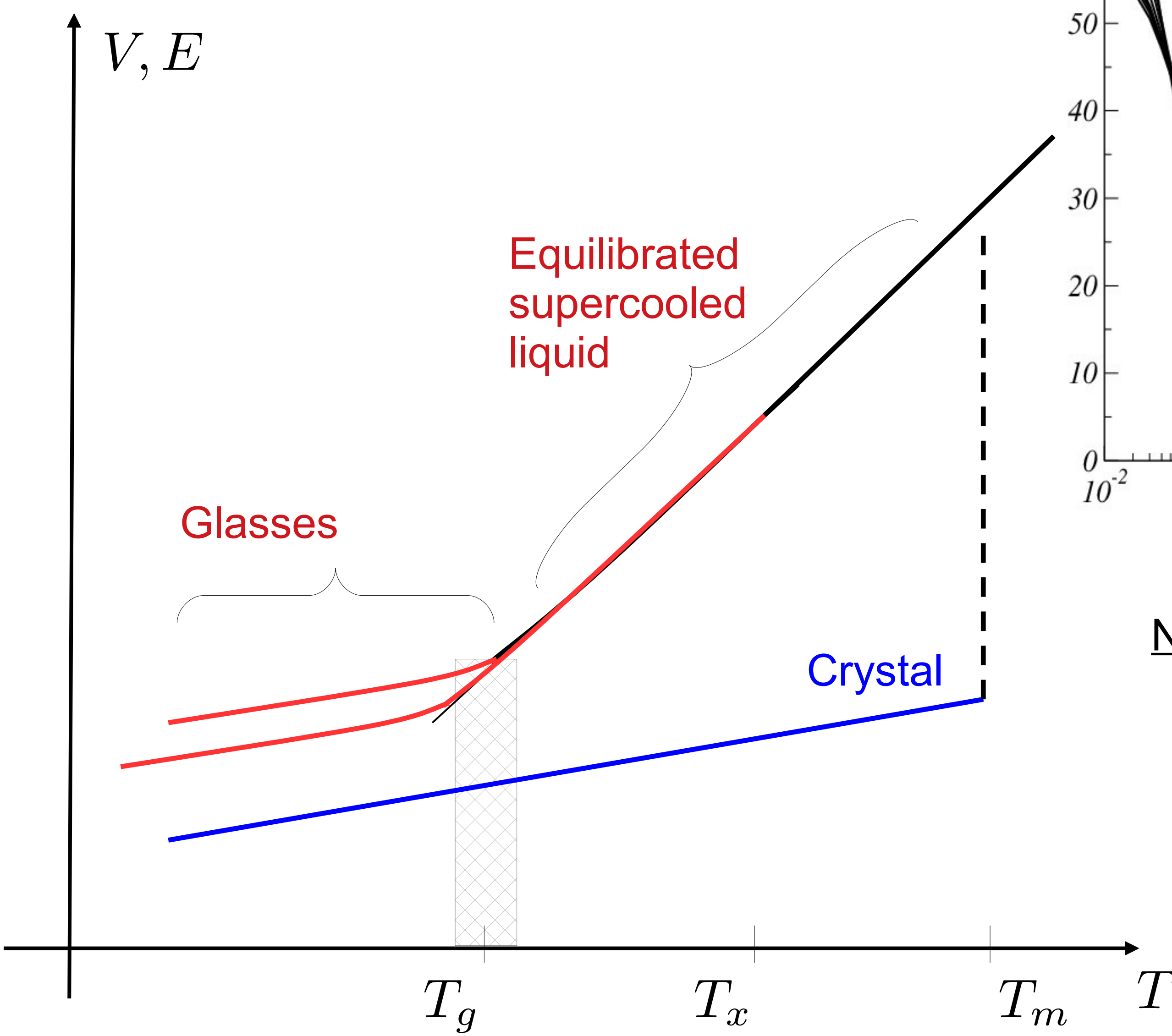
The glass transition

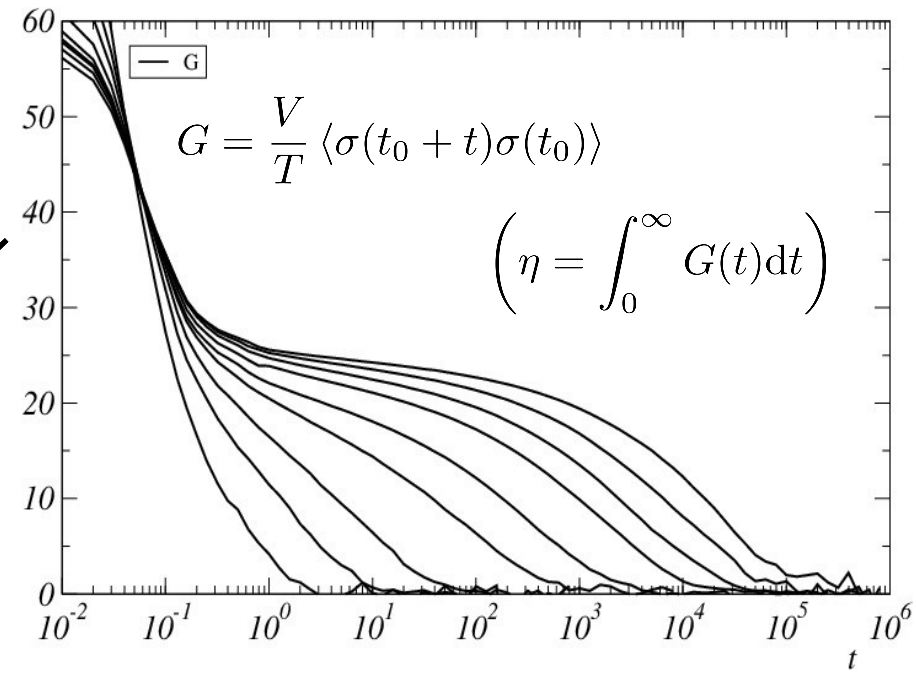




Noticeable SL properties:
- non-Arrhenius behaviour (fragility)
- diffusive plateau (caging)

The glass transition

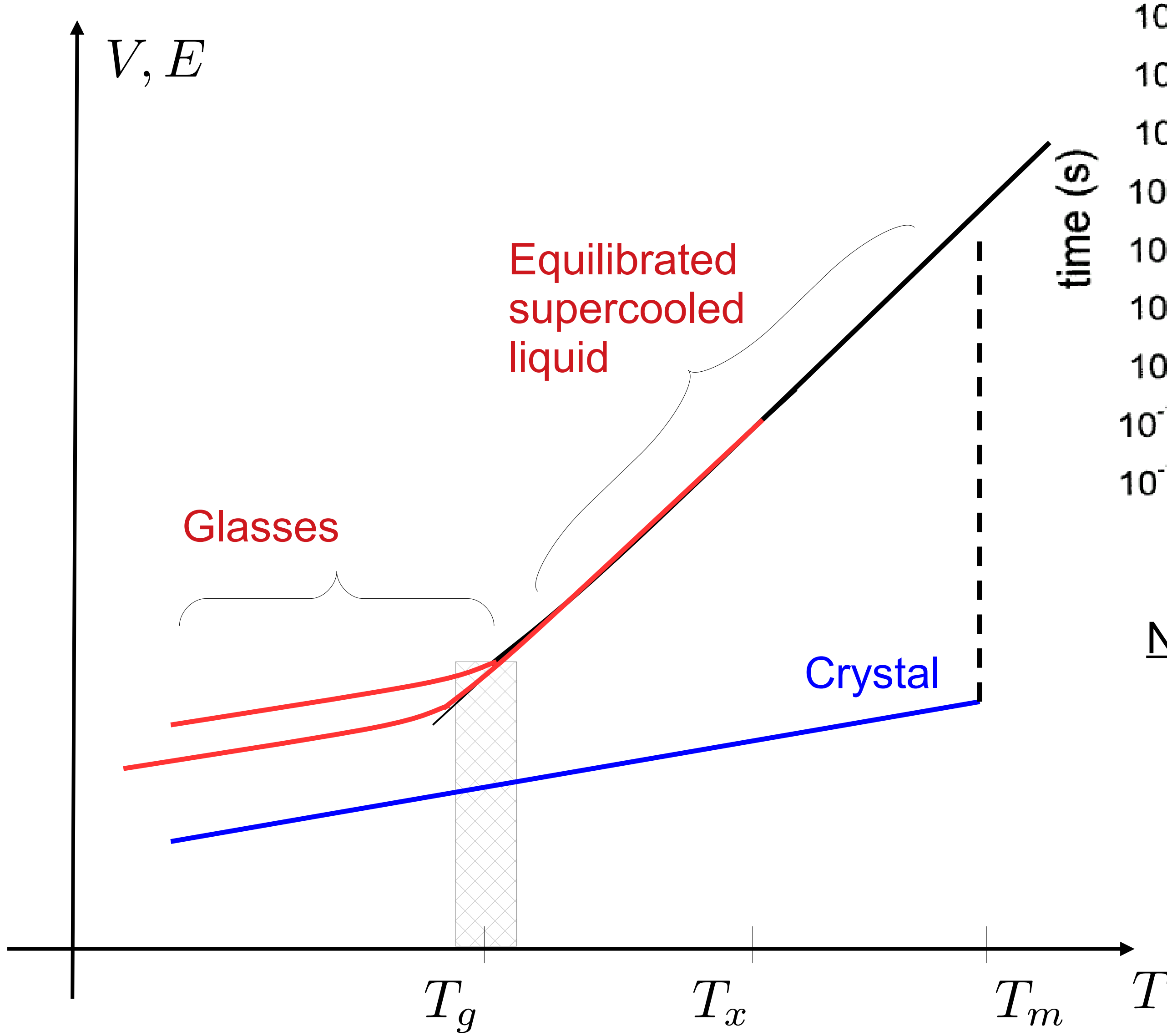


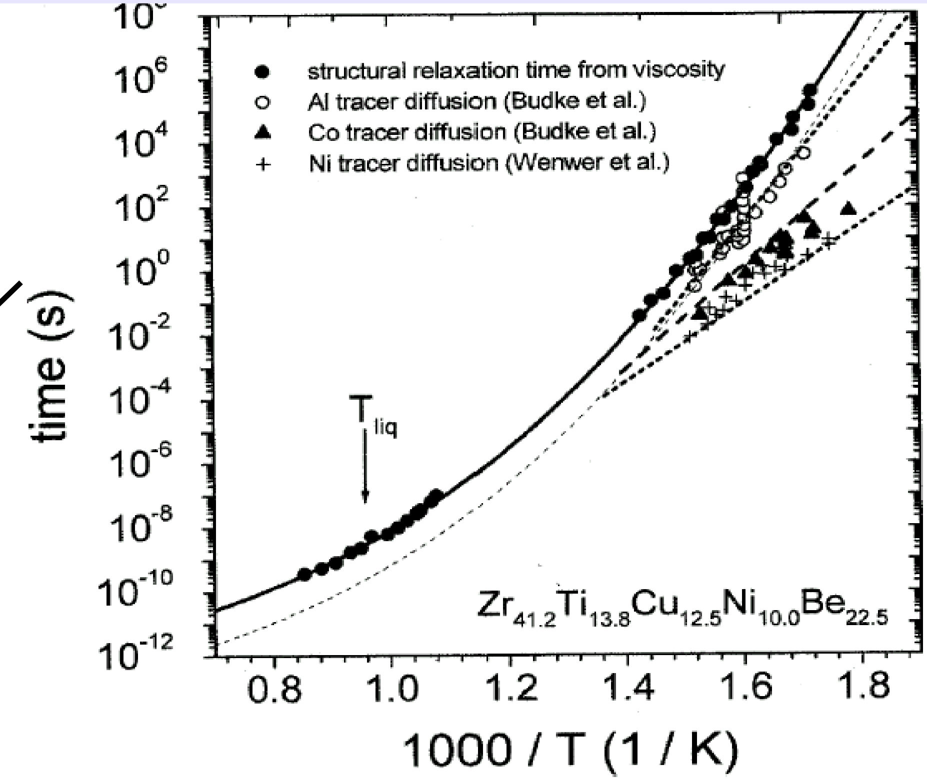


<u>Noticeable SL properties:</u>

- non-Arrhenius behaviour (fragility)
- diffusive plateau (caging)
- stretched exponential relaxation

The glass transition





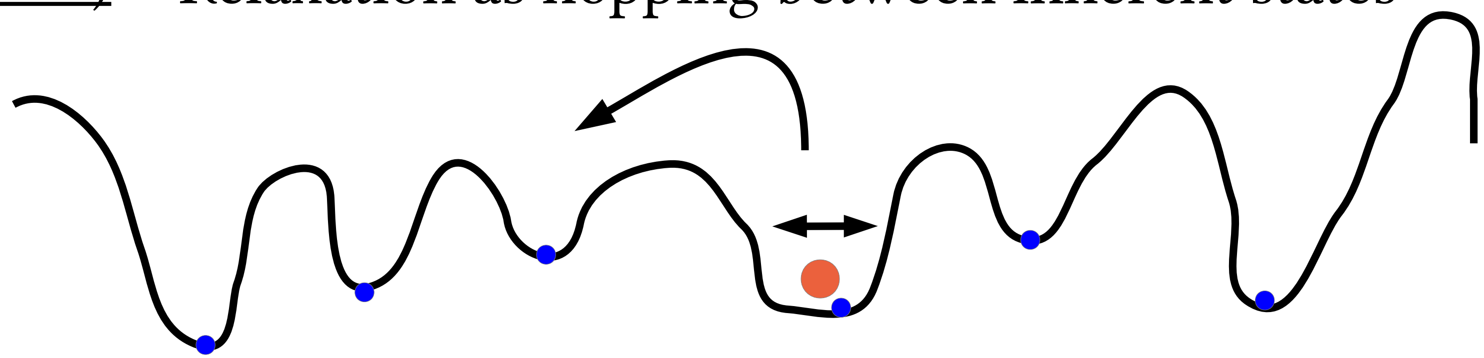
Noticeable SL properties:

- non-Arrhenius behaviour (fragility)
- diffusive plateau (caging)
- stretched exponential relaxation
- decoupling & break-down of Stokes-Einstein's relation

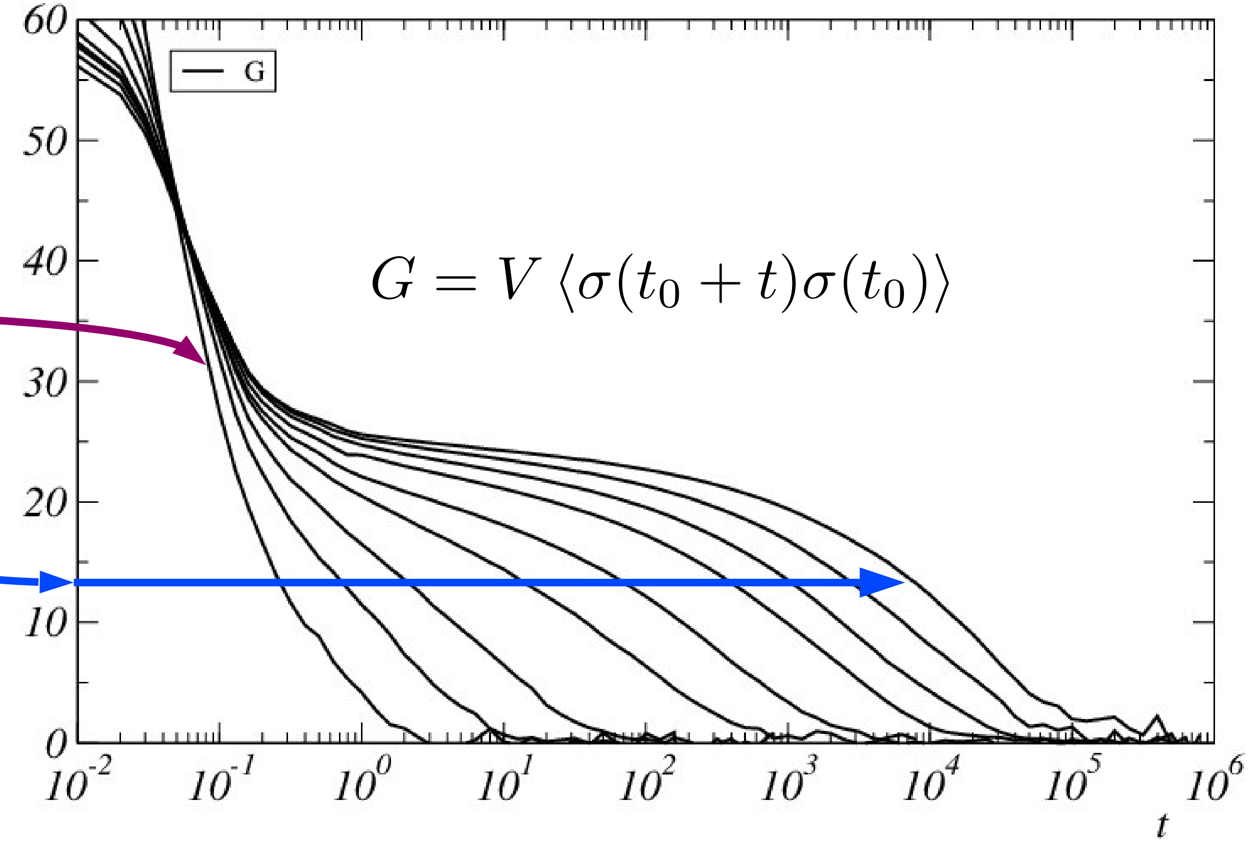
$$D/T \sim \eta^{-\zeta}$$

Hopping between inherent states

Goldstein (1969) Relaxation as hopping between inherent states



$$\boxed{\eta \simeq G^\star \tau_\alpha}$$



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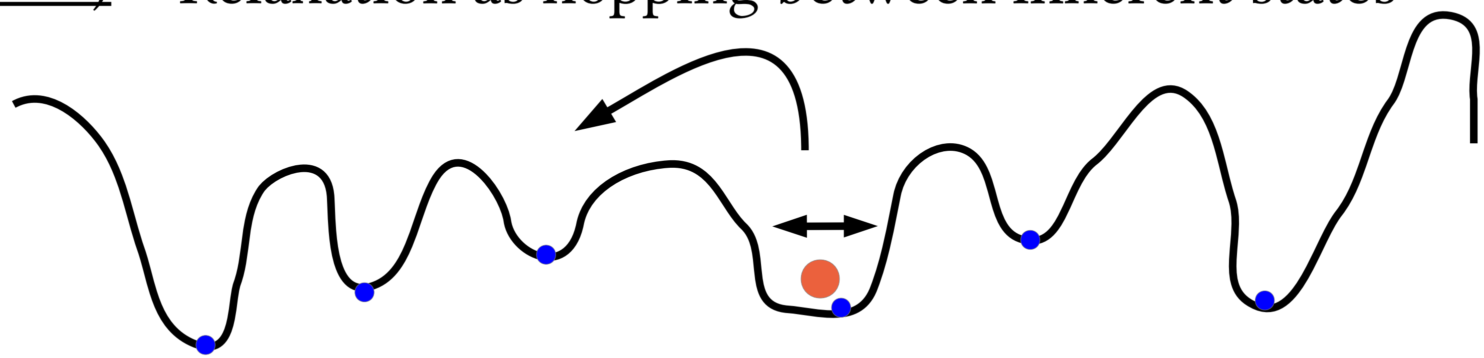
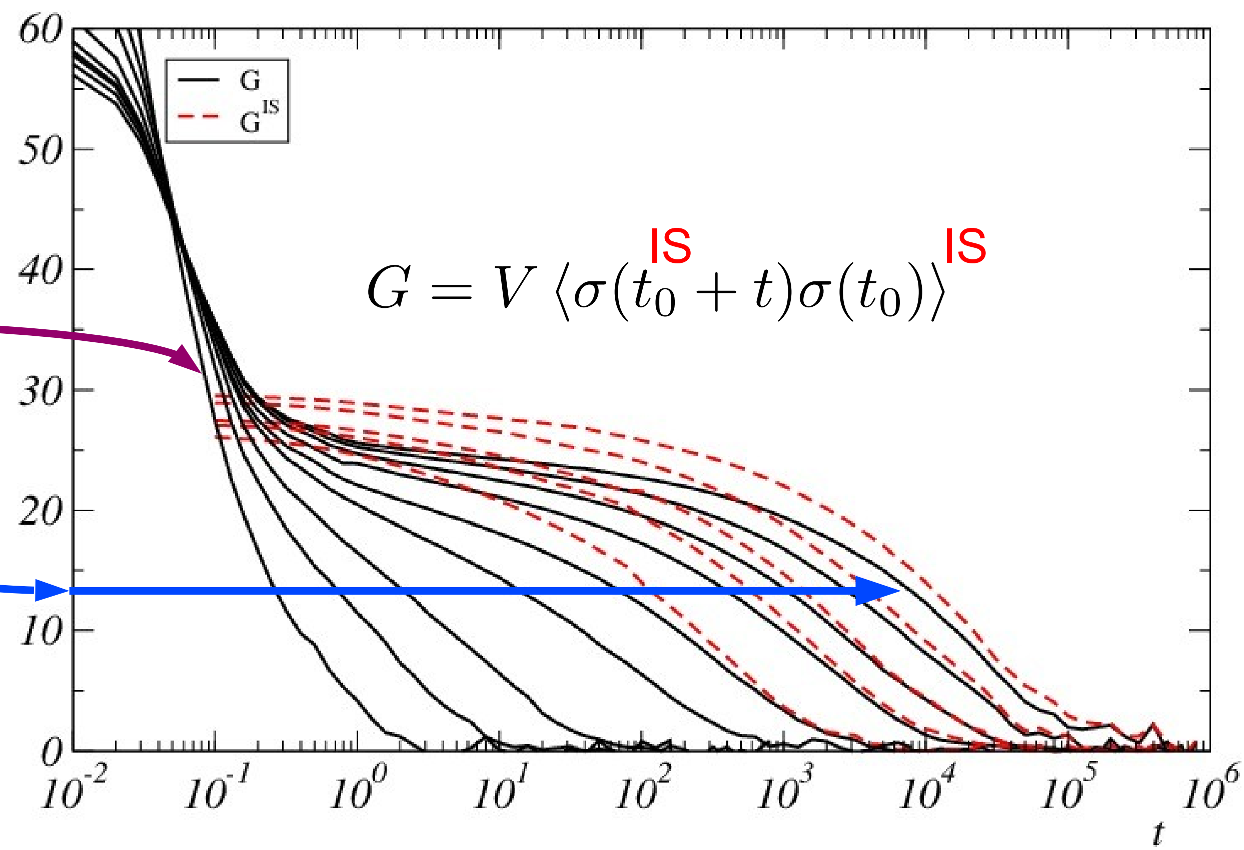




$$\boxed{\eta \simeq G^\star \tau_\alpha}$$

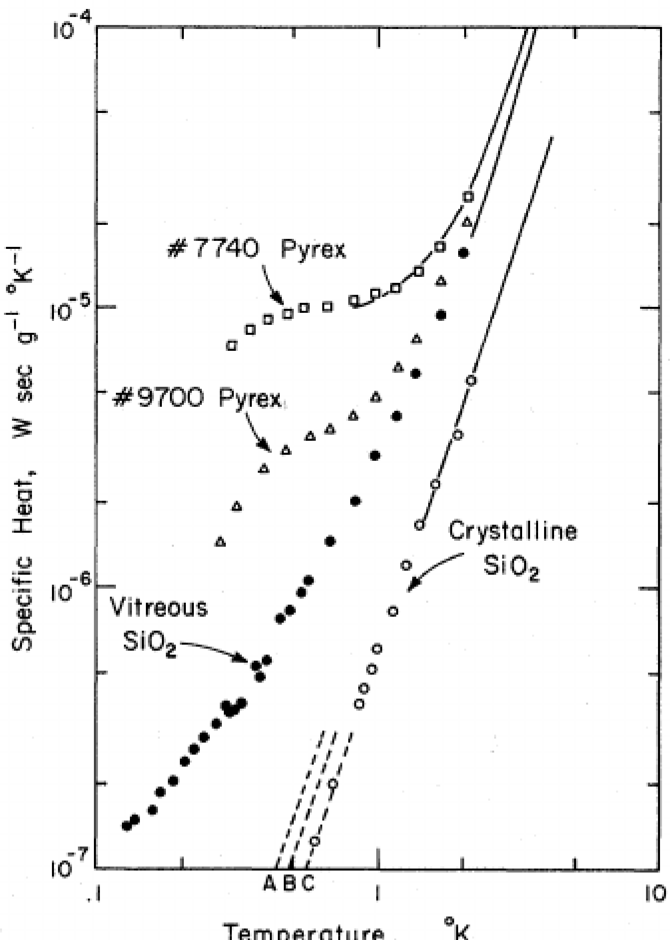
The glassy state

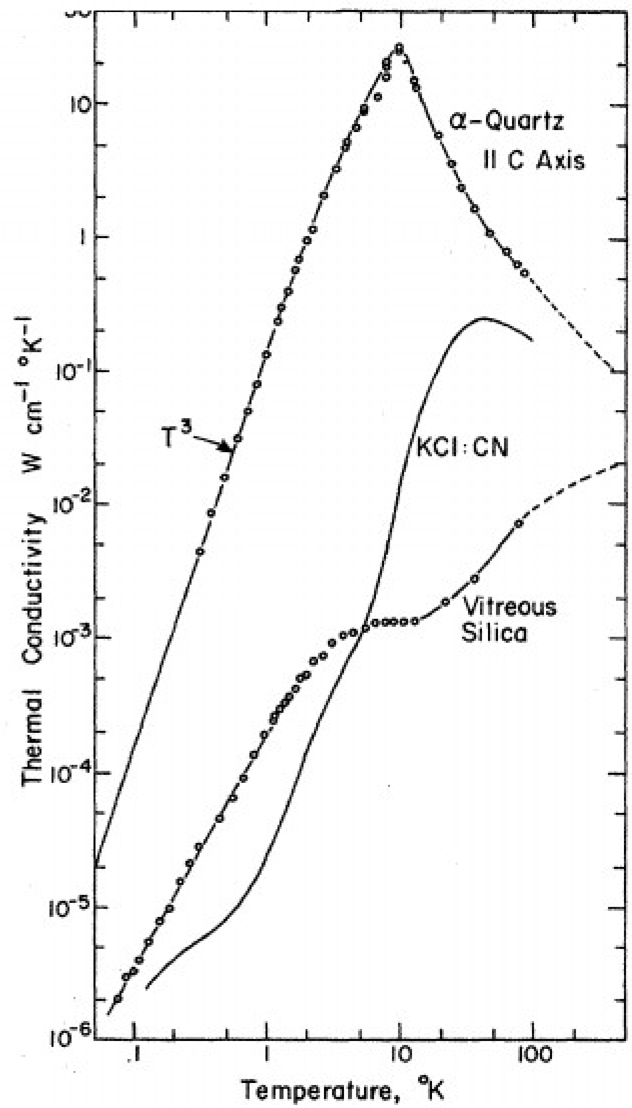
Thermal Conductivity and Specific Heat of Noncrystalline Solids*

R. C. Zeller† and R. O. Pohl
Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, New York 14850
(Received 28 May 1971)

Debye: $C_v \sim T^3$

$$K = \frac{1}{3} C_v v \ell$$

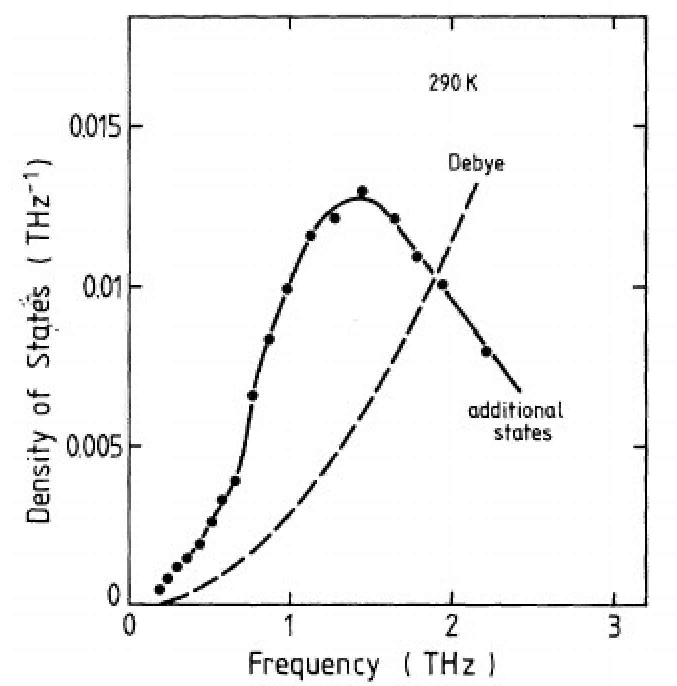




Excess of modes ↔ local defects?

Anderson et al (1972)
Phillips (1972)
Buchenau, Parshin, Schober,...

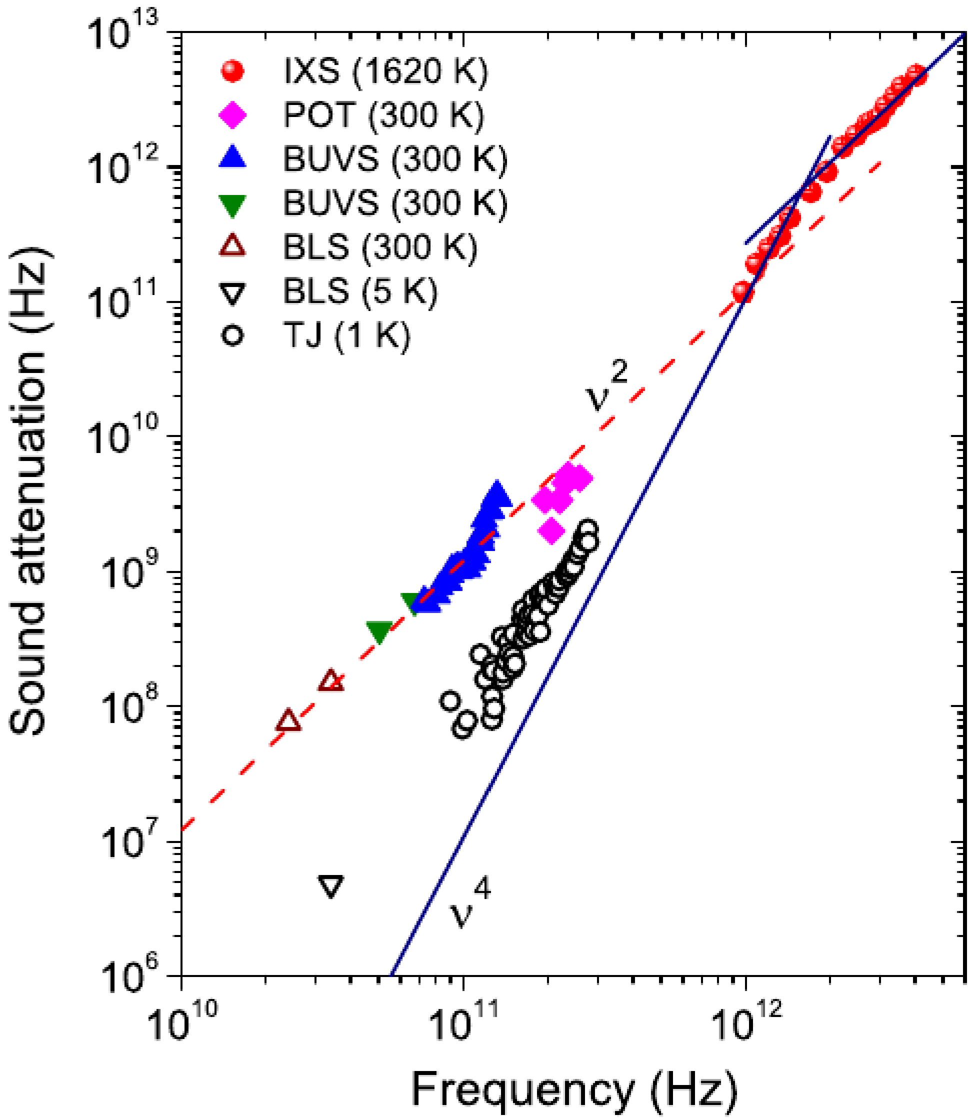
Buchenau (1986)
Malinovsky & Sokolov (1986)



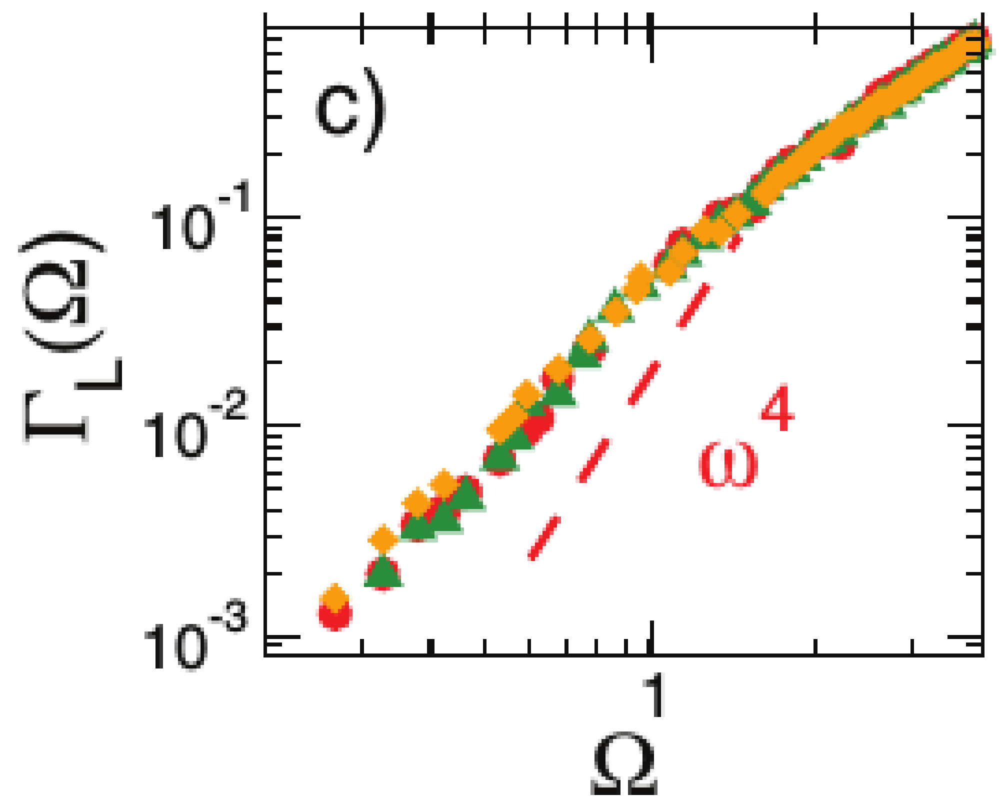
Vitreous silica,
Buchenau *et al* (1984)

Rayleigh scattering $\Gamma \sim k^{d+1}$ **?...**

Baldi et al PRL (2010)



Marruzzo et al Sc. Rep. (2013)

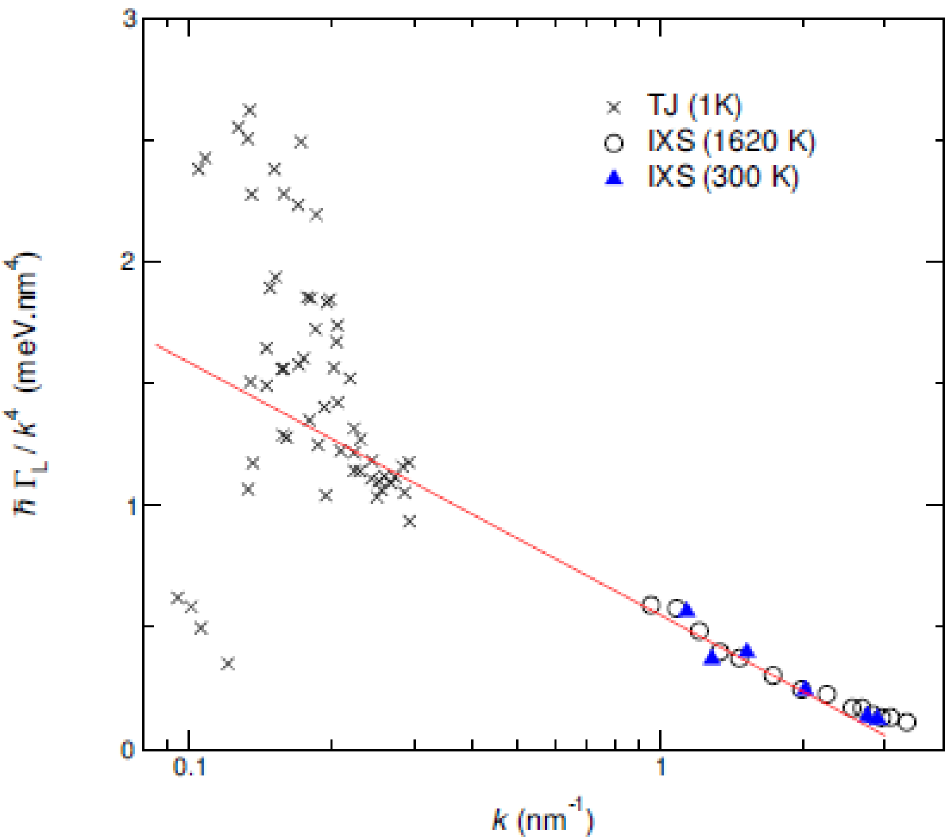


The glassy state

… or non-Rayleigh scattering $\Gamma \sim -k^{d+1} \ln k$

Gelin et al Nature Mat. (2016)

From Baldi et al PRL (2010)



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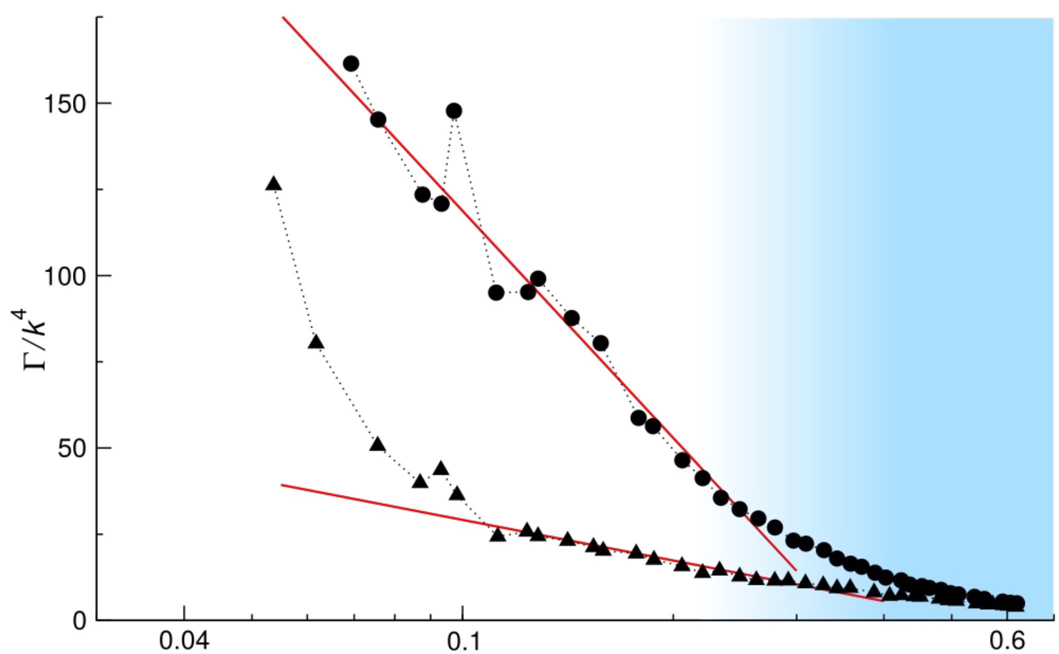


Inherent states are elastic solids

Inherent state

=

Local minimum

=

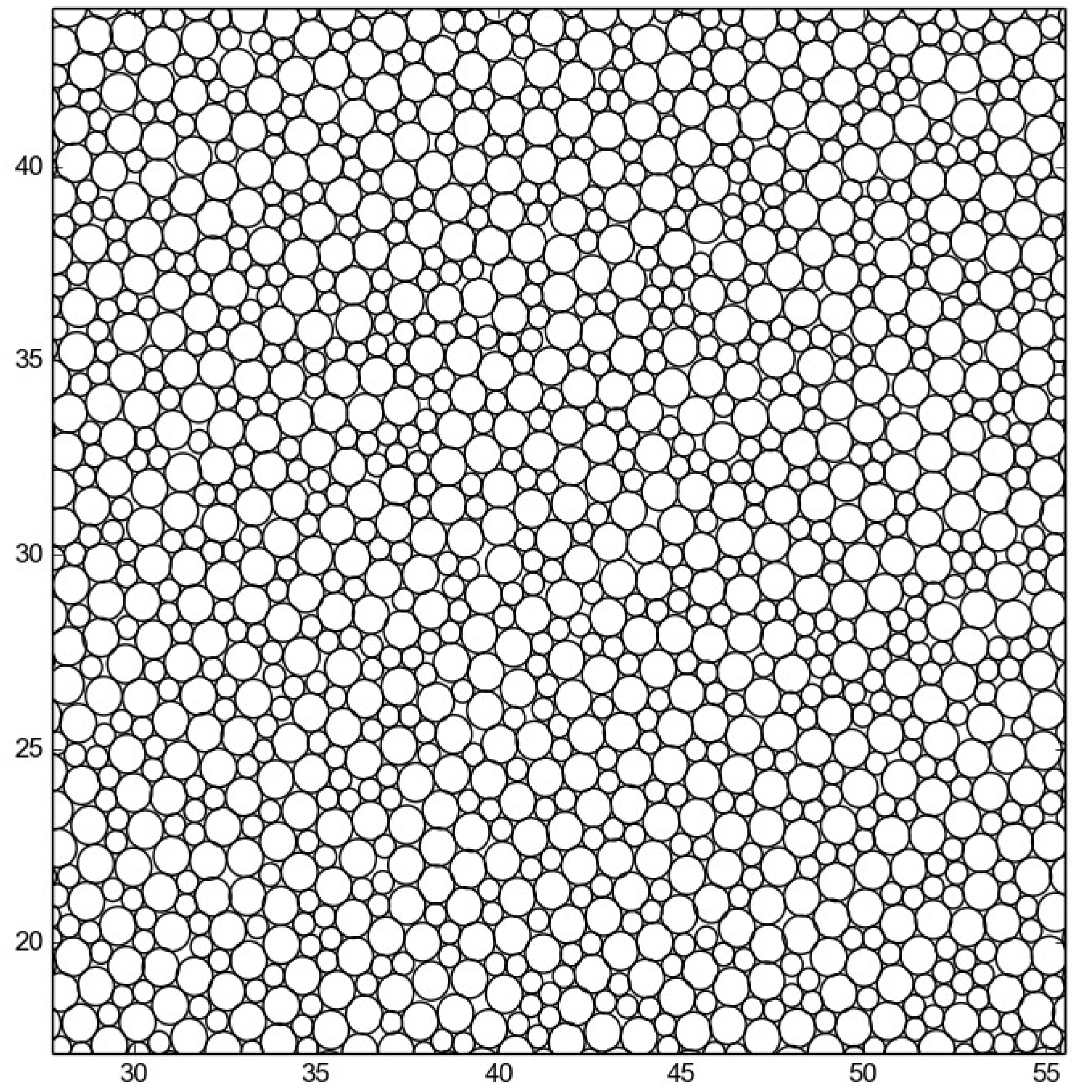
Mechanically stable state

=

Elastic solid

2D, Bidisperse
Lennard-Jones

$$\mathcal{U} = \sum_{i<j} V(r_{ij})$$



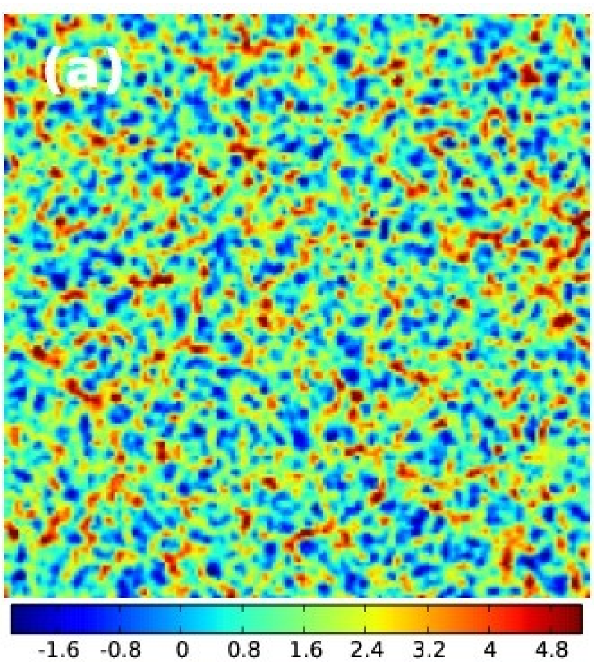
The local IS stress field

$$\widehat{\sigma}_{\alpha\beta\ \underline{k}} = \sum_{i<j} f_{ij}^{\alpha}\ r_{ij}^{\beta}\ \frac{e^{-i\underline{k}\cdot\underline{r}_i} - e^{-i\underline{k}\cdot\underline{r}_j}}{i\underline{k}\cdot\underline{r}_{ij}}$$

$$\begin{aligned} i\underline{k}\cdot\underline{\underline{\widehat{\sigma}}}_{\underline{k}} &= \sum_{i<j} \underline{f}_{ij}\left(e^{-\underline{k}\cdot\underline{r}_i} - e^{-\underline{k}\cdot\underline{r}_j}\right) \\ &= \sum_{i} e^{-\underline{k}\cdot\underline{r}_i}\ \underline{f}_i \ = 0 \end{aligned}$$

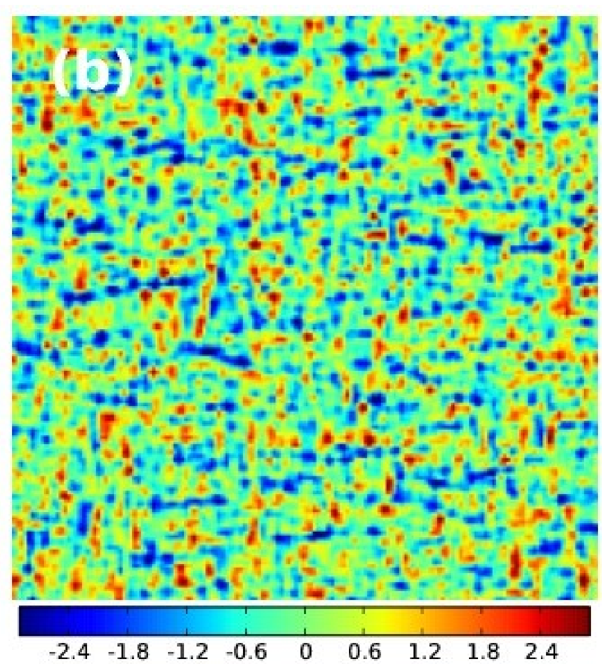
Pressure

$$\sigma_1 \equiv -\frac{1}{2}(\sigma_{xx} + \sigma_{yy})$$



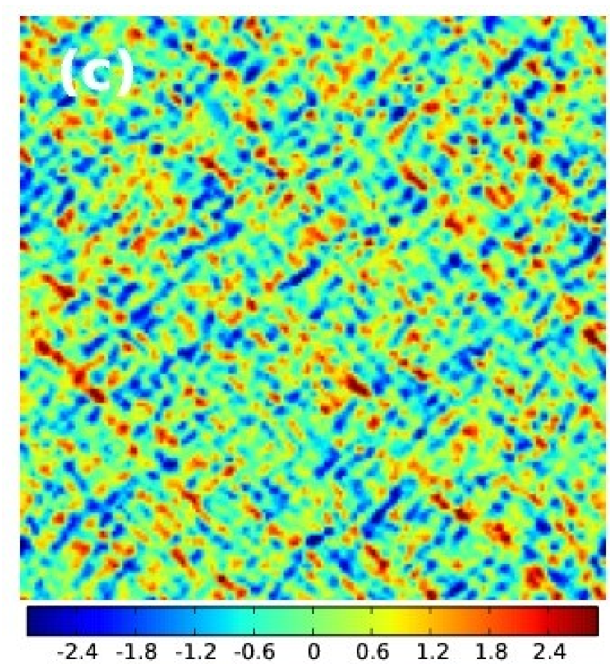
Normal

$$\sigma_2 \equiv \frac{1}{2}(\sigma_{xx} - \sigma_{yy})$$



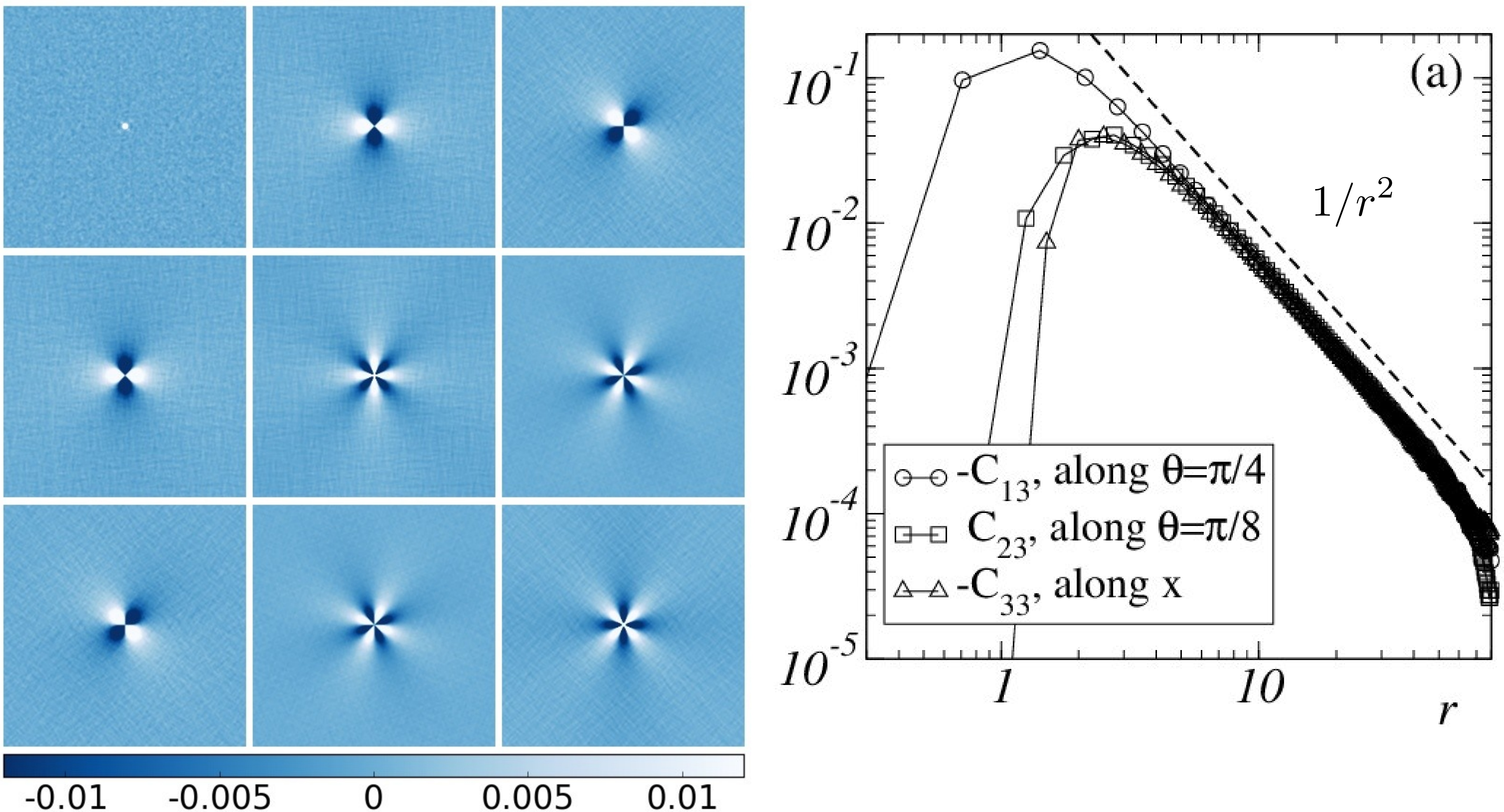
Shear

$$\sigma_3 \equiv \sigma_{xy}$$



Real space stress correlations

$$C_{ab}(\underline{r}) \equiv \langle \sigma_a(\underline{r}_0)\sigma_b(\underline{r}_0 + \underline{r})\rangle$$



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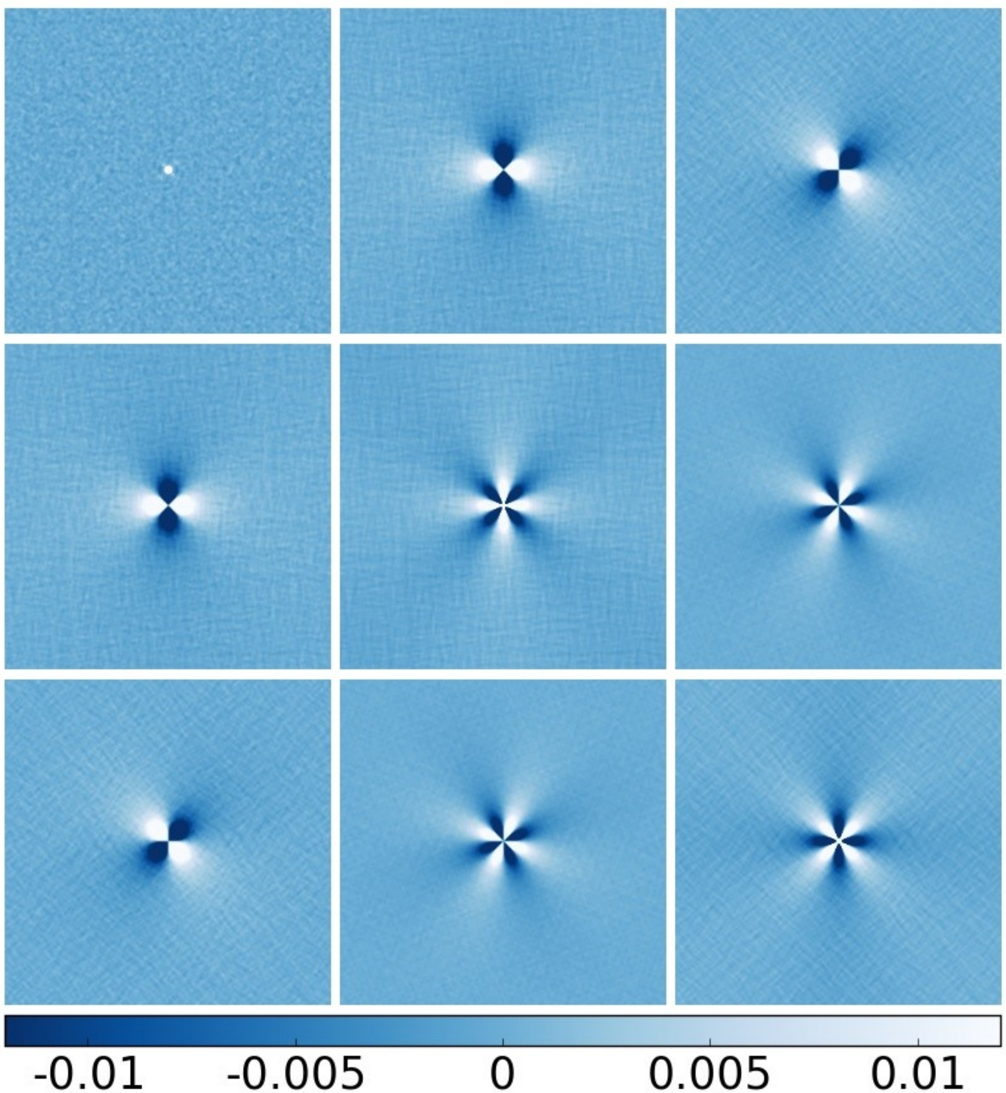


Observations:

- anisotropy
- $1/r^d$ decay in 2D & 3D

Cause? Elasticity??

Glass ~
elastic continuum
+ random sources

Problems:

1) the IS stress cannot be described via an elastic response problem

2) Henkes&Chakraborty: correlations near jamming / interpret via Edwards theory

A general result

Take:

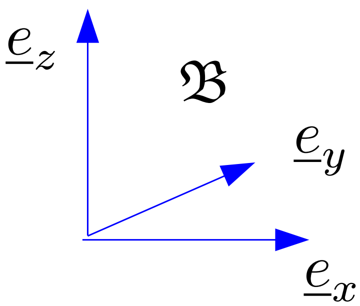
- an ensemble of mechanically balanced states
- materially isotropic
- with normal stress fluctuations (to be specified)

Then:

- the stress autocorrelation presents isotropic and anisotropic terms
- its anisotropic part decays at long range as $1/r^d$

Applies both in
2D [AL, PRE, 96, 052101 (2017)]
3D [AL, JCP, 149, 104107 (2018)]

Tensors and rotations



$$\xrightarrow{\text{Rotation } \underline{\underline{R}}} \quad \mathfrak{B}^{\underline{\underline{R}}} = \{\underline{\underline{R}}^T \cdot \underline{e}_x, \underline{\underline{R}}^T \cdot \underline{e}_y, \underline{\underline{R}}^T \cdot \underline{e}_z\}$$

$$\underline{r} \longrightarrow \underline{r}' = \underline{\underline{R}} \cdot \underline{r}$$

$$\underline{\underline{\sigma}} \longrightarrow \underline{\underline{\sigma}}' = \underline{\underline{R}} \cdot \underline{\underline{\sigma}} \cdot \underline{\underline{R}}^T$$

A vector representation for stress

$$\underset{\sim}{\sigma} \longrightarrow \underset{\sim}{\sigma}' = \mathcal{D} \cdot \underset{\sim}{\sigma}$$

Analogous to Wigner-D matrix

$$\underset{\approx}{C}(\underline{r}) \equiv \langle \underset{\sim}{\sigma}(\underline{r}_0 + \underline{r})\, \underset{\sim}{\sigma}(\underline{r}_0) \rangle_c \longrightarrow \mathcal{D} \cdot \underset{\approx}{C}\,(\underline{r}) \cdot \mathcal{D}^T$$

A vector representation for stress

“Magnetic” & azimuthal numbers

$$\underset{\sim}{\sigma} = \left\{ \begin{aligned} \sigma_1 &= -\frac{1}{\sqrt{3}} \left(\sigma_{xx} + \sigma_{yy} + \sigma_{zz}\right) \\ \sigma_2 &= -\frac{1}{\sqrt{6}} \left(\sigma_{xx} + \sigma_{yy} - 2\,\sigma_{zz}\right) \\ \sigma_3 &= \sqrt{2}\,\sigma_{yz} \\ \sigma_4 &= \sqrt{2}\,\sigma_{xz} \\ \sigma_5 &= \sqrt{2}\,\sigma_{xy} \\ \sigma_6 &= \frac{1}{\sqrt{2}} \left(\sigma_{xx} - \sigma_{yy}\right) \end{aligned} \right.$$

$\ell = 0$: σ_1

$m = 0$: σ_1, σ_2

$m = \pm 1$: σ_3, σ_4

$m = \pm 2$: σ_5, σ_6

$\ell = 2$: $\sigma_2, \ldots, \sigma_6$

$$D^z(\phi) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & \cos\phi & \sin\phi & 0 & 0 \\ 0 & 0 & -\sin\phi & \cos\phi & 0 & 0 \\ 0 & 0 & 0 & 0 & \cos 2\phi & \sin 2\phi \\ 0 & 0 & 0 & 0 & -\sin 2\phi & \cos 2\phi \end{pmatrix}$$

A vector representation for stress

"Magnetic" & azimuthal numbers

$$
\underset{\sim}{\sigma} = \left\{
\begin{aligned}
&\left.\begin{aligned}
\sigma_1 &= -\frac{1}{\sqrt{3}}\,(\sigma_{xx}+\sigma_{yy}+\sigma_{zz}) \\
\sigma_2 &= -\frac{1}{\sqrt{6}}\,(\sigma_{xx}+\sigma_{yy}-2\,\sigma_{zz})
\end{aligned}\right\} m = 0 \\
&\left.\begin{aligned}
\sigma_3 &= \sqrt{2}\,\sigma_{yz} \\
\sigma_4 &= \sqrt{2}\,\sigma_{xz}
\end{aligned}\right\} m = \pm 1 \\
&\left.\begin{aligned}
\sigma_5 &= \sqrt{2}\,\sigma_{xy} \\
\sigma_6 &= \frac{1}{\sqrt{2}}\,(\sigma_{xx}-\sigma_{yy})
\end{aligned}\right\} m = \pm 2
\end{aligned}\right.
$$

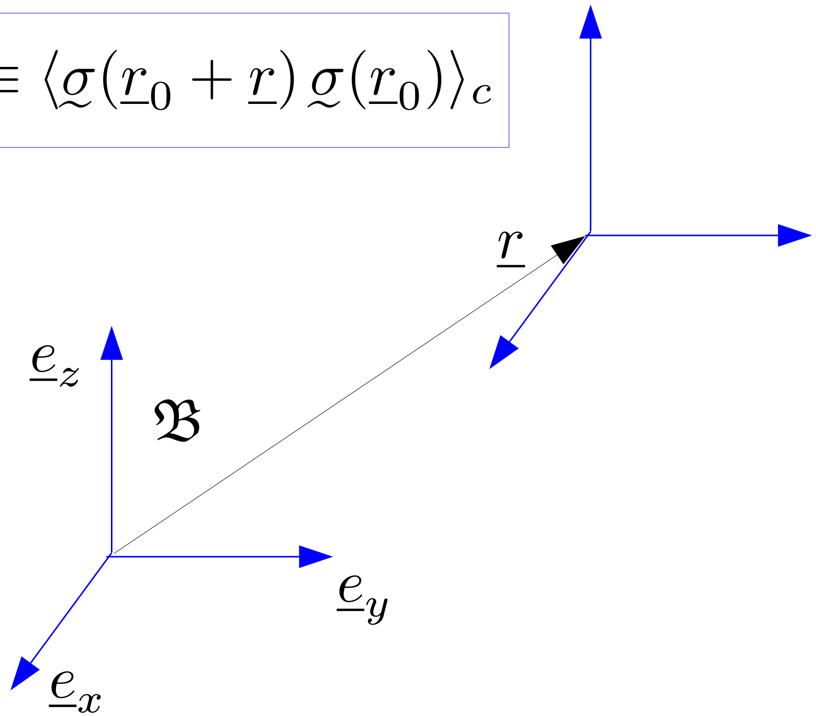
$\ell = 0$ (σ_1)

$\ell = 2$ (σ_2 to σ_6)

$$
D^y(\theta) = \begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{3}{2}\cos^2\theta - \frac{1}{2} & 0 & -\frac{\sqrt{3}}{2}\sin 2\theta & 0 & \frac{\sqrt{3}}{2}\sin^2\theta \\
0 & 0 & \cos\theta & 0 & -\sin\theta & 0 \\
0 & \frac{\sqrt{3}}{2}\sin 2\theta & 0 & \cos 2\theta & 0 & -\frac{1}{2}\sin 2\theta \\
0 & 0 & \sin\theta & 0 & \cos\theta & 0 \\
0 & \frac{\sqrt{3}}{2}\sin^2\theta & 0 & \frac{1}{2}\sin 2\theta & 0 & \frac{1}{2}\cos^2\theta + \frac{1}{2}
\end{pmatrix}
$$

The stress autocorrelation

$$\underset{\approx}{C}(\underline{r}) \equiv \langle \underset{\sim}{\sigma}(\underline{r}_0 + \underline{r})\, \underset{\sim}{\sigma}(\underline{r}_0) \rangle_c$$



Assume:

- translation invariance $C_{ab}(\underline{r}) = C_{ba}(-\underline{r})$
- spatial inversion symmetry $C_{ab}(\underline{r}) = C_{ab}(-\underline{r})$

$$C_{ab} = C_{ba}$$

21 coefficients

The stress autocorrelation

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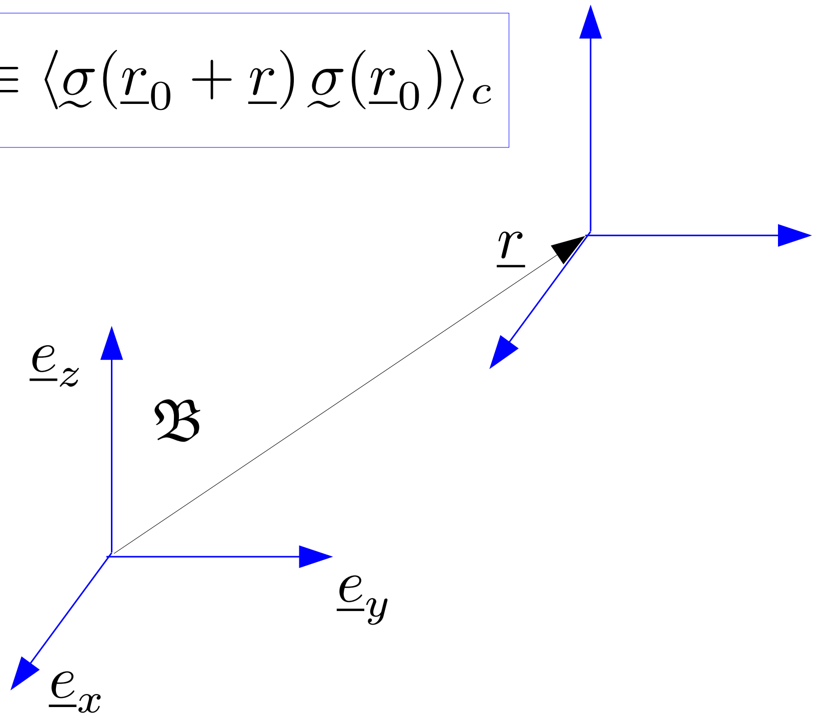

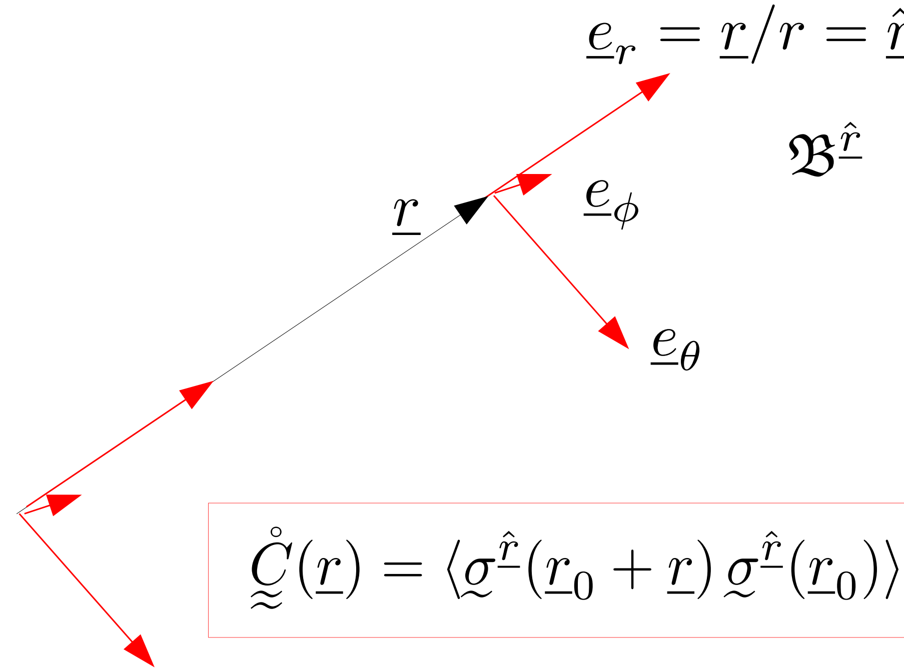

$$\mathring{\underset{\approx}{C}}(\underline{r}) = \langle \underset{\sim}{\sigma}^{\hat{\underline{r}}}(\underline{r}_0 + \underline{r})\, \underset{\sim}{\sigma}^{\hat{\underline{r}}}(\underline{r}_0) \rangle_c$$

Assume:

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$$C_{ab} = C_{ba}$$

21 coefficients

Material isotropy implies:

$$\mathring{\underset{\approx}{C}}(\underline{r}) = \mathring{\underset{\approx}{C}}(r)$$

$$= \underset{\approx}{C}(r\underline{e}_x)$$

Material isotropy

$$\underset{\approx}{C}(\underline{r}) \equiv \langle \underset{\sim}{\sigma}(\underline{r}_0 + \underline{r})\, \underset{\sim}{\sigma}(\underline{r}_0) \rangle_c$$

must have the same functional form in all bases

Take any $\underline{\underline{R}}$, and write the stress autocorrelation in $\mathfrak{B}^{\underline{\underline{R}}}$

$$\underline{r} \longrightarrow \underline{\underline{R}} \cdot \underline{r} \qquad \boxed{\underset{\approx}{C}(\underline{\underline{R}} \cdot \underline{r}) = \mathcal{D} \cdot \underset{\approx}{C}\,(\underline{r}) \cdot \mathcal{D}^T}$$

Case 1: Take any point $\underline{r}$

Define $\underline{\underline{R}} \equiv \underline{\underline{R}}^{\hat{\underline{r}}}$: $\mathfrak{B} \longrightarrow \{\underline{e}_\theta, \underline{e}_\phi, \underline{e}_r\}$

$\underline{r} \longrightarrow (0, 0, 1)$

$$\boxed{\underset{\approx}{C}(0, 0, r) = \underset{\approx}{C}(r\underline{e}_z) = \mathcal{D}^{\hat{\underline{r}}} \cdot \underset{\approx}{C}\,(\underline{r}) \cdot \left(\mathcal{D}^{\hat{\underline{r}}}\right)^T \equiv \underset{\approx}{\mathring{C}}(\underline{r})}$$

Case 2: Take $\underline{r} = r\underline{e}_z$

and $\underline{\underline{R}} \equiv \underline{\underline{R}}^z(\theta)$

$$\boxed{\underset{\approx}{\mathring{C}}(r) = \underset{\approx}{C}(r\underline{e}_z) = \mathcal{D}^z(\theta) \cdot \underset{\approx}{\mathring{C}}(r) \cdot \mathcal{D}^z(-\theta)}$$

Material isotropy

Prop. 1: $\boxed{\underset{\approx}{\mathring{C}}(\underline{r}) = \underset{\approx}{\mathring{C}}(r)}$

$$\underset{\approx}{C}\,(\underline{r}) = \left(\mathcal{D}^{\underline{\hat{r}}}\right)^{T} \cdot \underset{\approx}{\mathring{C}}(r) \cdot \mathcal{D}^{\underline{\hat{r}}}$$

Prop. 2: $\boxed{\underset{\approx}{\mathring{C}}(r) = \mathcal{D}^{z}(\theta) \cdot \underset{\approx}{\mathring{C}}(r) \cdot \mathcal{D}^{z}(-\theta)}$

recalling

$$D^{z}(\phi) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & \cos\phi & \sin\phi & 0 & 0 \\ 0 & 0 & -\sin\phi & \cos\phi & 0 & 0 \\ 0 & 0 & 0 & 0 & \cos 2\phi & \sin 2\phi \\ 0 & 0 & 0 & 0 & -\sin 2\phi & \cos 2\phi \end{pmatrix}$$

it implies that:

$$\underset{\approx}{\mathring{C}}(\underline{r}) = \begin{pmatrix} \mathring{C}_1(r) & \mathring{C}_2(r) & 0 & 0 & 0 & 0 \\ \mathring{C}_2(r) & \mathring{C}_3(r) & 0 & 0 & 0 & 0 \\ 0 & 0 & \mathring{C}_4(r) & 0 & 0 & 0 \\ 0 & 0 & 0 & \mathring{C}_4(r) & 0 & 0 \\ 0 & 0 & 0 & 0 & \mathring{C}_5(r) & 0 \\ 0 & 0 & 0 & 0 & 0 & \mathring{C}_5(r) \end{pmatrix}$$

In Fourier space

The stress autocorrelation $\widehat{\underset{\approx}{C}}(\underline{k}) = \dfrac{1}{(2\pi)^3} \left\langle \widehat{\underset{\sim}{\sigma}}(\underline{k})\ \left(\widehat{\underset{\sim}{\sigma}}(\underline{k})\right)^* \right\rangle_c$

Its radial form: $$\mathring{\widehat{\underset{\approx}{C}}}(k) = \frac{1}{(2\pi)^3} \left\langle \widehat{\underset{\sim}{\sigma}}^{\underline{\hat{k}}}(\underline{k})\ \left(\widehat{\underset{\sim}{\sigma}}^{\underline{\hat{k}}}(\underline{k})\right)^* \right\rangle_c$$

are related by: $$\widehat{\underset{\approx}{C}}(\underline{k}) = (\mathcal{D}^{\underline{\hat{k}}})^T \cdot \mathring{\widehat{\underset{\approx}{C}}}(\underline{\hat{k}}) \cdot \mathcal{D}^{\underline{\hat{k}}}$$

Prop 1: $\boxed{\mathring{\widehat{\underset{\approx}{C}}}(\underline{k}) = \mathring{\widehat{\underset{\approx}{C}}}(k)}$

Prop 2:
$$\mathring{\widehat{\underset{\approx}{C}}}(\underline{k}) = \begin{pmatrix} \mathring{\widehat{C}}_1(k) & \mathring{\widehat{C}}_2(k) & 0 & 0 & 0 & 0 \\ \mathring{\widehat{C}}_2(k) & \mathring{\widehat{C}}_3(k) & 0 & 0 & 0 & 0 \\ 0 & 0 & \mathring{\widehat{C}}_4(k) & 0 & 0 & 0 \\ 0 & 0 & 0 & \mathring{\widehat{C}}_4(k) & 0 & 0 \\ 0 & 0 & 0 & 0 & \mathring{\widehat{C}}_5(k) & 0 \\ 0 & 0 & 0 & 0 & 0 & \mathring{\widehat{C}}_5(k) \end{pmatrix}$$

Mechanical balance

$$i\underline{k} \cdot \underline{\underline{\widehat{\sigma}}} = 0$$

$$\Leftrightarrow$$

$$\forall k \neq 0 \quad \begin{cases} \widehat{\sigma}_{kk} = 0 \\ \widehat{\sigma}_{k\vartheta} = 0 \\ \widehat{\sigma}_{k\varphi} = 0 \end{cases}$$

$$\Leftrightarrow$$

$$\forall \underline{k} \neq \underline{0} \quad \begin{cases} \widehat{\sigma}_2^{\hat{k}}(\underline{k}) = \dfrac{1}{\sqrt{2}}\, \widehat{\sigma}_1^{\hat{k}}(\underline{k}) \\ \widehat{\sigma}_3^{\hat{k}}(\underline{k}) = \widehat{\sigma}_4^{\hat{k}}(\underline{k}) = 0 \end{cases}$$

$$\underset{\sim}{\widehat{\sigma}} = \begin{cases} -\dfrac{1}{\sqrt{3}}\,(\sigma_{\vartheta\vartheta} + \sigma_{\varphi\varphi} + \sigma_{kk}) \\ -\dfrac{1}{\sqrt{6}}\,(\sigma_{\vartheta\vartheta} + \sigma_{\varphi\varphi} - 2\,\sigma_{kk}) \\ \sqrt{2}\,\sigma_{\varphi k} \\ \sqrt{2}\,\sigma_{\vartheta k} \\ \sqrt{2}\,\sigma_{\vartheta\varphi} \\ \dfrac{1}{\sqrt{2}}\,(\sigma_{\vartheta\vartheta} - \sigma_{\varphi\varphi}) \end{cases}$$

$$\forall \underline{k} \neq \underline{0} \qquad \underset{\approx}{\hat{\mathring{C}}}(\underline{k}) = \begin{pmatrix} \hat{\mathring{C}}_1(k) & \frac{1}{\sqrt{2}}\,\hat{\mathring{C}}_1(k) & 0 & 0 & 0 & 0 \\ \frac{1}{\sqrt{2}}\,\hat{\mathring{C}}_1(k) & \frac{1}{2}\,\hat{\mathring{C}}_1(k) & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \hat{\mathring{C}}_5(k) & 0 \\ 0 & 0 & 0 & 0 & 0 & \hat{\mathring{C}}_5(k) \end{pmatrix}$$

Cartesian and Radial, in real and Fourier spaces

$$C_{ab}(\underline{r}) \equiv \langle \sigma_a(\underline{r}_0)\, \sigma_b(\underline{r}_0 + \underline{r}) \rangle_c$$

$$\boxed{\mathring{C}_{ab}(\underline{r}) \equiv \langle \sigma_a^{\underline{\hat{r}}}(\underline{r}_0)\, \sigma_b^{\underline{\hat{r}}}(\underline{r}_0 + \underline{r}) \rangle_c}$$

$$\underset{\approx}{\mathring{C}} = \mathcal{D}_{\underline{\hat{r}}} \cdot \underset{\approx}{C} \cdot \mathcal{D}_{\underline{\hat{r}}}^T$$

$$\mathcal{F}$$

$$\widehat{C}_{ab}(\underline{k}) \equiv \frac{1}{(2\pi)^2} \left\langle \widehat{\sigma}_{a\,\underline{k}}\, \left(\widehat{\sigma}_{b\,\underline{k}}\right)^* \right\rangle_c$$

$$\boxed{\mathring{\widehat{C}}_{ab}(\underline{k}) \equiv \frac{1}{(2\pi)^2} \left\langle \widehat{\sigma}^{\underline{\hat{k}}}_{a\,\underline{k}} \left(\widehat{\sigma}^{\underline{\hat{k}}}_{b\,\underline{k}}\right)^* \right\rangle_c}$$

$$\underset{\approx}{\mathring{\widehat{C}}} = \mathcal{D}_{\underline{\hat{k}}} \cdot \underset{\approx}{\widehat{C}} \cdot \mathcal{D}_{\underline{\hat{k}}}^T$$

After a bit of algebra...

$$
\begin{cases}
\mathring{C}_1(r) = \mathring{C}_1^{(0)} \\
\mathring{C}_2(r) = -\dfrac{\sqrt{2}}{2}\,\mathring{C}_1^{(2)} \\
\mathring{C}_3(r) = \dfrac{\mathring{C}_1^{(0)} + 4\mathring{C}_5^{(0)}}{10} - \dfrac{\mathring{C}_1^{(2)} - 4\mathring{C}_5^{(2)}}{7} + \dfrac{9\mathring{C}_1^{(4)} + 6\mathring{C}_5^{(4)}}{35} \\
\mathring{C}_4(r) = \dfrac{\mathring{C}_1^{(0)} + 4\mathring{C}_5^{(0)}}{10} - \dfrac{\mathring{C}_1^{(2)} - 4\mathring{C}_5^{(2)}}{14} - \dfrac{6\mathring{C}_1^{(4)} + 4\mathring{C}_5^{(4)}}{35} \\
\mathring{C}_5(r) = \dfrac{\mathring{C}_1^{(0)} + 4\mathring{C}_5^{(0)}}{10} + \dfrac{\mathring{C}_1^{(2)} - 4\mathring{C}_5^{(2)}}{7} + \dfrac{3\mathring{C}_1^{(4)} + 2\mathring{C}_5^{(4)}}{70}
\end{cases}
$$

where $\mathring{C}^{(m)}(r) = (2\pi)^{-3/2} \int_0^\infty \mathrm{d}k\; k^2\, \hat{\mathring{C}}(k)\, \dfrac{J_{m+\frac{1}{2}}(kr)}{\sqrt{kr}}$

or, $$\boxed{\mathring{C}^{(m)}(r) = (2\pi)^m\, r^m\, \mathcal{F}^{-1}_{2m+3}\left[\frac{\hat{\mathring{C}}(\|\underline{k}\|)}{\|\underline{k}\|^m}\right]}$$

since $f(r) = (2\pi)^{-d/2} \int_0^\infty \mathrm{d}k\; \dfrac{k^{d/2}}{r^{d/2-1}}\, \widehat{f}(k)\, J_{\frac{d}{2}-1}(kr)$

After a bit of algebra...

$$
\begin{cases}
\mathring{C}_1(r) = \mathring{C}_1^{(0)} \\
\mathring{C}_2(r) = -\dfrac{\sqrt{2}}{2}\,\mathring{C}_1^{(2)} \\
\mathring{C}_3(r) = \dfrac{\mathring{C}_1^{(0)} + 4\mathring{C}_5^{(0)}}{10} - \dfrac{\mathring{C}_1^{(2)} - 4\mathring{C}_5^{(2)}}{7} + \dfrac{9\mathring{C}_1^{(4)} + 6\mathring{C}_5^{(4)}}{35} \\
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\mathring{C}_5(r) = \dfrac{\mathring{C}_1^{(0)} + 4\mathring{C}_5^{(0)}}{10} + \dfrac{\mathring{C}_1^{(2)} - 4\mathring{C}_5^{(2)}}{7} + \dfrac{3\mathring{C}_1^{(4)} + 2\mathring{C}_5^{(4)}}{70}
\end{cases}
$$

where $\boxed{\mathring{C}^{(m)}(r) = (2\pi)^m\, r^m\, \mathcal{F}^{-1}_{2m+3}\left[\dfrac{\hat{\mathring{C}}(\|\underline{k}\|)}{\|\underline{k}\|^m}\right]}$

We will show Continuity in k=0

- does not exclude a singularity in $\hat{\mathring{C}}_1(k)$ or $\hat{\mathring{C}}_5(k)$
- yet, for all $m \neq 0$, $1/k^m$ leading singularity (under the inverse transform)

$$\mathring{C}^{(m)} \sim 1/r^3 \text{ at long range}$$

Isotropic tensors

Definition: an isotropic tensor = a tensor invariant under all rotations
in the case of rank four tensors, it means:

$$\underset{\approx}{C} = \mathcal{D} \cdot \underset{\approx}{C} \cdot \mathcal{D}^T$$

Schur:

$$\underset{\approx}{C} = \begin{pmatrix} C_0 & 0 & 0 & 0 & 0 & 0 \\ 0 & C_0' & 0 & 0 & 0 & 0 \\ 0 & 0 & C_0' & 0 & 0 & 0 \\ 0 & 0 & 0 & C_0' & 0 & 0 \\ 0 & 0 & 0 & 0 & C_0' & 0 \\ 0 & 0 & 0 & 0 & 0 & C_0' \end{pmatrix}$$

Take any $\underset{\approx}{C}(\underline{r})$

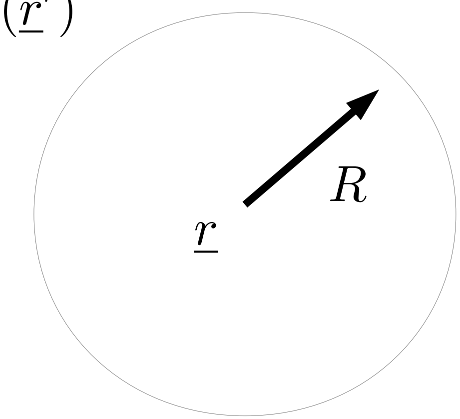
Define its isotropic part $\mathrm{I}\textsc{so}\left[\underset{\approx}{C}\right]$ as the isotropic tensor with:

$$C_0 \equiv C_{11}$$

$$C_0' \equiv \frac{1}{5}\left(\mathrm{Tr}\left[\underset{\approx}{C}\right] - C_{11}\right)$$

Local stress fluctuations

In an infinite medium,
the window-averaged stress: $$\overline{\underset{\sim}{\sigma}}(\underline{r};R) = \frac{1}{\Omega_R} \int_{\|\underline{r}'-\underline{r}\|<R} \mathrm{d}^2\underline{r}' \ \underset{\sim}{\sigma}(\underline{r}')$$



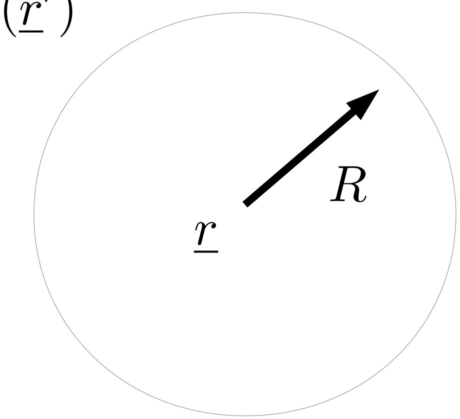
Its fluctuation matrix: $J_{ab}(R) = \langle \overline{\sigma}_a(\underline{r};R)\overline{\sigma}_b(\underline{r};R)\rangle_c$

Check that $\underset{\approx}{J}(R) = \dfrac{1}{\Omega_R^2} \displaystyle\int_{r_1<R} \mathrm{d}^3\underline{r}_1 \int_{r_2<R} \mathrm{d}^3\underline{r}_2 \ \underset{\approx}{C}\,(\underline{r}_2 - \underline{r}_1)$
is an isotropic tensor

Local stress fluctuations

In an infinite medium,
the window-averaged stress:

$$\overline{\underset{\sim}{\sigma}}(\underline{r};R) = \frac{1}{\Omega_R} \int_{\|\underline{r}'-\underline{r}\|<R} \mathrm{d}^2\underline{r}'\ \underset{\sim}{\sigma}(\underline{r}')$$



Its fluctuation matrix: $J_{ab}(R) = \langle \overline{\sigma}_a(\underline{r};R)\overline{\sigma}_b(\underline{r};R)\rangle_c$

Check that $\underset{\approx}{J}(R) = \dfrac{1}{\Omega_R^2} \displaystyle\int_{r_1<R} \mathrm{d}^3\underline{r}_1 \int_{r_2<R} \mathrm{d}^3\underline{r}_2\ \underset{\approx}{C}\left(\underline{r}_2 - \underline{r}_1\right)$
is an isotropic tensor

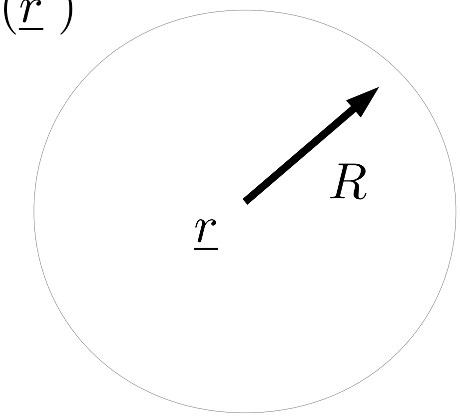
Normal fluctuations means that:

$$\Omega_R\, \underset{\approx}{J}(R) \longrightarrow \text{ finite when } R \to \infty$$

Local stress fluctuations

In an infinite medium,
the window-averaged stress:

$$\overline{\underset{\sim}{\sigma}}(\underline{r};R) = \frac{1}{\Omega_R} \int_{\|\underline{r}'-\underline{r}\|<R} \mathrm{d}^2\underline{r}'\ \underset{\sim}{\sigma}(\underline{r}')$$



Its fluctuation matrix: $J_{ab}(R) = \langle \overline{\sigma}_a(\underline{r};R)\overline{\sigma}_b(\underline{r};R)\rangle_c$

Check that $\underset{\approx}{J}(R) = \dfrac{1}{\Omega_R^2} \displaystyle\int_{r_1<R} \mathrm{d}^3\underline{r}_1 \int_{r_2<R} \mathrm{d}^3\underline{r}_2\ \underset{\approx}{C}\left(\underline{r}_2 - \underline{r}_1\right)$
is an isotropic tensor

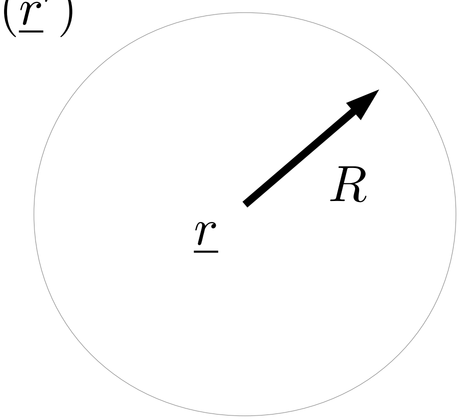
Hence:
$$\begin{aligned}\underset{\approx}{J}(R) &= \mathrm{Iso}\underset{\approx}{J}(R) \\ &= \frac{1}{\Omega_R^2} \int_{r_1<R} \mathrm{d}^3\underline{r}_1 \int_{r_2<R} \mathrm{d}^3\underline{r}_2\ \mathrm{Iso}\left[\underset{\approx}{C}\right]\left(\|\underline{r}_2 - \underline{r}_1\|\right) \\ &= \frac{1}{\Omega_R} \int \frac{\mathrm{d}^3\underline{k}}{(2\pi)^3}\, \widehat{\alpha}(\underline{k};R)\, \mathrm{Iso}\left[\widehat{\underset{\approx}{C}}\right](\underline{k})\end{aligned}$$

Where $\widehat{\alpha}$ (the scaled intersection volume function) is real-valued, positive, and

$$\widehat{\alpha} \to (2\pi)^3\, \delta^3(\underline{k}) \quad \text{when} \quad R \to \infty$$

Local stress fluctuations

In an infinite medium,
the window-averaged stress: $\overline{\underset{\sim}{\sigma}}(\underline{r};R) = \dfrac{1}{\Omega_R} \displaystyle\int_{\|\underline{r}'-\underline{r}\|<R} \mathrm{d}^2\underline{r}' \; \underset{\sim}{\sigma}(\underline{r}')$



Its fluctuation matrix: $J_{ab}(R) = \langle \overline{\sigma}_a(\underline{r};R)\overline{\sigma}_b(\underline{r};R)\rangle_c$

Check that $\underset{\approx}{J}(R) = \dfrac{1}{\Omega_R^2} \displaystyle\int_{r_1<R} \mathrm{d}^3\underline{r}_1 \int_{r_2<R} \mathrm{d}^3\underline{r}_2 \; \underset{\approx}{C}\,(\underline{r}_2 - \underline{r}_1)$
is an isotropic tensor

Hence: $\underset{\approx}{J}(R) = \mathrm{Iso}\underset{\approx}{J}(R)$

$$= \frac{1}{\Omega_R^2} \int_{r_1<R} \mathrm{d}^3\underline{r}_1 \int_{r_2<R} \mathrm{d}^3\underline{r}_2 \; \mathrm{Iso}\left[\underset{\approx}{C}\right](\|\underline{r}_2 - \underline{r}_1\|)$$

$$= \frac{1}{\Omega_R} \int \frac{\mathrm{d}^3\underline{k}}{(2\pi)^3}\, \widehat{\alpha}(\underline{k};R)\,\mathrm{Iso}\left[\widehat{\underset{\approx}{C}}\right](\underline{k})$$

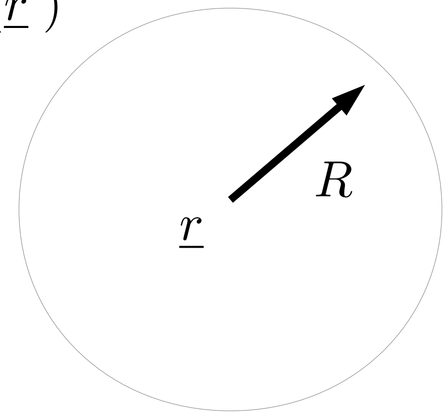
continuous at k=0

Where $\widehat{\alpha}$ (the scaled intersection volume function) is real-valued, positive, and

$$\widehat{\alpha} \to (2\pi)^3\,\delta^3(\underline{k}) \;\text{ when }\; R \to \infty$$

Local stress fluctuations

In an infinite medium,
the window-averaged stress: $\overline{\underset{\sim}{\sigma}}(\underline{r};R) = \dfrac{1}{\Omega_R} \displaystyle\int_{\|\underline{r}'-\underline{r}\|<R} \mathrm{d}^2\underline{r}' \ \underset{\sim}{\sigma}(\underline{r}')$



Its fluctuation matrix: $J_{ab}(R) = \langle \overline{\sigma}_a(\underline{r};R)\overline{\sigma}_b(\underline{r};R)\rangle_c$

Check that $\underset{\approx}{J}(R) = \dfrac{1}{\Omega_R^2} \displaystyle\int_{r_1<R} \mathrm{d}^3\underline{r}_1 \int_{r_2<R} \mathrm{d}^3\underline{r}_2 \ \underset{\approx}{C}\left(\underline{r}_2 - \underline{r}_1\right)$
is an isotropic tensor

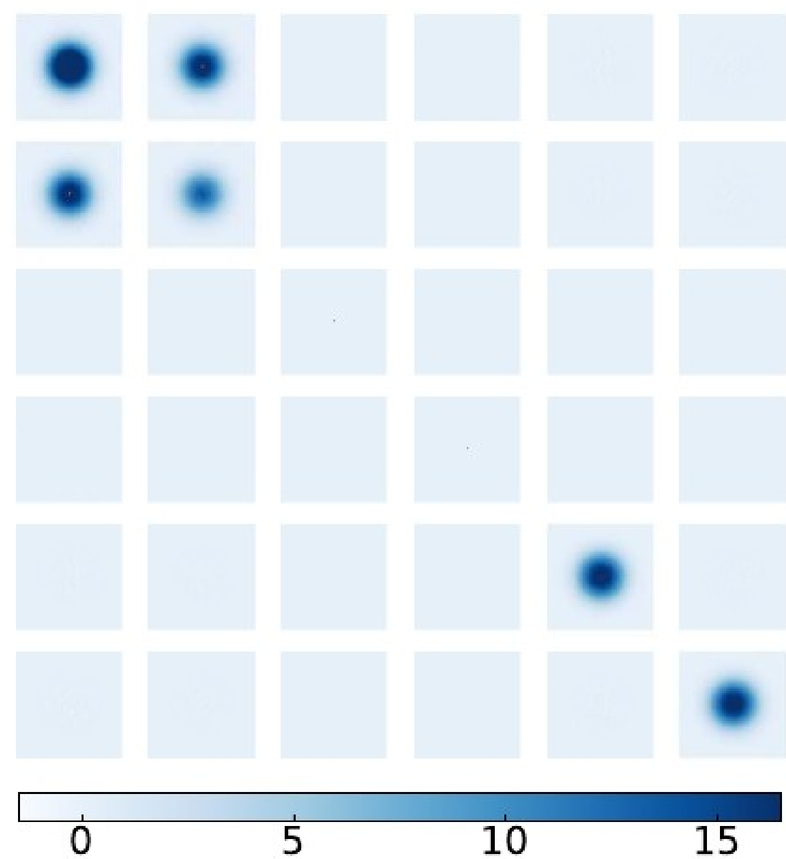
Normal fluctuations means that:

$$\Omega_R\, \underset{\approx}{J}(R) \underset{R\to\infty}{\longrightarrow} \mathrm{Iso}\ \underset{\approx}{\widehat{C}}(\underline{0}) = \begin{pmatrix} \widehat{C}_0(0) & 0 & 0 & 0 & 0 & 0 \\ 0 & \widehat{C}_0'(0) & 0 & 0 & 0 & 0 \\ 0 & 0 & \widehat{C}_0'(0) & 0 & 0 & 0 \\ 0 & 0 & 0 & \widehat{C}_0'(0) & 0 & 0 \\ 0 & 0 & 0 & 0 & \widehat{C}_0'(0) & 0 \\ 0 & 0 & 0 & 0 & 0 & \widehat{C}_0'(0) \end{pmatrix}$$

$$\widehat{C}_0(k) = \mathring{\widehat{C}}_1(k) \qquad \widehat{C}_0'(k) = \frac{1}{10}\,\mathring{\widehat{C}}_1(k) + \frac{2}{5}\,\mathring{\widehat{C}}_5(k)$$

Numerical data

$$\forall \underline{k} \neq \underline{0} \qquad \underset{\approx}{\hat{\mathring{C}}}(\underline{k}) = \begin{pmatrix} \hat{\mathring{C}}_1(k) & \frac{1}{\sqrt{2}}\,\hat{\mathring{C}}_1(k) & 0 & 0 & 0 & 0 \\ \frac{1}{\sqrt{2}}\,\hat{\mathring{C}}_1(k) & \frac{1}{2}\,\hat{\mathring{C}}_1(k) & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \hat{\mathring{C}}_5(k) & 0 \\ 0 & 0 & 0 & 0 & 0 & \hat{\mathring{C}}_5(k) \end{pmatrix}$$

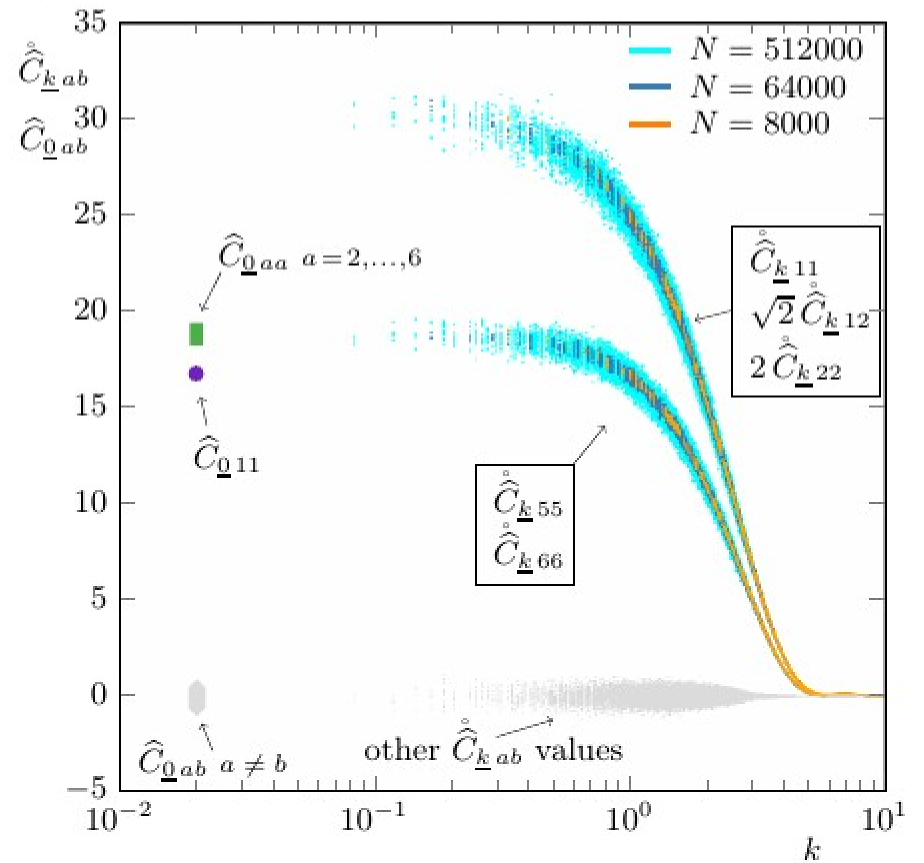


Numerical data

$$\forall \underline{k} \neq \underline{0} \qquad \underset{\approx}{\mathring{\widehat{C}}}(\underline{k}) = \begin{pmatrix} \mathring{\widehat{C}}_1(k) & \frac{1}{\sqrt{2}}\,\mathring{\widehat{C}}_1(k) & 0 & 0 & 0 & 0 \\ \frac{1}{\sqrt{2}}\,\mathring{\widehat{C}}_1(k) & \frac{1}{2}\,\mathring{\widehat{C}}_1(k) & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \mathring{\widehat{C}}_5(k) & 0 \\ 0 & 0 & 0 & 0 & 0 & \mathring{\widehat{C}}_5(k) \end{pmatrix}$$

$$\underset{\approx}{\widehat{C}}_{k \to \underline{0}} \neq \underset{\approx}{\widehat{C}}_{\underline{k} = \underline{0}}$$

$$\underbrace{\text{Fluctuations on a sphere in the infinite medium} \neq \text{Fluctuations in the whole cell}}_{\textbf{Invalidity of spatial ergodicity}}$$



Conclusions

Proven:

$$\left.\begin{array}{l}\text{Material isotropy}\\ \text{Mechanical balance}\\ \text{Normality of local fluctuations}\end{array}\right\} \Longrightarrow \begin{array}{l}\text{Long-range correlations}\\ \sim \text{elastic Green functions}\end{array}$$

2D [AL, PRE, 96, 052101 (2017)]
3D [AL, JCP, 149, 104107 (2018)]

Observed:

Normal fluctuations, local and macroscopic, (fully expected)

Ergodicity breaking

Associated with correlation background (homogeneous term) in real-space
Impacts the value of stress fluctuations