ACOUSTIC-LIKE EXCITATIONS IN STRUCTURAL GLASSES BY A MEAN FIELD APPROACH

Rayleigh Scattering and disorder-induced mixing of polarizations

Workshop ‘Interaction, Disorder, Elasticity’
École de Physique des Houches
Les Houches, April 3-7, 2023

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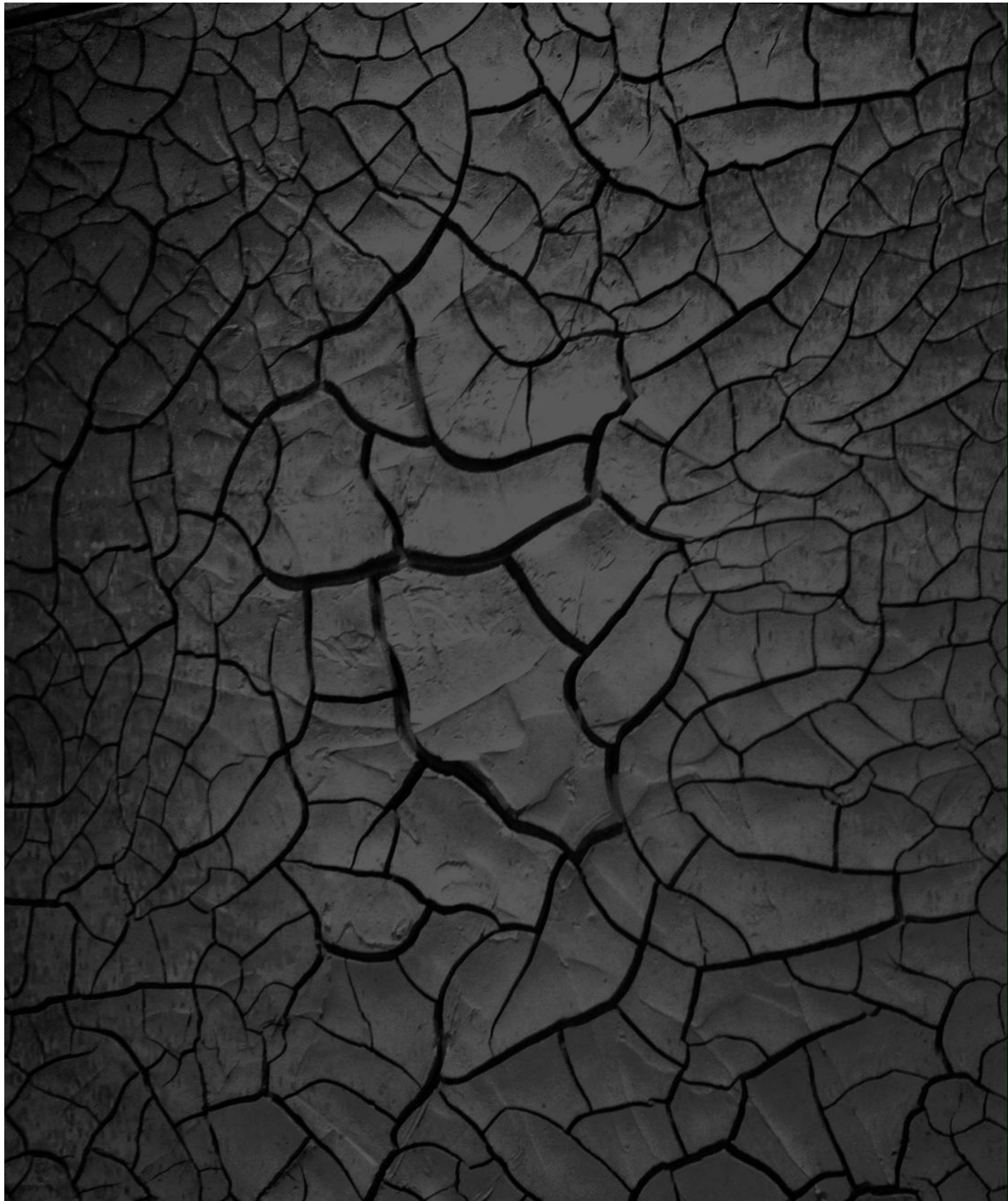
SISSA



Alberto Burri, Cretto G1 (1975) Galleria Nazionale D’Arte Moderna e Contemporanea, Roma

- M. G. Izzo, G. Ruocco, and S. Cazzato, ‘The Mixing of Polarizations in the Acoustic Excitations of Disordered Media With Local Isotropy’ Front. Phys. 6, 108 (2018)
- M. G. Izzo, B. Wehinger, S. Cazzato, A. Matic, C. Masciovecchio, A. Gessini, and G. Ruocco, ‘Rayleigh scattering and disorder-induced mixing of polarizations in amorphous solids at the nanoscale: 1-octyl-3-methylimidazolium chloride glass’ Phys. Rev. B 102, 214309 (2020)
- https://github.com/mariagraziaizzo/Generalized-Born-Approximation (work in progress)

The dynamic structure factor of structural glasses: atomistic and mean field description in the harmonic approximation

$$S_i(\mathbf{q},\omega) \propto (\frac{q}{\omega})^2 \int d^3r e^{i\mathbf{q}\cdot\mathbf{r}} \int dt e^{i\omega t} < \mathbf{j}_i(\mathbf{r},t)\mathbf{j}(\mathbf{0},0) >$$

i=L,T

MICROSCOPIC DESCRIPTION

$$S_L(\mathbf{q},\omega) \propto \frac{q^2}{\omega^2} T \sum_\alpha \delta(\omega-\Omega_\alpha) \sum_{ij} < (\hat{q}\cdot\mathbf{e}_i^\alpha)(\hat{q}\cdot\mathbf{e}_j^\alpha) e^{i(\mathbf{r}_i-\mathbf{r}_j)\cdot\mathbf{q}} >$$

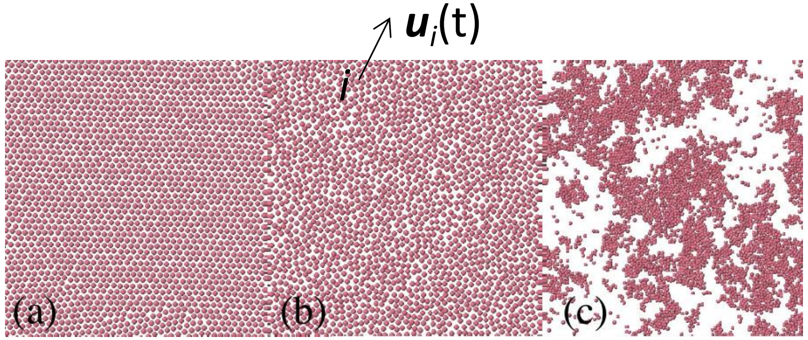
$$e^{\alpha'}_{i(s')} D_{ij(s's)} e^{\alpha}_{j(s)} = \Omega_\alpha^2 \delta_{\alpha\alpha'}$$

NORMAL MODES

D: DYNAMICAL MATRIX

$$\ddot{\mathbf{u}}_i(t) = \sum_{j=1}^N D_{ij}\mathbf{u}_j \quad j_L(\mathbf{q},t) = \sum_{i=1}^N \mathbf{q}\cdot\dot{\mathbf{u}}_i$$

- THE LOCALIZED SOFT MODES: a special class of non-Goldstone vibrational normal modes of glasses with a large value of the inverse partecipation ratio and Ω_α <<1.



[1] H. Mizuno, H. Shiba and A. Ikeda, PNAS 114 (46) E9767 (2017)

[2] L. Berthier, *Physics* 4, 42 (2011)

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$$S_i(\mathbf{q},\omega) \propto (\frac{q}{\omega})^2 \int d^3 r e^{i\mathbf{q}\cdot\mathbf{r}} \int dt e^{i\omega t} < \mathbf{j}_i(\mathbf{r},t)\mathbf{j}(\mathbf{0},0) >$$ i=L,T

MEAN FIELD DESCRIPTION

$$S_L(\mathbf{q},\omega) \propto \frac{q^2}{\omega} Im\{< G_L(\mathbf{q},\omega) >\}$$

DYSON EQUATION:

$$G^0(\mathbf{q},\omega) = \frac{1}{\mathbf{q}^2 - c^2\omega^2}$$

$$<G_L(\mathbf{q},\omega) >= \frac{1}{G^0_L(\mathbf{q},\omega) - \Sigma_L(\mathbf{q},\omega)}$$

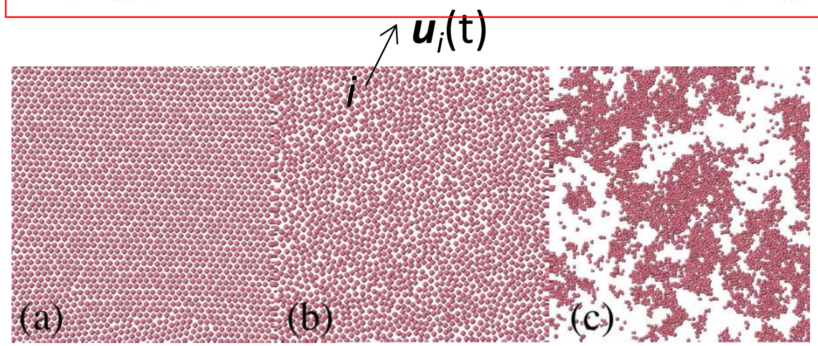
$\Sigma(\mathbf{q},\omega)$: SELF-ENERGY

PERTURBATIVE SERIES EXPANSION

It constitutes the starting point for smoothing methods or approximations.

auto-correlation function of the elastic tensor

$$R_{\gamma\alpha jl\beta ki\delta}(\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2) = \langle \delta C_{\gamma\alpha jl}(\mathbf{r}_1)\delta C_{\beta ki\delta}(\mathbf{r}_2)\rangle$$



FROM DISORDER TO SPATIAL INHOMOGENEITY OF THE ELASTIC TENSOR

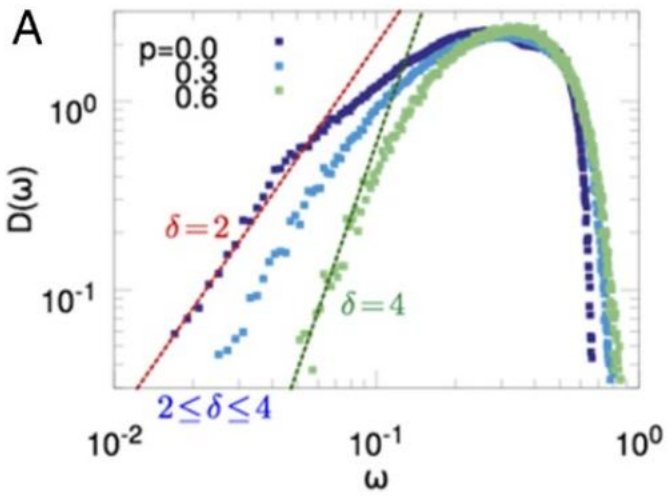
[2] L. Berthier, *Physics* 4, 42 (2011)

The dynamic structure factor of structural glasses: atomistic and mean field description in the harmonic approximation

Rayleigh scattering (ω^4 trend in VDOS):

MICROSCOPIC DESCRIPTION

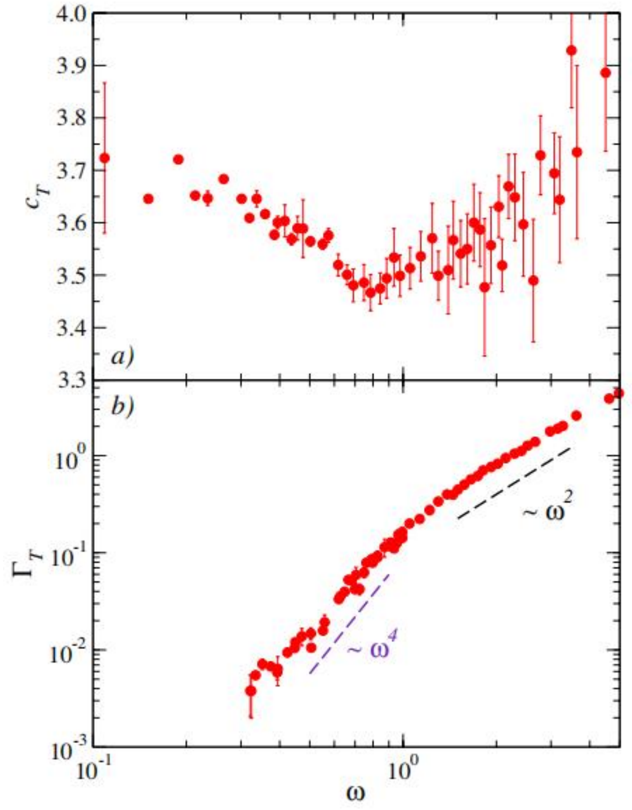
LOCALIZED SOFT MODES → ω^4 TREND OF LOW-ω VDOS



[3] L. Angelani, M. Paoluzzi, G. Parisi, and G. Ruocco, PNAS 115, 8700 (2018)

MEAN FIELD DESCRIPTION

RAYLEIGH SCATTERING FROM ELASTIC INHOMOGENEITIES → $\Gamma(\Omega) \propto \Omega^4=(cq)^4$



[4] G. Monaco and S. Mossa, PNAS 106, 16907 (2009)

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$$S_i(\mathbf{q},\omega) \propto (\frac{q}{\omega})^2 \int d^3r e^{i\mathbf{q}\cdot\mathbf{r}} \int dt e^{i\omega t} < \mathbf{j}_i(\mathbf{r},t)\mathbf{j}(\mathbf{0},0) >$$

MICROSCOPIC DESCRIPTION

$$S_L(\mathbf{q},\omega) \propto \frac{q^2}{\omega^2} T \sum_\alpha \delta(\omega - \Omega_\alpha) \sum_{ij} < (\hat{q}\cdot\mathbf{e}_i^\alpha)(\hat{q}\cdot\mathbf{e}_j^\alpha) e^{i(\mathbf{r}_i - \mathbf{r}_j)\cdot\mathbf{q}} >$$

MEAN FIELD DESCRIPTION

$$S_L(\mathbf{q},\omega) \propto \frac{q^2}{\omega} Im\{< G_L(\mathbf{q},\omega) >\}$$

partial biliography:

[5] S. N. Taraskin, and S. R. Elliot, Phys. Rev. B 56, 8605 (1997)
[6] E. Lerner, G. During, E. Bouchbinder, Phys. Rev. Lett. 117, 035501 (2016)
[7] M. Baity-Jesi, V. Martin-Mayor, G. Parisi, S. Perez-Gaviro, Phys. Rev. Lett. 115, 267205 (2015)
[8] L. Wang, A. Ninarello, P. Guan, L. Berthier, G. Szamel, and E. Flenner, Nat. Commun. 10, 26 (2019)
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[10] S. Bonfanti, R. Guerra, C. Mondal, I. Procaccia, and S. Zapperi, Phys. Rev. Lett. 125, 085501 (2020)
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[12] S. Kohler, G. Ruocco, W. Schirmacher, Phys Rev B 88, 064203 (2013)
[13] R. H. Kraichnan, J Math Phy. 2, 124 (1961)
[14] J. Kim and S. Torquato,New J.Phys. 22 (2020) 123050

The dynamic structure factor of structural glasses: atomistic and mean field description in the harmonic approximation

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MEAN FIELD DESCRIPTION

$$S_L(\mathbf{q},\omega) \propto \frac{q^2}{\omega} Im\{< G_L(\mathbf{q},\omega) >\}$$

amorphization transition: enhancing localization of normal modes ⟷ setting up spatial elastic fluctuations

[13] H. Mizuno, S. Mossa, and J.-L. Barrat, Phys. Rev. B **94**, 144303 (2016)
[14] H. Mizuno, S. Mossa and J.-L. Barrat, Phys. Rev. E 87, 042306 (2013)

Localized soft modes in the Euclidean Random Matrix model ⟷ Corresponding Self-energy expressions, e.g. in the Self-Consistent Born Approximation (SCBA)

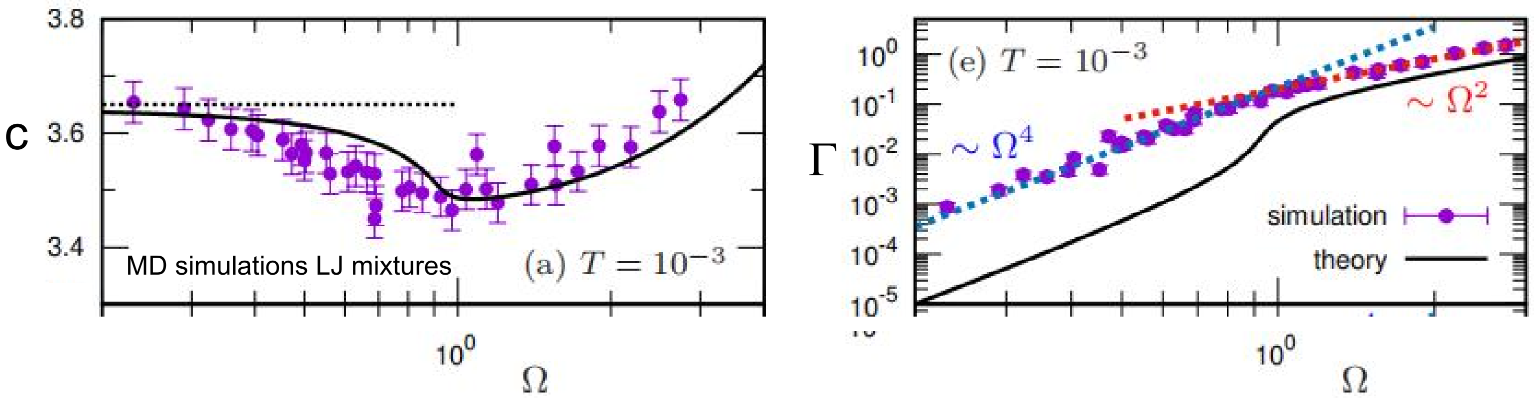
[15] M. Mezard, G. Parisi and A. Zee, Nucl. Phys. B 559, 689 (1999)
[16] T. S. Grigera, V. Martin-Mayor, G. Parisi, P. Urbani and P. Verrocchio, J. Stat. Mech. P02015 (2011)
[17] C. Ganter and W. Schirmacher, Phys. Rev. B 82, 094205 (2010)
[18] E. Bouchbinder, E. Lerner, C. Rainone, P. Urbani, and F. Zamponi, Phys. Rev. B 103, 174202 (2021)

The dynamic structure factor of structural glasses: atomistic and mean field description in the harmonic approximation

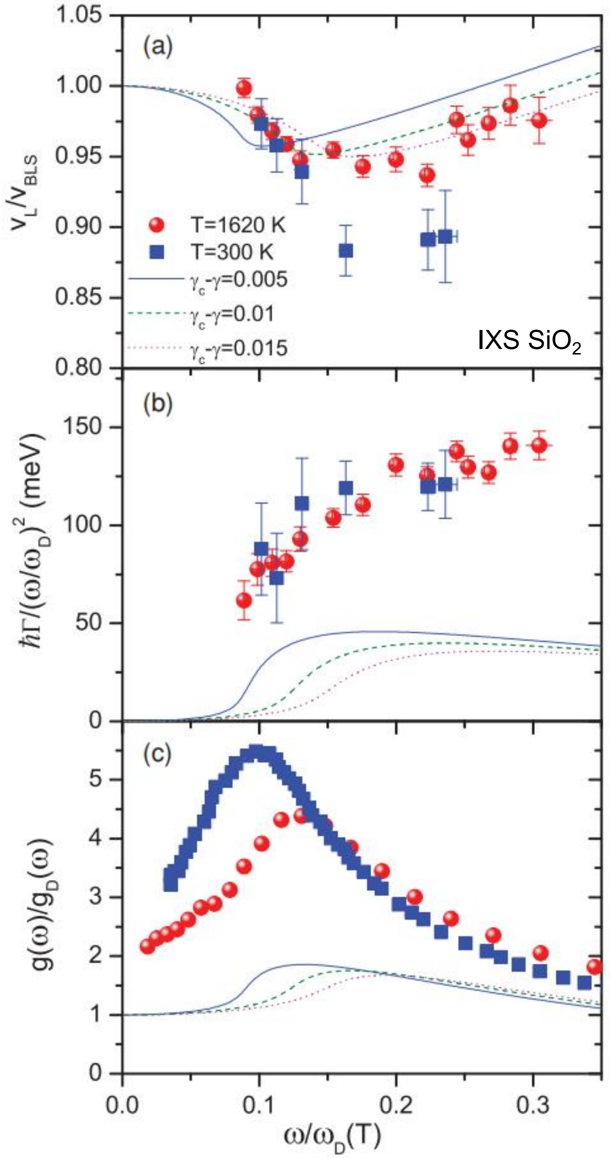
- Can a Random Media theory allow to achieve a realistic description of the features of $S(\mathbf{q},\omega)$ in a structural glasses related to the presence of elastic inhomogeneities?

Comparing Random Media Theories with real systems behavior

- Mean field RMTs qualitatively but not quantitatively reproduce the Rayleigh scattering.
- The degree of elastic inhomogeneity measured by MD simulations is larger than the Self-Consistent Born Approximation (SCBA) edge of stability [18].



[18] H. Mizuno, S. Mossa, Cond. Mat. Phys., **22**, 43604 (2019)



[19] G. Baldi, V. M. Giordano, and G. Monaco, Phys. Rev. B **83**, 174203 (2011)

- How the spatial elastic inhomogeneity affects the polarization properties of acoustic-like excitations in glasses?

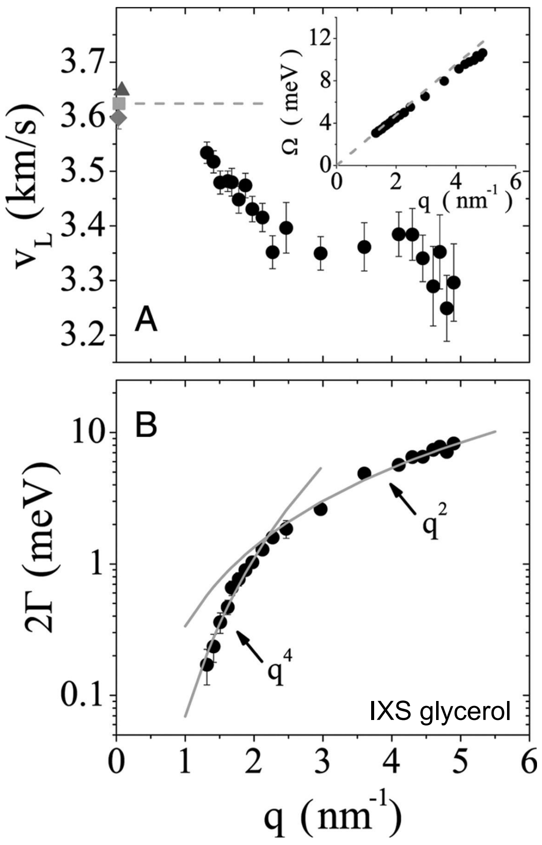
✓ Phase velocity
✓ Amplitude
Polarization

Rayleigh scattering

Comparing Random Media Theories with real systems behavior

IXS experiments and MD simulations:

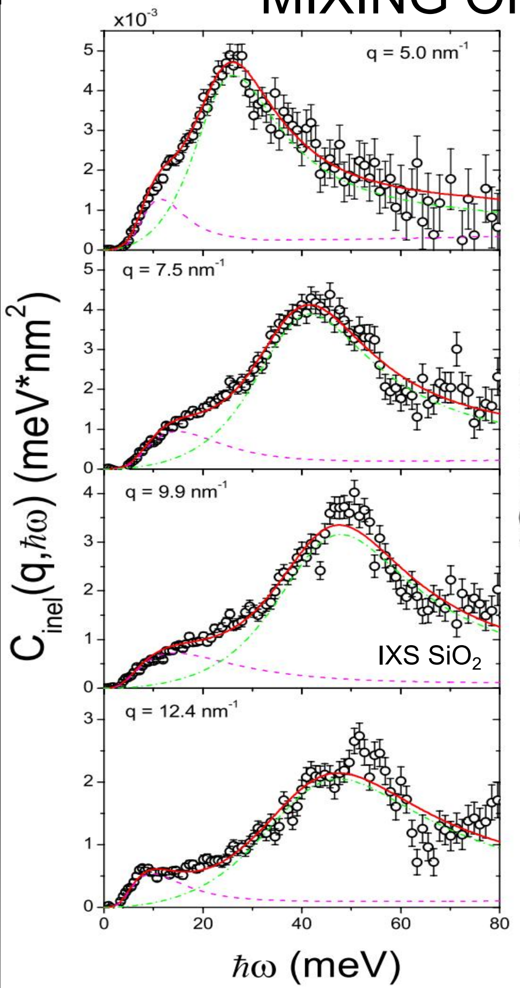
RAYLEIGH SCATTERING

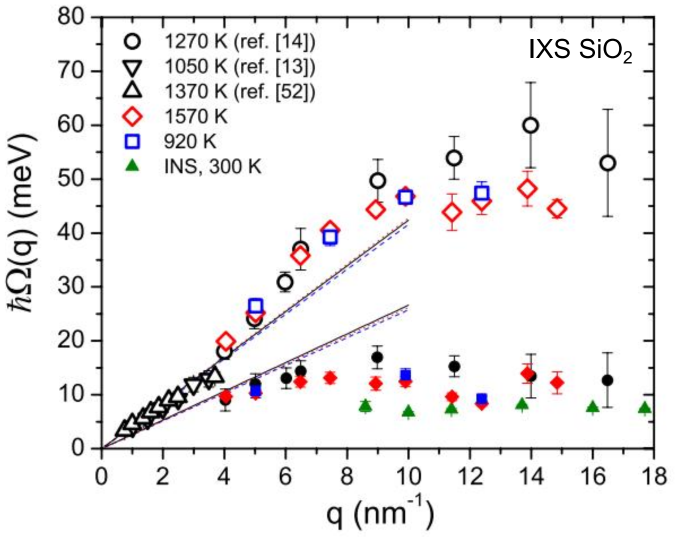


[20] Monaco G, Giordano V. *PNAS* **106,** 3659 (2009)

[21] C. Ferrante et al., Nat Commun. **4**, 1793 (2013)
[22] B. Rufflé, D. A. Parshin, E. Courtens, R. Vacher, Phys. Rev. Lett. **100**, 014204 (2008)
[23] B. Ruta, G. Baldi, F. Scarponi, D. Fioretto, V. M. Giordano, and G. Monaco, J. Chem. Phys. **137**, 214502 (2012)
[24] G. Baldi, V. M. Giordano, G. Monaco, and B. Ruta, Phys. Rev. Lett. **104**, 195501 (2010)

MIXING OF POLARIZATIONS





[25] G. Baldi, V. M. Giordano, G. Monaco, F. Sette, E. Fabiani, A. Fontana, and G. Ruocco, Phys. Rev. B 77, 214309 (2008)

[26] B. Ruzicka, T. Scopigno et al., Phys. Rev. B 69, 100201(R) (2004)
[27] F. Bencivenga and D. Antonangeli, Phys. Rev. B 90, 134310 (2014)
[28] A. Cimatoribus, S. Saccani, F. Bencivenga, A. Gessini, M. G. Izzo, and C. Masciovecchio, New J. Phys. 12, 053008 (2010)
[29] M. C. C. Ribeiro, J. Chem. Phys. 139, 114505 (2013)

From the STOCHASTIC HELMHOLTZ EQUATION to the DYSON EQUATION: finding a formal expression for <**G**(**x**,**x'**,t)>

The stochastic Helmholtz equation: $\{\hat{L}^0_{ki}(\mathbf{x},t) + \hat{L}^s_{ki}(\mathbf{x},t)\}G_{ij}(\mathbf{x},\mathbf{x}',t) = \delta_{kj}\delta(\mathbf{x}-\mathbf{x}')\delta(t)$

- Deterministic differential operator: $\hat{L}^0_{ki}(\mathbf{x},t) = -\delta_{ki}\rho_0\frac{\partial^2}{\partial t^2} + \lambda_0\frac{\partial}{\partial x_k}\frac{\partial}{\partial x_i} + \mu_0\left[\frac{\partial}{\partial x_k}\frac{\partial}{\partial x_i} + \delta_{ki}\frac{\partial}{\partial x_l}\frac{\partial}{\partial x_l}\right]$

- Stochastic differential operator:

$$\hat{L}^s_{ki}(\mathbf{x},t) = -\delta_{ki}\delta\rho(\mathbf{x})\frac{\partial^2}{\partial t^2} + \frac{\partial}{\partial x_k}\delta\lambda(\mathbf{x})\frac{\partial}{\partial x_i} + \frac{\partial}{\partial x_k}\delta\mu(\mathbf{x})\frac{\partial}{\partial x_i} + \delta_{ki}\frac{\partial}{\partial x_l}\delta\mu(\mathbf{x})\frac{\partial}{\partial x_l}$$

RANDOM FIELD: $\delta\mu(\mathbf{x},\gamma);\ \gamma\in\Gamma$

From the STOCHASTIC HELMHOLTZ EQUATION to the DYSON EQUATION: finding a formal expression for <**G**(**x**,**x'**,t)>

A case in point,

the scalar stochastic Helmholtz equation: $\hat{L}^0 G(\mathbf{x},\mathbf{x}_0) + k^2 C(\mathbf{x}) = \nabla^2 G(\mathbf{x},\mathbf{x}_0) + k^2[1 + C(\mathbf{x})] = \delta(\mathbf{x}-\mathbf{x}_0)$

$$< C(\mathbf{x}) >= 0$$

$$G_0(\mathbf{x},\mathbf{x}_0,t) = \frac{e^{ik|\mathbf{x}-\mathbf{x}_0|}}{-4\pi|\mathbf{x}-\mathbf{x}_0|} e^{\pm i\omega t}$$

FREE SPACE WAVEVECTOR $k = \frac{\omega}{c}$

From the STOCHASTIC HELMHOLTZ EQUATION to the DYSON EQUATION: finding a formal expression for <**G**(**x**,**x'**,t)>

The scalar stochastic Helmholtz equation: $G(\mathbf{x},\mathbf{x}_0) = (\hat{L}^0)^{-1}\delta(\mathbf{x}-\mathbf{x}_0) - (\hat{L}^0)^{-1}k^2 C(\mathbf{x}) G(\mathbf{x},\mathbf{x}_0)$

$$< C(\mathbf{x}_1) >= 0$$

$$(\hat{L}^0)^{-1} f(x) = \int G^0(\mathbf{x},\mathbf{x}')f(\mathbf{x}')d^3x'$$

....

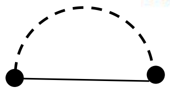
$$< G(\mathbf{x},\mathbf{x}_0) = G^0(\mathbf{x},\mathbf{x}_0) - k^2\int G^0(\mathbf{x},\mathbf{x}_1)C(\mathbf{x}_1)G^0(\mathbf{x}_1,\mathbf{x}_0)d^3x_1 + (-k^2)^2\int G^0(\mathbf{x},\mathbf{x}_1)C(\mathbf{x}_1)G^0(\mathbf{x}_1,\mathbf{x}_2)C(\mathbf{x}_2)G^0(\mathbf{x}_2,\mathbf{x}_0)d^3x_1 d^3x_2 + \ldots >$$

- Hypothesis of Gaussian random field: $< C(\mathbf{x}_1)\ldots C(\mathbf{x}_{2n})) >= \sum_{p.p.} R(\mathbf{x}_\alpha,\mathbf{x}_\beta)\ldots R(\mathbf{x}_\gamma,\mathbf{x}_\delta)$

$$R(\mathbf{x}_\alpha,\mathbf{x}_\beta) =< C(\mathbf{x}_\alpha)C(\mathbf{x}_\beta) >\simeq \epsilon_0^2 e^{-\frac{|\mathbf{x}_\alpha - \mathbf{x}_\beta|}{a}}$$

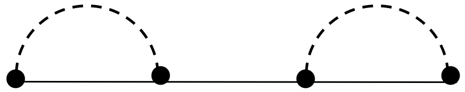
Irreducible diagram:

$k^4 R(\mathbf{x}_i,\mathbf{x}_j)$



$G^0(\mathbf{x}_i,\mathbf{x}_j)$

Reducible diagram:

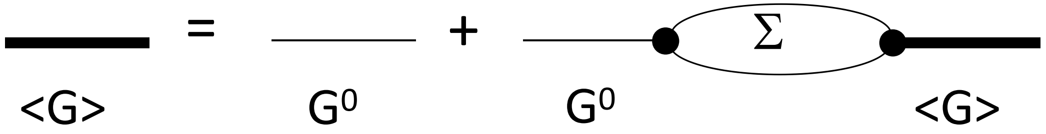


[30] K. Sobczyk, ‘Stochastic wave propagation’, Elsevier, Warszawa (1985)
[31] S. M. Rytov, Y. A. Kravtsov, ‘Principles of statistical radiophysics 4 – Wave propagation trough random media’ Springer-Verlag, Berlin (1989)

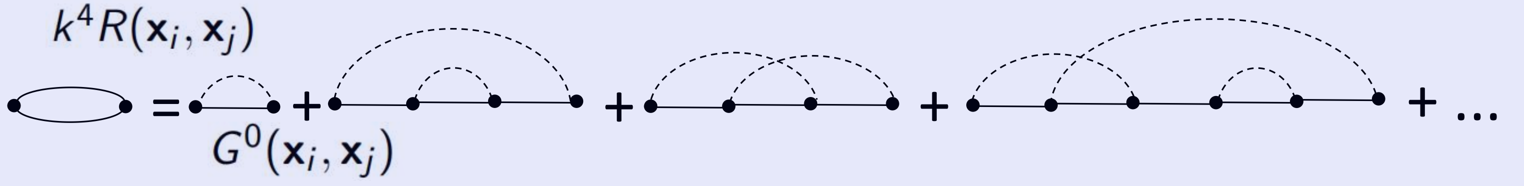
From the STOCHASTIC HELMHOLTZ EQUATION to the DYSON EQUATION: finding a formal expression for <**G**(**x**,**x'**,t)>

The Dyson equation:

- In real space: $$< \mathbf{G}(\mathbf{x}-\mathbf{x}_0) >= \mathbf{G}^0(\mathbf{x}-\mathbf{x}_0) + \int \mathbf{G}^0(\mathbf{x}-\mathbf{x}_1)\mathbf{\Sigma}(\mathbf{x}_1-\mathbf{x}_2) < \mathbf{G}(\mathbf{x}_2-\mathbf{x}_0) > d^3x_1 d^3x_2$$
- Diagramatic representation:



PERTURBTIVE SERIES EXPANSION OF Σ:



- In Fourier conjugate space:

$$< \mathbf{G}(\mathbf{q},\omega)> = \frac{1}{\mathbf{G}^0(\mathbf{q},\omega)^{-1} - \mathbf{\Sigma}(\mathbf{q},\omega)}$$

$$\mathbf{q}\cdot(\mathbf{x}-\mathbf{x}_0) = 2\pi$$
$$\omega t = 2\pi$$

'BARE' MEDIUM → $\mathbf{G}^0(\mathbf{q},\omega)^{-1}$

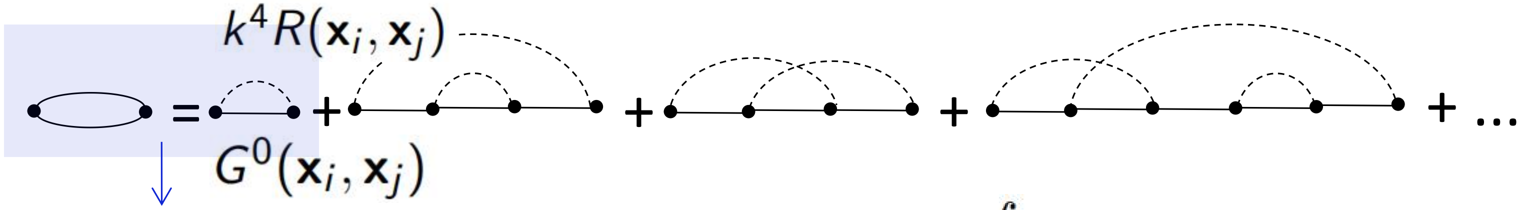
DISORDER → $\mathbf{\Sigma}(\mathbf{q},\omega)$

An approximate expression, truncation or closure procedure is needed to obtain a working definition of Σ

[31] S. M. Rytov, Y. A. Kravtsov, 'Principles of statistical radiophysics 4 – Wave propagation trough random media' Springer-Verlag, Berlin (1989)

The Born Approximation

The Born Approximation: a LOCAL approximation of Σ



$$\Sigma^B(|\mathbf{x}_i - \mathbf{x}_j|) = k^4 R(|\mathbf{x}_i - \mathbf{x}_j|) G^0(|\mathbf{x}_i - \mathbf{x}_j|) \longleftrightarrow \Sigma^B(q) = k^4 \int dq' R(q) G^0(q - q') dq'$$

- The term $\propto$ k^4 is the leading term in the perturbative series expansion.
- The Born (or Bourret) closure procedure : LOCAL INDEPENDENCE HYPOTHESIS

$$< \; G(\mathbf{x}, \mathbf{x}_0) = G^0(\mathbf{x}, \mathbf{x}_0) - k^4 \int G^0(\mathbf{x}, \mathbf{x}_1) C(\mathbf{x}_1) G^0(\mathbf{x}_1, \mathbf{x}_2) C(\mathbf{x}_2) G(\mathbf{x}_2, \mathbf{x}_0) d^3x_1 d^3x_2 \; >$$

CLOSURE: $< C(\mathbf{x}_1) C(\mathbf{x}_2) G(\mathbf{x}_2, \mathbf{x}_0) > = < C(\mathbf{x}_1) C(\mathbf{x}_2) > < G(\mathbf{x}_2, \mathbf{x}_0) > = R(\mathbf{x}_1, \mathbf{x}_2) < G(\mathbf{x}_2, \mathbf{x}_0) >$

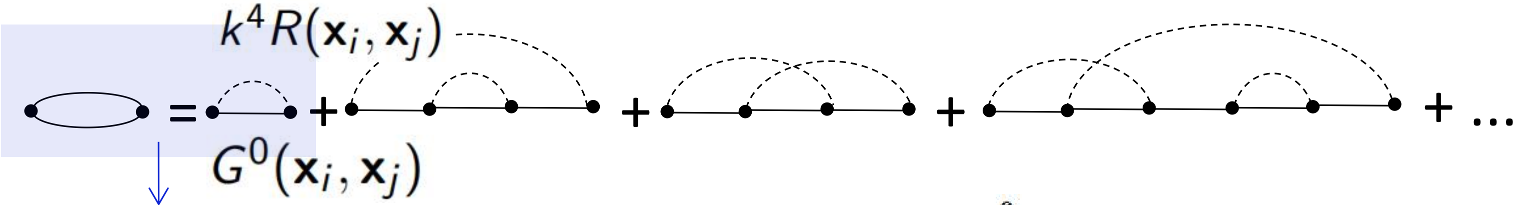
$$< G(\mathbf{x}, \mathbf{x}_0) > = G^0(\mathbf{x}, \mathbf{x}_0) - \int G^0(\mathbf{x}, \mathbf{x}_1) \underbrace{k^4 R(\mathbf{x}_1, \mathbf{x}_2) G^0(\mathbf{x}_1, \mathbf{x}_2)}_{\Sigma^B(\mathbf{x}_1, \mathbf{x}_2)} < G(\mathbf{x}_2, \mathbf{x}_0) > d^3x_1 d^3x_2$$

The local field $G(\mathbf{x}_2, \mathbf{x}_0)$ is statistically independent from the perturbation $C(\mathbf{x}_1)C(\mathbf{x}_2)$

[30] K. Sobczyk, ‘Stochastic wave propagation’, Elsevier, Warszawa (1985)
[31] S. M. Rytov, Y. A. Kravtsov, ‘Principles of statistical radiophysics 4 – Wave propagation trough random media’ Springer-Verlag, Berlin (1989)

The Born Approximation

The Born Approximation: a LOCAL approximation of Σ

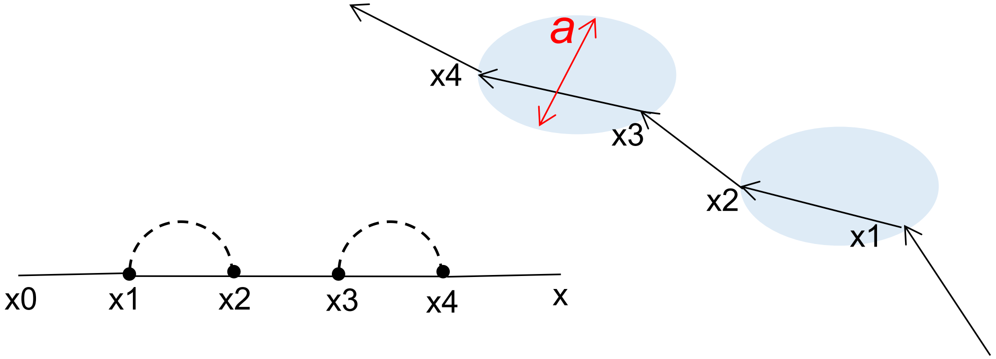


$$\Sigma^B(|\mathbf{x}_i - \mathbf{x}_j|) = k^4 R(|\mathbf{x}_i - \mathbf{x}_j|) G^0(|\mathbf{x}_i - \mathbf{x}_j|) \longleftrightarrow \Sigma^B(q) = k^4 \int dq' R(q) G^0(q - q') dq'$$

$$R(\mathbf{x}_\alpha, \mathbf{x}_\beta) = < C(\mathbf{x}_\alpha) C(\mathbf{x}_\beta) > \simeq \epsilon_0^2 e^{-\frac{|\mathbf{x}_\alpha - \mathbf{x}_\beta|}{a}}$$

- Corresponding SCATTERING EVENTS:

k<<1 $\rightarrow$ the effect of the elastic perturbation on <G> is cumulative throughout a large region. The local details of the scattering event are irrelevant. Scattering forward and back from the same inhomogeneity is neglected.



- The Born Approximation describes the Rayleigh scattering qualitatively.

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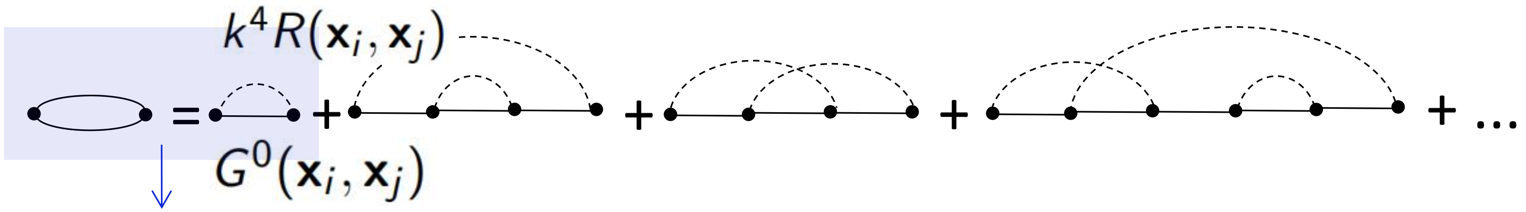
[30] K. Sobczyk, ‘Stochastic wave propagation’, Elsevier, Warszawa (1985)
[31] S. M. Rytov, Y. A. Kravtsov, ‘Principles of statistical radiophysics 4 – Wave propagation trough random media’ Springer-Verlag, Berlin (1989)

The Born Approximation : from scalar to vector

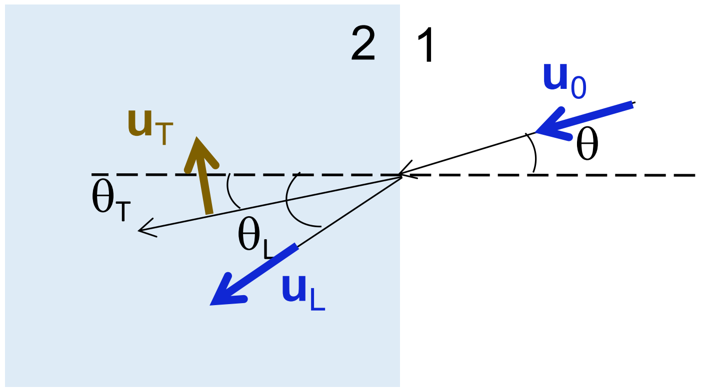


$$R_{\gamma\alpha jl\beta ki\delta}(\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2) = \langle \delta C_{\gamma\alpha jl}(\mathbf{r}_1)\delta C_{\beta ki\delta}(\mathbf{r}_2)\rangle$$

$$< \mathbf{G}(\mathbf{q},\omega) > = < g_L(\mathbf{q},\omega) > \hat{q}\hat{q} + < g_T(\mathbf{q},\omega) > (I - \hat{q}\hat{q})$$

$$\Sigma^B_{kk}(\mathbf{q},\omega) = \hat{L}^1_{kkii}\mathbf{G}^0_{ii} \xrightarrow[kk,ii=L,T]{} \Sigma_{L(T)} = \Sigma_{LL(TT)} + \Sigma_{LT(TL)}$$

<u>The mixing of polarization in an elementary scattering event of a purely longitudinal elastic wave</u>:



$$\frac{\sin(\theta)}{\sin(\theta_L)} = \frac{c_{L1}}{c_{L2}}$$

$$\frac{\sin(\theta)}{\sin(\theta_T)} = \frac{c_{L1}}{c_{T2}}$$

- Necessary condition of validity of the vector Born approximation: $\mathbf{q} \sim \mathbf{k}$

  under this condition the amplitude of the 'spurious' polarization refracted wave is negligible

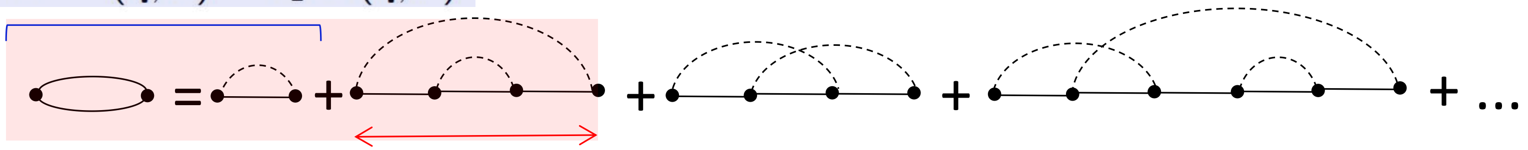
[32] L. D. Landau and E. M. Lifshitz, Theory of Elasticity (Pergamon, Oxford, 1959).

The Generalized Born Approximation

A NON-LOCAL approximation of Σ:

$$\Sigma^2(\mathbf{q},\omega) = \hat{L}_1 < G^1(\mathbf{q},\omega) >$$

$$\Sigma^{1(B)}(\mathbf{q},\omega) = \hat{L}_1 G^0(\mathbf{q},\omega)$$

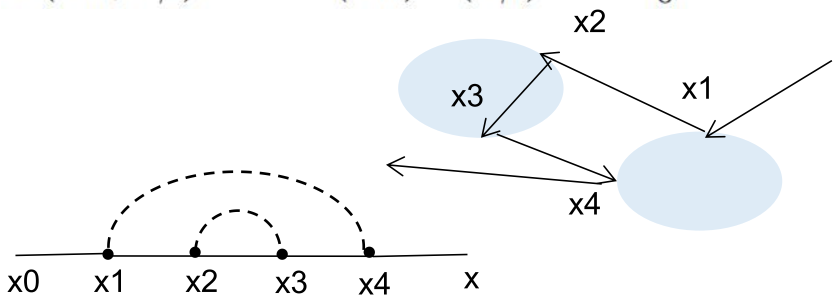


$G^0(\mathbf{x}_i,\mathbf{x}_j)$ $< G^1(\mathbf{x}_i,\mathbf{x}_j) >$

- Terms $\propto k^8$ in the perturbative series expansion are considered.

- Corresponding SCATTERING EVENTS:

$$R(\mathbf{x}_\alpha,\mathbf{x}_\beta) =< C(\mathbf{x}_\alpha)C(\mathbf{x}_\beta) >\simeq \epsilon_0^2 e^{-\frac{|\mathbf{x}_\alpha-\mathbf{x}_\beta|}{a}}$$



k~1: non-local approximation of the perturbation-field interaction. The explicit q-dependence of $<G^1(\mathbf{q},\omega)>$ should be retained. Local details of the scattering event become relevant.

One correlated double scattering event (forward and back from the same inhomogeneity) is included.

[35] M. G. Izzo, G. Ruocco, and S. Cazzato, 'The Mixing of Polarizations in the Acoustic Excitations of Disordered Media With Local Isotropy' Front. Phys. 6, 108 (2018)
[36] M. G. Izzo, B. Wehinger, S. Cazzato, A. Matic, C. Masciovecchio, A. Gessini, and G. Ruocco, 'Rayleigh scattering and disorder-induced mixing of polarizations in amorphous solids at the nanoscale: 1-octyl-3-methylimidazolium chloride glass' Phys. Rev. B 102, 214309 (2020)

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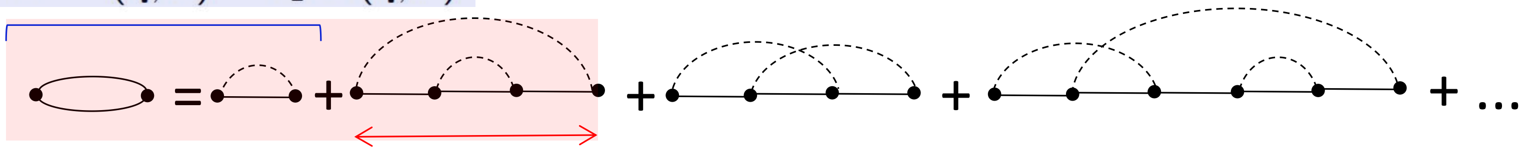


$G^0(\mathbf{x}_i,\mathbf{x}_j)$ $< G^1(\mathbf{x}_i,\mathbf{x}_j) >$

$$\langle G_{ii}(\mathbf{q},\omega)\rangle^1 = \lim_{\eta\to 0^+} \frac{1}{\tilde{c}_i^2}\left\{\frac{1}{\tilde{q}_{0i,\eta}^2 - q^2 - q^2\frac{\epsilon^2}{\tilde{c}_i^2}\Delta\tilde{\Sigma}_{ii}^1(\mathbf{q},\omega_\eta)}\right\}$$

$$\lim_{\eta\to 0^+}\sum_{n=0}^{\infty}\frac{[\frac{\epsilon^2}{\tilde{c}_i^2}q^2\Delta\tilde{\Sigma}_{ii}^1(\mathbf{q},\omega_\eta)]^n}{[\tilde{q}_{0i,\eta}^2 - q^2]^{n+1}}$$

k~1: non-local approximation of the perturbation-field interaction. The explicit q-dependence of $<G^1(\mathbf{q},\omega)>$ should be retained.

$$\tilde{q}_{0i,\eta} = \frac{\omega_\eta}{\tilde{c}_i}\,;\quad \omega_\eta = \omega + i\eta\,;$$

$$\tilde{c}_i = [(c_i^0)^2 + \epsilon^2\tilde{\Sigma}_{ii}^1(0,0)]^{1/2}$$

$$\Delta\tilde{\Sigma}_{ii}^1(\mathbf{q},\omega) = (\epsilon^2 q^2)^{-1}[\Sigma_{iijj}^1(\mathbf{q},\omega) - \Sigma_{iijj}^1(0,0)]$$

Theorem:

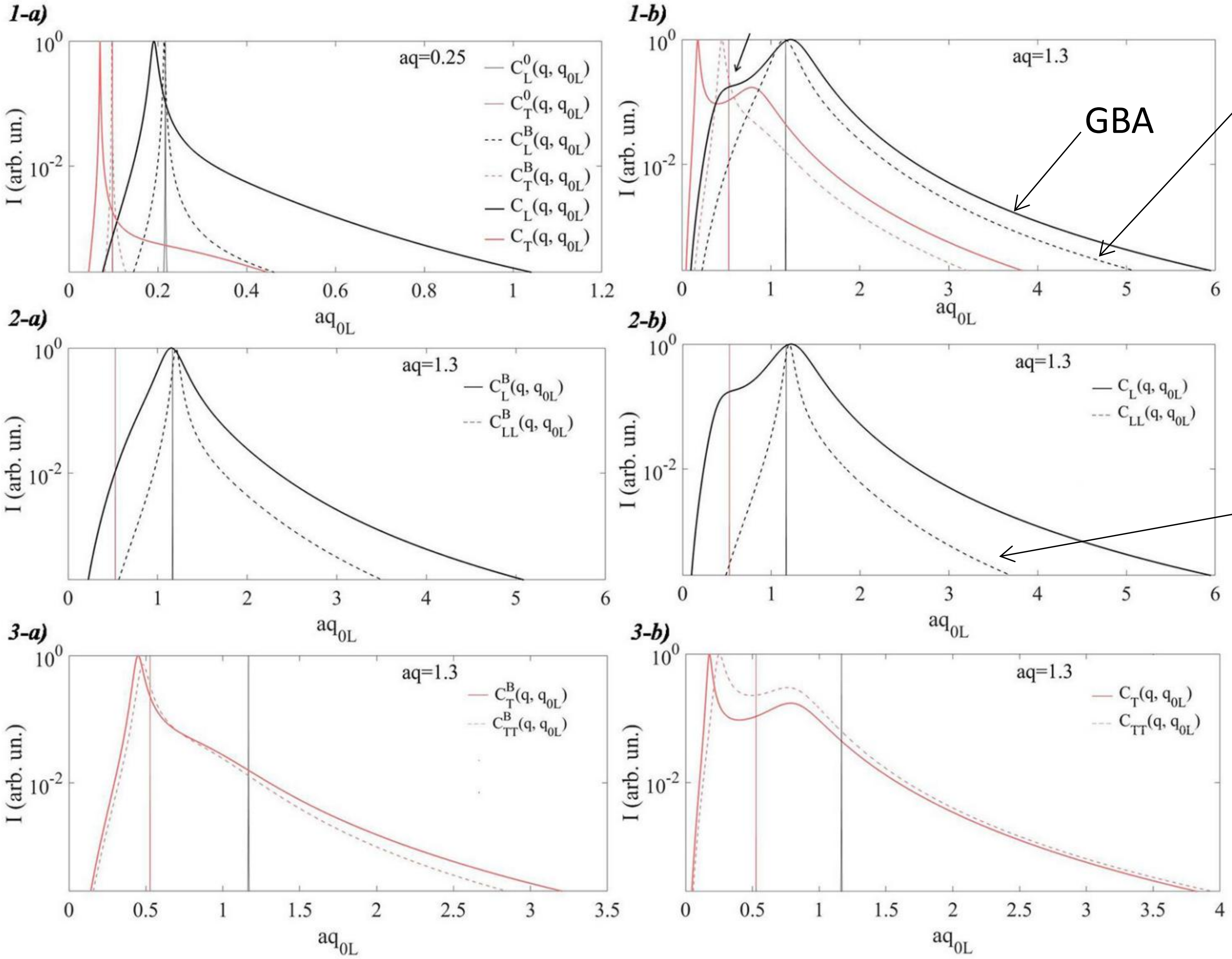
- The Taylor series is convergent almost everywhere for (q ,ω):

$$\mathrm{Im}[\Delta\tilde{\Sigma}_{ii}^1(\mathbf{q},\omega)] > 0;\quad \frac{\epsilon^2}{\tilde{c}_i^2}|\Delta\tilde{\Sigma}_{ii}^1(\mathbf{q},\omega)| < 1$$

[35] M. G. Izzo, G. Ruocco, and S. Cazzato, 'The Mixing of Polarizations in the Acoustic Excitations of Disordered Media With Local Isotropy' Front. Phys. 6, 108 (2018)

The Mixing of Polarizations in the Born and Generalized Born Approximations

Born Approx.



Born Approx.

GBA

GBA

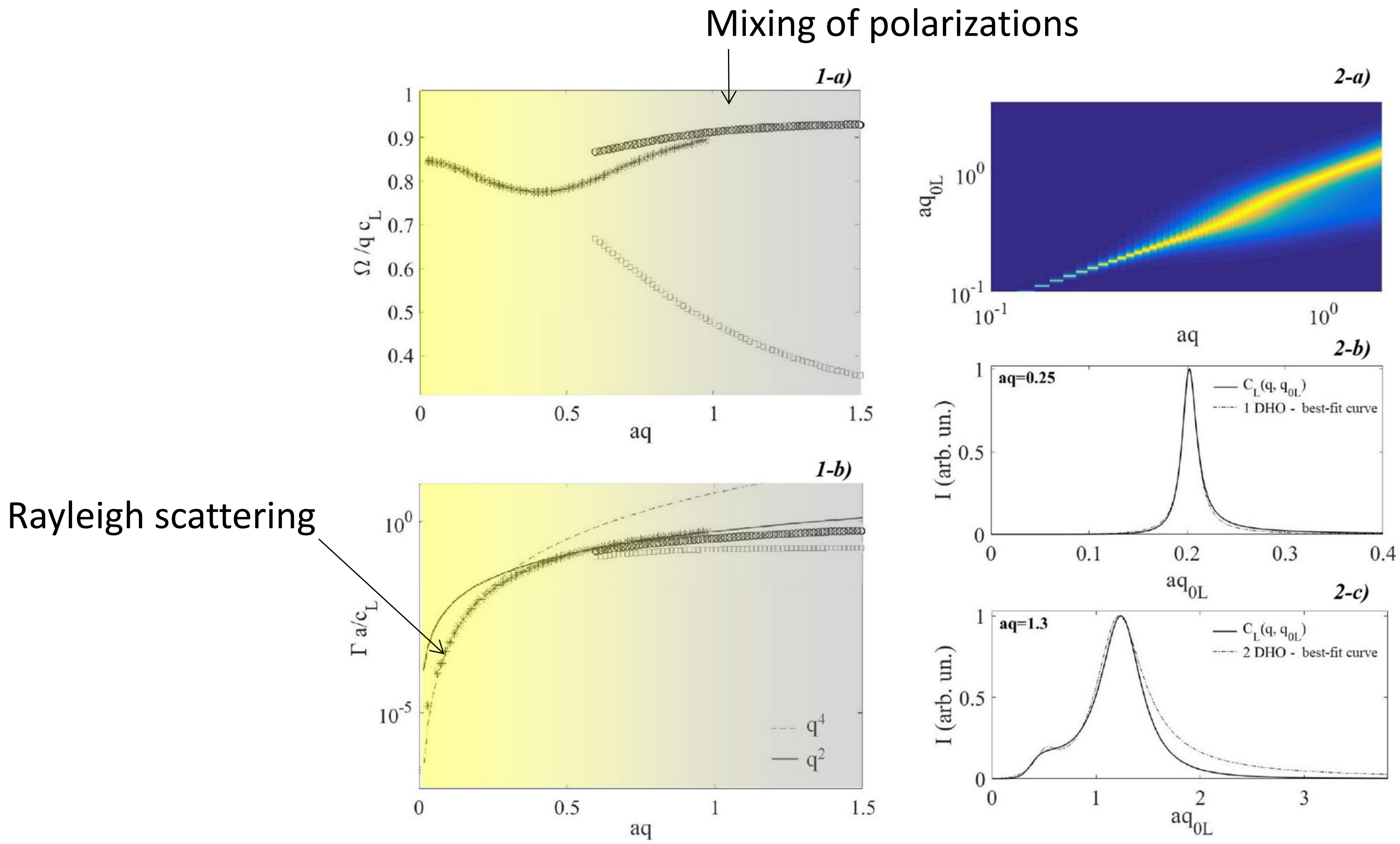
$$\Sigma_L = \Sigma_{LL} + \Sigma_{LT}$$

$$C_i(\mathbf{q}, \omega) \propto \frac{\omega^2}{q^2} S_i(q, \omega)$$

i=L,T

[35] M. G. Izzo, G. Ruocco, and S. Cazzato, Front. Phys. 6, 108 (2018)

Features of the Acoustic Dynamics in the Generalized Born Approximation



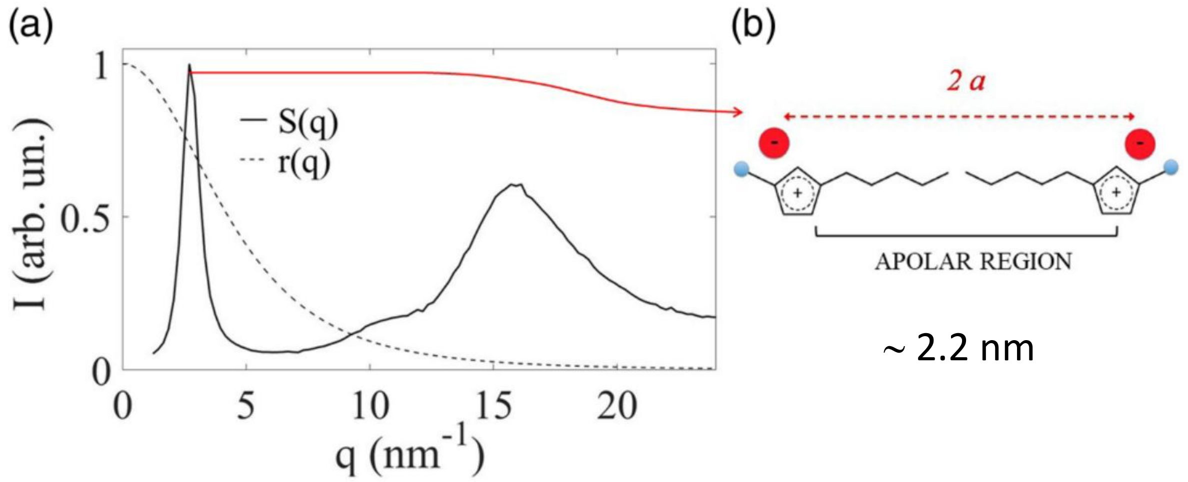
[35] M. G. Izzo, G. Ruocco, and S. Cazzato, Front. Phys. 6, 108 (2018)

Modeling [C8MIM]Cl glass as an elastically random medium

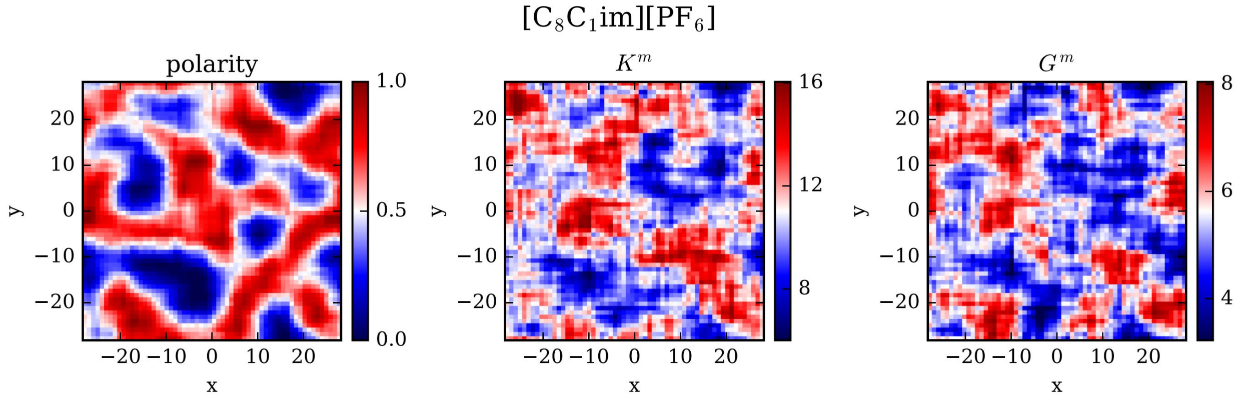
MODEL INPUT: → Mean field Random Media Theories

$$R_{\mu\mu}(r) = < \delta\mu(\mathbf{x})\delta\mu(\mathbf{y}) > = \epsilon^2 \cdot e^{-r/a}$$

[C8MIM]Cl glass and its nanoscale elastic heterogeneity:



~ 2.2 nm

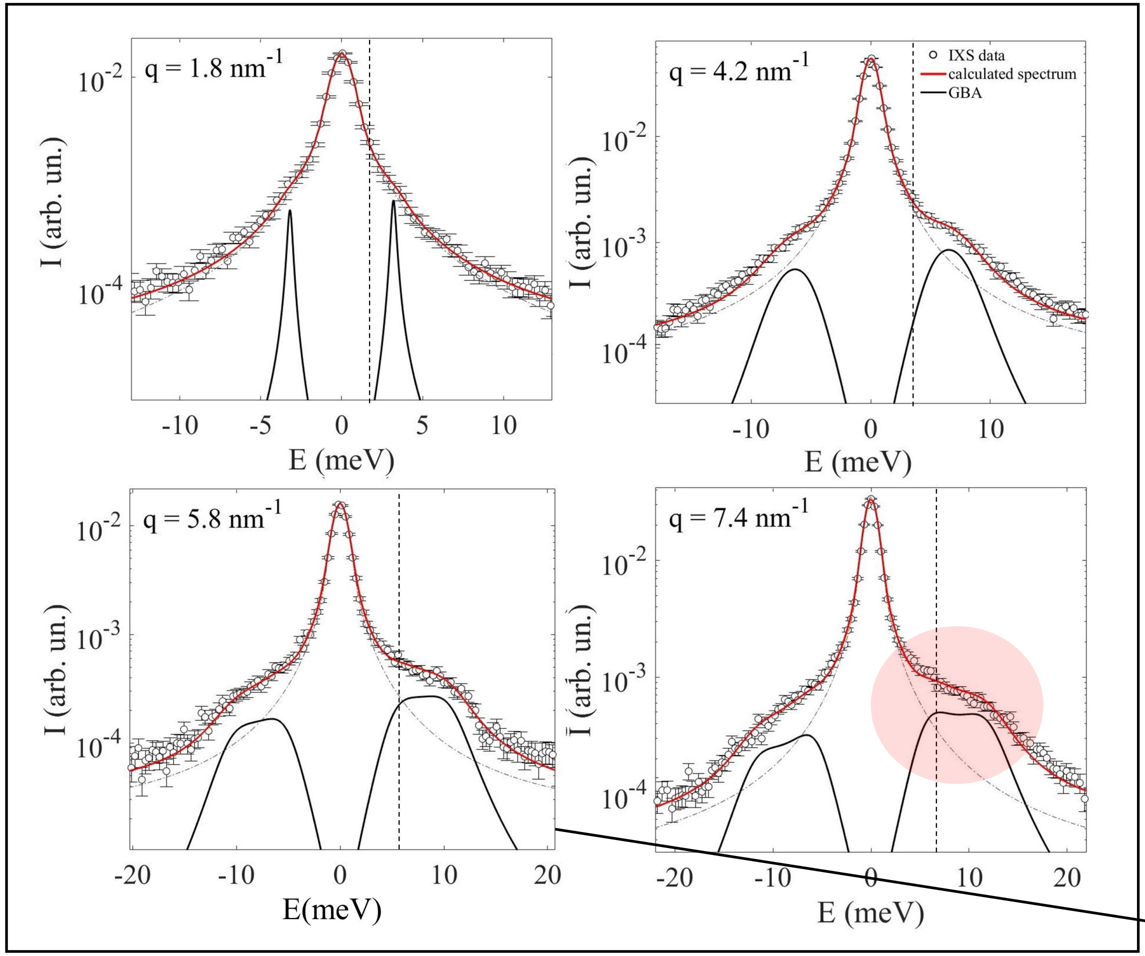


- In ionic glasses the elastic heterogeneity is defined by the alternation of polar (stiffer) and nonpolar (softer) domains, which remains well defined in ILs with sufficiently long alkyl chains.
- There exists a correlation between elastic heterogeneity and local topology, which is easily experimentally accessible.

[37] A. A. Veldhoest and M. C. C. Ribeiro, J. Chem. Phys. 148, 193803 (2018)

Generalized Born Approximation vs. Inelastic X-ray Scattering experiment

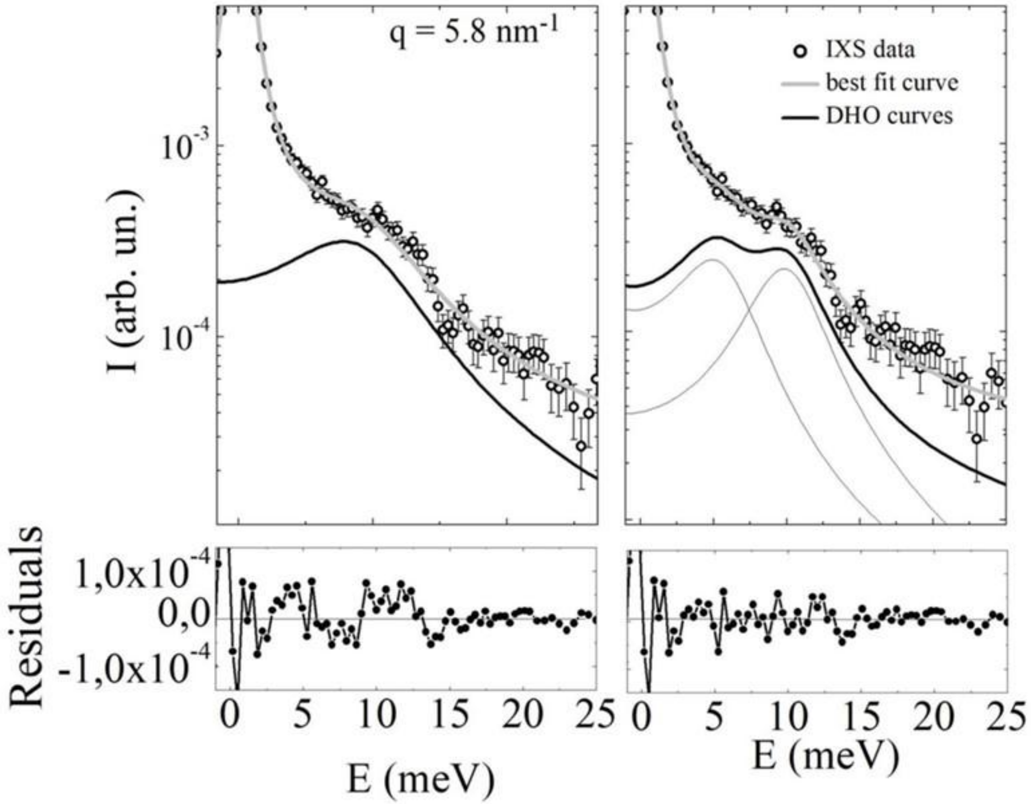
IXS SPECTRA vs GENERALIZED BORN APPROXIMATION



$$I(q,E) = A(q)\left[E\frac{n(E)+1}{k_B T}S_L(q,E)\right]\otimes R(E) + c(q)$$

Damped Harmonic Oscillators (DHOs):

$$S_L(q,E) = \sum_n \frac{\tilde{I}_{L(n)}(q)\Gamma_{L(n)}(q)\Omega^2_{L(n)}(q)}{\left[\Omega^2_{L(n)}(q) - E^2\right]^2 + E^2\Gamma^2_{L(n)}(q)}$$

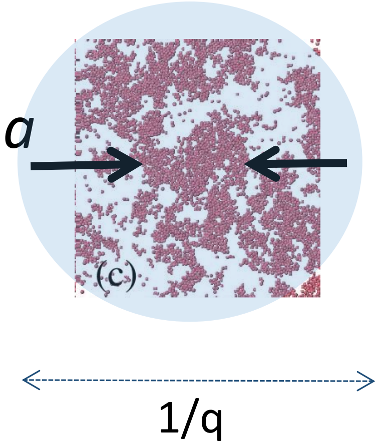


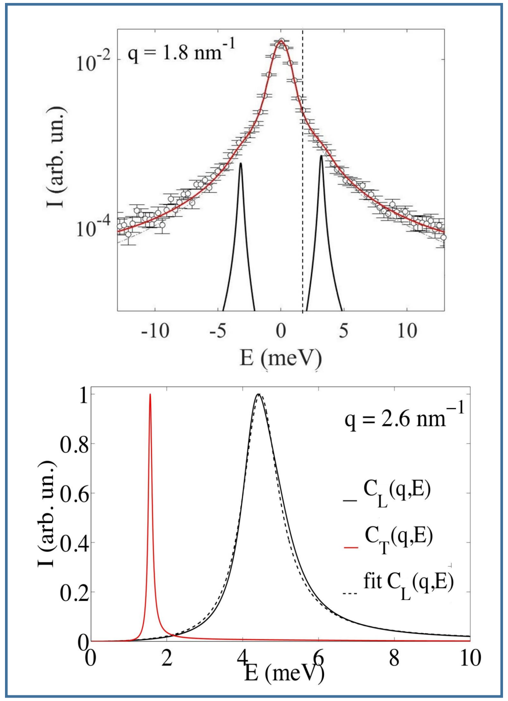
[36] M. G. Izzo, B. Wehinger, S. Cazzato, A. Matic, C. Masciovecchio, A. Gessini, and G. Ruocco, Phys. Rev. B 102, 214309 (2020)

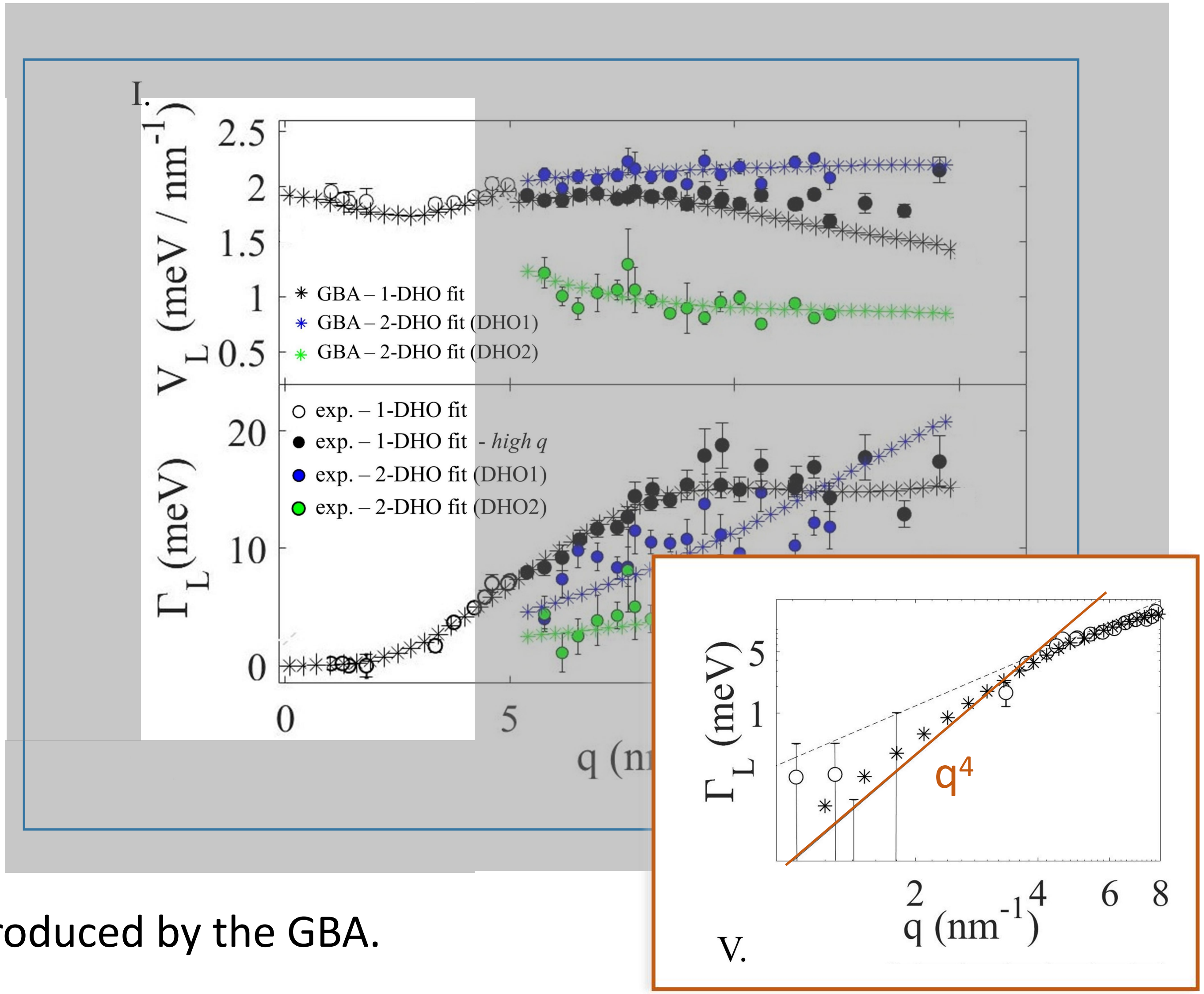
The Rayleigh scattering in GBA and IXS experiment

Rayleigh region: $q \ll a^{-1}$

- The dynamic structure factors are characterized by a well-defined inelastic excitation.





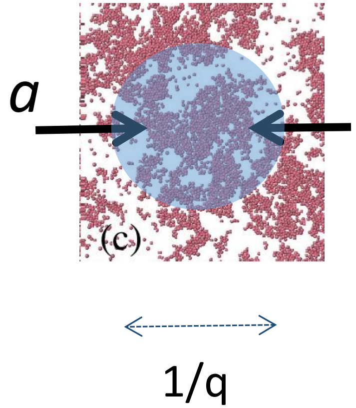


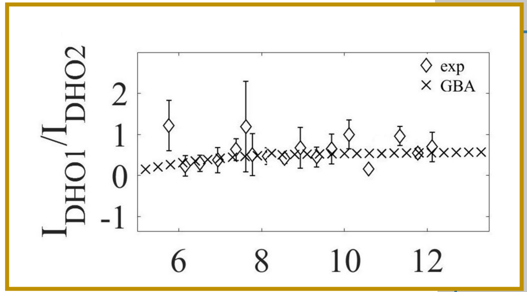
- The Rayleigh scattering is *quantitatively* reproduced by the GBA.

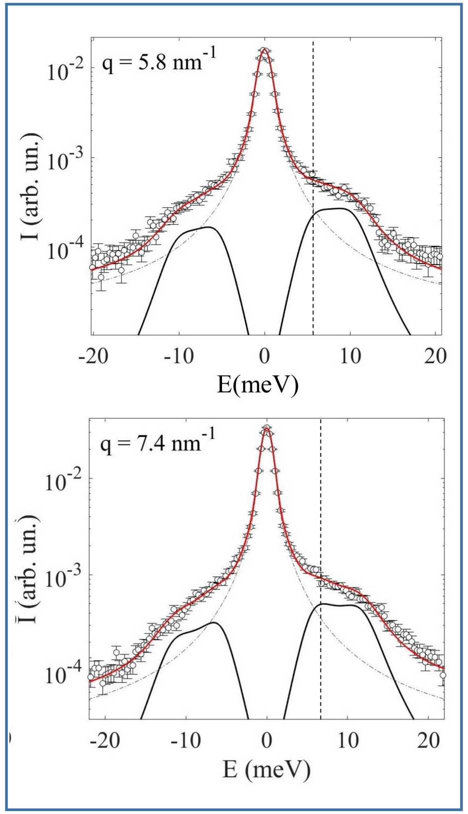
[36] M. G. Izzo, B. Wehinger, S. Cazzato, A. Matic, C. Masciovecchio, A. Gessini, and G. Ruocco, Phys. Rev. B 102, 214309 (2020)

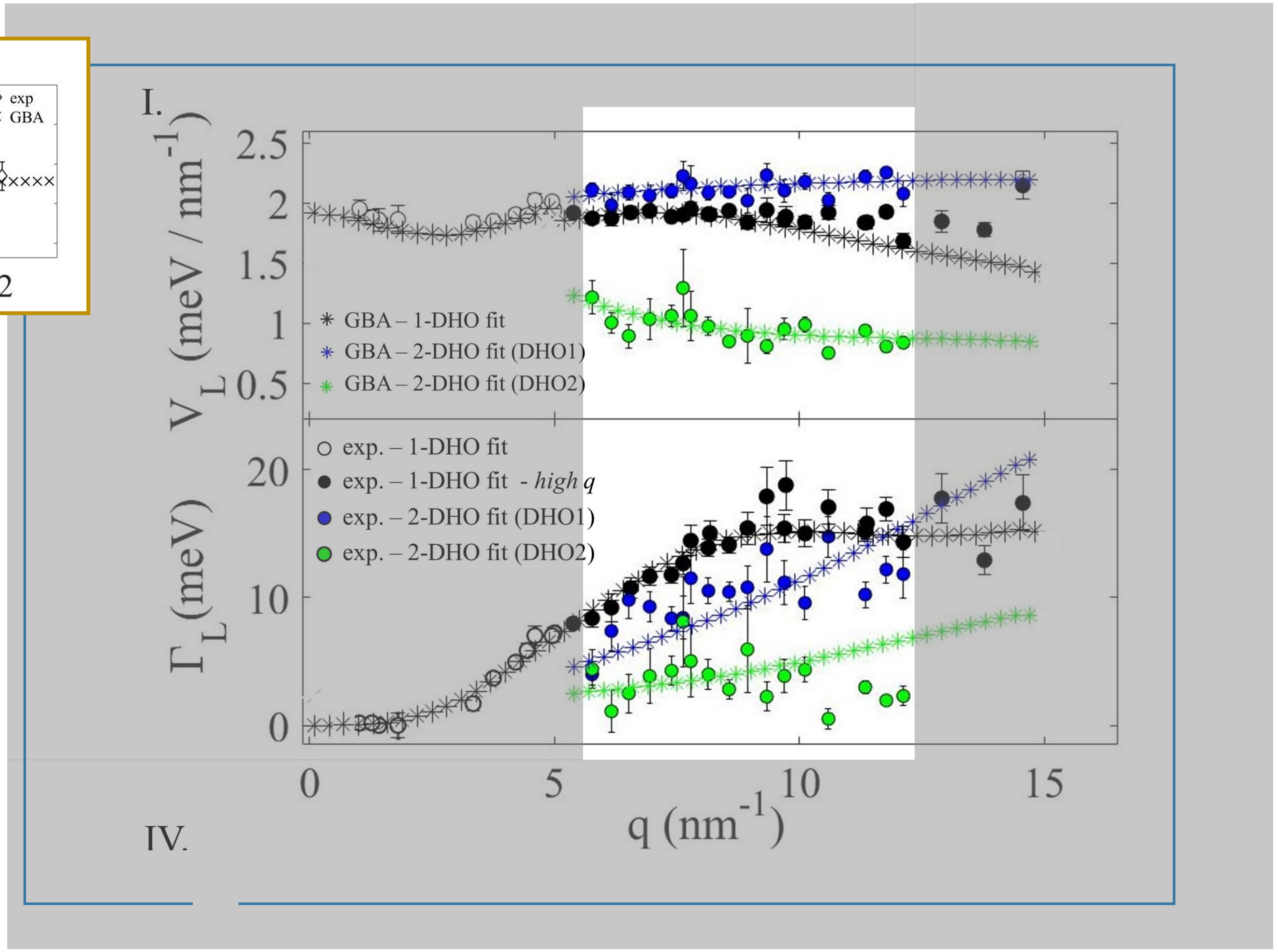
The mixing of polarizations in GBA and IXS experiment

Beyond the Rayleigh region: $\boldsymbol{q \sim a^{-1}}$









[37] M. G. Izzo, B. Wehinger, S. Cazzato, A. Matic, C. Masciovecchio, A. Gessini, and G. Ruocco, Phys. Rev. B 102, 214309 (2020)

CONCLUSIONS

- By a Random Media Theory approach the Generalized Born Approximation allows for both *quantitative* account of Rayleigh scattering and mixing of polarizations.

- A *vector* field and *non-local* effects accounted by second order terms of the perturbative series expansion are needed in mean field approach in order to achieve a realistic description of acoustic-like features in glasses in the first pseudo-Brillouin zone.

- The Rayleigh scattering and the mixing of poloarizations in glasses are phenomena interconnected.

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