# Dynamical structure factor

# in glassy systems

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A study of the high frequency dynamics of *topologically desordered* solids.

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1. The problem
2. The field theory
3. Comparison with numerics
4. Outlooks

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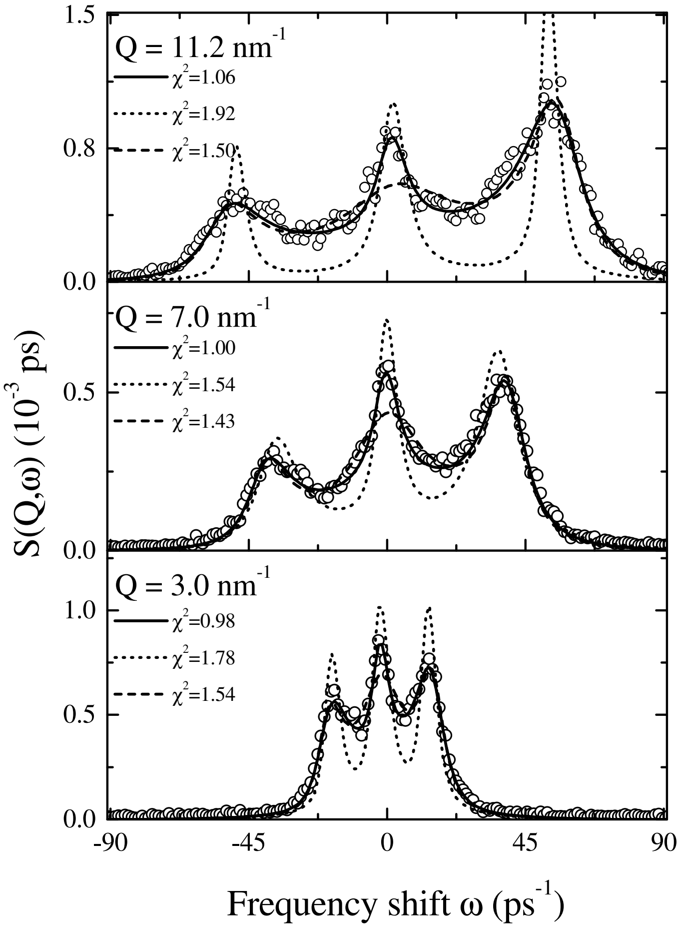
# The problem

Inelastic X-ray scattering (IXS) experiments provide information on the short time dynamics of amorphous solids, such as structural glasses or supercooled liquids.

An example:



A peak is observed in the high frequency region of the spectrum ($> 0.1$ THz). It is usually interpreted in terms of propagation of quasi-elastic sound waves, the so-called high frequency sound.

## Properties

- Position:
  In the region $0.1p^* - 1.0p^*$ ($p^*$ being the position of the first maximum in the static structure factor), the frequency at the peak depends linerly on the momentum $p$.

- Broadening:
  The width of the spectral line, $\Gamma$ is:

$$\Gamma(p) = Ap^x \quad , \quad x \approx 2 \, , \qquad (1)$$

  with $A$ displaying a very mild (if any) temperature dependence.

The wavelength of the plane wave is comparable with the inter-particle distance.
$\Longrightarrow$ No hydrodynamical origin

Harmonic approximation: $\vec{r}_i = \vec{x}_i + \vec{u}_i$

$$H = -\frac{1}{2} \sum_{ij,\mu\nu}^{N} M_{ij;\mu\nu} u_i^{\mu} u_j^{\nu} \qquad (2)$$

$\vec{x}$ = quenched positions

$\vec{u}$ = fluctuations

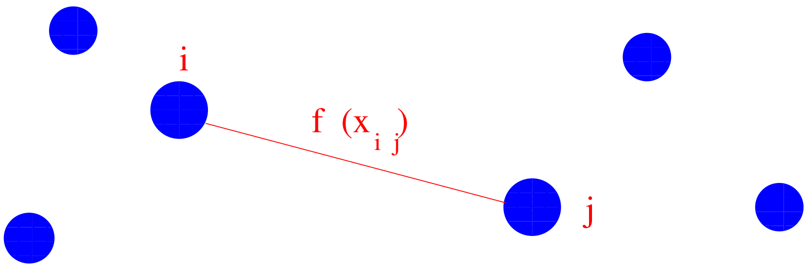
$\mathbf{M}$ = Hessian (Euclidean random matrix)

Disorder $\Longrightarrow P\left[\{\vec{x}\}\right]$

## The model

- particle displacements all collinear
- quenched positions uncorrelated
- $N, V \to \infty, \;\; \rho$ fixed

$$M_{ij} \equiv \delta_{ij} \sum_{k=1}^{N} f(x_{ik}) - f(x_{ij}) \qquad (3)$$



All the dynamical properties are encoded in the Hessian matrix.

The experimental spectra are proportional to the the dynamical structure factor, given by

$$S_E(p,E) = \overline{\sum_n Q_n(p)\delta(E-E_n)}\,, \qquad (4)$$

$$Q_n(p) = \frac{1}{N}\left|\sum_{i=1}^{N} e_n(i)\mathrm{e}^{\mathrm{i}p\cdot x_i}\right|^2\,, \qquad (5)$$

$E_n$ = eigenvalues

$e_n(i)$ = eigenvectors

$\overline{(\ldots)}$ = average over the disorder

From energy to frequency domain: $E = \omega^2$

We shall compute the resolvent:

$$G(p,z) = \overline{\frac{1}{N}\sum_{ij} e^{ip(x_{ij})}\left[\frac{1}{z-M}\right]_{ij}} \qquad (6)$$

$$S_E(p,E) = -\frac{Im}{\pi}\lim_{\eta\to 0^+} G(p,z)\,, \quad z \equiv E + \mathrm{i}\eta \qquad (7)$$

## The field theory

The resolvent is the propagator of the Gaussian variables $\vec{\phi}$ (N-dimensional).

$$G(p,z) = \frac{1}{N}\sum_{ij}\frac{\delta^2}{\delta J_i \delta J_j}\overline{e^{ip(x_{ij})}\ln \mathcal{Z}[J]}\Big|_{J=0} \tag{8}$$

$$\mathcal{Z}[J] \equiv \int \prod_k d\phi_k \, e^{\left(-\frac{1}{2}\vec{\phi}(z-M)\vec{\phi}+\vec{\phi}\cdot\vec{J}\right)} \tag{9}$$

Replica trick:

$$\ln \mathcal{Z}[J] = \lim_{n\to 0}\frac{1}{n}\left(\mathcal{Z}^n[J]-1\right) . \tag{10}$$

$$\vec{\phi} \Longrightarrow \vec{\phi}^{(a)} \quad a = 1, \ldots n$$

Bosonic fields:

$$\rho(x) \equiv \sum_i \delta(x-x_i) \tag{11}$$

$$\chi(x) \equiv \sum_{i,a}(\phi_i^{(a)})^2\delta(x-x_i) \tag{12}$$

$$\psi^{(a)}(x) \equiv \sum_i \phi_i^{(a)}\delta(x-x_i) \tag{13}$$

Lagrange multipliers: $\tilde{\rho}(x), \tilde{\psi}^{(a)}(x), \tilde{\chi}(x)$.

Average over the disorder $\Longrightarrow$

$$G(p,z) = \lim_{n\to 0}\left[\frac{1}{\rho\tilde{f}(p)} - \frac{1}{\rho\tilde{f}^2(p)}\int d^dx d^dy \; e^{ip(x-y)}\langle\tilde{\psi}^{(1)}(x)\tilde{\psi}^{(1)}(y)\rangle\right] \quad (14)$$

with the measure:

$$\mathcal{Z}\left[\rho,z\right] = \int D[\psi^{\tilde{(a)}},\chi,\tilde{\chi}]\exp\left(S_0+S_1\right) \,, \quad (15)$$

$$S_0 \equiv \int d^dx\chi(x)\tilde{\chi}(x) - \frac{1}{2}\sum_{a=1,n}\int d^dx d^dy \; \tilde{\psi}^{(a)}(x)f^{(-1)}(x-y)\tilde{\psi}^{(a)}(y) \quad (16)$$

$$S_1 \equiv \rho\int d^dx \; \left(\exp\Phi(x)-1\right) \quad (17)$$

$$\Phi(x) \equiv +i\int d^dy f(y-x)\chi(y) - \frac{1}{2}\frac{\sum_{a=1,n}\left(\tilde{\psi}^{(a)}(x)\right)^2}{z+\tilde{\chi}(x)} \quad (18)$$

The interaction is exponential !!!

Some scheme of approximation is needed.
The expansion $\exp \Phi(x) - 1 \sim \Phi(x)$ yields the leading order term:

$$\begin{aligned} G(p,z) &= \frac{1}{z - \rho\tilde{f}(0) - \rho\tilde{f}(p)} \quad \Longrightarrow \\ S(p,E) &= \delta\left(E - \rho\tilde{f}(0) - \rho\tilde{f}(p))\right) \end{aligned} \qquad (19)$$

- in frequency domain $\omega_P \propto p$ at *small* $p$
- <u>no</u> broadening

The result is exact at $\rho \to \infty$.

## **Beyond leading order**

Including higher powers of $\Phi$ new terms arise.
The Dyson resummation of generic L-loops terms adds a complex self-energy:

$$G(p,z) = \frac{1}{z - \rho\tilde{f}(0) - \rho\tilde{f}(p) - \Sigma(p,z)} \qquad (20)$$

The peak has a lorentzian shape.
$Re\Sigma$ set out the position, $Im\Sigma$ the width.

A generic L-loops term gives a contribute $\propto \frac{1}{\rho^L}$ to the self-energy

- The one-loop contribute to self-energy is:

$$\Sigma_1 = \frac{1}{\rho} \int \frac{d^d q}{(2\pi)^d} G_0(q,z) \left[\rho \tilde{f}(p-q) - \rho \tilde{f}(q)\right]^2 \tag{21}$$

- Many integrals belong to two-loops contribute.

What does the theory predict?

## The gaussian case

Our choice for the function $f$ shall be the following:

$$\tilde{f}(p) = (2\pi\sigma^2)^{d/2}\, \mathrm{e}^{-\sigma^2 \frac{p^2}{2}} \tag{22}$$

The parameter $\sigma$ sets our length-scale, and for phenomenological purposes might be identified with the inverse of the first maximum of the static structure factor

Within the Gaussian case, the real and the imaginary parts can be computed numerically in a straighforward way for any value of $p$.
In order to investigate the scaling laws of the position and the broadening of the acoustic peak, we studied analitycally the low momentum regime.

$$\boxed{\sigma p << 1}$$

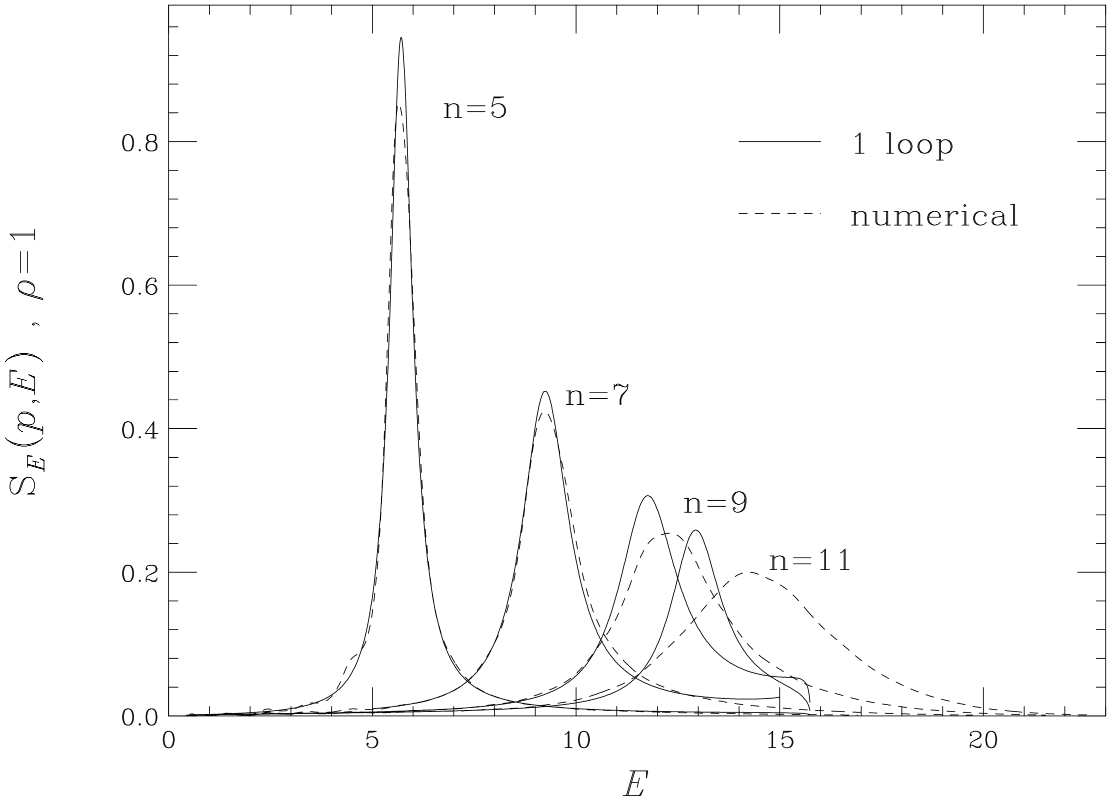
- $\omega_P \propto p$
- – one-loop: $\Gamma = A_1\, p^4$
  – two-loops: $\Gamma = A_2\, p^2$
  – No clear scaling law!
  there is a cross-over among the two regimes at a value $p_c$ which depends on the density.

$$(\sigma p_c)^2 = \frac{A_2}{A_1} \frac{1}{\rho \sigma^3} \qquad (23)$$

## Comparison with numerical simulations

Gaussian case:

$N = 32^3, \quad \sigma^3 \rho = 1, \quad \sigma p = 0.19 n$



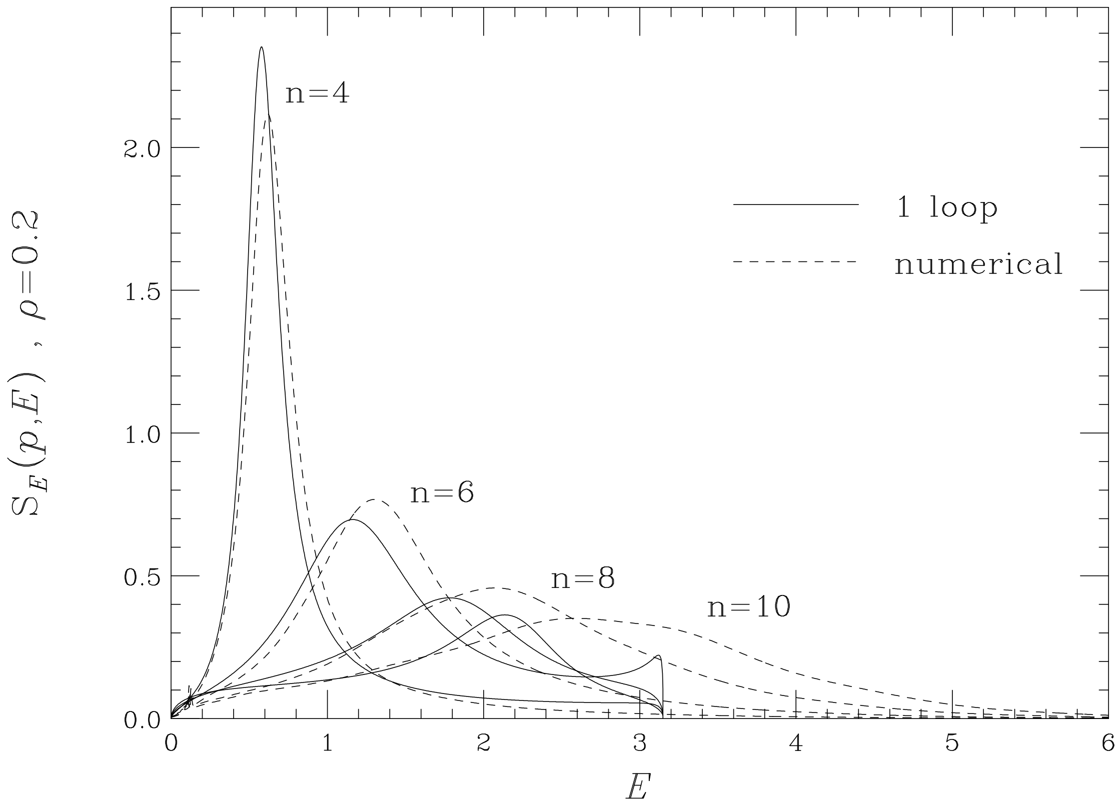

For $n < 5$ the statistics is very poor.

The smallest $p$ is not in the $\sigma p << 1$ region

$\sigma p_c = 0.31$ (not observable!!)

## Gaussian case:

$N = 32^3, \quad \sigma^3\rho = 0.2, \quad \sigma p = 0.19n$




Though the high density expansion holds for $\sigma^3\rho > 1$, the agreement is still quite good.

# Outlooks

What about realistic systems?

- The quenched positions are correlated
- $f(r) = \frac{d^2V(r)}{dr^2} - \frac{1}{r}\frac{dV(r)}{dr}$
  (No Fourier transform for real potentials)

Let us take:

$$f(r) \Longrightarrow f'(r) = f(r)g(r)$$

The correlations are taken into account and everything is mathematically well defined