

Re: Report 2 submitted on 2023-01-06 on scipost 202211 00007v1.

Title: "Quasi-localized vibrational modes, Boson peak and sound attenuation in model mass-spring networks"

Authors: Shivam Mahajan and Massimo Pica Ciamarra

Dear Editor,

We thank Reviewer 2 for the supportive comments and provide below a detailed answer to the Reviewer's remarks and a list of changes.

We hope that our revised manuscript is now fully suitable for publication in Sci Post, and thank you for your consideration.

Your sincerely,
Massimo Pica Ciamarra

List of changes:

1. Following the reviewer's suggestions, we have added data for the distribution of the local shear modulus.
2. We have investigated the spatial correlation function of the local shear modulus, as suggested by the referee. This study was particularly useful as it evidenced constant elastic correlation length.
3. We explain in the manuscript the increase in shear modulus with f stems from an increase in its affine component and a decrement of its non-affine one.
4. We discuss in the manuscript how our algorithm affects the strength of the boson peak.

Referee #2:

Although the method is too artificial, the results seem to be reasonable. The relation between local heterogeneities and vibrational properties is an important issue, and the present works can contribute to this issue. I think the paper could be considered for publication, if the authors could address issues and questions below.

Reply: We thank the reviewer for acknowledging that our work contributes to understanding the relationship between elastic heterogeneities and vibrational properties. Our method is certainly artificial: its value is in that it creates mass-spring networks with diverse elastic heterogeneities at fixed connectivity and prestress (we added more data to highlight this point in the revised manuscript), allowing us to elucidate how these heterogeneities influence the vibrational properties.

Fluctuations of elastic properties are central quantities in this work. So, the authors should present distribution of local stiffness. What is the functional form of distribution? The fluctuating theory assumes several different functional forms of distributions (please see PHYSICAL REVIEW B 88, 064203 (2013)). The authors could discuss numerical results with the theoretical assumption.

Reply: We show the local elastic properties distribution in Fig. R1a. Different curves refer to different values of the swapping fraction f . The distributions have a Gaussian core and asymmetric fat tails at the considered length scales. We reported a similar shape in three dimensions in model three dimensional glasses in Phys. Rev. Lett. 127, 215504. The uniform, power-law, truncated Gaussian and log-normal distribution considered in the article mentioned by reviewer do not describe the distribution we find.

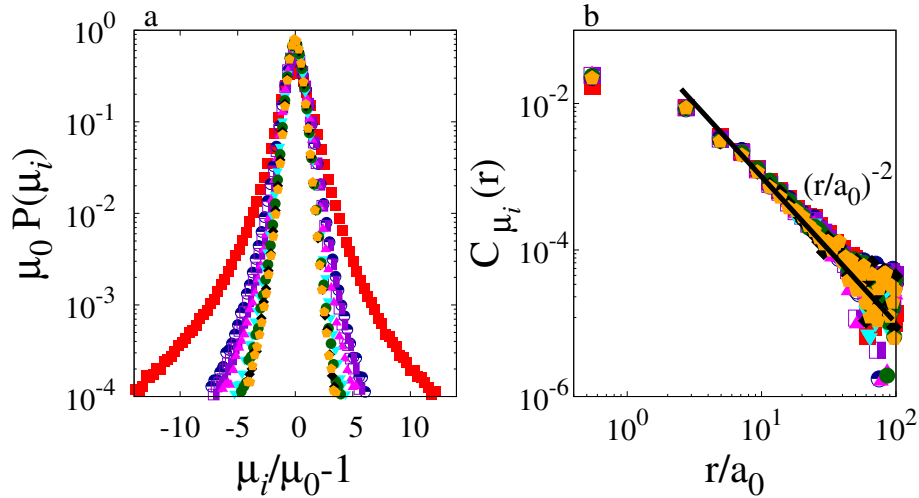


Figure R1: Distribution at microscopic level coarse-grained at different w .

If I correctly understand, the correlation length ξ_e is measured as the coarse-grained length that the disorder parameter converges. But, a more honest way to measure the correlation length is to calculate the spatial correlation function of the local stiffness. The authors could check the correlation function decays with the distance ξ_e .

Reply: We thanks the reviewer for this comment that suggested us to critically reconsider the approach we used to extract the correlation length. We have investigated the radial correlation function of the local shear modulus, taking into account the expected quadrupolar symmetry. Fig. R1b shows that the correlation function is f independent, indicating that our algorithm does not influence any microscopic length scale. This finding agree with another observation reported in our manuscript, namely that the size of the QLMs is also f independent.

What is the meaning of the scale of $\xi_e \sim \gamma^{1/2}$?

Reply: In the revised manuscript, we clarify that ξ_e is constant, indicating that in our system γ is only affected by changes in the variance of the distribution of the single particle shear modulus (as we verify in Fig. b in the main text). As such, our revised analysis do not support the relation $\xi_e \sim \gamma^{1/2}$, in the system we have considered. This relation holds when comparing systems only differing the in the correlation length of the local shear modulus. When this is the case, by virtue of the central limit theorem, the fluctuations of the coarse-grained shear modulus scales as the correlation volume. Hence, $\gamma \sim \xi_e^2$ in two spatial dimensions.

This work considers only the shear modulus. How about the bulk modulus? If the bulk modulus is much larger than the shear modulus, it can not be important for low-frequency vibrational properties. The authors should add this point on discussion.

Reply: We understand the reviewer's concern concerning the bulk modulus. In dense glasses, the bulk modulus is sensibly larger than the shear modulus and does not contribute to low-frequency vibrational properties. Our systems estimate that the bulk modulus is four to five times larger than the shear modulus.

In fig2c, the shear modulus increases from 60 to 90. I do not yet understand why the modulus is change so much, by the algorithm of swapping. The prestress shows only a tiny change, so I guess change of the connectivity leads to the increase of shear modulus. Is this correct? The authors would put comments on this point with some figure of connectivity.

Reply: The change in shear modulus does not originate from a change in connectivity. Indeed, our algorithm does not influence the connectivity as it acts by swapping the stiffness and rest length of randomly selected bonds. Similarly, the change in shear modulus does not originate from the change in prestress, as the reviewer notices. We demonstrate this point in a clearer manner in the revised manuscript by comparing systems with the same prestress.

To rationalize the physical origin of the observed increase of the shear modulus, we consider that the modulus has an affine ($\mu_a > 0$) and a non-affine ($\mu_{na} \geq 0$) contribution

$$\mu = \mu_a - \mu_{na}.$$

In the absence of swapping, we find $\mu_{na}/\mu_a \simeq 0.5$. On increasing f , the affine contribution increases (up to 12%) and the non-affine one decreases (up to 20%). These changes drive the observed increase in the shear modulus.

While the non-affine contribution is of difficult analytical estimation, the variation of the affine contribution is easily determined. Indeed, at fixed connectivity, $\mu_a \propto \langle k(L^2 - 3/4Ll_0) \rangle$, with L the length of a bond, l_0 its rest length, and k its stiffness.

The authors study the boson peak frequency, but it is good to study the boson peak strength as well. The boson peak strength is measured as $D(\omega_{BP})/D_{debye}(\omega_{BP})$ (where $D_{debye}(\omega)$ is the Debye DOS), which is also described by the fluctuating theory. How is the elasticity fluctuation (or disorder parameter γ) related to the BP strength?

Reply: We find the Boson peak strength increases with the degree of disorder, e.g., at smaller f . As we find $D(\omega_{bp})\omega_{bp}^{-1}$ to growth with γ , in agreement with theoretical predictions. Since γ only varies in a small range, it is arduous to establish a quantitative relationship.

In Fig. 6, crossover between ω^3 and ω^2 seems to vanish as f increases (fluctuations become small). Why so? Is this consistent with the theoretical prediction?

Reply: Increasing f leads to more stable systems with a smaller sound attenuation parameter. The crossover between the two regimes persists as f increases but shifts to higher frequencies. We have added guiding lines to Fig 8 to put this crossover in evidence.