Nonphononic spectrum of two-dimensional structural glasses

Lerner, E.; Bouchbinder, E.

DOI
10.1063/5.0120115

Publication date
2022

Document Version
Final published version

Published in
Journal of Chemical Physics

License
CC BY

Citation for published version (APA):
Nonphononic spectrum of two-dimensional structural glasses

Cite as: J. Chem. Phys. 157, 166101 (2022); https://doi.org/10.1063/5.0120115
Submitted: 11 August 2022 • Accepted: 27 September 2022 • Published Online: 24 October 2022
Published open access through an agreement with Universiteit van Amsterdam Instituut voor Fysica

Edan Lerner and Eran Bouchbinder

ARTICLES YOU MAY BE INTERESTED IN

Low-energy quasilocalized excitations in structural glasses
The Journal of Chemical Physics 155, 200901 (2021); https://doi.org/10.1063/5.0069477

Elastic moduli fluctuations predict wave attenuation rates in glasses
The Journal of Chemical Physics 154, 081101 (2021); https://doi.org/10.1063/5.0038710

Microscopic observation of two-level systems in a metallic glass model
The Journal of Chemical Physics 158, 014501 (2023); https://doi.org/10.1063/5.0128820
Nonphononic spectrum of two-dimensional structural glasses

Cite as: J. Chem. Phys. 157, 166101 (2022); doi: 10.1063/5.0120115
Submitted: 11 August 2022 • Accepted: 27 September 2022 •
Published Online: 24 October 2022

Edan Lerner and Eran Bouchbinder

AFFILIATIONS
1 Institute of Theoretical Physics, University of Amsterdam, Science Park 904, 1098 XH Amsterdam, The Netherlands
2 Chemical and Biological Physics Department, Weizmann Institute of Science, Rehovot 7610001, Israel

© 2022 Author(s). All article content, except where otherwise noted, is licensed under a Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by/4.0/). https://doi.org/10.1063/5.0120115

Extensive numerical work from recent years has established that the low-frequency nonphononic vibrational spectrum of structural glasses follows a \( \sim \omega^4 \) scaling with angular frequency \( \omega \). This universal quartic \( \sim \omega^4 \) law featured by the nonphononic spectrum has been shown to be independent of the details of the interparticle interaction potential, glass formation protocol, and spatial dimensions \( d \geq 2 \). Furthermore, indirect evidence for the quartic scaling of the nonphononic spectrum of two-dimensional structural glasses was presented in Refs. 1 and 6–8. In Refs. 4 and 7, it was shown that in two-dimensional structural glasses, the prefactor \( \omega^4_c \) of the quartic \( \sim \omega^4 \) law is \( N \)-dependent, scaling as \( \omega^4_c \sim (\sqrt{\log N})^5 \), where \( N \) denotes the number of particles in a glass. At the same time, deviations from the quartic scaling of the nonphononic spectrum were reported for three-dimensional (3D) structural glasses in Refs. 9 and 10 depending on the system size and formation protocol of the glasses studied. These previous works associated these deviations with a glassy length scale \( \xi \) that features the universal quartic law \( \sim \omega^4 \). The length \( \xi \) has been shown to be glass-formation-protocol dependent—decreasing for lower-energy, more stable glasses—fully consistent with previously observed deviations in the exponent \( \beta \) of the nonphononic spectrum \( \sim \omega^\beta \) from the apparently universal value \( \beta = 4 \).

Recently, in Refs. 11 and 12, it has been argued that the nonphononic spectrum of two-dimensional (2D) structural glasses rather follows \( \sim \omega^\beta \) with \( \beta < 4 \), presumably casting doubt on the validity of previous observations and claims. Here, we study the nonphononic spectrum of two-dimensional structural glasses and show that (i) the exponent \( \beta \) is glass-formation-protocol and system-size dependent, as seen previously for structural glasses in three dimensions, and (ii) the scaling \( \omega^4_c \sim 1/\sqrt{\log N} \) put forward in Refs. 4 and 7 is consistent with numerical observations presented below.

We simulate a generic glass-forming model in 2D—also studied in Refs. 11 and 12—in which point-like particles interact via an inverse-power-law potential that is smoothed at a cutoff distance up to two derivatives; see, e.g., Ref. 7 for the model’s details. We prepare ensembles of glasses by (i) instantaneously quenching high-temperature liquid states to zero temperature (as done in Refs. 11 and 12) and (ii) by annealing liquids for 10 simulational time units (described, e.g., in Ref. 7) at temperature \( T = 0.5 \), which is approximately the (computer) glass transition temperature of our studied glass-forming model. Each of these annealing runs are followed by an instantaneous quench to zero temperature to form a glass (termed “well-annealed” in Fig. 1). The ensemble sizes can be found in Ref. 13.

In Fig. 1, we present our results; Figs. 1(a) and 1(c) show the raw vibrational spectra \( D(\omega;N) \) of our pair of glass ensembles, respectively, as indicated in the legends. A clear system-size dependence is apparent in both ensembles. We further find that the exponent featured by the low-frequency power-law regime of \( D(\omega;N) \) drops below 4 for smaller, quickly quenched glasses, cf. Fig. 1(c), consistent with observations in 3D. That is, we find that \( \beta(N) < 4 \) increases with the system size \( N \) from \( \beta = 3.2 \) for \( N = 36 \) to \( \beta = 3.6 \) for \( N = 1600 \). In Figs. 1(b) and 1(d), we show that rescaling both axes according to the \( N \) dependence of the nonphononic-excitations’ characteristic scale \( \sim 1/\sqrt{\log N} \) as put forward in Refs. 4 and 7 leads to a convincing data collapse, confirming that the nonphononic
FIG. 1. (a) The VDoS $D(\omega;N)$ of well-annealed computer glasses (see the text for details) vs $\omega/\omega_0$ for various system sizes $N$ (see the legend), where $\omega_0 \equiv c_s/a_0$, with $c_s$ being the shear wave speed and $a_0$ being an interparticle distance. Note that the 4:1 and 3.6:1 scaling triangles correspond to the lines going through the $N = 1600$ and $N = 36$ data, respectively, demonstrating a systematic variation of the exponent $\beta$ with $N$. (b) The same data as in (a), but here plotting $(\omega_0/\sqrt{\log N}) D(\omega;N)$ vs $\omega/(\omega_0/\sqrt{\log N})$. (c) The same as (a), but for glasses formed by an infinitely fast quench, $\dot{T} \to \infty$. Note that the 3.6:1 and 3.2:1 scaling triangles correspond to the lines going through the $N = 1600$ and $N = 36$ data, respectively, demonstrating again a systematic variation of the exponent $\beta$ with $N$. (d) The same as (b), but for the data shown in (c). VDoS of 2D glasses is, indeed, $N$ dependent. In Fig. 2, we present the cumulative distributions $C(\omega) \equiv \int_{\omega_0}^{\omega} D(\omega') d\omega'$, showing again that $\beta$ features both glass-formation protocol and system-size dependencies. We note that the $N$ dependence of the exponent $\beta(N)$ also appears to be consistent with the results presented in the supplementary material file of Refs. 11 and 12 (which can be found in Ref. 14). For example, in Fig. 2(b), therein, the cumulative density of states normalized by $\omega^{4.5}$ is presented for various system sizes.

FIG. 2. (a) The cumulative distributions $C(\omega/\omega_0) \equiv \int_{\omega_0}^{\omega} D(\omega'/\omega_0) d(\omega'/\omega_0)$ of well-annealed computer glasses plotted vs $\omega/\omega_0$ for various system sizes as indicated in the legend. (b) The same data as in (a), but here plotting $(\omega/\omega_0)^{-4.5} C(\omega/\omega_0)$ vs $\omega/(\omega_0/\sqrt{\log N})$. (c) The same as (a), but for glasses formed by an infinitely fast quench, $\dot{T} \to \infty$. (d) Here, we plot $(\omega/\omega_0)^{-4.2} C(\omega/\omega_0)$ vs $\omega/(\omega_0/\sqrt{\log N})$ for the data shown in (c). A clear $N$-dependence of the exponent $\beta$ is seen in this representation.
Our data demonstrate the difficulty in accurately determining the value of the exponent $\beta$ appearing in the low-frequency $-\omega^\beta$ scaling of the nonphononic spectrum of two-dimensional structural glasses. The proper determination of $\beta$ in the thermodynamic limit requires careful finite-size tests (see, e.g., Ref. 10 for three-dimensional glasses), which are particularly hard to conduct in two-dimensions due to the abundance of low-frequency phononic modes that obscure the nonphononic spectrum (see elaborate discussion on this issue in Ref. 15). In this context, we note that in Ref. 1, systems of $N = 25\,600$ particles were employed—together with a nonlinear-excitation analysis—in order to show (via simulations and extreme-value-statistics arguments) that $\beta = 4$ in two-dimensional glasses, even if the latter were formed by an instantaneous quench from high-temperature liquid states. Our results, taken together with the data presented in Refs. 1, 4, 6, and 7, support that $\beta = 4$ is the universal value characterizing the nonphononic spectrum of structural glasses in the thermodynamic limit, including in two dimensions.

Discussions with Lijin Wang, Elijah Flenner, and Grzegorz Szamel are acknowledged.

**AUTHOR DECLARATIONS**

**Conflict of Interest**

The authors have no conflicts to disclose.

**Author Contributions**

Edan Lerner: Conceptualization (equal); Investigation (equal); Writing – original draft (equal). Eran Bouchbinder: Conceptualization (equal); Writing – original draft (equal).

**DATA AVAILABILITY**

The data that support the findings of this study are available from the corresponding author upon reasonable request.

**REFERENCES**

13. We created about 3.8M, 2.1M, 427K, and 94K independent, well-annealed glassy samples and about 14M, 12M, 6.8M, and 2.8M independent, instantaneously quenched glassy samples of sizes $N = 36, 64, 196, \text{ and } 1600$, respectively.