Statistics and Properties of Low-Frequency Vibrational Modes in Structural Glasses

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Erratum: Statistics and Properties of Low-Frequency Vibrational Modes in Structural Glasses [Phys. Rev. Lett. 117, 035501 (2016)]

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In the Numerical Methods section of the Supplemental Material, the following detail regarding the preparation protocol of the glassy samples studied in our work was unintentionally omitted: for the KABLJ and 3DIPL models, after an equilibration run in the high temperature regime, short annealing runs were carried out before employing a nonlinear conjugate gradient minimization algorithm to create athermal glassy samples. These annealing runs were carried out to prevent numerical instabilities that would occur from time to time when attempting to minimize the energy of high temperature configurations using a nonlinear conjugate gradient algorithm. They lasted for a duration of $50.0\tau_0$ at temperature $T = 0.45\varepsilon/k_B$ for the KABLJ model, and for $100.0\tau_0$ at temperature $T = 0.5\varepsilon/k_B$ for the 3DIPL model. Here ε and τ_0 are the microscopic units of energy and time, respectively, and k_B is the Boltzmann constant. We note that the structural relaxation time at the annealing temperatures is several orders of magnitude longer than the duration of the annealing runs.

In subsequent work by some of us [1] it became apparent that this unintentionally-omitted detail is likely to have important physical implications. It was found that instantaneous quenches used to create a computer glass may have a significant effect on its density of vibrational modes. In particular, fully overdamped quenches from high temperatures result in solids that exhibit an enhanced number of low-frequency modes, described by a density of vibrational modes that grows as ω^β with $\beta \leq 4$, and ω denoting the frequency. The findings of [1] suggest that the presence of inertia during the cooling process of glassy samples—which is universally present in every realistic cooling process of real glasses—can suppress the occurrence of low-frequency glassy modes, and produce the ω^4 scaling of the density of vibrational modes. We hypothesize that the annealing runs (that involve inertial dynamics) performed in the preparation of the glassy samples analyzed in our Letter could be responsible for the observed ω^4 scaling of their density of vibrational modes.

Annealing runs as described above were not performed for the harmonic soft spheres model; however, those systems were quenched from high temperature configurations using the FIRE algorithm (fast inertial relaxation engine [2]), which, as implied by its name, intrinsically contains an inertial component in its dynamics that could lead to an uncontrolled degree of structural relaxation beyond what is possible using fully overdamped dynamics.

[1] E. Lerner and E. Bouchbinder, Phys. Rev. E **96**, 020104(R) (2017).
[2] E. Bitzek, P. Koskinen, F. Gähler, M. Moseler, and P. Gumbsch, Phys. Rev. Lett. **97**, 170201 (2006).

