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Numerical study of the equilibrium Kauzmann transition between a liquid and a disordered glass

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Collaboration: G. Biroli (LPENS)

Scientific context: Most liquids gradually solidify at low temperature via a physical process called the glass transition towards a non-equilibrium disordered state of matter [1]. This process is well-known experimentally at the macroscopic scale. At the fundamental level, however, the statistical mechanics description of the phenomenon is much less advanced, as it took several decades of difficult analytic work to 'only' derive a solid mean-field transition of the liquid-glass transition, which is now reaching completion [2]. The effect of fluctuations in disordered systems is typically very important but theory is for now unable to capture them. In the last 10 years, considerable progress was also made to develop simple yet realistic atomistic models for glass transition studies, as well as numerical methods to more efficiently sample the configuration space which is known to be highly complex [3].

State-of-the-art theory and simulations suggest that an equilibrium phase transition between liquid and glass states could exist in model liquids in finite dimensions [4], but demonstrating the existence of the transition and studying the associated properties (universality, exponents, characteristic lengthscales) has not been possible so far, leading some researchers to claim that this is an impossibly difficult task.

We wish to solve this difficult problem.

Description of the thesis: In this thesis, we will develop and combine numerical approaches to systematically investigate the statistical mechanics nature of the transition between liquid and glass states in equilibrium conditions. By carefully choosing simple glass models, and starting with modest system sizes, we will develop and benchmark various computational approaches to very efficiently explore complex energy landscapes (population annealing, swap Monte Carlo, non-equilibrium hybrid Monte Carlo simulations, etc.) and cross the equilibrium liquid-glass Kauzmann transition for bulk systems. In a second step, varying the system size gradually, we shall investigate whether the findings in small systems extend to larger ones, in order to eventually develop finite size scaling methods to approach the thermodynamic limit. Ultimately, this work will provide a definitive answer to a mystery that has haunted the field of disordered systems for more than fifty years by demonstrating whether a glass state of matter can truly be defined in three-dimensional glass-forming liquids.

Supervision: The project will take place at Gulliver (ESPCI UMR 7083 CNRS) and be supervised by L. Berthier (DR, CNRS). The lab has developed well-known expertise for the study of disordered and non-equilibrium materials, and has a large experience regarding the numerical simulations of these systems [4]. The work will also be performed in close collaborarion with G. Biroli (LPENS, UMR 8023). Berthier and Biroli have (very) often collaborated on this topic in the past [1, 5].

Références :

[1] L. Berthier and G. Biroli, *Theoretical perspective on the glass transition and amorphous materials*, Rev. Mod. Phys. 83, 587 (2011).

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[4] B. Guiselin, G. Tarjus, and L. Berthier, *Is glass a state of matter?* Phys. Chem. Glasses 63, 136 (2022)

[5] G. Jung, G. Biroli, and L. Berthier, *Predicting dynamic heterogeneity in glass-forming liquids by physics-informed machine learning*, Phys. Rev. Lett. 130, 238202 (2023)