Configurational entropy of glass-forming systems from graph isomorphism

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— The configurational entropy plays a central role in the thermodynamic scenarios of glass transition, such as Adam-Gibbs theory and random first-order transition theory. By definition, the configurational entropy $S_c$ is the difference between the entropy of liquid and the vibrational entropy with structural rearrangement restricted, both of which can be obtained by means of thermodynamic integration. On the other hand, $S_c$ is essentially a measure of the number of basins in the energy landscape, and therefore it can also be estimated by explicitly enumerating inherent structures. To this end, we first coarse-grain the vibrational motions by mapping configurations to Voronoi diagrams and then categorize them using canonical labelling. The Voronoi graph entropy is calculated as $S_G/k_B = -\sum p_i \log(p_i)$, where $p_i$ is the probability of finding distinct graph $i$. We find for an $n$-particle subsystem of glass-forming hard-disk/sphere fluids, $S_G(n)$ scales linearly with $n$, and $S_c$ can be estimated from the slope.

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