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Transition rates in the Lennard-Jones binary mixture[1] YASHENG YANG, BULBUL CHAKRABORTY, JANÉ KONDEV, Martin Fisher School of Physics, Brandeis University — The slow relaxation in glass forming liquids approaching the glass transition is often described by the Vogel-Fulcher-Tammann (VFT) equation which predicts a diverging viscosity at a non-zero temperature. The origin of this anomalously slow relaxation is an outstanding problem. Recent work (PRE 70, 060501(R) (2004)) shows that a system will obey the VFT equation near a critical point if the transition rates between different macrostates have an asymmetric form: energy lowering rates depend only on the entropy change and energy raising rates depend only on the energy change. Here we investigate this mechanism for glassy dynamics in the the Lennard-Jones binary mixture (LJBM); a well-known glass former. The transition rates between different inherent structures (local minima of the potential energy) are calculated using the interval-bisection method. We find that the energy lowering transition rates are not temperature-sensitive, while the energy raising ones depend on the temperature. The dynamics in the IS energy space is however, non Markovian. We discuss these findings in light of the proposed mechanism for glassy relaxation characterized by a VFT form.

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