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Quantum Effects in the Glass Transition and Anomalous Dynamics of Water

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Abstract:

The glass transition phenomenon remains one of the most challenging topic in condensed matter physics. All these studies usually neglect any quantum effects in structural relaxation of glass forming systems. However, low Tg liquids of light molecules might have significant contribution of quantum effects. We show [1] that quantum effects should lead to a significant decrease of the glass transition temperature T_g with respect to the melting temperature T_m, so that the ratio T_g/T_m can be much lower than the typical value of 2/3. Furthermore, the viscosity or structural relaxation time should exhibit highly unusual temperature dependence, namely a decrease of the apparent activation energy upon approaching T_g, instead of traditional increase (i.e. sub-Arrhenius dependence instead of usual super-Arrhenius). Combining neutron scattering and dielectric relaxation spectroscopy we show that quantum fluctuations are indeed not negligible in deeply supercooled water, the lightest molecule that exists in a liquid state at ambient conditions. Our dielectric measurements revealed an anomalously weak temperature dependence of structural relaxation in water at T close to its T_g ~136K. Moreover, we discovered unusually large isotope effect in Tg of water [2]. We demonstrate that this anomalous behavior can be explained well by quantum effects in structural relaxation. We speculate that the apparent fragile-to-strong crossover in water, and its low value of T_g/T_m~0.5 can be explained by quantum effects. At the end, we discuss criteria that define the importance of quantum effects in the glass transition.

1. Novikov, V. N. & Sokolov, A. P. Role of quantum effects in the glass transition. **Phys. Rev. Lett. 110**, 065701, (2013).
2. C. Gainaru, et al., **PNAS** (2014, in print).