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Takeshi Egami

University of Tennessee Oak Ridge National Laboratory, USA

Atomic dynamics in liquid in real space and time: Towards the liquid-state-physics

The science of liquid and glass is seriously under-developed compared to that of crystalline solids, because most of the theoretical tools of condensed-matter-physics assume lattice periodicity, and thus are powerless for liquid and glass in which the structure has no periodicity and many-body correlations dominate. However, owing to recent advances in computational power and experimental tools we are making significant progress. We found that the origin of viscosity in high-temperature liquid is the local topological excitation, the elementary excitation to change the local topology of atomic connectivity which we named anankeon, and gave the direct experimental proof of this mechanism for water through the inelastic x-ray scattering (IXS). The results of the IXS were double-Fourier transformed into the van Hove function, g(r, t), which describes the two-body atomic correlation in real space and time (Fig. 1). We have also determined the van Hove function by inelastic neutron scattering (INS) for liquid metals and superfluid helium. Whereas Landau explained superfluidity from the energy dissipation side, the real space mechanism has not been known. Using INS we have determined a new real space mechanism of superfluidity in terms of coherent atomic tunneling. On the theoretical side we are developing a new statistical mechanics of liquid in terms of topological identification of the state using the graph theory, which greatly simplifies the statistics and make it possible to evaluate the configurationally entropy. These advances are making the creation of the field of liquid-state-physics a real possibility.



Figure 1: The van Hove function of water at room temperature determined by inelastic x-ray scattering. Time = 0 gives the same-time (snap-shot) correlation. Merging of the first and second peaks show the time-scale of topological excitation.

Biography

Takeshi Egami has completed his PhD from University of Pennsylvania, and Postdoctoral studies from University of Sussex and Max-Planck Institute in Sttutgart. After teaching at Penn for 30 years he moved to the University of Tennessee/Oak Ridge National Laboratory as Distinguished Scientist. He was the Director of Joint Institute for Neutron Sciences. He has published more than 500 papers and one book, gave more than 300 invited presentations at conferences, and was cited more than 18000 times. He has been the Editor of Advances in Physics and Division Associate Editor of Physical Review Letters

egami@utk.edu