Entropy Scaling of the Transport Properties of Simple and Not-so-Simple Fluids

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At its core, entropy scaling is the notion of an intimate relationship between the residual (or excess) entropy (a measure of structure of the fluid phase) and the macroscopically scaled transport properties. This relationship was first noticed by Rosenfeld in 1977 based upon a small database of molecular dynamics simulations for very “simple” fluids (hard sphere, Lennard-Jones, etc.). Recent years have seen empirical modifications of this approach applied to real fluids, but this talk focuses on “simple” systems more comprehensively than the work of Rosenfeld. This talk summarizes a few recent results related to entropy scaling of “simple” fluids: 1) if the scaled transport properties are multiplied by the appropriate factor of residual entropy, the dilute-gas divergence can be removed without causing non-monovariability in the liquid phase scaling 2) the residual entropy appears to be connected with the transition from liquid-like to gas-like behavior in supercritical phases in a similar notion to Widom curves 3) for model glassformers, entropy scaling appears to still hold, with the density scaling exponent capturing the deviation from a quasi-universal relationship. In short, understanding residual entropy teaches us many things about transport properties.