Velocity Auto-correlation Functions in the Dense Regime

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Various functional forms of velocity auto-correlation functions (VACF) have been proposed for ease in fitting molecular dynamics data. The VACFs range from hard-sphere models to complicated oscillatory behaviors. Benefits of fitting functions range from extracting diffusion data as well as vibrational density of states. In this work we show how to arrive at a functional form for VACFs that includes secular behavior in the dense regime, i.e. includes a $t^{-\frac{3}{2}}$ term. This new form is applied to a equimolar carbon and hydrogen mixture at $20\,\mathrm{eV}$ and $10\,\mathrm{g/cc}$. This new functional form captures the $t^{-\frac{3}{2}}$ behavior in the dense regime. Additionally, we show how to separate the VACF into solid and gas portions amenable to an ionic entropy calculation akin to Refs. [1, 2]

[1] E. R. Meyer, C. Ticknor, J. D. Kress, and L. A. Collins, Phys. Rev. E **93**, 042119 (2016).
[2] M. P. Desjarlais, Phys. Rev. E **88**, 062145 (2013).