

Abstract Submitted  
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**Direct measurement of negative square gradient coefficients for density fluctuations in all-atom simulations of common liquids** COLIN DENNISTON, LINGTI KONG, DAN VRIESINGA, University of Western Ontario — We perform all-atom simulations of common liquids such as water (TIP3P) and organic liquids such as short-chain olefins. We show that square gradient coefficients for the mass density can be measured directly in a linear response measurement to sinusoidal forces at several different wavelengths. Surprisingly, in all fluids measured, the square gradient coefficient is negative implying that density gradients lower the free energy of the system. However, stability is maintained at any wavelength greater than the separation between molecules due to the global mass conservation constraint. We suggest that this provides a mechanism for the molecular scale cut-off of pressure singularities that arise in situations such as droplet pinch-off.

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