Renormalization Contributions to get Accurate Results Closer to Gas-Liquid and Liquid-Liquid Critical Points than is Easily Achieved by Simply using Molecular Dynamics Methods

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Molecular dynamic methods applied to spherical molecules interacting with hard cores and suitably adjusted soft repulsive shoulders next to attractive square wells have given results that are in reasonably good agreement with measurements on several single component fluids both far from gas-liquid critical points and reasonably close to their critical points. But when quite close to a critical point, highly accurate results require larger and larger numbers of particles in the calculations, owing to the important role played then by density fluctuations of increasingly long wavelengths. Because calculations with very large numbers of particles can become prohibitively expensive and time consuming, it may be of interest to see whether "global" renormalization-group additions to easily achievable molecular dynamics results for fewer particles can result in substantial improvements in predicting behavior in the near vicinity of critical points. Some results, using essentially the method described in J. A. White, J. Chem. Phys. 112 (2000) 3236, will be reported for near critical point behavior in the vicinity of the gas-liquid critical point for water, and to explore what might be expected near its possible second, low-density high-density liquid-liquid critical point below the normal freezing point.