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Putting water on a lattice: The importance of long wavelength density fluctuations in theories of hydrophobic and interfacial phenomena. SURIYANARAYANAN VAIKUNTANATHAN, PHILLIP GEISSLER, University of California, Berkeley — The physics of air-water interfaces plays a central role in modern theories of the hydrophobic effect such as the Lum-Chandler-Weeks (LCW) theory. Implementing these theories, however, has been hampered by the difficulty of addressing fluctuations in the shape of such soft interfaces. We show that this challenge is a fundamental consequence of mapping long wavelength density variations onto discrete degrees of freedom. Specifically, through an analysis of the lattice gas model and related approximations, we identify a narrow parameter regime in which the lattice gas model can optimally be used to describe long wavelength liquid density fluctuations such as the capillary modes at a liquid-vapor interface. Coupling fluctuations in the lattice model to fluctuations on finer molecular scales through the least complicated realization of the LCW perspective, we obtain an effective Hamiltonian for lattice occupation variables in the presence of a hydrophobic solute. We show that this Hamiltonian - with no unknown parameters - in fact suffices to describe quantitatively the the solvation of hydrophobic objects with various shapes and sizes. This model is uniquely well suited for exploring hydrophobic and interfacial phenomena that involve disparate length scales.

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