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Microscopic theories of the structure and glassy dynamics of ultra-dense hard sphere fluids RYAN JADRICH, KENNETH SCHWEIZER, University of Illinois at Urbana-Champaign — We construct a new thermodynamically self-consistent integral equation theory (IET) for the equilibrium metastable fluid structure of monodisperse hard spheres that incorporates key features of the jamming transition. A two Yukawa generalized mean spherical IET closure for the direct correlation function tail is employed to model the distinctive short and long range contributions for highly compressed fluids. The exact behavior of the contact value of the radial distribution function (RDF) and isothermal compressibility are enforced, as well as an approximate theory for the RDF contact derivative. Comparison of the theoretical results for the real and Fourier space structure with nonequilibrium jammed simulations reveals many similarities, but also differences as expected. The new structural theory is used as input into the nonlinear Langevin equation (NLE) theory of activated single particle dynamics to study the alpha relaxation time, and good agreement with recent experiments and simulations is found. We demonstrate it is crucial to accurately describe the very high wave vector Fourier space to reliably extract the dynamical predictions of NLE theory, and structural precursors of jamming play an important role in determining entropic barriers.

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