B. Molecular Dynamics Simulations

Classical molecular dynamics (MD) simulations were used to study the model fluid described in the previous subsection. $N = 500$ identical, structureless particles of mass m were confined in a cubic box, of volume V, with periodic boundary conditions in all directions. All MD simulations were performed in the canonical (NVT) ensemble with a time step of $0.002\sigma\sqrt{m/\epsilon}$. A Nosé-Hoover thermostat with the coupling parameter equals to 2 was used to maintain the temperature. All simulations were initialized with the system in a face centered cubic configuration and further equilibrated over 250 000 steps for each temperature, T, and density, $\rho = N/V$. After the equilibration period was over, additional 500 000 steps were used to sample the system. A cutoff radius $r_c = 3.5\sigma$ was employed for the potential Eq. (4). Diffusivities were computed using the Einstein relation. At each state point, 100 configurations were sampled and used to construct the instantaneous normal mode spectra and associated quantities. We repeated the calculation for some state points using 500 configurations and found no significant difference.

C. Density, Diffusional and Structural Anomalies

Figure 1 illustrates the regions associated with the density, diffusional and structural anomalies of the model fluid studied here in the density-temperature planes. The region of density anomaly corresponds to state points for which $(\partial\rho/\partial T)_P > 0$ and is bounded by the locus of points for which the thermal expansion coefficient is zero. The translational diffusion coefficient as a function of $\rho^* = \rho\sigma^3$ goes as follows. For the low temperature isotherms, the diffusivity increases as the density is lowered, reaches a maximum at $\rho_{D\max}$ and decreases until it reaches a minimum at $\rho_{D\min}$. The locus of extrema in the $D(\rho)$ curve mark the boundaries of the region of diffusional anomaly, as shown in Figure 1 using dashed lines.

The region of structural anomaly of core-softened fluids is defined most simply using the translational or pair correlation order metric, defined as[14]

$$t \equiv \int_0^{\xi_c} |g(\xi) - 1| d\xi, \tag{5}$$

where $\xi \equiv r\rho^{1/3}$ is the interparticle separation scaled by the mean interparticle distance, $g(\xi)$ is the radial distribution function and ξ_c is a scaled cut-off distance. In this work, we use