

Supplementary Information

Noether-Constrained Correlations in Equilibrium Liquids

Florian Sammüller, Sophie Hermann, Daniel de las Heras, and Matthias Schmidt

Theoretische Physik II, Physikalisches Institut, Universität Bayreuth, D-95447 Bayreuth, Germany

(Dated: 7 June 2023, www.mschiidt.uni-bayreuth.de)

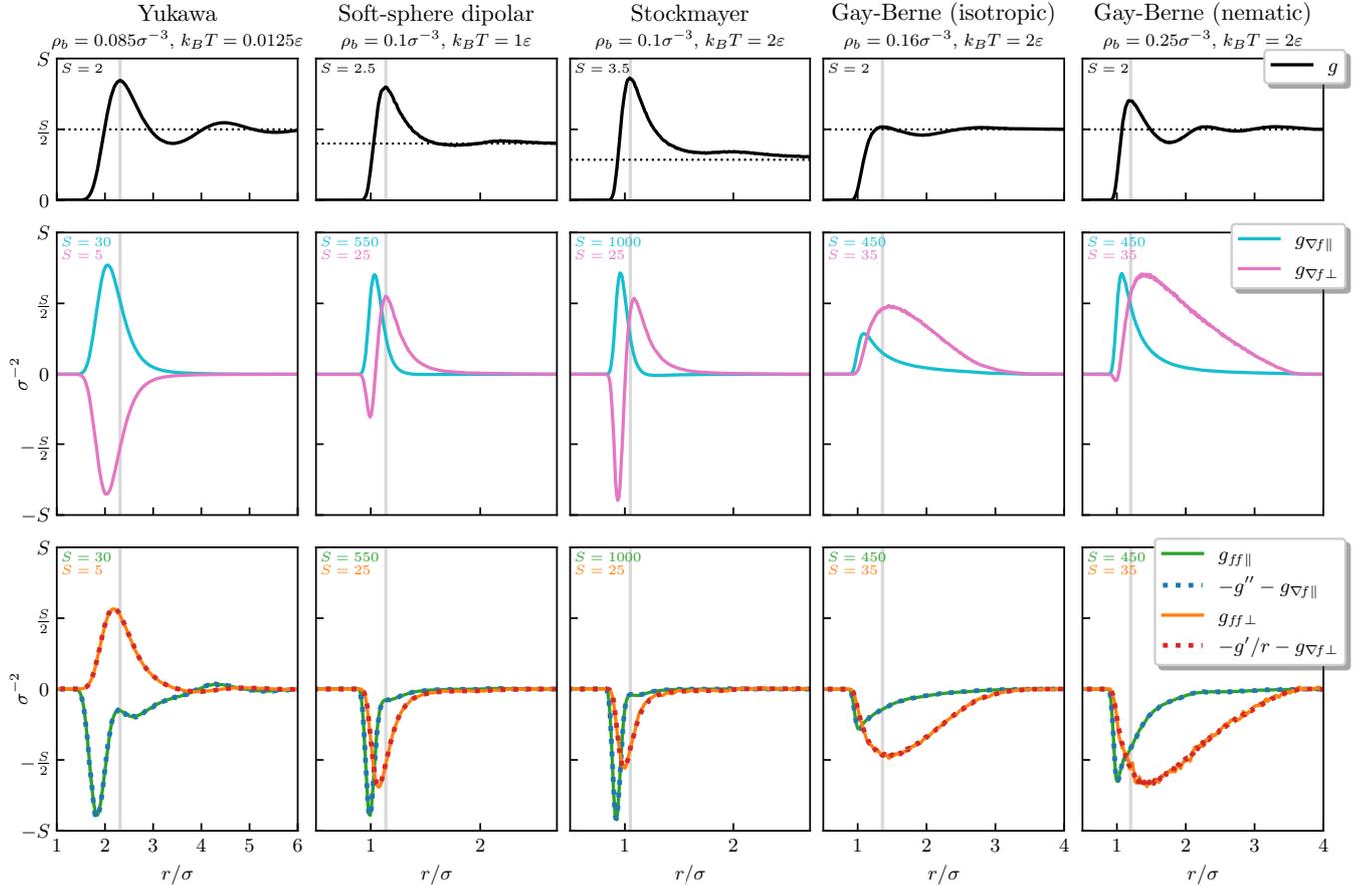


FIG. 3: Correlation functions analogous to Fig. 2 of the main text, but for the Yukawa liquid (first column), the soft-sphere dipolar fluid (second column), the Stockmayer fluid (third column), and the Gay-Berne model in the isotropic (fourth column) and nematic phase (fifth column). The results for the anisotropic models are obtained from canonical Monte Carlo simulations, and they are averaged over the microscopic orientations; the simulation box volume is $V = (20\sigma)^3$ and the long-ranged interactions are cut off at radial distance 10σ . Shown are results for the pair correlation function $g(r)$ (first row) and for the radial (\parallel) and transversal (\perp) components of the two-body force-gradient correlator $\mathbf{g}_{\nabla f}(r)$ (second row) and the force-force pair correlator $\mathbf{g}_{ff}(r)$ (third row). The respective vertical scale factor S is given in the top left corner of each panel and the scaled values for bulk density ρ_b and temperature T are indicated for each model fluid above the respective column. The results for the Yukawa liquid with inverse screening parameter $\kappa = 2/\sigma$ are qualitatively similar to those of the WCA liquid (second column Fig. 2 of the main text) but here with much longer-ranged decay behaviour. For identical dipolar strength $\mu/\sqrt{\epsilon\sigma^3} = 2$ the results for $g_{\nabla f\perp}(r)$ for both the soft-sphere dipolar fluid [58] and the Stockmayer fluid show strong signatures of chain formation, similar to the behaviour of the three-body gel former (fourth column of Fig. 2 of the main text). The Gay-Berne model (with parameters $\kappa = 3.8, \kappa' = 5$ [62]) features positive-valued $g_{\nabla f\perp}(r)$, which contrasts the behaviour of all other models and which we take to indicate interlocked arrangements of neighboring anisotropic molecules.

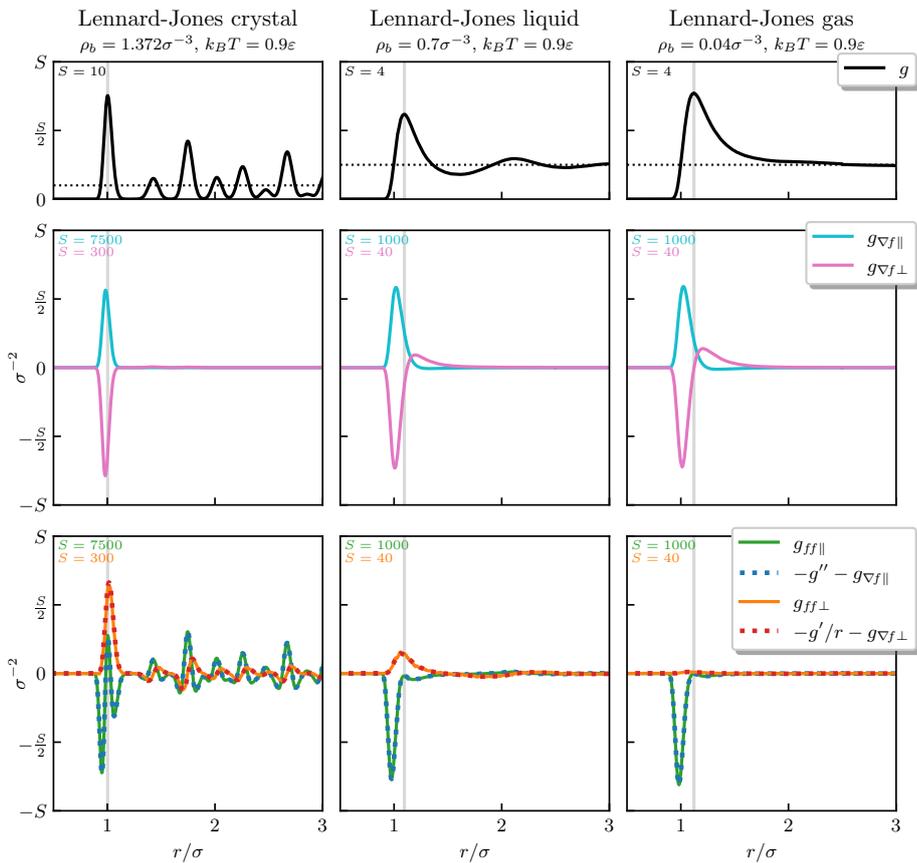


FIG. 4: Comparison of correlation functions for the LJ system in the fcc crystal phase (first column), the liquid (second column), and the gas phase (third column). Shown are the pair correlation function $g(r)$ (top row), the force-gradient correlator $\mathbf{g}_{\nabla f}(r)$ (middle row), and the force-force correlator $\mathbf{g}_{ff}(r)$ (bottom row). The plot style is analogous to Fig. 2 of the main text and to Fig. 3 of this SI. While the results for the gas and for the liquid carry the full structural two-body information, the correlators for the crystal are resolved only as a function of the radial distance r . This representation constitutes an average over global translations and rotations of the general inhomogeneous Noether sum rule, see Eq. (11) of the main text with $|\mathbf{r} - \mathbf{r}'|$ kept fixed. The reduced Noether identities (13) and (14) continue to hold in this averaged sense, as is demonstrated by the data collapse in the lower left panel. This perfect agreement serves as an indirect indication of the validity of the more general Eq. (11), which is applicable in the full inhomogeneous geometry.