A Generalized Ornstein-Zernike Approach for the Triplet Correlation Function.

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Warm dense matter (WDM) is characterized by strong Coulomb correlations, where the structure factor—traditionally derived from the Ornstein-Zernike (OZ) equation—governs transport properties. However, a complete description requires knowledge of three-body correlations, which are inaccessible to standard linear response theory.

This work presents two interconnected advances. First, numerical results for the structure factor are obtained within the Mean Spherical Approximation (MSA) and applied to transport properties, demonstrating the necessity of going beyond the ideal plasma model. Second, and most importantly, the OZ formalism is systematically extended to three-body correlations. By taking the second functional derivative of the free energy with respect to the interaction potential, a new integral equation for the triplet correlation function is derived, paralleling the classic OZ equation for pairs.

Crucially, we highlight the experimental pathway enabled by modern coherent X-ray sources (e.g., XFELs). While pair correlations manifest in the linear density response, three-body correlations are encoded in the nonlinear density response of the system. The derived equation provides the necessary theoretical framework to extract the three-body direct correlation function C_3 from future nonlinear scattering experiments, where measurements of the second and third harmonics of the density perturbation directly probe higher-order correlation functions. This establishes a direct link between advanced statistical mechanics and the diagnostics of WDM at high-intensity laser facilities.