Collective modes in strongly coupled 2D and 3D binary systems

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We report on a systematic MD and theoretical study of 2D and 3D binary Yukawa liquids whose objective has been to map the collective mode structures of binary systems over the parameter space of the relevant mixing parameters, including the liquid, crystalline and disordered lattice phases. In the first phase of the study we concentrated on mixtures of components with different masses and with different concentrations, but with identical charges. We observe the formation of acoustic and optic modes: the latter being the hallmark of the presence of more than one component.

The sound speeds associated with the longitudinal and transverse acoustic modes exhibit a remarkable coupling (Gamma)-dependence. For weak coupling, the RPA predicted dominance of the lighter mass species should prevail. For higher coupling however, the QLCA predicts the formation of virtual atom-s that results in the reversal of roles and the dominance of the heavy mass species. MD simulations show clearly the transition from the intermediate coupling to the strong coupling regime both in the liquid and in the crystalline or disordered solid phase and fully corroborate the QLCA result.

In the second phase we investigated the combined charge ratio (Z) and concentration ratio (c) dependence of the collective modes. This question is closely related to the existence of a variety of structural phases in a (zero temperature) binary system: for a chosen lattice structure phonon softening marks the phase boundary of the structure in the Z - c plane. The number of optic modes depends on the concentration ratios and on the crystal structure that can accommodate the chosen concentrations. We show that in all cases the mode frequencies satisfy a generalized Kohn sum rule.

We have focused on simple structures for c=1, c=2 (2D) and c=3 (3D) mixtures in compatible Z-domains. We have identified an invariant mode, independent of the mass ratio, as a universal phenomenon in these structures. . In the liquid state only one longitudinal and one (2D) or two (3D) transverse optic modes survive which, however, are not necessarily in correspondence with the optic modes of the lattice. While further studies are still needed, the QLCA seems to be a good predictor for the wave-dispersion of these modes.