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The origin of the roton minimum[1] G.J. KALMAN, Boston College, S. KYRKOS, Le Moyne College, K.I. GOLDEN, U. of Vermont, P. HARTMANN, Z. DONKO, Hungarian Acad. of Sciences — The roton minimum is a deep minimum in the collective excitation spectrum of the liquid, forming around fairly high k-values. We have discovered, through MD simulations, that this appears to be a general feature of strongly coupled liquids and is ubiquitous in 2D and 3D Yukawa liquids. We suggest that the physical origin of the roton minimum has to be sought in the quasi-localization of particles in a strongly correlated liquid and in the ensuing formation of local microcrystals whose averaged frequency dispersion would show roton minimum-like feature. Focusing on the phonon dispersion in a 2D crystal lattice, the position of the roton minimum is coincident with that of the closest point on the Brillouin zone boundary. To show how this leads to the development of the roton minimum, we have constructed a model for the dynamical structure function $S(\mathbf{k},\omega)$ of a 2D lattice system. By using the classical fluctuation dissipation theorem we obtain $S(\mathbf{k},\omega)$ through a lattice model for the density response function $\chi(\mathbf{k},\omega)$, where the liquid behavior is emulated by a phenomenological collision frequency. The liquid dispersion relation is calculated through angular averaging. We examine its behavior in the vicinity of the Brillouin zone boundaries, and compare the results with MD simulations.

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