Microscopic collective dynamics in equilibrium fluids. Self-consistent relaxation theory, molecular dynamics simulations, inelastic neutron and X-ray scattering

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Exhaustive information about the microscopic collective dynamics in equilibrium fluids can be obtained by inelastic neutron and X-ray scattering experiments. These experiments reveal a number of effects which cannot be explained by the well-known hydrodynamic theory. The self-consistent relaxation theory of the collective dynamics of particles in liquids has been developed within the concept of time correlation functions. The theory agrees with well known results for both short-wavelenth limit (dynamics of a free-moving particle) and long-wavelength (hydrodynamic) limit. The analytical expressions for the dynamic structural factor and the spectral density of the transverse current realized over a wide range of wave numbers are obtained. The theory reproduces the transition from a regime with typical equilibrium fluid dynamics to a regime with collective particle dynamics in which solid-like properties are manifested: effective shear stiffness, transverse (shear) acoustic waves. The theoretical results are compared with the results of molecular dynamics simulations and experimental data on inelastic scattering of neutrons and X-rays in metallic melts.

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