Self-dynamic response in simple liquids as resolved by Vibration-Transit theory GIULIA DELORENZI-VENNERI, ERIC CHISOLM, DUANE WALLACE, Los Alamos National Laboratory — The dynamic response in a simple liquid is described within the approach of Vibration- Transit theory. In this theory the zeroth-order Hamiltonian describes the vibrational motion in a single random valley. This Hamiltonian is tractable, is evaluated *a priori* for monatomic liquids, and the same Hamiltonian is used for equilibrium and nonequilibrium theory. When applied to the self intermediate scattering function $F^s(q,t)$ in liquid sodium, it is found that the vibrational contribution is in perfect agreement with Molecular Dynamics through short and intermediate times, at all q. This is direct confirmation that normal mode vibrational correlations are present in the motion of the liquid state. The primary transit effect is diffusive motion of the vibrational equilibrium positions, as the liquid transits rapidly among random valleys. A model of the transit motion as a standard random walk results in a theoretical $F^s(q,t)$ in excellent agreement with molecular dynamics results at all q and t. The present approach provides a decisive improvement over traditional non- equilibrium theories.

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