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Elementary excitations and flow in the liquid[1]

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A new mode of excitation is introduced to elucidate the dynamics in simple liquids at the atomic scale. Some properties of liquid defy easy explanations. For instance, in liquids phonons are overdamped with a very short lifetime. Nevertheless the Dulong-Petit law ($C_V \sim 3k_B$) is widely observed at high temperatures. As temperature is reduced the specific heat markedly increases in the supercooled state, only to drop down sharply at the glass transition. Viscosity shows an Arrhenian behavior at high temperatures, but increases rapidly toward the glass transition in the supercooled state. We suggest that these perplexing observations can be naturally explained in terms of the local configurational excitations (LCE's) which locally change the atomic connectivity by an atom losing or gaining one nearest neighbor. We show that the lifetime of LCE, τ_{LC}, is equal to the Maxwell relaxation time, τ_M, at temperatures above the crossover temperature, T_A. Above T_A the phonon mean-free path, $\xi = c_T \tau_{LC}$, where c_T is the transverse sound velocity, becomes shorter than the interatomic distance, resulting in phonon localization. Therefore LCE's are the elementary excitations in the liquid. They are independent of each other above T_A, but below T_A LCE's interact through phonon exchange, resulting in the rapid increase in τ_M, culminating in the glass transition. LCE's are also the mechanism of flow at low temperature under strong shear stress. In this case, however, losing and gaining of the neighbors are strongly coupled, so that $\tau_M = \tau_{LC}$ /2 [1]. We also discuss dynamic heterogeneity in terms of LCE interactions.

[1] T. Iwashita and T. Egami, *Phys. Rev. Lett.*, **108,** 196001 (2012).

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