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Improved model for the transit entropy of monatomic liquids ERIC CHISOLM, NICOLAS BOCK, DUANE WALLACE, Los Alamos National Laboratory — In the original formulation of vibration-transit (V-T) theory for monatomic liquid dynamics, the transit contribution to entropy was taken to be a universal constant, calibrated to the constant-volume entropy of melting. This implied that the transit contribution to energy vanishes, which is incorrect. Here we develop a new formulation that corrects this deficiency. The theory contains two nuclear motion contributions: (a) the dominant vibrational contribution $S_{vib}(T/\theta_0)$, where T is temperature and θ_0 is the vibrational characteristic temperature, and (b) the transit contribution $S_{tr}(T/\theta_{tr})$, where θ_{tr} is a scaling temperature for each liquid. The appearance of a common functional form of S_{tr} for all the liquids studied is deduced from the experimental data, when analyzed via the V-T formula. The theoretical entropy of melting is derived, in a single formula applying to normal and anomalous melting alike. An *ab initio* calculation of θ_0 for Na and Cu, based on density functional theory, provides verification of our analysis and V-T theory. In view of the present results, techniques currently being applied in *ab initio* simulations of liquid properties can be employed to advantage in the further testing and development of V-T theory.

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