New theoretical model for partition function and configurational entropy in non-equilibrium states

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Abstract

New model of non-equilibrium thermodynamic states has been investigated. It is well known that once well-defined partition functions are calculated in equilibrium, all the thermodynamic variables can be calculated from them. On the other hand, any standard definition of partition function in non-equilibrium has not established yet, which hinders the derivation of thermodynamic variables from them. To overcome this problem, the concept of temperature is extended in a new style. It is also well known that unique value temperature can be defined for each system only in equilibrium. In contrast, in this paper, configurational temperature apart from kinetic (phonon) temperature is defined as a function of energy fragment. In other words, each fragment decomposed from the whole system has its own configurational temperature. Such definition allows the description of thermodynamic states either in equilibrium or in non-equilibrium. In addition, new formulation of non-canonical partition function, internal energy and entropy are derived on the basis of the new definition of temperature. On the basis of this new model, computational experiments are performed on simple non-interacting systems to investigate the cooling and relaxation effects in terms of the time profile of partition function, internal energy and configurational entropy. It is concluded that the new formulation has gained a foot in applying it to a variety of non-equilibrium systems.

Keywords: configurational entropy, thermodynamics, statistical mechanics, computer simulation

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