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Flux and storage of energy in non-equilibrium stationary states

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A system kept out of equilibrium in the stationary state by the external source of energy stores an energy in excess over its value at equilibrium. We determine this excess energy, U for two model systems: the ideal gas and the Lennard-Jones liquid. We show that in order to describe non-equilibrium states an external energy source must be explicitly included in the analysis. The final non-equilibrium, stationary state depends not only on the total flux of energy, J_U , but also on the mode of energy transfer into the system. In both systems we study three scenarios of energy transfer: (1) the energy flux per unit volume is constant; (2) the energy flux per unit volume is proportional to the local temperature (3) the energy flux per unit volume is proportional to the local density. Similarly as in equilibrium thermodynamics we introduce internal, adiabatic constraints in the system and find that $U/J_U = \tau$ is minimized in the stationary (unconstrained) state. τ is the characteristic time scale of energy outflow from the system immediately after shut-down of energy flux into the system. Finally we perform MD simulations of 2D Rayleigh-Benard system (RB) of hard discs to check this variational principle for two competing stationary states (conductive and convective). We find that the stable state has smaller value of U/J_U .

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