

Abstract Submitted
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Negating Negative Heat Capacity in Nanoclusters KARO MICHAELIAN, Instituto de Fisica, Universidad Nacional Autonoma de Mexico, IVAN SANTAMARIA-HOLEK, Facultad de Ciencias, Universidad Nacional Autonoma de Mexico — It is shown that “negative heat capacity” in nanoclusters is an artifact of applying equilibrium thermodynamic formalism on a “small” system trapped out of equilibrium in a particular structural motif representing only part of the energetically available phase space volume. Trapping may occur in either the canonical or microcanonical ensemble, but it is unavoidable in the microcanonical. A more general consequence of trapping is that all macroscopic quantities determined for nanoclusters will depend on the initial conditions.

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