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Origin of Apparent Negative Heat Capacity in Constrained Microcanonical Modeling of Excited Nuclear Systems MICHAEL QUINLAN, JAN TÕKE, IWONA PAWELCZAK, Department of Chemistry, University of Rochester, Rochester, New York 14627, WOLF-UDO SCHRÖDER, Departments of Chemistry and Physics, University of Rochester, Rochester, New York 14627 — The origin of negative heat capacity in certain classes of microcanonical models of phase transitions in small systems is studied. It is demonstrated that the domain of negative heat capacity appears in such calculations as a result of an unphysical discontinuity in the model phase space and, specifically, the exclusion of energetically (microcanonically) allowed micro-states filling the space between the domains corresponding to different phases. It is also shown that already a crude filling of these unphysical gaps in the model phase space results in a restoration of the concavity of the entropic curve S(E*) and thus in an elimination of the faux negative heat capacity in the phase transition region.

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