Unleashing the Power of Microcanonical Inflection-Point Analysis: The Principle of Minimal Sensitivity

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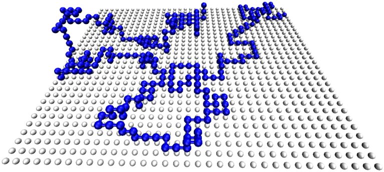

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   - Microcanonical Inflection-Point (IP) Analysis
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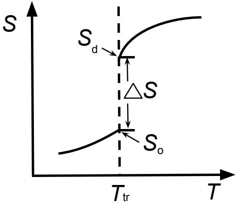
Canonical Analysis

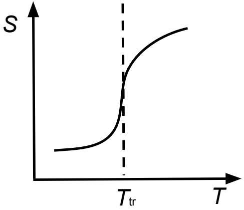
- **Classification of Phase Transitions by Ehrenfest**
  uniquely identify T_{tr} in the thermoldynamic limit $(N \to \infty)$
  *n***th order:** discontinuity or divergence in $\left(\frac{\partial^{(n)} F}{\partial T^{(n)}}\right)_{T_0}$
  Free Energy F(T,V,N): $S = -\left(\frac{\partial F}{\partial T}\right)_{V,N}$; $C_{\mathrm{v}} = -T\left(\frac{\partial^2 F}{\partial T^2}\right)_{V,N}$

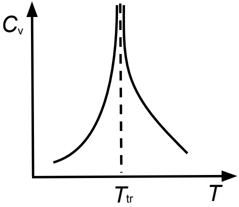
1st:

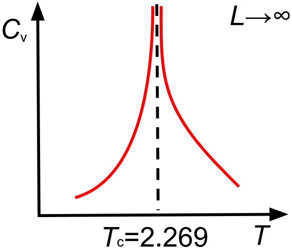


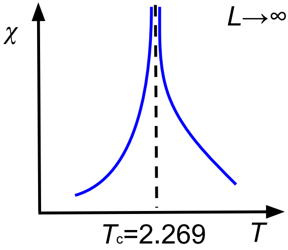
$\Delta S = \Delta Q / T_{\mathrm{tr}}$ (ΔQ is the latent heat)

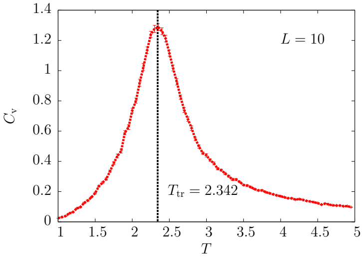
2nd:

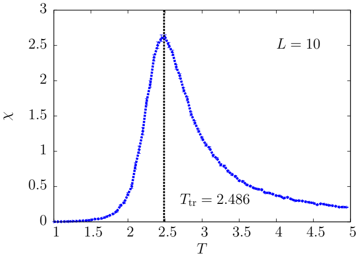






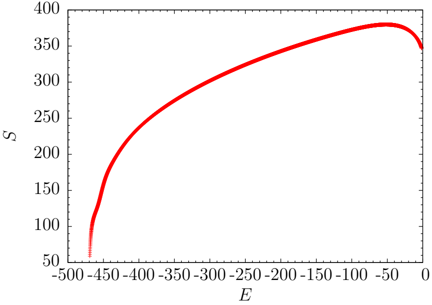




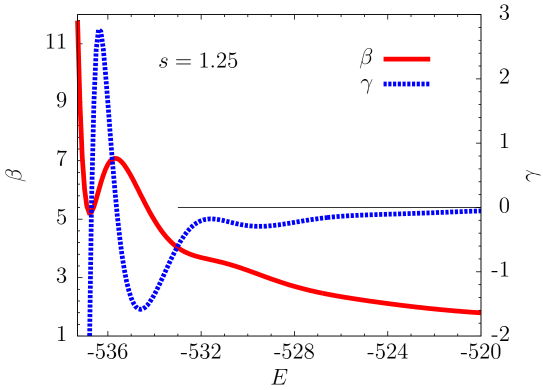


- **Problem:** fails to identify unique $T_{\rm tr}$ in finite system
  example: Ising model on finite lattice

Microcanonical Inflection-Point (IP) Analysis



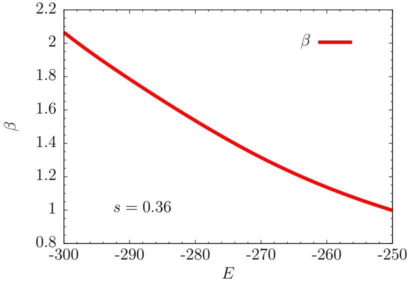
- **Density of States:** $g(E)$
- **Microcanonical Entropy:** $S(E) = k_{\mathrm{B}} \ln g(E)$
- **Inverse Temperature:** $\beta(E) \equiv T^{-1}(E) = \frac{dS(E)}{dE}$

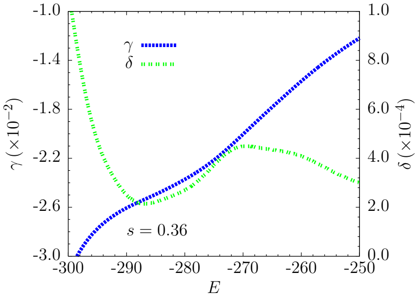


- **Strategy:** employing the principle of minimal sensitivity (PMS)
- **1st order:** backbending in $\beta(E)$; $\gamma(E) = d\beta/dE > 0$ peak
- **2nd order:** IP in $\beta(E)$; $\gamma(E) < 0$ peak

P. M. Stevenson, Phys. Rev. D **23**, 2916 (1981).

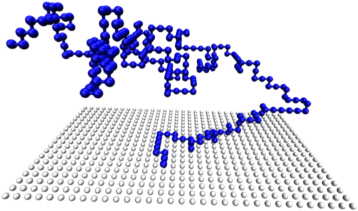
S. Schnabel, D. T. Seaton, D. P. Landau, and M. Bachmann, Phys. Rev. E **84**, 011127 (2011).

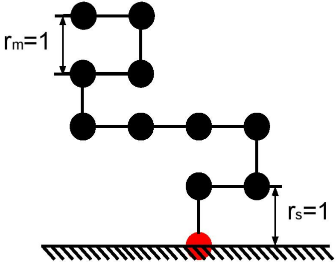




- **3nd order:** IP in $\gamma(E)$; $\delta(E) = d\gamma/dE > 0$ valley
- **Advantages:** identify transitions and transition temperatures systematically and uniquely for finite systems

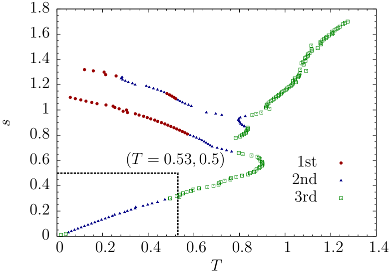
Model & Simulation Method





- **Model:** grafted simple-cubic lattice polymer (250-mer)
- **Energy:** $E(n_s, n_m) = -\varepsilon_0(n_s + sn_m)$
  n_s: number of monomer-substrate contacts
  n_m: number of nonadjacent monomer-monomer contacts
  s: reciprocal solubility
- **Simulation Method:** contact-density chain-growth algorithm

M. Bachmann and W. Janke, Phys. Rev. Lett. **91**, 208105 (2003).



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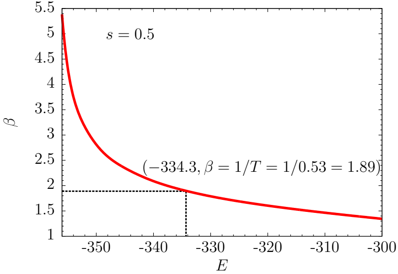
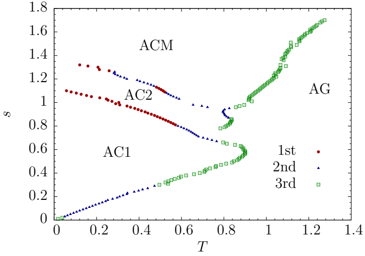
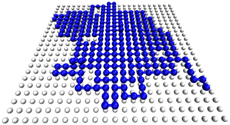
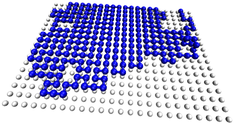


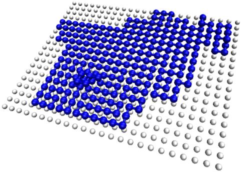
- **Procedure of Finding Configurations:**
  1. Determine s and T
  2. $T(E) \longrightarrow \beta = 1/T(E) \longrightarrow E$
  3. Identify configurations of energy E for a given value of s

- **AC1:** adsorbed, compact, 1 layer

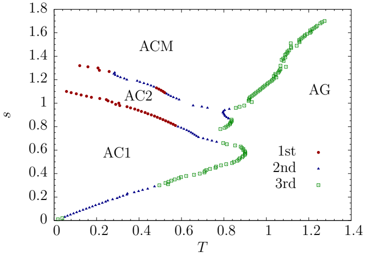


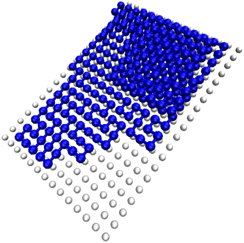


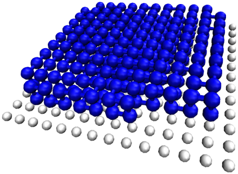


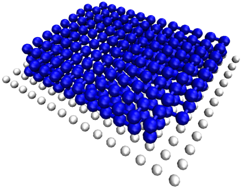


- **AC2:** adsorbed, compact, 2 layers

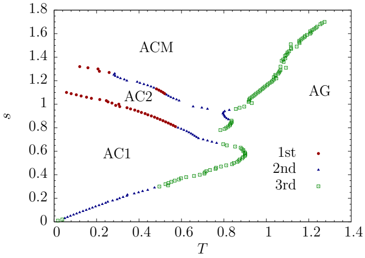


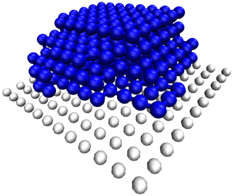


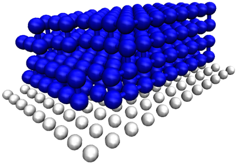


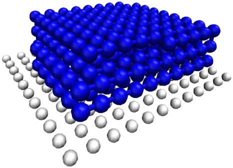


- **ACM:** adsorbed, compact, multiple layers

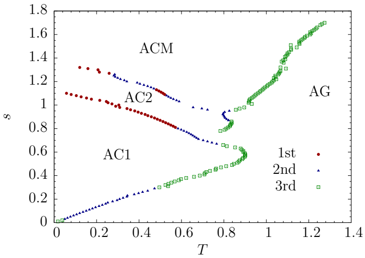


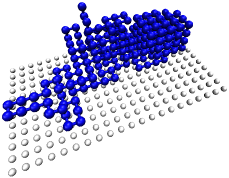


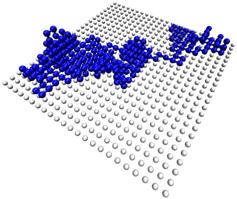


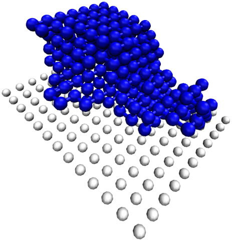


- **AG:** adsorbed, globular









Summary

- **Novel approach to the classification of phase transitions:**
  1. combination of microcanonical inflection-point (IP) analysis and principle of minimal sensitivity
  2. classify transitions:
     1st $\rightarrow$ backbending in β, $\gamma = d^2S/dE^2 > 0$ peak
     2nd $\rightarrow$ IP in β, $\gamma = d^2S/dE^2 < 0$ peak
     3rd $\rightarrow$ IP in γ, $\delta = d^3S/dE^3 > 0$ valley
  3. advantages: applies to finite systems and allows to locate unique transition temperatures
- **Application:**
  1. adsorption of a grafted, simple-cubic lattice polymer model
  2. complete "phase" diagram constructed by means of microcanonical IP analysis