the origin of thermodynamic singularities: topology and analyticity

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central issue:

relation between nonanalytic points of thermodynamic functions and the topology of certain configuration space submanifolds

hope:

- efficient description of the essential physics
- additional insights due to an unconventional perspective

outline

- motivation: an exactly solvable example
- configuration space topology
- relation between nonanalyticities and topology changes
  - finite systems
  - infinite systems
- physical consequences,. . .
- résumé

the kinetic mean-field spherical model

as a motivation to discuss the relation between nonanalytic points and configuration space topology:

$$\mathcal{H} = \frac{1}{2}\sum_{i=1}^{N}\dot{\sigma}_i^2 - \frac{1}{2N}\sum_{i,j=1}^{N}\sigma_i\sigma_j \qquad \text{with} \quad \sum_{i=1}^{N}\sigma_i^2 = N \quad \text{and} \quad \sum_{i=1}^{N}\sigma_i\dot{\sigma}_i = 0$$

features:

- interacting
- phase transition in the thermodynamic limit
- continuous configuration space
- simple!

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exact solution for finite N:

$$\Omega_N(\varepsilon) \propto \int_{\mathbb{R}^N} \mathrm{d}\sigma \int_{\mathbb{R}^N} \mathrm{d}\dot{\sigma}\, \delta\left(\sum_{i=1}^{N}\sigma_i^2 - N\right)\, \delta\left(\sum_{i=1}^{N}\sigma_i\dot{\sigma}_i\right)\, \delta\left(\frac{1}{2}\sum_{i=1}^{N}\dot{\sigma}_i^2 - \frac{1}{2N}\sum_{i,j=1}^{N}\sigma_i\sigma_j - N\varepsilon\right)$$

$$\vdots$$

$$\propto \int_0^1 \mathrm{d}y\, y^{-1/2}\,(1-y)^{(N-3)/2}\,(2\varepsilon+y)^{(N-3)/2}\,\Theta\,(2\varepsilon+y)$$

(L. Casetti and M. Kastner, cond-mat/0605399)

nonanalyticities of the entropy I

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↙ ↘

finite systems | **infinite system**

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finite systems

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Boltzmann entropy:

$$s_N(\varepsilon) = \frac{1}{N} \ln \Omega_N(\varepsilon)$$

nonanalyticity at
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finite systems	infinite system

Boltzmann entropy:

$$s_N(\varepsilon) = \frac{1}{N} \ln \Omega_N(\varepsilon)$$

$$s_\infty(\varepsilon) = \lim_{N\to\infty} \frac{1}{N} \ln \Omega_N(\varepsilon)$$

$$= \begin{cases} \ln \frac{1+2\varepsilon}{2} & \text{for } \varepsilon \leqslant \frac{1}{2} \\ \frac{1}{2} \ln 2\varepsilon & \text{for } \varepsilon > \frac{1}{2} \end{cases}$$

nonanalyticity at $\varepsilon_c^{\text{finite}} = 0$

nonanalyticity at $\varepsilon_c^{\text{infinite}} = \frac{1}{2}$

nonanalyticities of the entropy II

findings are remarkable because:

- thermodynamic functions of finite systems are found to be nonanalytic in general

- *locus* of the nonanalyticity jumps discontinuously in the thermodynamic limit

- Both the nonanalyticilies at $\varepsilon_c^{\text{finite}} = 0$ and $\varepsilon_c^{\text{infinite}} = \frac{1}{2}$ are consequences of the same topology change in configuration space

- typically even more complex: $\mathcal{O}(N)$ or even $\mathcal{O}(\mathrm{e}^N)$ nonanalytic points in finite systems (becoming dense in the thermodynamic limit), most of which do not correspond to phase transitions in the infinite system

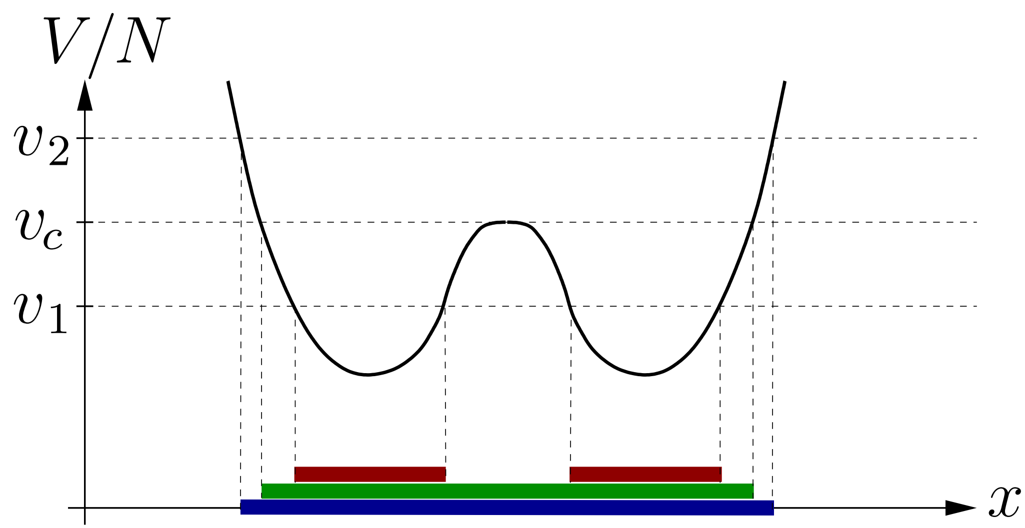
configuration space topology

Hamiltonian function $\mathcal{H} = \frac{1}{2}\sum_{i=1}^{N} p_i^2 + V(x)$
with potential V and $x = (q_1, \ldots, q_N) \in \Gamma_N \subseteq \mathbb{R}^N$.

family $\{\mathcal{M}_v\}_{v\in\mathbb{R}}$ of submanifolds

$$\mathcal{M}_v = \left\{x \in \Gamma_N \,\middle|\, V(x) \leqslant Nv\right\},$$

topology change at v_c if $\{\mathcal{M}_v\}_{v \lesssim v_c} \not\approx \{\mathcal{M}_v\}_{v \gtrsim v_c}$.



Morse theory

How to compute topological quantities?

A tool from differential topology:

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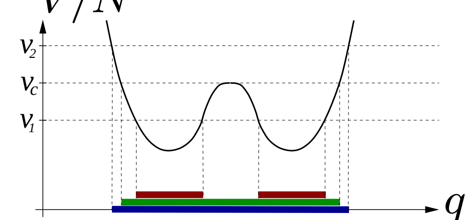
idea:

- consider submanifolds $\mathcal{M}_v = \{x \in \Gamma \mid V(x) \leqslant Nv\}$
- topology of the $\mathcal{M}_v$ is changed only at critical values $v_c = V(x_c)/N$, where $\mathrm{d}V(x_c) = 0$.



- the nature of the topology change is determined by the eigenvalues of the Hessian of V at x_c.

topology and nonanalyticities

topology changes in the potenial energy submanifolds $\mathcal{M}_v$	$\longleftrightarrow$	nonanalyticities in thermodynamic functions

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$\swarrow$ $\searrow$

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- finite systems
  - canonically: no non-analytic points
  - microcanonically: nonanalytic points at every critical level
- infinite systems

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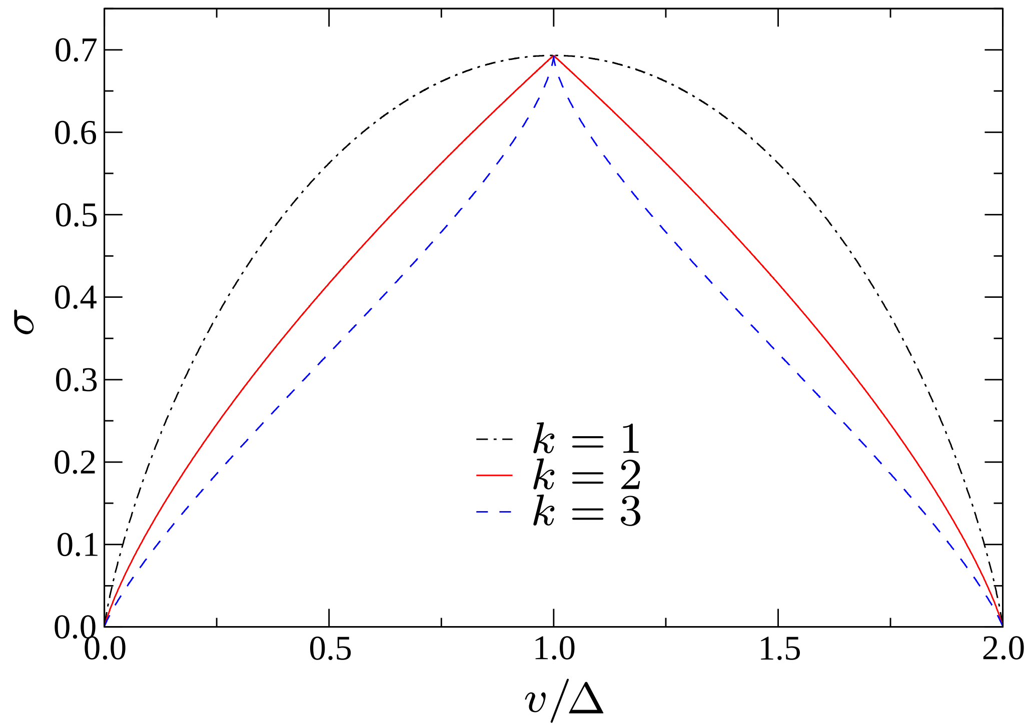
↘ infinite systems

- ↓ more complicated...

infinite system nonanalyticities I

observation:

topology changes of $\mathcal{M}_v$ are related to phase transitions



(example: mean-field k-trigonometric model)

- many topology changes, dense on the energy axis in the thermodynamic limit
- $\exists$ a signature of the phase transition in a purely topological quantity

infinite system nonanalyticities II

assumptions on the potential:

- V smooth and confining,
- interparticle interactions of short range.

theorem:

(R. Franzosi and M. Pettini 2004)

A topology change of the $\mathcal{M}_v$ at $v = v_c$ is necessary for a phase transition to take place at v_c.

infinite system nonanalyticities II

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hypothesis:

as in the theorem (topology change of the $\mathcal{M}_v$ at $v = v_c$ necessary for a phase transitions at v_c), but for arbitrary potentials V.

hypothesis and sufficiency criterion I

Q1: Is the “topological hypothesis” true in general?

Q2: When are topology changes sufficiently “strong” to effect a phase transition?

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M. Kastner, PRL **93**, 150601 (2004)

D. A. Garanin, R. Schilling, and A. Scala, PRE **70**, 036125 (2004)

I. Hahn and M. Kastner, PRE **72**, 056134 (2005)

not necessarily a drawback, but:

a challenge! there's something to understand!

a counterexample

mean-field φ^4-model (long range interactions!)

$$V = -\frac{J}{2N}\Big(\sum_{i=1}^{N} q_i\Big)^2 + \sum_{i=1}^{N}\left(-\tfrac{1}{2}q_i^2 + \tfrac{1}{4}q_i^4\right), \qquad q_i \in \mathbb{R}$$

critical energy $v_c \neq$ energies of the topology changes

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microcanonical entropy: (I. Hahn and M. Kastner 2005)

$s(v,m)$	analytic function
$s(v) = \sup_m s(v,m)$	nonanalytic function

$\Longrightarrow$ singularity from a finite dimensional maximization over an analytic function

- exclusively in long range systems
- classical critical exponents (if continuous)

hypothesis and sufficiency criterion II

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hypothesis and sufficiency criterion II

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A1: No, the situation is more complex!

Q2: When are topology changes sufficiently “strong” to effect a phase transition?

A2: work in progress!

separation of “topological” and “non-topological” contributions to the thermodynamic functions by means of Morse theory

$\Longrightarrow$ conditions on the density of (Morse) critical points of the potential

$\Longrightarrow$ sufficiency criterion on the topology change for the occurrence of a phase transition

(M. Kastner and S. Schreiber, in preparation)

back to the spherical model

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- nonanalyticities in $s_N(\varepsilon)$ at $\varepsilon_c^{\text{finite}} = 0$ and $\varepsilon_c^{\text{infinite}} = \frac{1}{2}$, respectively,
- topology change of the $\mathcal{M}_v$ at $v = 0$.

relation between nonanalyticities and topology changes?

- finite system:

$$\Omega(\varepsilon) = \int_0^\infty \mathrm{d}t\, \Omega_k(t)\Omega_c(\varepsilon - t)$$

- infinite system:

$$\Omega(\varepsilon) = \Omega_k\left(\varepsilon - \langle v\rangle(\varepsilon)\right)\Omega_c\left(\langle v\rangle(\varepsilon)\right)$$

. . . but the situation is much more intricate in other models. . .

résumé

- idea: concepts from topology to (efficiently?) describe physical phenomena
- $\exists$ nonanalyticities in the finite system entropy, caused by topology changes in the $\mathcal{M}_v$
  (phase transitions in finite systems?)
- configuration space topology
  - is related to phase transitions in infinite systems in the case of (well-behaved) short-range potentials
  - can be supplemented by phase transitions from a “maximization” in long-range systems

what is the origin of a thermodynamic singularity?