Effective long-range interactions in driven systems

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Systems with long range interactions

two-body interaction

$$v(r) \propto \frac{1}{r^{d+\sigma}}$$

in d dimensions

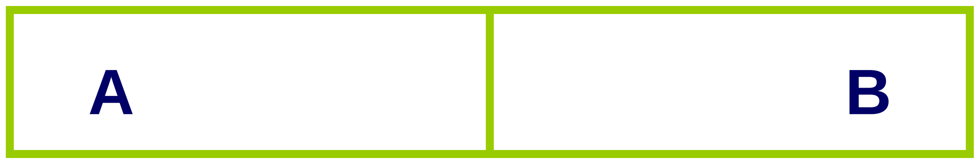
for $\sigma<0$

$$E \propto VR^{-\sigma} \propto V^{1-\sigma/d}$$

and the energy is not extensive

self gravitating systems	$(1/r)$	$\sigma=-2$
ferromagnets	$(1/r^3)$	$\sigma=0$
2d vortices	$\log(r)$	$\sigma=-2$

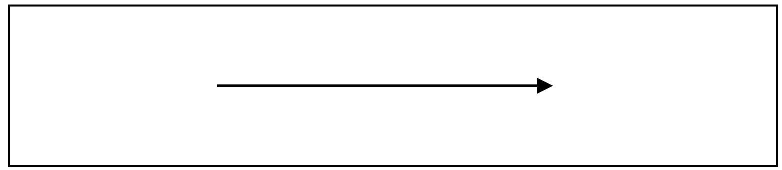
These systems are non-additive $F \neq F_A + F_B$



As a result, many of the common properties of typical systems with short range interactions are not shared by these systems.

Driven systems

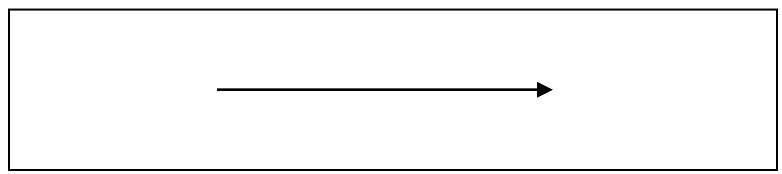
heat current T_1



T_2

$T_1 > T_2$

charge current



E

- Local and stochastic dynamics
- No detailed balance (non-vanishing current)
- What is the nature of the steady state?

drive in conserving systems result in many cases in long range correlations leading, in some cases, to spontaneous symmetry breaking and condensation transition even in one dimension.

What can be learned from systems with long-range interactions on steady state properties of driven systems?

Systems with long range interactions

Free Energy: $F = E - TS$

since $E \propto V^{1-\sigma/d}$, $S \propto V$

$S << E$ the entropy may be neglected in the thermodynamic limit.

In finite systems, although E>>S, if T is high enough E may be comparable to TS, and the full free energy need to be considered. (Self gravitating systems, e.g. globular clusters) one may implement the large T limit by rescaling the Hamiltonian

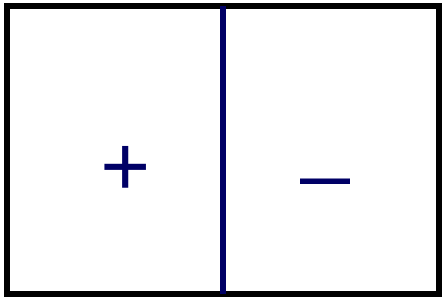
$$H \to V^{\sigma/d} H \quad \Rightarrow \quad E \propto V$$

$$F = E - TS$$

Mean-field type interactions is an extreme case with σ=-d.
for example, consider the Ising model:

$$H = -\frac{J}{2N}\left(\sum_{i=1}^{N} S_i\right)^2 \qquad S_i = \pm 1$$

Although the canonical thermodynamic functions (free energy, entropy etc) are extensive, the system is non-additive



$$E = 0 \qquad E_+ = E_- = -JN/4$$

$$E \neq E_1 + E_2$$

Features which result from non-additivity

Thermodynamics

- Negative specific heat in microcanonical ensemble
- Inequivalence of microcanonical (MCE) and canonical (CE) ensembles
- Temperature discontinuity in MCE

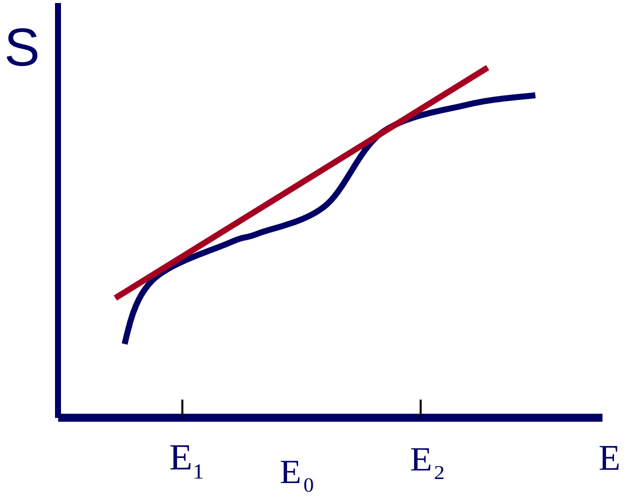
Dynamics

- Breaking of ergodicity in microcanonical ensemble
- Slow dynamics, diverging relaxation time

Some general considerations

Negative specific heat in microcanonical ensemble of non-additive systems.

Antonov (1962); Lynden-Bell & Wood (1968); Thirring (1970), Thirring & Posch

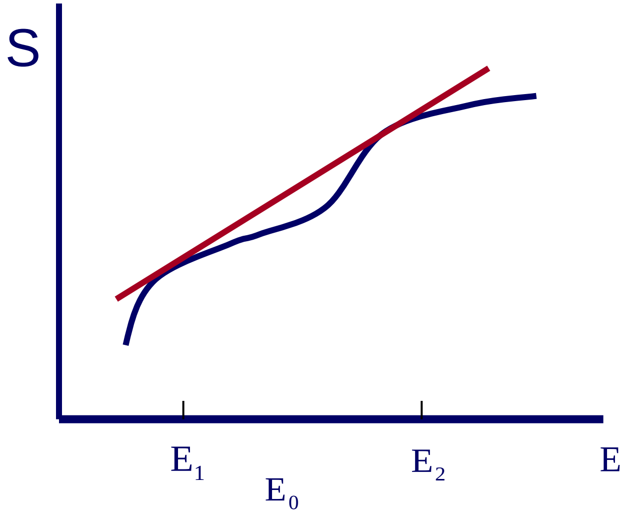


coexistence region
in systems with short range interactions

$$E_0 = xE_1 + (1-x)E_2$$
$$S_0 = xS_1 + (1-x)S_2$$

hence S is concave and the microcanonical specific heat is non-negative

On the other hand in systems with long range interactions (non-additive), in the region $E_1<E<E_2$



$S_0 = xS_1 + (1-x)S_2$

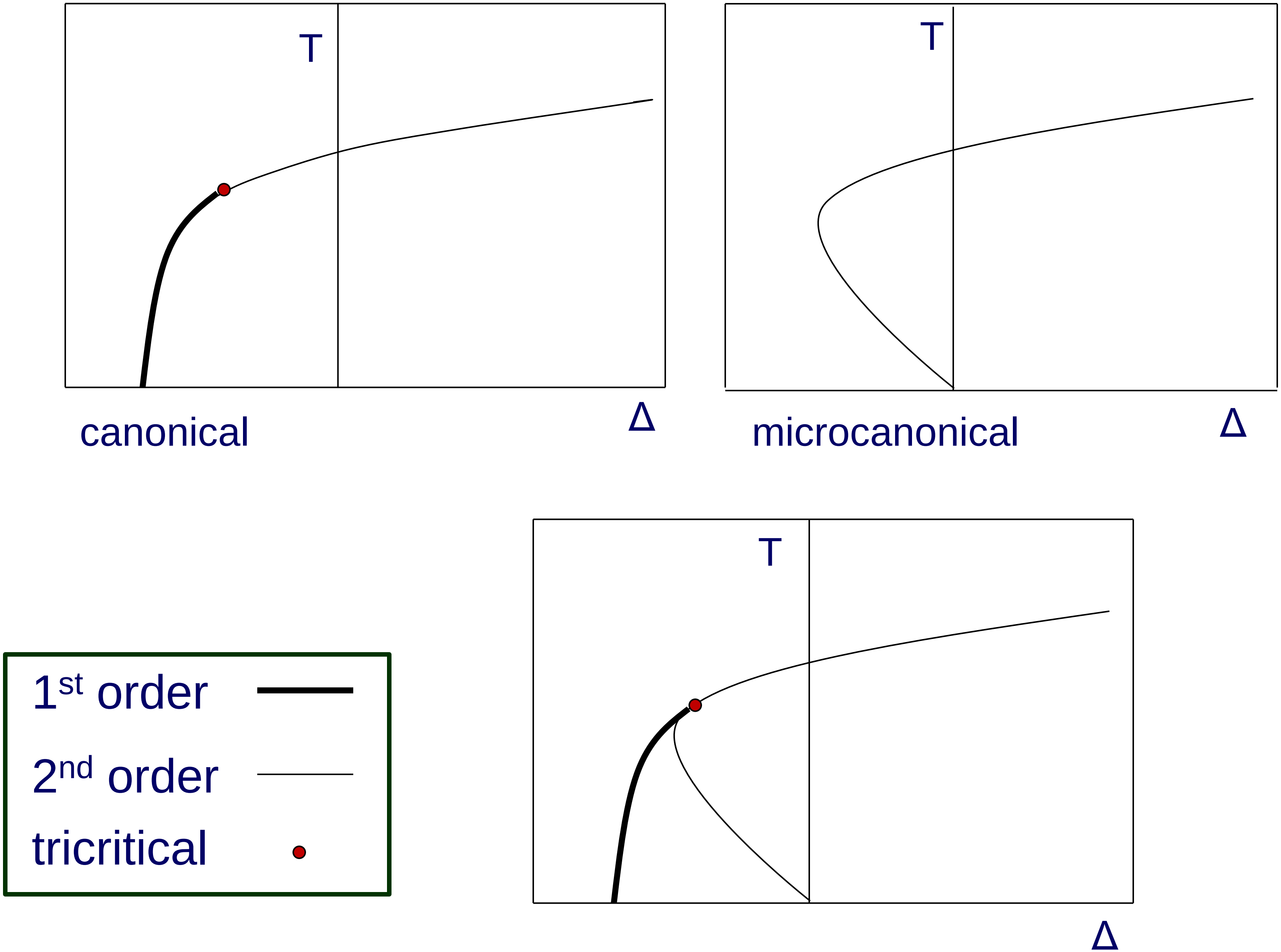
$E_0 \neq xE_1 + (1-x)E_2$

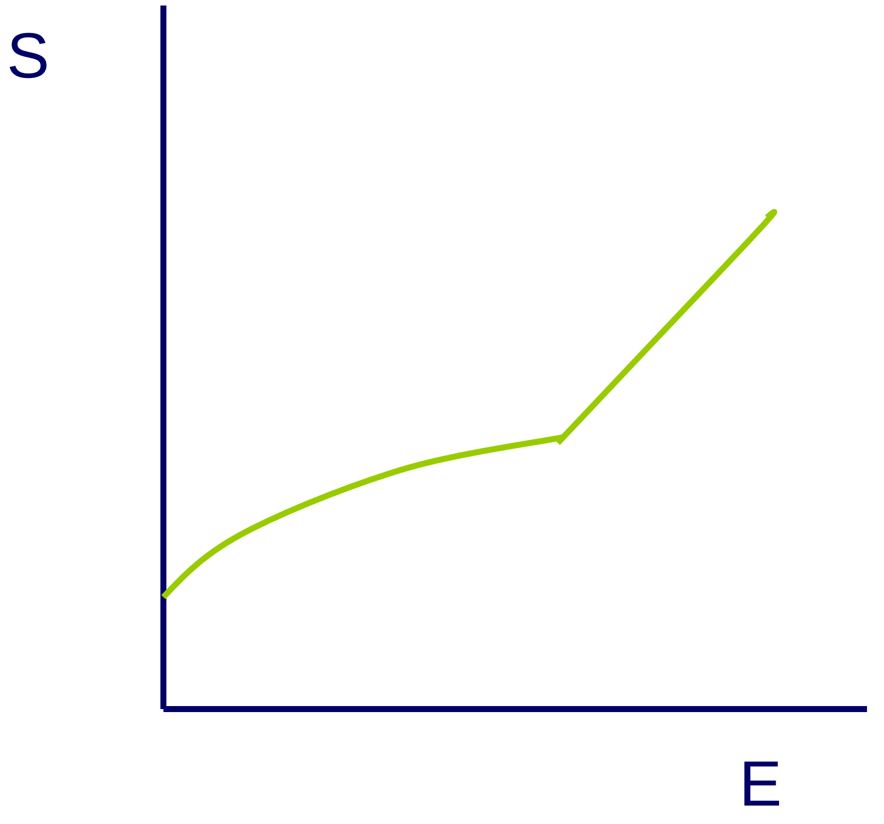
The entropy may thus follow the homogeneous system curve, the entropy is not concave. and the microcanonical specific heat becomes Negative $C_V<0$.

compared with canonical ensemble where

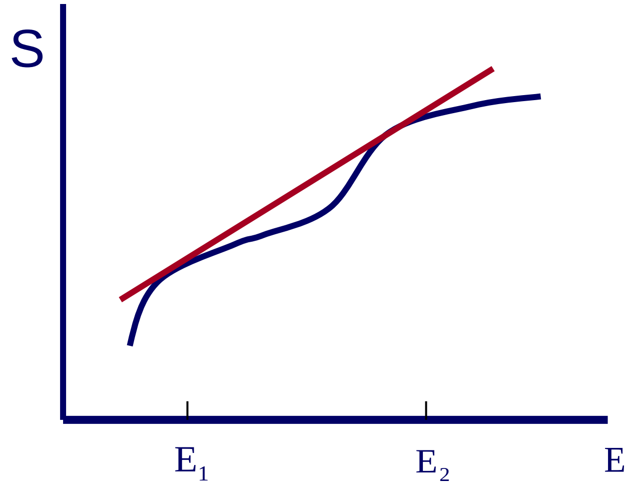
$$T^2 C_V = <E^2> - <E>^2 \geq 0$$

Typical (but not exclusive) resulting phase diagrams




S
E

In general it is expected that whenever the canonical transition is first order the microcanonical and canonical ensembles differ from each other.



Dynamics

- Systems with long range interactions exhibit slow relaxation processes.
- This may result in quasi-stationary states (long lived non-equilibrium states whose relaxation time to the equilibrium state diverges with the system size).
- Non-additivity may facilitate breaking of ergodicity which could lead to trapping of systems in non-Equilibrium states.

Driven systems

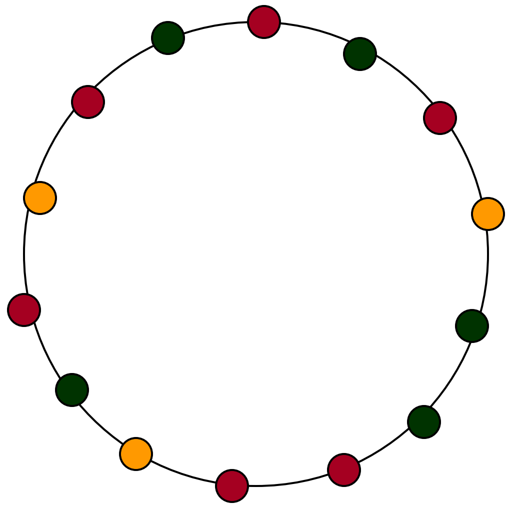
Long range correlations in driven systems

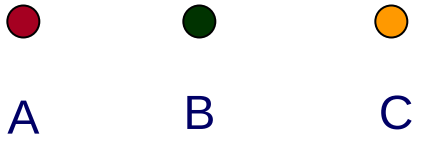
- Conserved variables tend to produce long range correlations.
- Thermal equilibrium states in short range systems are independent of the dynamics (e.g. Glauber and Kawasaki dynamics result in the same Boltzmann distribution)
- Non-equilibrium steady states depend on the dynamics (e.g. conserving or non-conserving)
- Conserving dynamics in driven, non-equilibrium systems may result in steady states with long range correlations even when the dynamics is local
- Can these correlations be viewed as resulting from effective long-range interactions?

ABC model

One dimensional driven model with stochastic local dynamics which results in phase separation (long range order) where the steady state can be expressed as a Boltzmann distribution of an effective energy with long-range interactions.

ABC Model





dynamics

$$AB \underset{1}{\overset{q}{\rightleftarrows}} BA$$

$$BC \underset{1}{\overset{q}{\rightleftarrows}} CB$$

$$CA \underset{1}{\overset{q}{\rightleftarrows}} AC$$

Evans,Kafri, Koduvely, Mukamel PRL 80, 425 (1998)
A model with similar features was discussed by Lahiri, Ramaswamy PRL 79, 1150 (1997)

Simple argument:

ACCCC → CCCCA

CBBBB → BBBBC

BAAAA → AAAAB

$$AB \underset{1}{\overset{q}{\rightleftharpoons}} BA$$

$$BC \underset{1}{\overset{q}{\rightleftharpoons}} CB$$

$$CA \underset{1}{\overset{q}{\rightleftharpoons}} AC$$

…AACBBBCCAAACBBBCCC…

↓ fast rearrangement

…AABBBCCCAAABBBCCCC…

↓ slow coarsening

…AAAAABBBBBCCCCCCAA…

The model reaches a phase separated steady state

- logarithmically slow coarsening

…AAAAABBBBBCCCCCCAA…

$$t \propto q^{-l} \qquad l \propto \ln t$$

- needs n>2 species to have phase separation
- Phase separation takes place for any q (except q=1)
- Phase separation takes place for any density N_A, N_B, N_C
- strong phase separation: no fluctuation in the bulk; only at the boundaries.

…AAAAAAAAAABBBBBBBBBBBBCCCCCCCCCCC…

Special case $N_A = N_B = N_C$

The argument presented before is general, independent of densities.

For the equal densities case the model has detailed balance for arbitrary q.

We will demonstrate that for any microscopic configuration {X}
One can define “energy” E({X}) such that the steady state
Distribution is

$$P(\{X\}) \propto q^{E(\{X\})}$$

AAAAAABBBBBBCCCCCC E=0

……AB….. $\longrightarrow$ ……BA….. E $\rightarrow$ E+1

……BC….. $\longrightarrow$ ……CB….. E $\rightarrow$ E+1

……CA….. $\longrightarrow$ ……AC….. E $\rightarrow$ E+1

With this weight one has:

$$\underbrace{W(AB \rightarrow BA)}_{=q} P(\ldots AB\ldots) = \underbrace{W(BA \rightarrow AB)}_{=1} P(\ldots BA\ldots)$$

$$P(\ldots BA\ldots)/P(\ldots AB\ldots) = q$$

This definition of “energy” is possible only for $N_A = N_B = N_C$

AAAAABBBBBCCCCC → AAAABBBBBCCCCC**A**

$E \rightarrow E + N_B - N_C$

$N_B = N_C$

Thus such “energy” can be defined only for $N_A=N_B=N_C$

AABBBBCCCAAAAABBBCCCC

The rates with which an A particle makes a full circle clockwise
And counterclockwise are equal

$$q^{N_B} = q^{N_C}$$

Hence no currents for any N.

For $N_B \neq N_C$ the current of A particles satisfies $J_A \propto q^{N_B} - q^{N_C}$

The current is non-vanishing for finite N. It vanishes only in the limit $N \to \infty$. Thus no detailed balance in this case.

The model exhibits strong phase separation

…AAAAAAAABBBABBBBBBCCCCCCCCCAA…

The probability of a particle to be at a distance l on the wrong side of the boundary is q^l

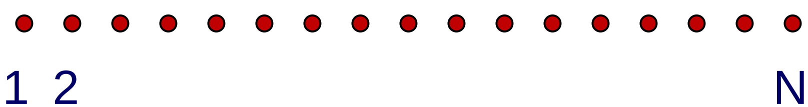
The width of the boundary layer is -1/lnq

$$N_A = N_B = N_C$$

$$P(\{x\}) = q^{E(\{x\})}$$

The "energy" E may be written as

$$E(\{x\}) = \sum_{i=1}^{N-1} \sum_{k=1}^{N-i} \left(C_i B_{i+k} + A_i C_{i+k} + B_i A_{i+k} \right) - (N/3)^2$$



(mean-field like interaction with σ=-d)

Alternatively, in a manifestly translational invariant form:

$$E(\{x\}) = \sum_{i=1}^{N} \sum_{k=1}^{N-1} \left(1 - \frac{k}{N} \right) \left(C_i B_{i+k} + A_i C_{i+k} + B_i A_{i+k} \right)$$

$$P(\{x\}) = q^{E(\{x\})}$$

$$E(\{x\}) = \sum_{i=1}^{N-1} \sum_{k=1}^{N-i} \left(C_i B_{i+k} + A_i C_{i+k} + B_i A_{i+k} \right) - (N/3)^2$$

$$E(\{x\}) = \sum_{i=1}^{N} \sum_{k=1}^{N-1} \left(1 - \frac{k}{N} \right) \left(C_i B_{i+k} + A_i C_{i+k} + B_i A_{i+k} \right)$$

- Local dynamics
- Long range interaction

Partition sum

Excitations near a single interface: AAAAAAABBBBBB

$$Z_1(q) = \sum p(n) q^n$$

P(n)= degeneracy of the excitation with energy n

P(0)=1
P(1)=1
P(2)=2 (2, 1+1)
P(3)=3 (3, 2+1, 1+1+1)
P(4)=5 (4, 3+1, 2+2, 2+1+1, 1+1+1+1)

P(n)= no. of partitions of an integer n

$$p(n) \sim \frac{\exp(\pi\sqrt{2n/3})}{4n\sqrt{3}} \qquad n \to \infty$$

$$Z_1(q) = \sum p(n) q^n$$

$$Z_1(q) = \frac{1}{(1-q)(1-q^2)....}$$

$$(1+q+q^2+q^3+..)(1+q^2+q^4+..)(1+q^3+q^6+..)..$$

$$\Phi(q) = \prod_{k=1}^{\infty} (1-q^k)$$

(Euler's function)

Partition sum: $$Z(q) = N\left[\frac{1}{(1-q)(1-q^2)\ldots\ldots}\right]^3$$

Correlation function: $$\langle A_1 A_r \rangle \approx 1/3$$

with $$\langle A_1 \rangle \langle A_r \rangle = 1/9$$

for $$-1/\ln q < r < N/3$$

Weakly asymmetric ABC model

q=1 - homogeneous

q<1 - phase separation

consider $$q = e^{-\beta/N}$$

the model exhibits a phase transition at $\beta_c = 2\pi\sqrt{3}$
for the case of equal densities

$\beta < \beta_c$ homogeneous

$\beta > \beta_c$ phase separated

This feature persists at non-equal densities.

Clincy, Derrida, Evans, PRE 67, 066115 (2003)

The choice $q = e^{-\beta / N}$ amounts to rescaling the energy by 1/N

$$E(\{x\}) = \frac{1}{N} \sum_{i=1}^{N-1} \sum_{k=1}^{N-i} \left(C_i B_{i+k} + A_i C_{i+k} + B_i A_{i+k} \right) - N/9$$

effective rescaled “energy”

without rescaling:
energy is dominates the entropy, no transition $q = e^{-\beta}$

with rescaling:
energy and entropy are comparable, resulting in a transition $q = e^{-\beta / N}$

A brief summary of the ABC model

- Driven model with local dynamics
- Exhibits long range correlation (phase separation)
- It exhibits a phase transition in the weak bias limit
- In the case of equal densities its steady state may be expressed by an energy with long range interactions

Outline

- Generalize the model to study non-conserving processes
- Study the steady states in both cases
- The existence of effective long range interactions may lead to different steady states in both cases for equal densities
- Use this as a starting point to move into non-equal densities (where there is no detailed balance)

Generalized ABC model

- Add vacancies: A , B, C, 0; $N_A + N_B + N_C = N \quad , \quad N \leq L$

Dynamics

$$AB \underset{1}{\overset{q}{\rightleftharpoons}} BA$$

$$BC \underset{1}{\overset{q}{\rightleftharpoons}} CB$$

$$CA \underset{1}{\overset{q}{\rightleftharpoons}} AC$$

$$0X \underset{1}{\overset{1}{\rightleftharpoons}} 0X$$

X=A,B,C

Vacancies are "inert"

A. Lederhendler, D. Mukamel

For $N_A=N_B=N_C$ there is detailed balance

$$P(\{x\}) = q^{E(\{x\})} \qquad q = e^{-\beta/L}$$

$$E(\{x\}) = \sum_{i=1}^{L-1}\sum_{k=1}^{L-i}\left(C_i B_{i+k} + A_i C_{i+k} + B_i A_{i+k}\right) - N^2/9$$

not important

Non conserving processes

$$AB \underset{1}{\overset{q}{\rightleftharpoons}} BA$$

$$BC \underset{1}{\overset{q}{\rightleftharpoons}} CB$$

$$CA \underset{1}{\overset{q}{\rightleftharpoons}} AC$$

$$0X \underset{1}{\overset{1}{\rightleftharpoons}} 0X$$

X=A,B,C

$$ABC \underset{1}{\overset{q^{\theta}}{\rightleftharpoons}} 000$$

$$\theta = 3L\mu$$

…A000ACBABCCA00AACBBB00000CCC…

000

ABC

For $N_A=N_B=N_C$: there is detailed balance with respect to

$$E(\{x\}) = \left[\sum_{i=1}^{L-1} \sum_{k=1}^{L-i} \left(C_i B_{i+k} + A_i C_{i+k} + B_i A_{i+k} \right) - \frac{N^2}{6} \right] - \mu L N$$

$$P(\{X\}) \propto q^{E(\{X\})} \qquad q = e^{-\beta / L}$$

- $E(\{X\}, N+3) = E(\{X\}, N) - 3L\mu$

  irrespective of {X} and of where the deposition is made

  …A000ACBABCCA00AACBBB00000CCC…

  E(…B ABC…) = E(… ABC B…)

- The dynamics is local

continuum version of the model

$$F(\rho(x),T) = E - TS \ , \ q = e^{-\beta/L} \quad , \ \beta = 1/k_B T$$

$$E = \int_0^1 dx \int_0^{1-x} dz \left[\rho_B(x)\rho_A(x+z) + \rho_A(x)\rho_C(x+z) + \rho_C(x)\rho_B(x+z)\right] - \frac{1}{6}\left[\int_0^1 dx \rho(x)\right]^2$$

$$S = \int_0^1 dx \left[\rho_A(x)\ln \rho_A(x) + \rho_B(x)\ln \rho_B(x) + \rho_C(x)\ln \rho_C(x) + +\rho_0(x)\ln \rho_0(x)\right]$$

$$\rho(x) = \rho_A(x) + \rho_B(x) + \rho_C(\mathrm{x}) \quad , \quad \rho_0(x) = 1 - \rho(x)$$

Conserving dynamics corresponds to the canonical ensemble:

minimize $F(\rho(x),T)$ and the determine μ by taking the derivative.

$$\rho_A(x) = \frac{\rho}{3} + a_1 \cos 2\pi x + \ldots \qquad \rho = N/L$$

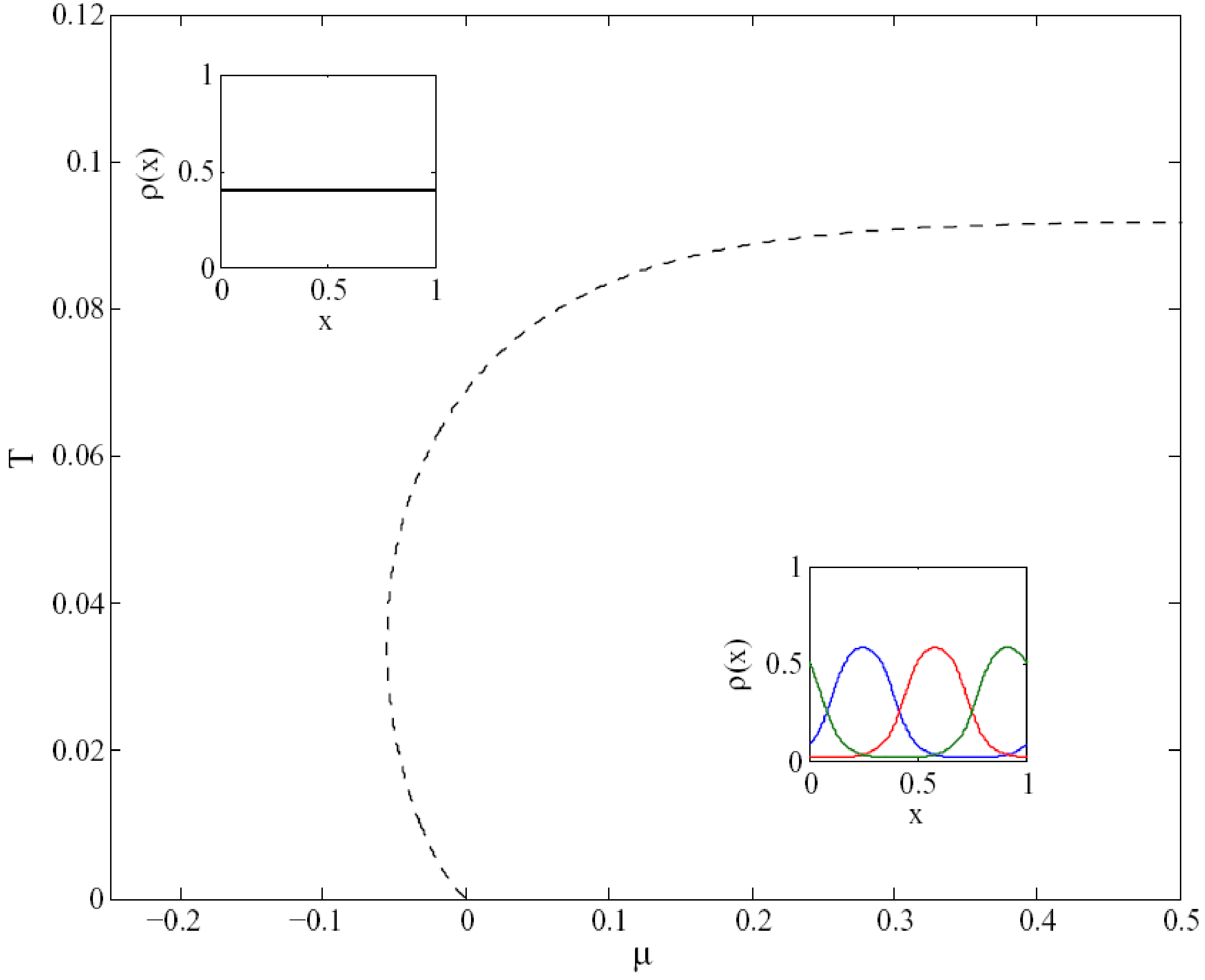
$$\rho_B(x) = \frac{\rho}{3} + b_1 \cos 2\pi (x - \frac{1}{3}) + \ldots$$

$$\rho_C(x) = \frac{\rho}{3} + c_1 \cos 2\pi (x - \frac{2}{3}) + \ldots$$

The model exhibits a transition from homogeneous to modulated structure at

$$\beta_c = 2\pi\sqrt{3}/\rho\,, \quad \mu = \frac{1}{\beta}\ln\frac{\rho}{3(1-\rho)}$$

Conserving dynamics



Non-conserving dynamics

$$AB \underset{1}{\overset{q}{\rightleftarrows}} BA$$

$$BC \underset{1}{\overset{q}{\rightleftarrows}} CB$$

$$CA \underset{1}{\overset{q}{\rightleftarrows}} AC$$

$$0X \underset{1}{\overset{1}{\rightleftarrows}} X0$$

X=A,B,C

$$ABC \underset{1}{\overset{q^{\theta}}{\rightleftarrows}} 000$$

$$\theta = 3L\mu$$

$$G(\mu, T; \rho(x)) = F(\rho(x), T) - \mu\rho$$

Grand canonical ensemble: minimize G with respect to ρ(x) at a given μ

$$G(\mu,T;\rho(x)) = F(\rho(x),T) - \mu\rho$$

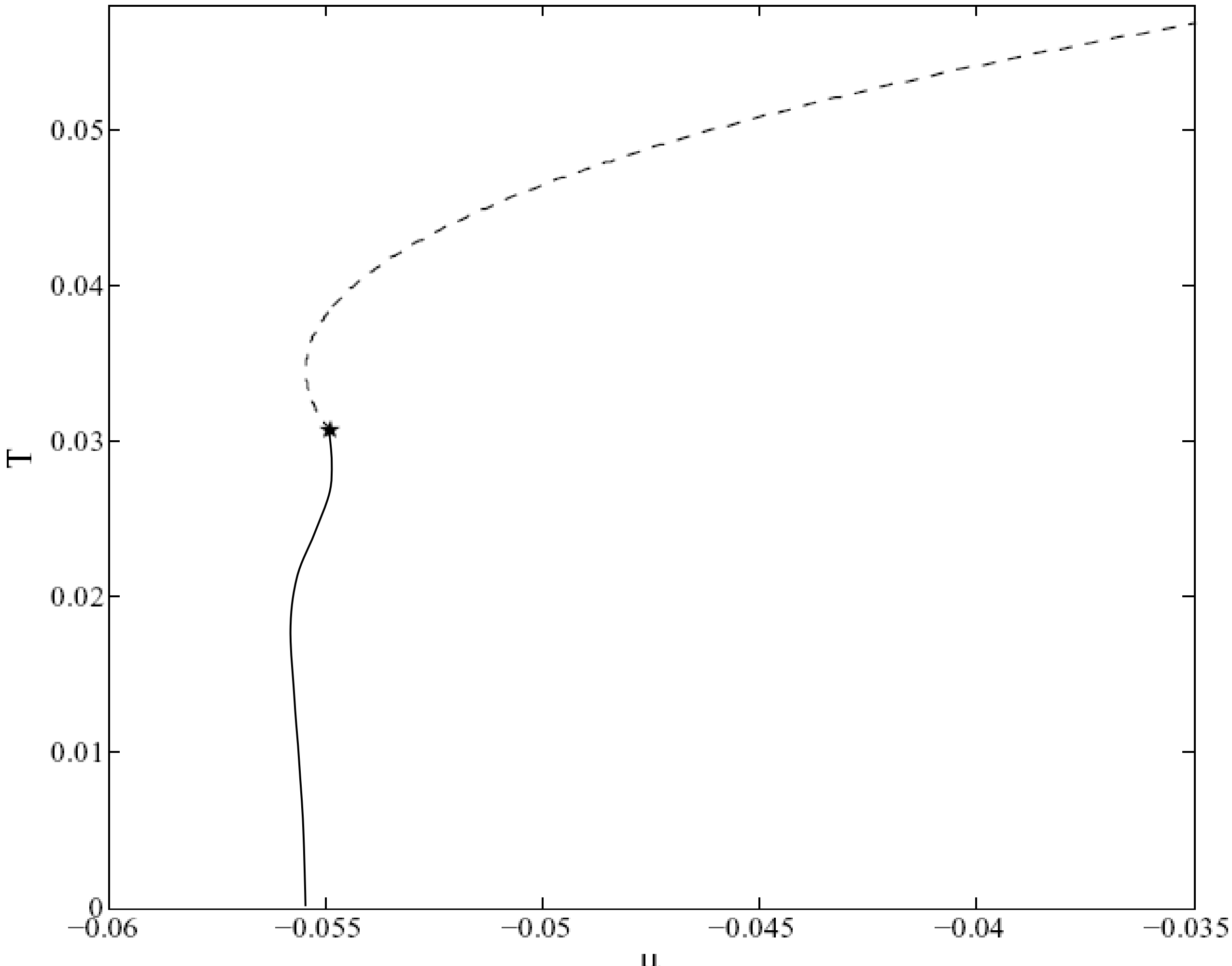
Grand canonical ensemble: minimize G with respect to ρ(x) at a given μ

One finds the same critical line as in the canonical ensemble

$$\beta_c = 2\pi\sqrt{3}/\rho\,, \quad \mu = \frac{1}{\beta}\ln\frac{\rho}{3(1-\rho)}$$

But with a tricritical point at $\rho_{TCP} = 1/3$ where the transition becomes first order

Non-conserving dynamics



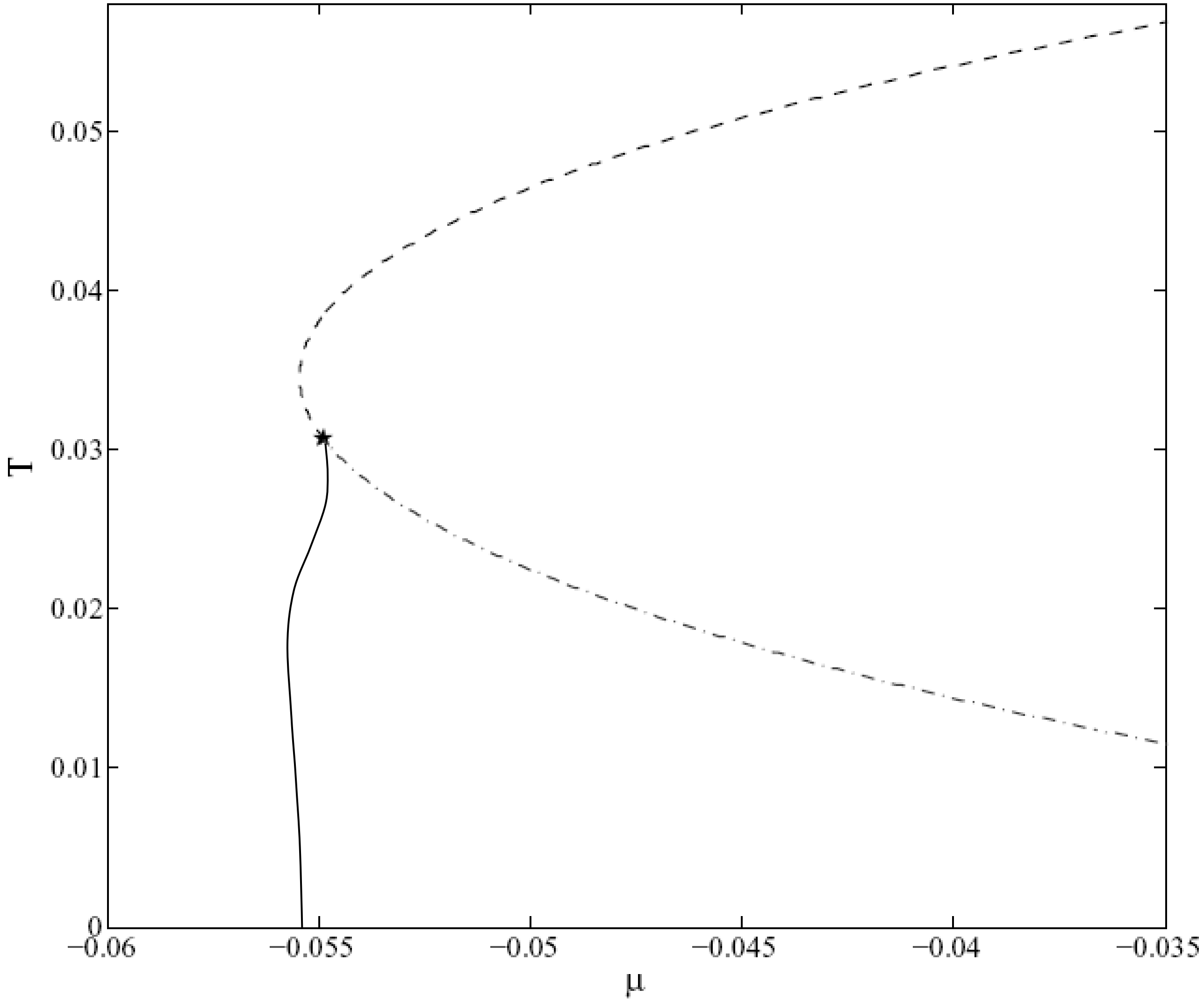
0000000 A..AB..BC..C

T=0

-1/18

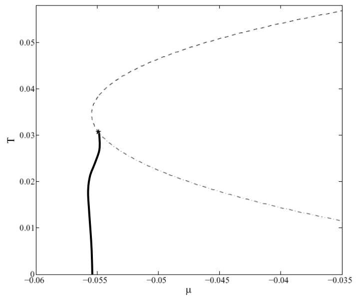
μ

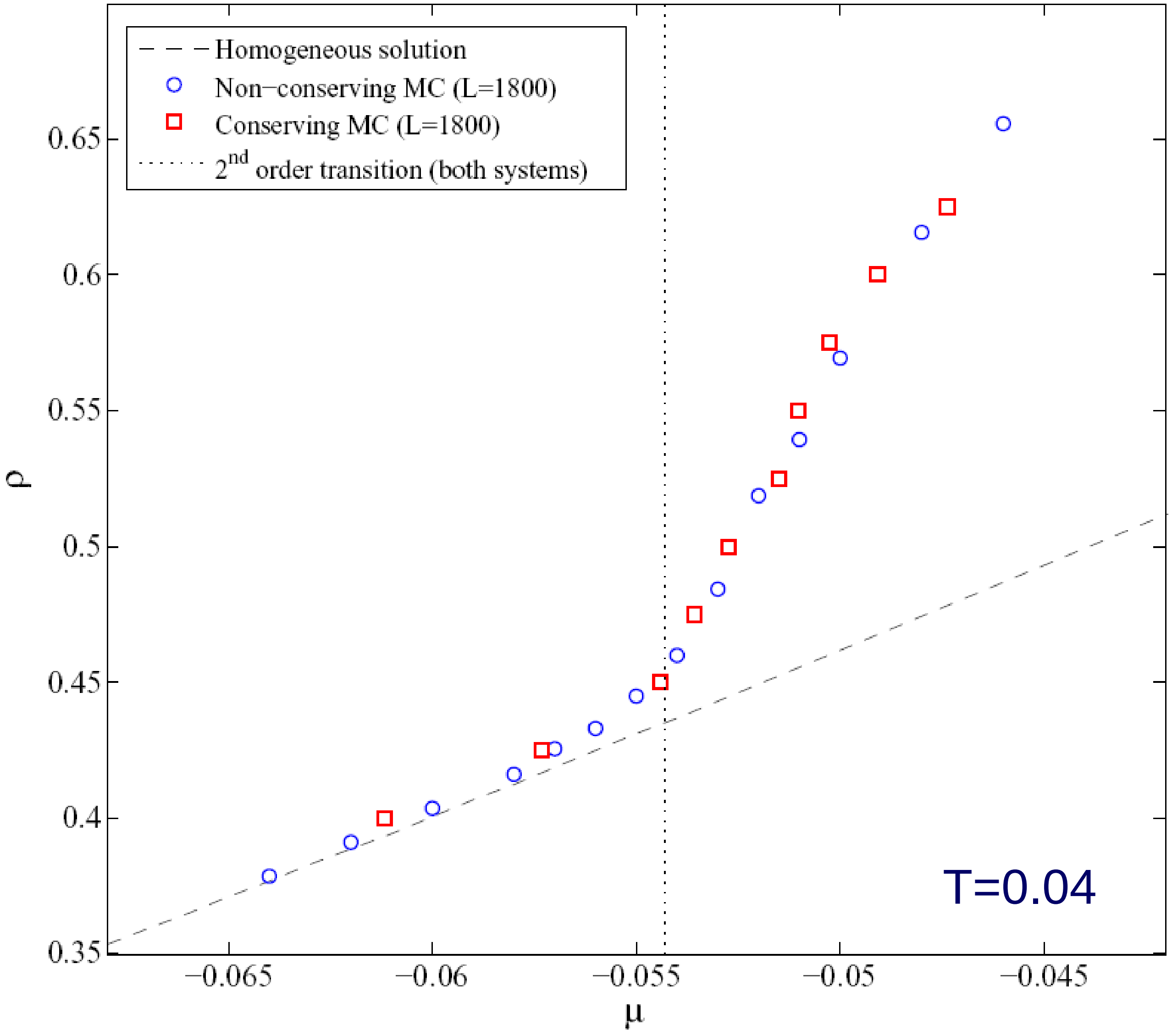
Canonical vs. grand-canonical phase diagrams



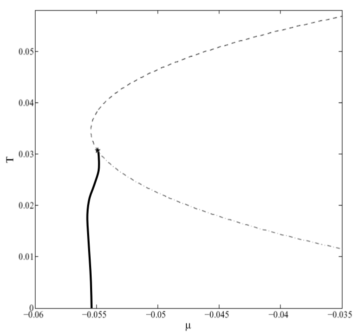
T=0

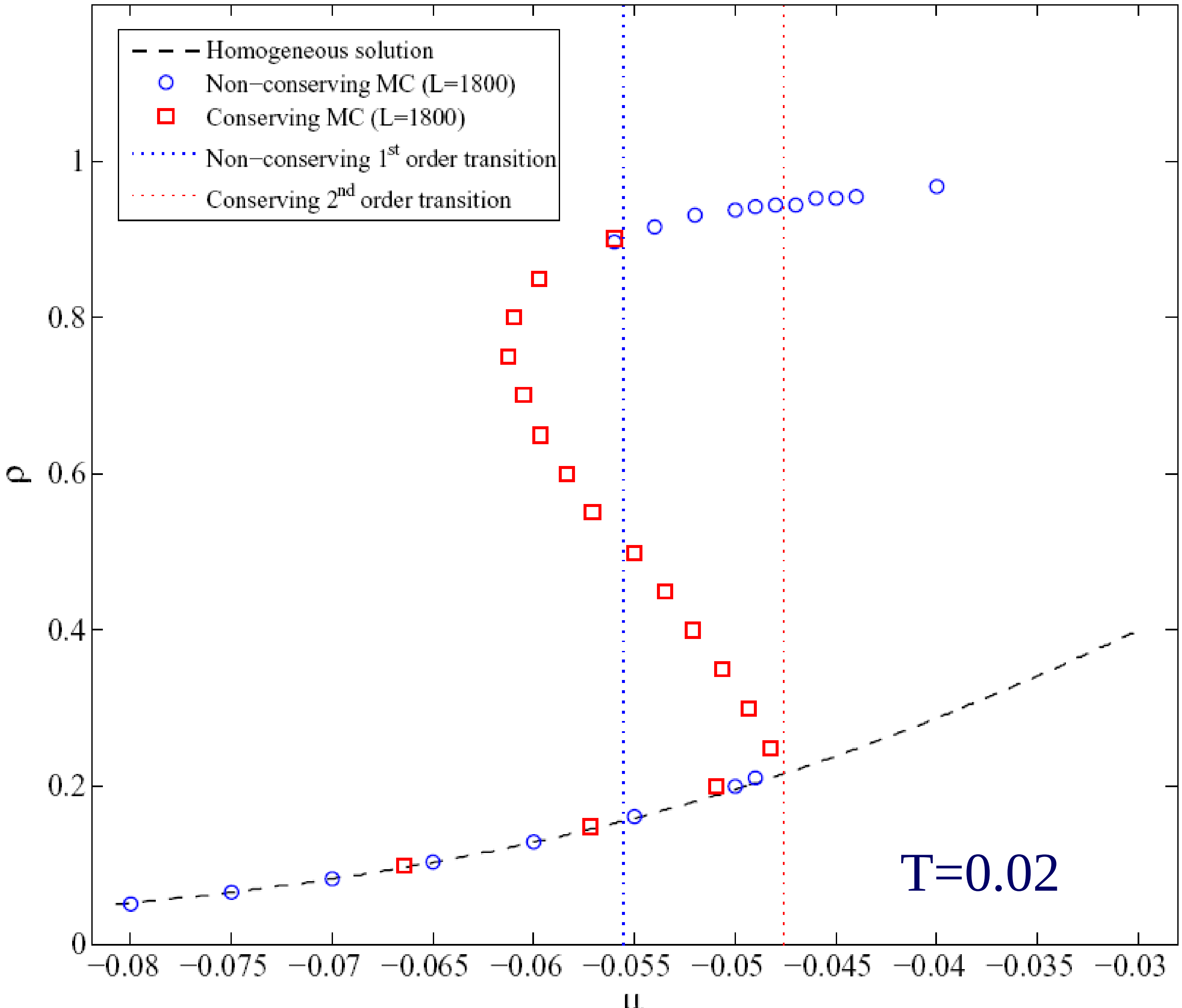
Conserving vs. non-conserving dynamics: 2^{nd} order line



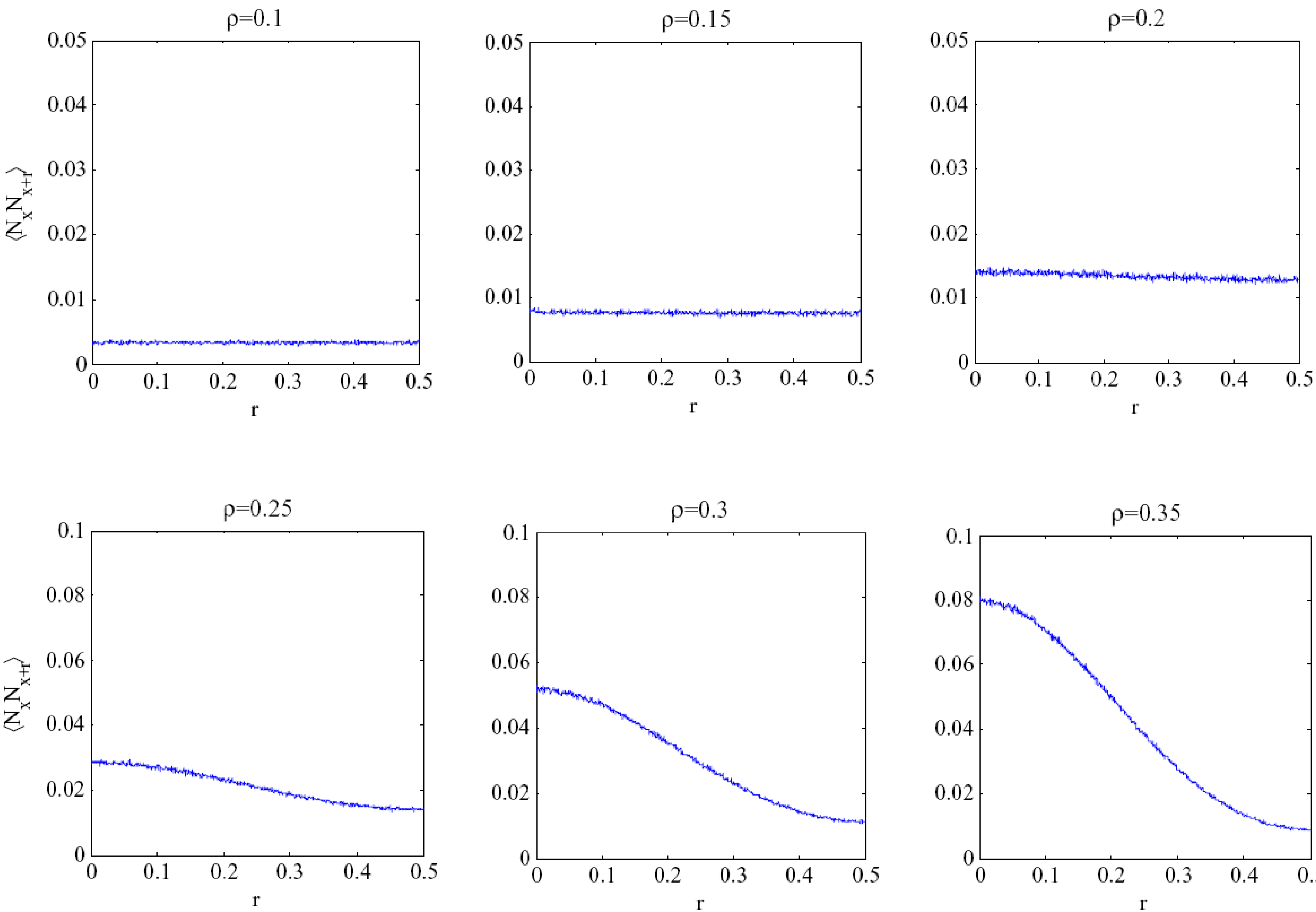


Conserving vs. non-conserving dynamics: 1st order line

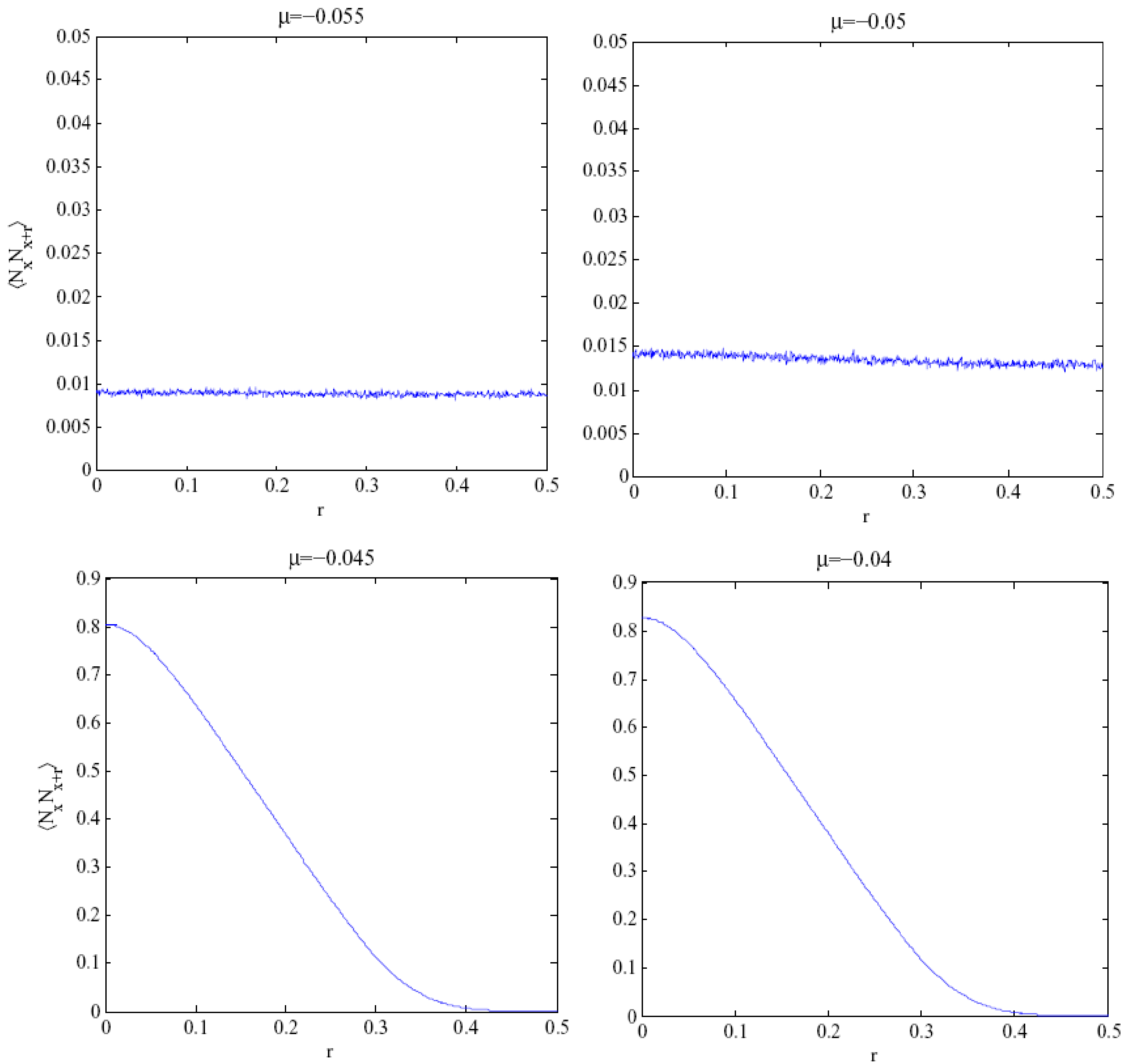




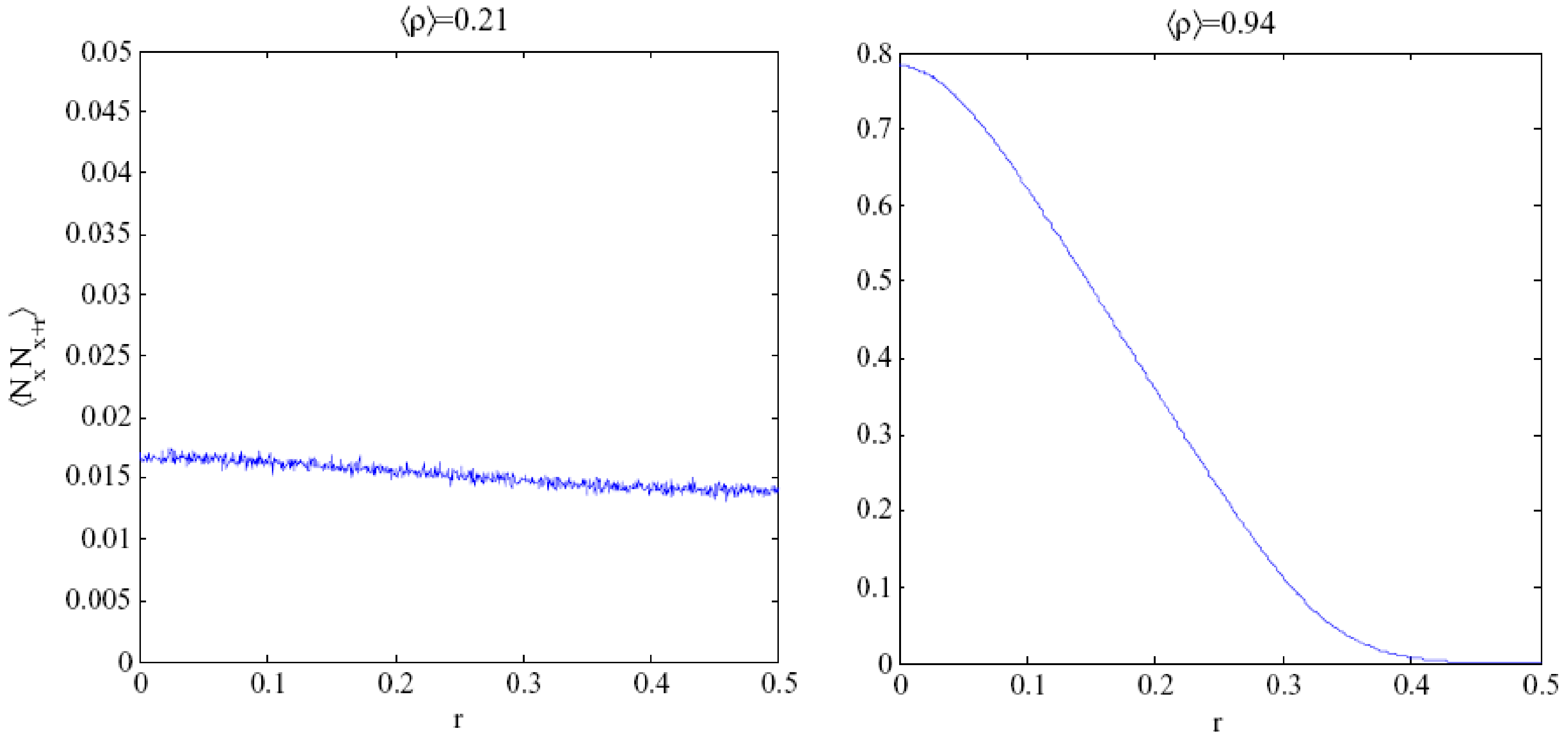
T=0.02, conserving dynamics – 2nd order transition at $\rho_c = 0.2177\ (\mu \approx -0.047)$



T=0.02, non-conserving dynamics – 1st order transition at



Correlations for both solutions with $\mu = -0.049$



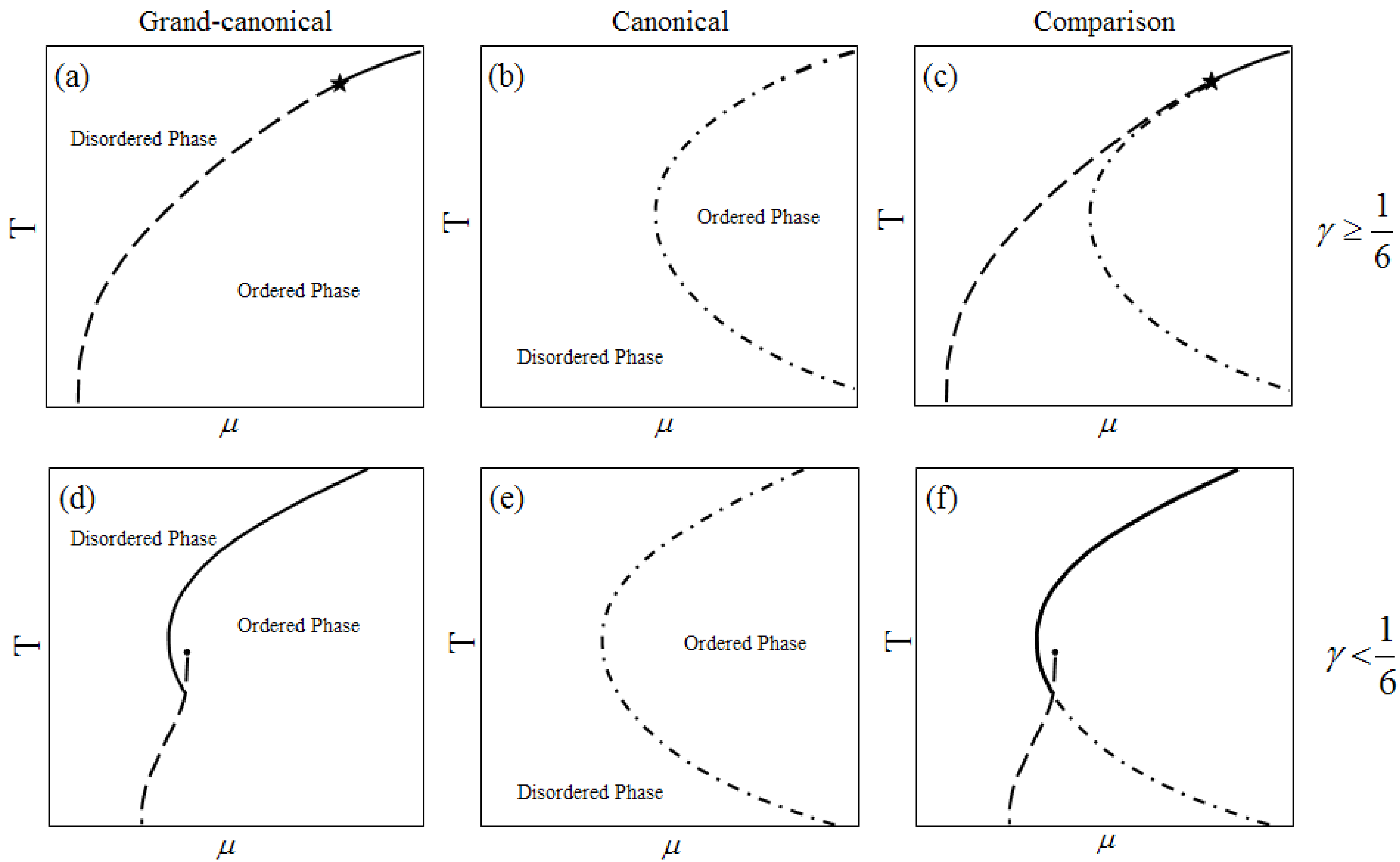
Further generalization

$$E(\{x\}) = \left[\sum_{i=1}^{L-1} \sum_{k=1}^{L-i} \left(C_i B_{i+k} + A_i C_{i+k} + B_i A_{i+k} \right) - \gamma N^2 \right] - \mu L N$$

This energy corresponds to the non-conserving process

$$ABC \underset{1}{\overset{q^{\theta}}{\rightleftharpoons}} 000 \qquad \vartheta = (6\gamma - 1)N + 3L\mu$$

This dynamics is non-local except for $\gamma = 1/6$



Grand-canonical
Canonical
Comparison
(a)
Disordered Phase
Ordered Phase
(b)
Ordered Phase
Disordered Phase
(c)
T
μ
$\gamma \geq \frac{1}{6}$
(d)
Disordered Phase
Ordered Phase
(e)
Ordered Phase
Disordered Phase
(f)
$\gamma < \frac{1}{6}$

Summary

- Local stochastic dynamics may result in effective long-range interactions in driven systems.
- This is manifested in the existence of phase transitions in one dimensional driven models.
- Existence of effective long range interactions can be explicitly demonstrated in the ABC model.
- The model exhibits phase separation for any drive $q \neq 1$
- Phase separation is a result of effective long-range interactions generated by the local dynamics.
- Inequivalence of ensembles in the driven model.