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Driven Diffusive Systems

a brief introduction

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Outline of the series

- Overview/Review "Equilibrium SM *vs.* Nonequilibrium SM"
- An Ising-like model in DDS "Shattered expectations"
- DDS in one-dimension "Bare bones NESM"
- Systems with more than one driven species "American football, Barber poles, and Clouds"
- Summary and Outlook "Come and join in the fun!"

Outline of the series

- Overview/Review "Equilibrium SM *vs.* Nonequilibrium SM"
  - What's Non-equilibrium Statistical Mechanics and why study it?
  - Equilibrium SM *vs.* two distinct classes of NESM
  - Master Equation, Probability Densities and Currents
  - What are Driven Diffusive Systems (DDS) and why study them?
- An Ising-like model in DDS "Shattered expectations"
- DDS in one-dimension "Bare bones NESM"
- Systems with more than one driven species "American football, Barber poles, and Clouds"
- Summary and Outlook "Come and join in the fun!"

Outline of the series

- Overview/Review "Equilibrium SM *vs.* Nonequilibrium SM"
- An Ising-like model in DDS "Shattered expectations"
  - What differences do the drive induce?
  - Surprises about T_c , above it, near it, and below it!
  - What we understand so far and what challenges remain.
- DDS in one-dimension "Bare bones NESM"
- Systems with more than one driven species "American football, Barber poles, and Clouds"
- Summary and Outlook "Come and join in the fun!"

Outline of the series

- Overview/Review "Equilibrium SM *vs.* Nonequilibrium SM"
- An Ising-like model in DDS "Shattered expectations"
- DDS in one-dimension "Bare bones NESM"
  - Interesting physics, despite just 1-D and "no interactions"
  - Potential applications - "mass transport"
  - Exact solutions and intractable extensions
- Systems with more than one driven species "American football, Barber poles, and Clouds"
- Summary and Outlook "Come and join in the fun!"

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- An Ising-like model in DDS "Shattered expectations"
- DDS in one-dimension "Bare bones NESM"
- Systems with more than one driven species "American football, Barber poles, and Clouds"
  - Variety of models with multiple species of particles
  - Surprises in "bare bones" NESM models with just two species
    - "Charged" particles driven in opposite directions
    - Phase transitions in the "ABC" model
- Summary and Outlook "Come and join in the fun!"

A personal view of the "spectrum" of physics

Statics
< "boring", do-able >

Dynamics
< exciting, undo-able >

Steady states, …
< interesting, do-able >

x = *constant* — full $x(t)$

$x = vt$, $A\cos(\omega t)$, $\Sigma_i A_i \cos(\omega_i t)$,…

electrostatics — full E&M

magnetostatics,
AC, power generation
radiation and waves,
⋮

equilibrium stat mech — *fearsome Fury*

---

equilibrium — *fearsome Fury*

time correlations in equilibrium
relaxation (fast or slow) into equilibrium
being caught in long-living,
metastable states
⋮
non-equilibrium stationary (steady) states

Two classes of NESM

…evolution according to rules that respect or violate detailed balance

What distinguishes equilibrium from non-equilibrium steady states?

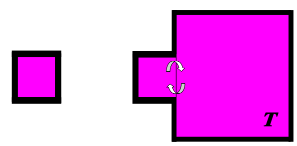
both time *independent* distributions !!

Boltzmann's fundamental hypothesis: $P^* \propto 1$
for an *isolated* system …

…led to highly successful description
of systems in thermal equilibrium

What distinguishes equilibrium from non-equilibrium steady states?

A pedantic picture



$P^*(\mathcal{C}) \propto \delta[E-\mathcal{H}(\mathcal{C})]$ $P^*(\mathcal{C}) \propto exp[-\beta\mathcal{H}]$

configuration

energy functional: "Hamiltonian"

What distinguishes equilibrium from non-equilibrium steady states?

Boltzmann's fundamental hypothesis: $P^* \propto 1$
for an *isolated* system …

- led to highly successful description of systems in thermal equilibrium
- no trace of dynamics here
- ***if*** you insist on "imposing" a dynamics via, say, a <u>*master equation*</u> for $P(\mathcal{C},t)$, then you had better respect **detailed balance** (or microscopic reversibility)

Master equation

$$\partial_t P(\mathcal{C},t) = \sum_{\mathcal{C}'} \{ R(\mathcal{C}' \to \mathcal{C})\, P(\mathcal{C}',t) - R(\mathcal{C} \to \mathcal{C}')\, P(\mathcal{C},t) \}$$

"Rates obey **detailed balance** if they satisfy…"

$$R(\mathcal{C}' \to \mathcal{C}) \,/\, R(\mathcal{C} \to \mathcal{C}') = exp[\beta\{\mathcal{H}(\mathcal{C}')-\mathcal{H}(\mathcal{C})\}]$$

- Stationary state satisfies $\partial_t P^*(\mathcal{C}) = 0$ …
- But **d.b.** R's implies $P^* \sim e^{-\beta\mathcal{H}}$ will do, since

$$R(\mathcal{C}' \to \mathcal{C})\, \underbrace{P^*(\mathcal{C}')}_{e^{-\beta\mathcal{H}(\mathcal{C}')}} - R(\mathcal{C} \to \mathcal{C}')\, \underbrace{P^*(\mathcal{C})}_{e^{-\beta\mathcal{H}(\mathcal{C})}} = 0$$

Take-home message:

If evolution rules (rates) respect detailed balance, the system is guaranteed to wind up eventually in equilibrium, with the Boltzmann distribution.

- *Furthermore*, in this stationary state, we have
- all net stationary currents *identically zero* :

$$R(\mathcal{C}' \to \mathcal{C})\, \boldsymbol{P}^*(\mathcal{C}') - R(\mathcal{C} \to \mathcal{C}')\, \boldsymbol{P}^*(\mathcal{C}) = 0$$

$\boxed{\textit{electrostatics !!}}$

What distinguishes equilibrium from non-equilibrium steady states?

- What if you insist on *violating* detailed balance
  (i.e., choose such rates in a master equation approach) ?

$$\partial_t \boldsymbol{P} = -\mathbb{L}\boldsymbol{P}$$

left eigenvector trivially exists, with eigenvalue zero,
right eigenvector is $\boldsymbol{P}^*$
uniqueness more tricky

What distinguishes equilibrium from non-equilibrium steady states?

- What if $\boldsymbol{K}^*$ ist on *violating* detailed balance
  (i.e., ...h rates in a master equation approach) ?
- Stationary state still exists.
- Net currents are *t-independent,* but can be *non-zero.*

…form non-trivial current ***loops.***

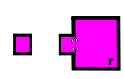
$\boxed{\textit{magnetostatics !!}}$

What distinguishes equilibrium from non-equilibrium steady states?

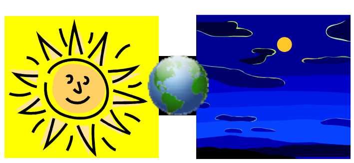
- What if you insist on *violating* detailed balance?
- Stationary state still exists.
- Net currents are *t-independent,* but can be *non-zero.*
- Do these P^*'s & K^*'s correspond to any physics?
- …and if so, how do you produce them?

…by coupling the system to ***more than one*** energy reservoir

What distinguishes equilibrium from non-equilibrium steady states?



$\boxed{\boldsymbol{K}^* \equiv 0}$



$\boldsymbol{P}^*, \boldsymbol{K}^* = ???$

Overview/Review

Equilibrium *vs.* Nonequilibrium Statistical Mechanics

- What's NESM?
- Where does it "belong"? and
- Why do we study it?

from curiosity-driven research… to dollar-driven research

from fun and games and
fundamental issues…
to practical applications and
long-term implications

curiosity-driven research…

fun and games

- computer games
  - simple (can be very simple)
  - surprising/unpredictable (can be very…)
  - e.g., Conway's "game of life"
  - models we "play with" (driven Ising!)

curiosity-driven research…

fun and games

- computer games
  - simple (can be very simple)
  - surprising/unpredictabl…
  - e.g., Conway's "game…
  - models we "play with" (driv…
- real life games
  - simple (can be very simple)
  - surprising/unpredictable (can be very…)
  - e.g., Bohr's kitchen

Come to my public lecture: July 15th

curiosity-driven research…

fundamental issues:

- Predict/hypothesize non-trivial ***P****'s
  (snow flakes, game of life and real life, …)
- Uniqueness of ***P**** , thermodynamic limit
  ("geometry dependent thermodynamics")
- Can the pair {***P****, ***K****} be the unique characterization of NESS?
  (like ***P**** alone fully determine an equilibrium state; Zia & Sxhmittmqnn, *JSTAT* P07012 2007)
- Equivalence classes of *R*'s (for the same {***P****, ***K****})
  (… generalization of "detailed balance" for equilibrium; *JSTAT* above)
- Universality classes – RG flow of ***K**** as well as ***P****?
  (Some NESS's display critical properties of an equil. system, others have "detailed balance violating" fixed points!)
- Understanding the implications of current loops … (Is there an underlying Gauge theory?)

  ⋮

- How do complex patterns of collective behavior ***emerge*** from simple rules for few particles?

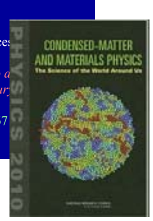
from curiosity-driven research… to dollar-driven research

Condensed-Matter and Materials Physics: The Science of the World Around Us

Committee on CMMP 2010, Solid State Sciences Committee, National Research Council, (US) National Academy of Sciences

"In this report, the Committee on CMMP 2010 looks ahead to a… are the prospects for CMMP in the early part of the 21st century…

http://www.nap.edu/catalog.php?record_id=11967



… dollar-driven research

CMMP 2010 … posed 6 challenges:

Three of them has something to do with the focus of this summer school!!

- How do complex phenomena ***emerge*** from simple ingredients?
- What happens ***far from equilibrium*** and why?
- What is the physics of ***life***?
- What new discoveries await us in the *nanoworld*?
- How will the *energy* demands of future generations be met?
- How will the *information technology* revolution be extended?

… dollar-driven research

DoE produced a similar report, with 5 “Grand Challenges”

Essentially identical to those of CMMP, except

…they used more words,

they are control freaks, and

they dropped ***life***!

http://www.sc.doe.gov/bes/reports/files/GC_rpt.pdf

Overview/Review

Equilibrium *vs.* Nonequilibrium Statistical Mechanics

- What’s NESM? Where does it “belong”? and Why do we study it?
- Master equation, detailed balance, and probability currents
- What are Driven Diffusive Systems (DDS) and why study them?

Master equation, Detailed Balance, Trees, and Irreversible Loops

What if you don’t know $\mathcal{H}$?

but have just a bunch of R’s ?

(e.g., a model for lions & lambs, or the stock market, or…)

$\mathcal{C}, t)$ }

$\mathcal{C})$}]

Does detailed balance still have meaning?

… and how would you know if

your set of R’s satisfy d.b. or not ?

What are the consequences?

Switch notation to simplify…

- Configurations of our system

  (discrete, finite for now): $C_i \quad \rightarrow \quad i$

- Probability to find system in C_i at time t :

  $P\,(C_i\,, t) \quad \rightarrow \quad P_i\,(t)$

- Master equation for evolution of $P_i\,(t)$:

$$\partial_t P_i\,(t) = \sum_{j \neq i} \left[w^j{}_i\, P_j\,(t) - w^i{}_j\, P_i\,(t) \right]$$

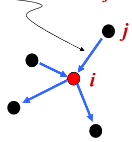
rate from i to j

instead of R($i \rightarrow j$)

Summary of notation and reminder

- Configurations: $C_i \quad i$
- Probability to find system: $P_i\,(t)$
- Master eqn: $\partial_t P_i\,(t) = \sum_{j \neq i} \left[w^j{}_i\, P_j\,(t) - w^i{}_j\, P_i\,(t) \right]$
- ***Net*** probability current… from j to i :

$$K^j{}_i\,(t) \;=\; w^j{}_i\, P_j\,(t) - w^i{}_j\, P_i\,(t)$$



Reminders …

- After long times, $P_i\,(t)$ settles to $P^*{}_i$, i.e. the *stationary* distribution, where $\partial_t P^*{}_i = 0$
- with *stationary* currents

$$\boxed{K^{*j}{}_i \;=\; w^j{}_i\, P^*{}_j - w^i{}_j\, P^*{}_i}$$

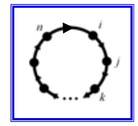
Reminders …

- At large t, $P_i\,(t)$ settles into a *stationary* P^*_i
- with *stationary* $K^{*j}_{\ i} = w^j_{\ i}\,P^*_j - w^i_{\ j}\,P^*_i$
- w's with detailed balance satisfy

$$w^i_{\ j}\,P^*(C_i) = w^j_{\ i}\,P^*(C_j)$$

$$K^* \equiv 0 \quad \Leftrightarrow \quad \text{detailed balance } \{w\}$$

- Detailed Balance was presented as



$$w^j_{\ i} / w^i_{\ j} = P^*_i / P^*_j$$

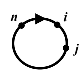
. . . which give the impression that it "depends" on a known stationary distribution P^* !

- But, DB is an "intrinsic" property of the dynamics (Kolmogorov criterion 1936!):
  - consider closed loops in configuration space:

$$\mathcal{L} \equiv i \to j \to k \ldots \to n \to i$$

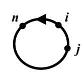
  - and the product of associated rates around the loop of the rates:

$$\Pi[\mathcal{L}] \equiv w^i_{\ j}\,w^j_{\ k} \ldots w^n_{\ i}$$



- as well as the product of associated rates around the loop *in reverse*:

$$\Pi[\mathcal{L}_{rev}] \equiv w^i_{\ n} \ldots w^k_{\ j}\,w^j_{\ i}$$



$$\Pi[\mathcal{L}] \equiv w^i_{\ j}\,w^j_{\ k} \ldots w^n_{\ i}$$

Kolmogorov criterion

…oduct of associated rates around …e:

$$\Pi[\mathcal{L}_{rev}] \equiv w^i_{\ n} \ldots w^k_{\ j}\,w^j_{\ i}$$

- Dynamics has **D**etailed **B**alance ***iff***

$$\Pi[\mathcal{L}] = \Pi[\mathcal{L}_{rev}] \qquad \textbf{\textit{for all loops!}}$$

- **I**rreversible **L**oops are key to NESS

Detailed Balance = Time reversal symmetry

- *Irreversible Loops* are key to NESS
- …but $K^* \neq 0$ is also key to NESS !
- Is there a link between IL's and $K^* \neq 0$?

YES! by way of "Trees"…

- P^*_i via "trees" well established (Hill 1966, but not widely known) route to any SS distribution

- Draw all directed trees with all k's, *s.t.* "root" is at i : $\mathcal{T}_{\alpha(i)}$
- Write product of all associated w's with each tree : $U[\mathcal{T}_{\alpha(i)}]$
- Then,

$$P^*_i = \Sigma_\alpha\, U[\mathcal{T}_{\alpha(i)}] \big/ \mathcal{Z}$$

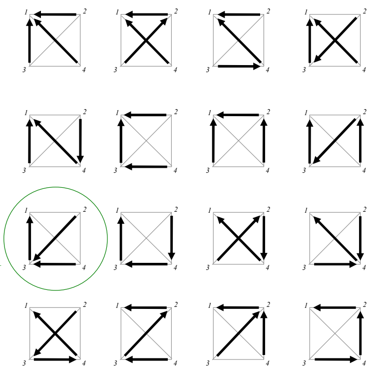
$\mathcal{Z}$ is a normalization factor: "super" partition function!!

A case with just 4 configurations

$i = 1,2,3,4$

Here are all 16 trees for P^*_1

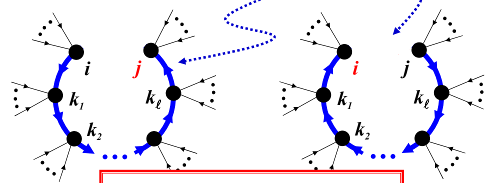
$U = w^4{}_3 w^2{}_3 w^3{}_1$



Starting with $K^{*\,j}{}_i = w^j{}_i P^*{}_j - w^i{}_j P^*{}_i$

see that the RHS is a sum over ***trees***

ONE tree in P^*_j



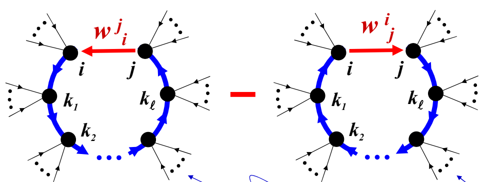
For each tree in P^*_j, there is just one in P^*_i that's the *SAME, EXCEPT* for …

reversing the direction of blue line

Next, look at the **combination**

Now, return to $K^{*\,j}{}_i = w^j{}_i P^*{}_j - w^i{}_j P^*{}_i$

and see that the RHS is a sum over



$\{\Pi[\mathcal{L}] - \Pi[\mathcal{L}_{rev}]\}$ {same product of w's}

Summary of DB, IL, & K^*'s

- Stationary probability currents (K^*)

  intimately related to

  Irreversible Loops (of w's) ***in*** $\{C_i\}$ ***space***
- K^*'s themselves must form ***current loops***
- Is there a simple relation between

  K^*-***loops*** and ***w-loops*** ???

  knowing that $IL \Leftrightarrow K^* \neq 0$
- K^* is a (probability current) distribution, from which we get averages of observables

  (e.g., energy flux ***through*** our system)

Other consequences (e.g., entropy production) and several explicit examples of K^* in "*Probability Currents*…" JSTAT P07012 (2007)

Overview/Review

Equilibrium *vs.* Nonequilibrium Statistical Mechanics

- What's NESM? Where does it "belong"? and Why do we study it?
- Master equation, detailed balance, and probability currents
- What are Driven Diffusive Systems (DDS) and why study them?

Overview/Review

Equilibrium *vs.* Nonequilibrium Statistical Mechanics

- That was a broad overview of NESM systems,
- esp. ones with detailed balance ***violating*** dynamics.
- Driven Diffusive Systems form a particularly interesting subset…
- teaching us many lessons about ***essentials*** of NESM (*fundamental problems*), and
- allowing us to build models for a wide range of natural phenomena (*applications*).

Driven Diffusive Systems

What are DDS? Why study them?

conservation laws crucial

…out of equilibrium !

using

direct drives, e.g., *E, g* fields

or random drives, e.g., multiple *T*'s

Driven Diffusive Systems

What are DDS? Why study them?

- Fundamental issues in NESM
- Physics of many ystems "all around us"
  - fast ionic conductors (which started this industry)
  - micro/macro biological systems
  - vehicular/pedestrian traffic, granular flow
  - social/economic networks
  - ⋮

Driven Diffusive Systems

What are DDS? Why study them?

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  - fast ionic conductors (which started this industry)
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But, real life is VERY COMPLEX!

Driven Diffusive Systems

Perhaps we can gain some insight through SIMPLE systems, like the Ising model

historic reminder :
The Lenz-Ising model was considered a theorists' "toy"!

Yet, we learned a great deal about EQUILIBRIUM SM through it.

Driven Diffusive Systems

Simple models and Potential applications

- Single species of particles (Ising lattice gas)
- Two or more species
- ***n*** dimensional objects embedded in ***d*** dim. space
- Variety of drives ("two temperature" models)
- (effects of) quenched disorder
- ⋮
- What's **not** DDS? ***Many, many*** other NE systems:
  - reaction-diffusion (birth-death) processes, with "serious" and/or "ordinary" interactions
  - percolation, directed percolation, BARW, persistence, …
  - epidemics, population dynamics, network dynamics, …
  - aging, glass, …

Simple Models and Applications

- Single species ($\boldsymbol{n},\boldsymbol{d}$) DDS

protein synthesis (0,1)
advection of passive particles (0,2)
fast ionic conductors (0,3)
transport thr polymeric membranes (0,3)
steps on vicinal surfaces (1,2)
flux lines in superconductors (1,3)
polymer sedimentation (1,3)
surface growth in MBE (2,3)

- Multi-species DDS

bio-molecular motors on microtubules
electrophoresis
vacancy mediated diffusion in alloys
vehicular/pedestrian traffic dynamics