Dynamical large deviations and glass transitions

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Dynamics is more than statics

Canonical example $\rightarrow$ glass transition problem

Statistical mechanics of trajectories rather than states/configurations

Dynamical large-deviations $\rightarrow$ s-ensemble method $\rightarrow$ glasses

\{Ruelle, Derrida, Lebowitz-Spohn, Gartner-Ellis, Donsker-Varadhan, ...\}

Applications in quantum many-body systems?
Stylised facts about the glass transition

#1: Slowdown w/o structural change

\[ t \ll \tau_\alpha \quad t \approx \tau_\alpha \quad t \gg \tau_\alpha \]

(e.g. 50:50 L-J mixture (Hedges 2009))

#2: Dynamical heterogeneity

#3: Anomalous response if driven out-of-equilibrium

\[
C_p \quad \text{cool -20 K/m} \quad \text{heat +20 K/m}
\]

\[
0.8 \quad 1.0 \quad 1.2 \quad 1.4 \quad 1.6 \quad 1.8 \quad 2.0
\]

\[
0.8 \quad 220 \quad 240 \quad 260 \quad T (K)
\]

\[
1.0 \quad 1.5 \quad 2.0 \quad 2.5 \quad 3.0 \quad 3.5 \quad 4.0 \quad 4.5
\]

\[
340 \quad 345 \quad 350 \quad 355 \quad 360 \quad 365 \quad 370 \quad 375 \quad 380 \quad \text{Temperature (K)}
\]
Perspectives on glass transition

**Thermodynamic**

Statics $\Rightarrow$ Dynamics

eg. RFOT

$\{\text{Parisi+Wolynes+many others}\}$

ideal models e.g. $p$-spin spin glass

**Dynamic**

Statics does not $\Rightarrow$ Dynamics

metric $\Rightarrow$ Dynamic facilitation

ideal models $K\text{CMs}$

$\{\text{Anderson+Andersen+Jackle+many others}\}$
#2: Dynamical heterogeneity

Cold/dense Lennard-Jones mixture
\{L. Hedges\}

\[ N_A = N_B = 10^4 \ (1:1.4) \]
\[ T = 1.1 < T_{\text{onset}} \]

Motion begets motion \(\rightarrow\) dynamical facilitation

Effective excitations are localised \{Keys-et-al, PRX 2011\}

Interesting structure in trajectories not in configurations/states
Dynamic facilitation $\rightarrow$ kinetically constrained models

$\partial_t |P\rangle = W |P\rangle \rightarrow W = \sum_i (n_{i-1} + \delta) \left[ \epsilon \sigma_i^+ + \sigma_i^- - \epsilon (1 - n_i) - n_i \right] + (i \leftrightarrow i - 1)$

constraint = operator valued rate

Trivial statics but heterogeneous & hierarchical dynamics

East model $\tau_{relax} \approx \tau_0 \exp \left( \frac{A}{T^2} + \frac{B}{T} \right)$ \quad \{Sollich-Evans 1999\}
Dynamic facilitation → kinetically constrained models

$\partial_t |P\rangle = \mathbb{W} |P\rangle$

$\exp \left( \frac{C}{T - T_0} \right)$

NB: no VFT


East model $\tau_{\text{relax}} \approx \tau_0 \exp \left( \frac{A}{T^2} + \frac{B}{T} \right)$  

{Sollich-Evans 1999}

$\frac{J}{T_0} \left( \frac{T_0}{T} - 1 \right)$  

{Elmatad-Chandler-JPG, JPCB 2009/2010}

$\log (\tau / \tau_0)$
“Thermodynamics” of trajectories: s-ensemble

- Time-integrated order parameter: $K = \text{activity}$
  - Active $K \gg 0$
  - Inactive $K \approx 0$
“Thermodynamics” of trajectories: s-ensemble

large-deviations of time-integrated observables

\[ P(K) \]

\[ P(K) \text{ against } K \text{ in the range from 0.02 to 0.04} \]

BMLJ

Time-integrated

East
“Thermodynamics” of trajectories: s-ensemble

\[ \text{time-integrated order parameter: } K = \text{activity} \]

\[ \text{active } K \gg 0 \]

\[ \text{inactive } K \approx 0 \]

\[ \text{large deviations} \]

\[ \text{Prob}(K) \approx e^{-t \varphi(K)} \]

\[ Z_t(s) \equiv \langle e^{-sK} \rangle \approx e^{t \theta(s)} \]

\[ s \leftrightarrow K \quad \varphi = \text{“entropy”} \quad \theta = \text{“free-energy”} \quad t = \text{“volume”} \]

\[ \mathbb{W} \rightarrow \mathbb{W}_s = \sum_i n_{i-1} \left[ e^{-s} (\epsilon \sigma_i^+ + \sigma_i^-) - \epsilon (1 - n_i) - n_i \right] \theta(s) \text{ largest eigenvalue} \]

\[ \mathbb{W}_s \text{ is “transfer matrix” of “partition sum” } Z_t(s) \]
“Thermodynamics” of trajectories: $s$-ensemble

**East model**

- **Order Parameter:**
  - $K(s)$
  - $\theta(s)$

**Graphs:**
- First-order dynamical transition at $s_c = 0$
- When $t_{obs} \to \infty$

**Equation:**
\[
W \to W_s = \sum_i n_{i-1} \left[ e^{-s} \left( \epsilon \sigma_i^+ + \sigma_i^- \right) - \epsilon (1 - n_i) - n_i \right] \theta(s) \quad \text{largest eigenvalue}
\]

- $W_s$ is “transfer matrix” of “partition sum” $Z_t(s)$

**Additional Notes:**
- Time-integrated order parameter: $K = \text{activity}$
- $K_0 = \text{inactive}$
- {e.g. Ruelle, Lebowitz-Spohn, Gartner-Ellis, Donsker-Varadhan, Lecomte+, many others}
- cf. Full Counting Statistics
“Thermodynamics” of trajectories: s-ensemble

\[ \text{Prob}(K) \approx e^{-sK} \]

\[ Z_t(s) \equiv \langle e^{-sK} \rangle \approx (s) \]

\[ s \leftrightarrow K \quad \varphi = \text{“entropy”} \]

\[ W \rightarrow W_s = \sum_i n_{i-1} \left[ e^{-s} \right] \]

\( W_s \) is “transfer matrix” of “partition sum”

\[ W_s(s) = \frac{1}{n} \sum_{i} \left[ e^{-s} \right] \]

BMLJ (MD/TPS, N=150)

activity vs. counting field

first-order dynamical transition

at \( s_c \gtrsim 0 \)

when \( t_{\text{obs}} \gg \tau \)

\( \text{ cf. Full Counting Statistics } \}

\{see also, 
Lecomte-Pitard-van Wijland 2011,
Speck-Chandler 2012
Speck-Malins-Royall 2012\}
“Thermodynamics” of trajectories: s-ensemble

**dynamical phase-diagram**

\[
(t_{\text{obs}} \to \infty, \, N \to \infty)
\]

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**equilibrium liquid**

**Active phase**

**Inactive phase**

**non-equilibrium “glass”**

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real dynamics \( s = 0 \rightarrow \text{can we access } s_c \gtrsim 0 ? \)

Accessible from normal dynamics via **cumulants** and **Lee-Yang zeros**

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\{Flindt-JPG, PRL 2013; Hickey-Flindt-JPG 2014\}
Preparing glasses with s-ensemble

{Keys-JPG-Chandler, PNAS 2013 and arXiv:1401.7206}

East model

{cf. Sollich-Evans 2003}

space-time bubbles (active & equil.)

space-time stripes (inactive & noneq.)

non-equilibrium characteristic length in glassy state
Preparing glasses with s-ensemble

{Keys-JPG-Chandler, PNAS 2013 and arXiv:1401.7206}

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non-equilibrium characteristic length in glassy state
Perspectives on glass transition

Thermodynamic

\[ F(\xi) \]

Statics \(\Rightarrow\) Dynamics

eg. RFOT

\{Parisi+Wolynes+many others\}

ideal models e.g. \(p\)-spin spin glass

low overlap (liquid) \(\rightarrow\) high overlap (glass)

{Franz-Parisi}

numerical evidence \{Berthier 2013, Parisi-Seoane 2013\}

Dynamic

Statics does not \(\Rightarrow\) Dynamics

metric \(\rightarrow\) Dynamic facilitation

ideal models KCMs

\{Anderson+Andersen+Jackle+many others\}

transition in space of trajectories

active (liquid) \(\rightarrow\) inactive (glass)
Triangular plaquette model (TPM):

\[ E = -\frac{J}{2} \sum_{\Delta} S_i S_j S_k \]

**Thermodynamics:**

1-1 mapping spins-plaquettes

free plaquettes \(\rightarrow\) free localised defects
\(\Rightarrow\) disordered \(\forall T\)

**Dynamics:** (effectively) kinetically constrained

Relaxation is hierarchical \(\longrightarrow\) \(\tau = e^{1/T^2}\)

cf. East facilitated model \{Sollich-Evans 1999\}

Statics trivial, dynamics complex & glassy, but singular only at \(T=0\) (cf. dynamic facilitation)
Two coupled TPMs (annealed):  

\[ E = -\frac{J}{2} \sum_{\Delta} (s_i^a s_j^a s_k^a + s_i^b s_j^b s_k^b) - \varepsilon \sum_i s_i^a s_i^b \]

{cf. Franz-Parisi}

Exact duality:

\[ Z(K_J, K_\varepsilon) = (\sinh 2K_J \sinh K_\varepsilon)^N Z(K_J^*, K_\varepsilon^*) \quad (2K_J = \beta J, \ K_\varepsilon = \beta \varepsilon) \]

\[ e^{-K_\varepsilon^*} = \tanh K_J, \quad \tanh K_J^* = e^{-K_\varepsilon} \]
Two coupled TPMs (annealed): \( E = -\frac{J}{2} \sum_{\Delta} (s_i^a s_j^a s_k^a + s_i^b s_j^b s_k^b) - \varepsilon \sum_i s_i^a s_i^b \)

Self-dual: \( \left( \sinh \frac{J}{T} \right) \left( \sinh \frac{\varepsilon}{T} \right) = 1 \)

Cf. TMP in field \{Sasa 2010\} & generalised Baxter-Wu \{Nienhuis 2010\}

1st order static transition at finite coupling ending at CP (*Ising*) \{Turner-Jack-JPG 2014\}

Transition vanishes at \( \varepsilon \to 0 \)
Classify trajectories of TPM according to dynamical activity $\rightarrow$ s-ensemble

1st order transition in activity & overlap

$E = -J \sum_{py} S_i S_j S_k S_l S_m$

spins-pyramids 1-1

same dualities as TPM
Similar features in tilings / dimer coverings / “spin-ice”-like systems

Eg. molecular random tilings
{Beton+Champness+Blunt+Whitelam+Stannard+...+JPG}

“mosaics” for real

free → confined defects
random tiled

ordered

\[ \text{dynamics facilitated by localised free defects} \]

\[ \text{free → confined defects} \]

\[ \text{random tiled} \]

\[ \text{ordered} \]

\[ \text{field} \]
Many-body localisation (MBL) transition:

\{Basko-Aleiner-Altshuler 2006, Huse+, many others\}

- Cf. Anderson localisation but for interacting system
- Singular change throughout spectrum
- Eigenstates change from “thermal” (ETH \{Deutsch, Sdrenicki\}) to MBL
- Observables do not relax in MBL phase
- Often thought of as “glass transition” but modelled with disorder

Can KCMs (as models for classical glasses) say anything about quantum MBL?
Recap: active-inactive “space-time” transitions in KCMs (eg. East/FA)

\[ \mathcal{W} \to \mathcal{W}_s = \sum_{i} n_{i-1} \left[ e^{-s} (\epsilon \sigma_i^+ + \sigma_i^-) - \epsilon (1 - n_i) - n_i \right] + (i \leftrightarrow i - 1) \]

Largest \( \epsilon \)/value = cumulant G.F. for activity \( \to \) 1st order phase transition

Can transform into **Hermitian** operator through equilibrium distribution

\[ H_s \equiv -\mathcal{P}^{-1} \mathcal{W}_s \mathcal{P} = -\sum_{i} n_{i-1} \left[ e^{-s} \sqrt{\epsilon} \sigma_i^x - \epsilon (1 - n_i) - n_i \right] + (i \leftrightarrow i - 1) \]

Consider as **Hamiltonian** and corresponding quantum unitary dynamics \( |\psi_t\rangle = e^{-itH_s} |\psi_0\rangle \)
KCMs and many-body localisation in closed quantum systems

\[ H_s = - \sum_i n_{i-1} \left[ e^{-s} \sqrt{\epsilon} \sigma_i^x - \epsilon (1 - n_i) - n_i \right] + (i \leftrightarrow i - 1) \quad |\psi_t\rangle = e^{-itH_s} |\psi_0\rangle \]

Signatures of MBP transition: (i) relaxation / non-relaxation of observables

\[ \langle M \rangle_t = \sum_i \langle \psi_t | \sigma_i^z | \psi_t \rangle \]

- does not relax on inactive side \( s > 0 \)
- relaxes on active side \( s < 0 \)
KCMs and many-body localisation in closed quantum systems

\[
\mathcal{H}_s = - \sum_i n_{i-1} \left[ e^{-s} \sqrt{\epsilon} \sigma_i^x - \epsilon (1 - n_i) - n_i \right] + (i \leftrightarrow i - 1) \quad |\psi_t\rangle = e^{-i \mathcal{H}_s t} |\psi_0\rangle
\]

Signatures of MBL transition: (ii) transitions throughout spectrum
KCMs and many-body localisation in closed quantum systems

\[ \mathcal{H}_s = -\sum_i n_{i-1} \left[ e^{-s} \sqrt{\epsilon} \sigma^x_i - \epsilon (1 - n_i) - n_i \right] + (i \leftrightarrow i - 1) \quad |\psi_t\rangle = e^{-it\mathcal{H}_s} |\psi_0\rangle \]

Signatures of MBL transition: (iii) level spacing statistics

Many symmetries in clean system

Can remove with site disorder:
\[ \epsilon \rightarrow |\epsilon - g\pi_i| \quad (g \ll \epsilon) \]

KCM dynamics unchanged

Many symmetries in clean system

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KCM dynamics unchanged
KCMs and many-body localisation in closed quantum systems

\[ \mathcal{H}_s = -\sum_i n_{i-1} \left[ e^{-s} \sqrt{\epsilon \sigma_i^x} - \epsilon(1-n_i) - n_i \right] + (i \leftrightarrow i-1) \quad |\psi_t\rangle = e^{-it\mathcal{H}_s}|\psi_0\rangle \]

Signatures of MBL transition: (iv) localisation onto classical basis

\[ \text{IPR} \]

\[ \text{LDOS} \]

\[ \Rightarrow \text{active-inactive transition} \rightarrow \text{1st order MBL transition in whole spectrum} \]

MBL transition without disorder
“Thermodynamics of trajectories” based on LD theory

Glass transition as a active/inactive transition in trajectory space

KCM glass models as models for MBL without disorder