Title: Thermalization in Quantum Systems - and its breakdown

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Abstract: <p>How does thermalization in quantum systems work? Naively, the unitary time evolution prevents thermalization, but one can easily show that in general quantum systems thermalize when brought into contact with a thermal bath. In noninteracting systems, the approach to the thermal value can be either ballistic or diffusive depending on particle statistics and bath temperature.</p>

<p> </p>

<p>However, many systems cannot be thermalized when placed in a bath: glasses.</p>

<p> </p>

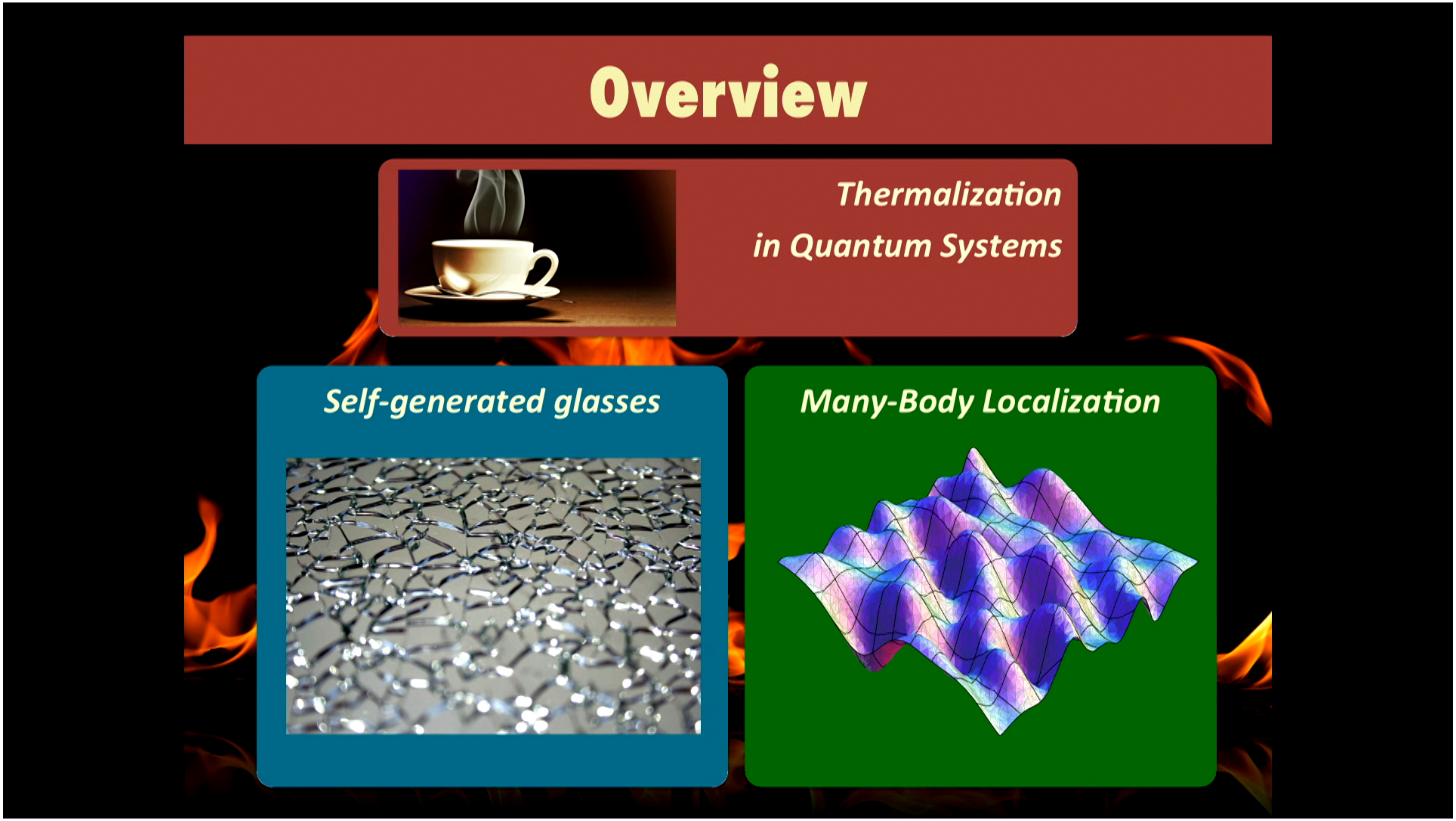
<p>I will discuss a disorderfree model of an organic electronic glass that is formed through rapid supercooling. Geometric frustration and long-range interactions cause the Arrhenius-type freezing.</p>

<p> </p>

<p>Quenched disorder can also lead to glassiness, a phenomenon known as many-body localization. In this case, thermalization is prevented by the existence of extensively many local integrals of motion. I will show how to compute these integrals of motion and their properties.</p>

Thermalization in Quantum Systems
and its breakdown

Louk Rademaker (KITP Santa Barbara)
Perimeter Institute, Wednesday 23 November 2016


Overview
Thermalization
in Quantum Systems
Self-generated glasses
Many-Body Localization

Foundations of Stat-Mech

Thermalization = **Loss** of **Memory** initial state information

In Quantum Mechanics there is **No Loss** due to **Unitary Time Evolution!**

How can Quantum Systems Thermalize?

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How can Quantum Systems Thermalize?

✧ **Eigenstate Thermalization Hypothesis** $\langle \psi_0 | \mathcal{A} | \psi_0 \rangle = Z^{-1} \mathrm{Tr}\, \mathcal{A} e^{-\beta H}$

Deutsch '91
Srednicki '94
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- **Quantum Chaos** Kitaev '15, Maldacena, Shenker, Stanford '15

  Out-of-time-ordered correlations (OTOC) $C_{WV}(t) = \langle [W(t), V(0)]^2 \rangle$

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  Polkovnikov '13

  Poissonian vs. Wigner-Dyson

- ✧ **Integrability / Conformal Field Theory**

  Existence of 'local density' integrals of motion

  Cardy, Calabrese '06
  Essler, Fagotti '16
  Doyon '15

19th Century Thermodynamics

Simpler question:

Two systems brought into contact.

Will they equilibrate?

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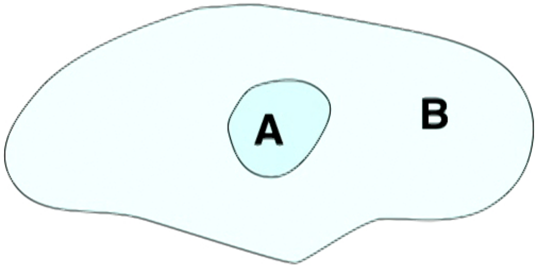
Example:

- Cup of tea/coffee in surrounding
- Superconducting sample in a fridge

In general:

- **'Hot' system A in 'cold' bath B** brought into contact at **t=0**



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Consider **Quantum system** with **A** at temperature $\mathbf{T_A}$ and **B** at temperature $\mathbf{T_B}$.

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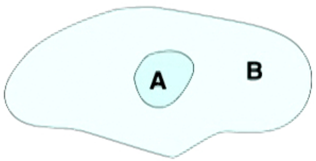

$$\mathcal{M}_0 = \beta_A H_A + \beta_B H_B + \log Z$$

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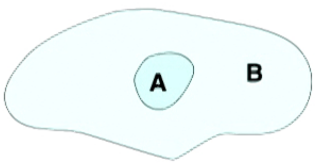

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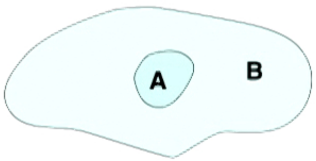

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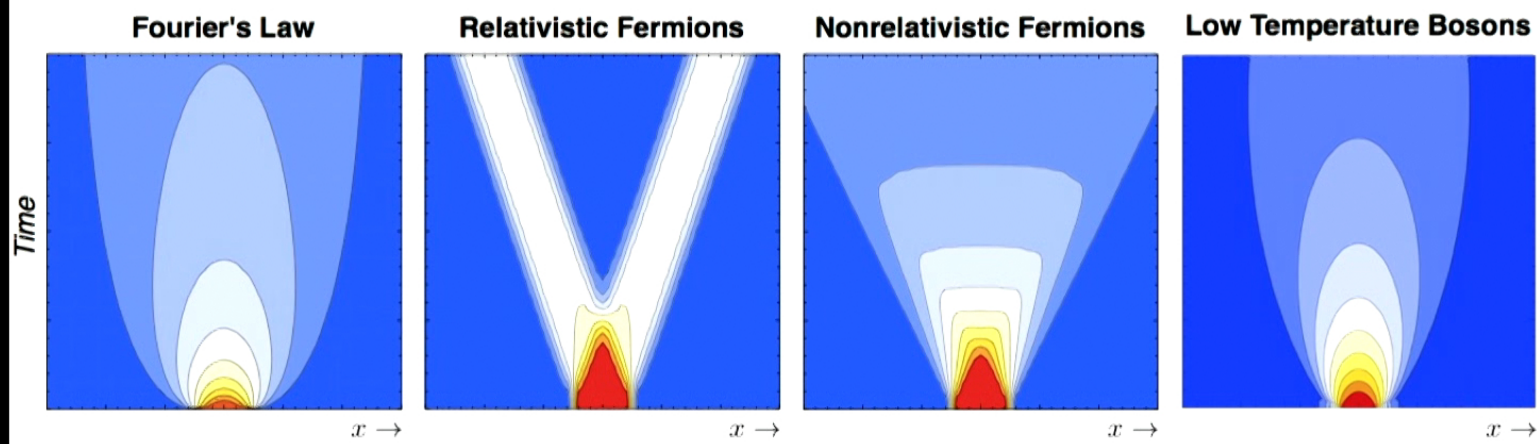
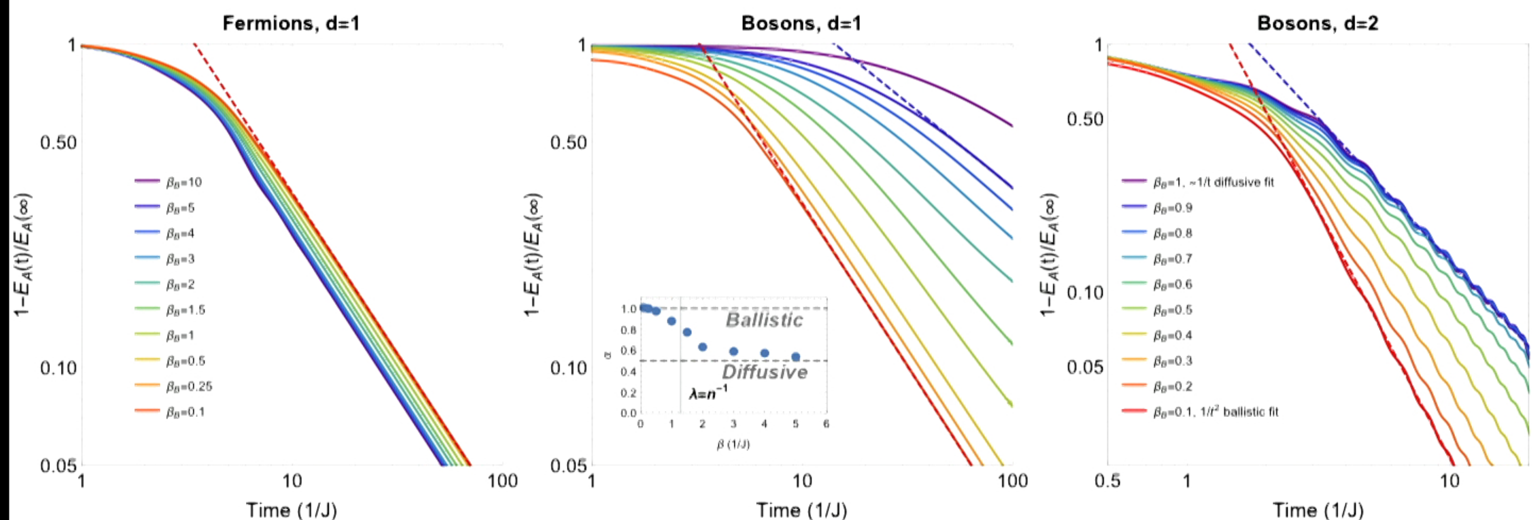
Hot flames



1. Classical expansion is **diffusive**, $\partial_t T = \mathcal{D}\nabla^2 T$, so $\Delta T \sim t^{-d/2}$
2. Relativistic fermions: **instantaneous** thermalization
3. Nonrelativistic noninteracting fermions thermalize **ballistically** $\Delta E \sim t^{-d}$
4. Bosons…

Approach to thermalization

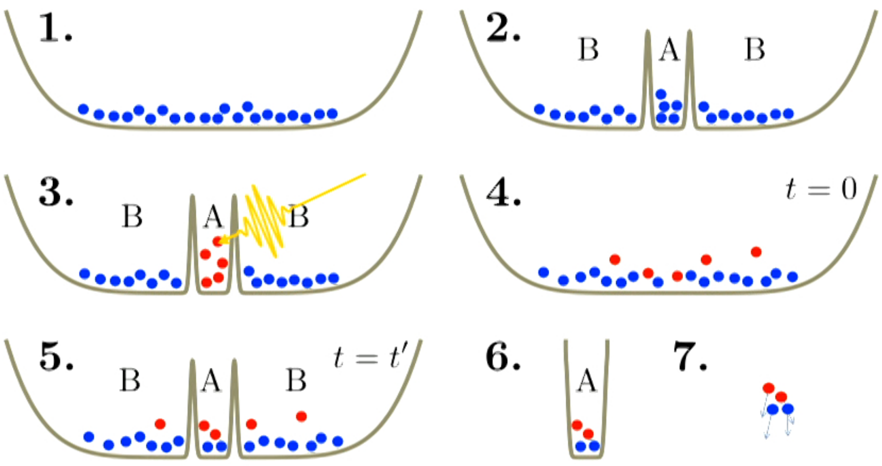


There is a **crossover** from ballistic to diffusive for bosons!

At **low temperatures**, when bosons overlap, diffusive **wave-like behavior** dominates $\partial_t \psi \sim \partial_x^2 \psi$

Experimental realization

Can test this **experimentally** with cold atoms:



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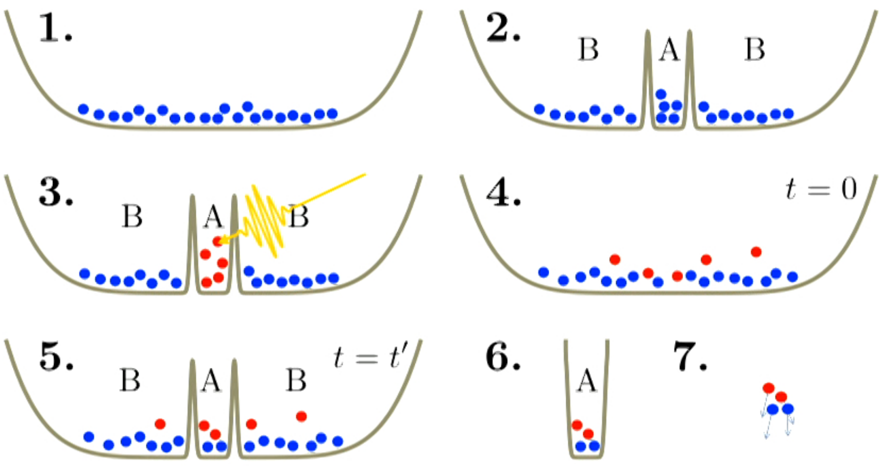

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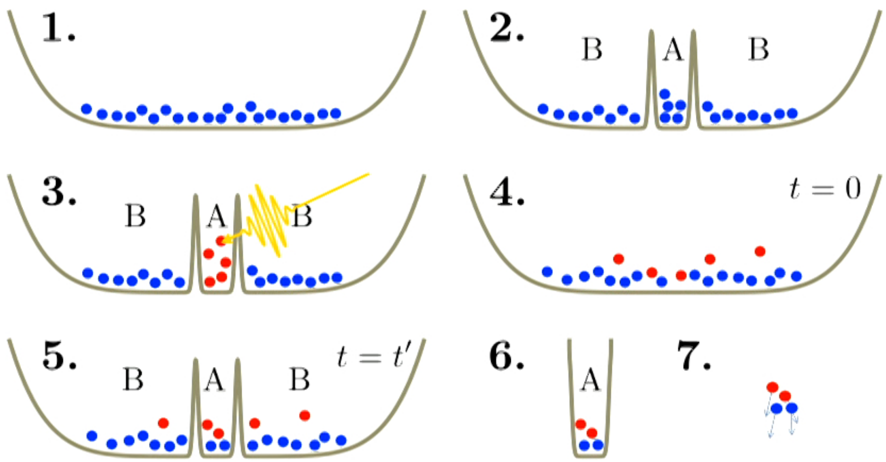

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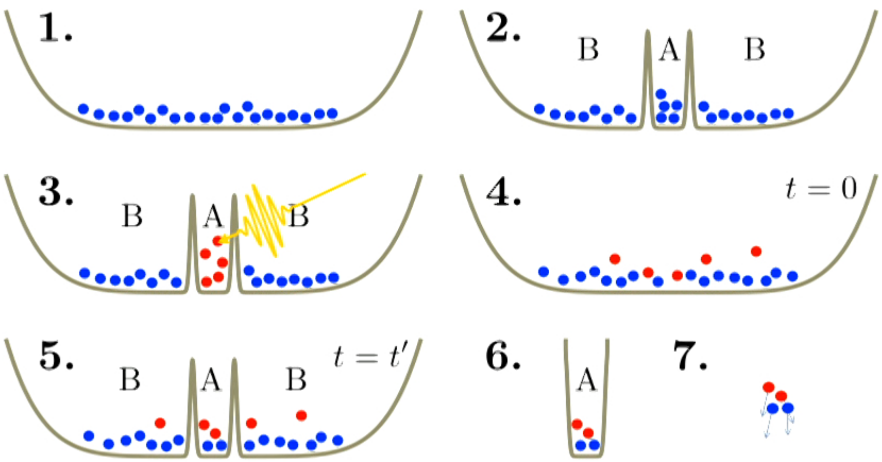

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Repeat with different 'end-times' to get $\Delta E(t)$

Thermalization - Outlook

What about **interacting nonintegrable systems**?

$$\mathcal{M}(t) = \sum_{ij} m^{(2)}_{ij}(t) b^\dagger_i b_j + \sum_{ijkl} m^{(4)}_{ijkl}(t) b^\dagger_i b^\dagger_j b_k b_l + \sum_{ijklmn} m^{(6)}_{ijklmn}(t) b^\dagger_i b^\dagger_j b^\dagger_k b_l b_m b_n + \ldots$$

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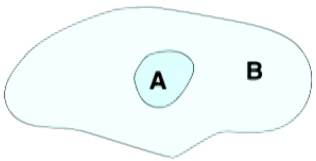

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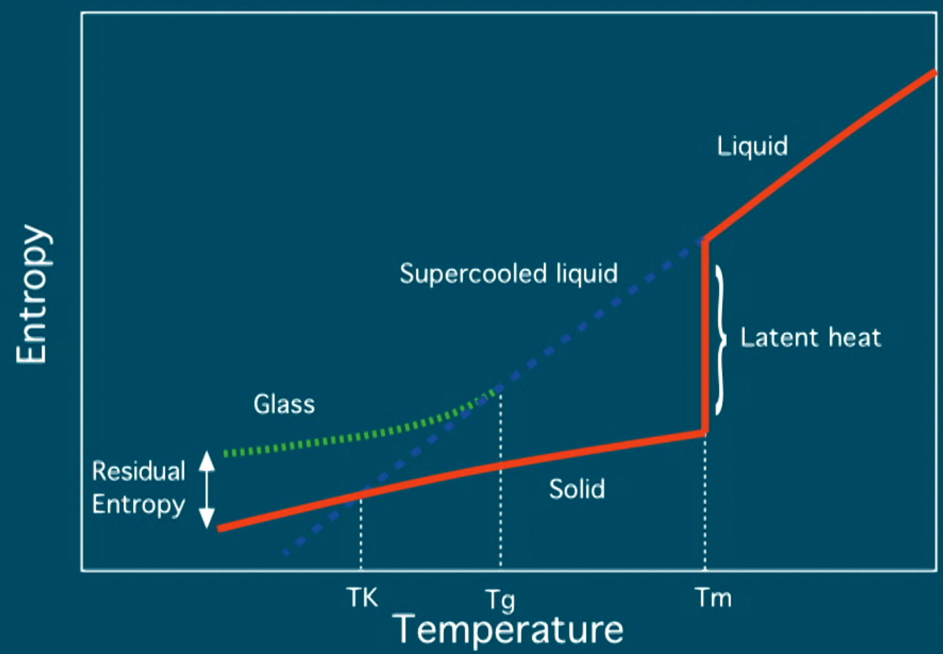
Self-generated Glasses

Fast cool to avoid a **First order transition** to make **supercool liquid**



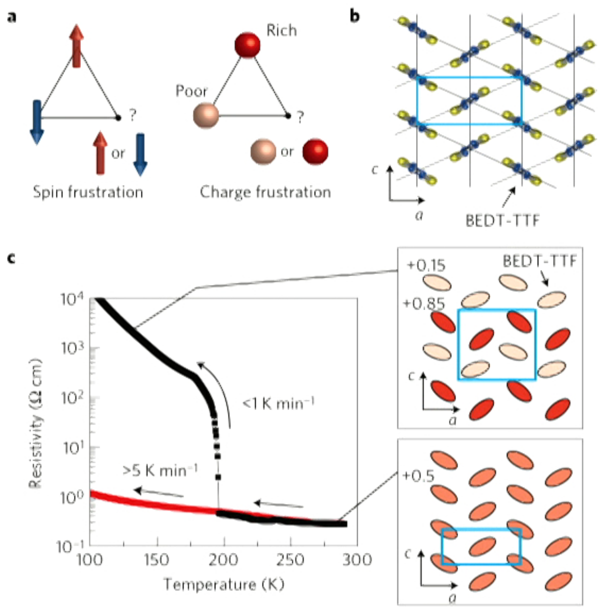
Liquid **slows down** to become **glass**

Electronic glass

Organic crystal θ-$(BEDT\text{-}TTF)_2RbZn(SCN)_4$

Low temperature electronic **stripe order**

Fast cooling: Glass with **Arrhenius dynamics**



Kagawa '14, Sato '15

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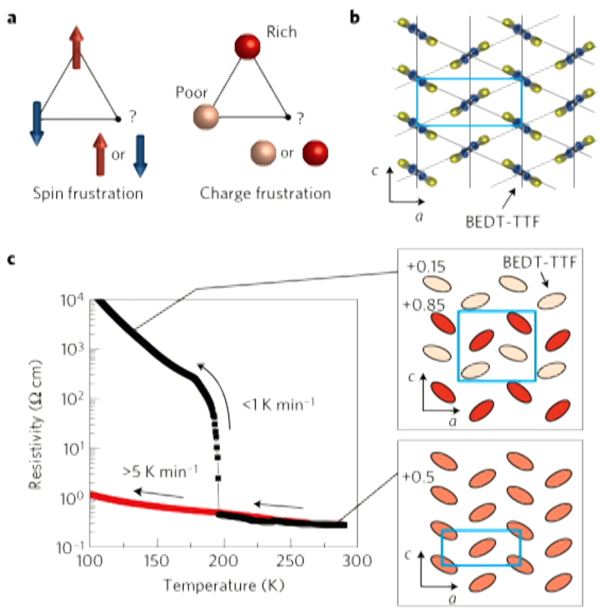

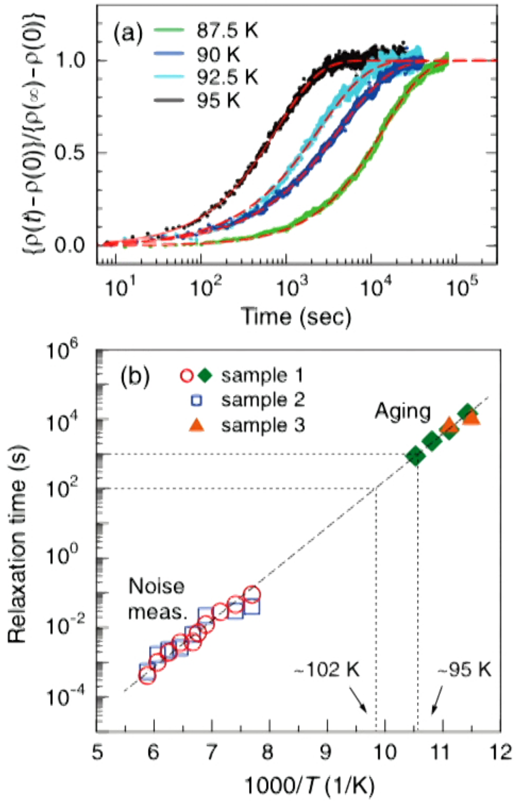

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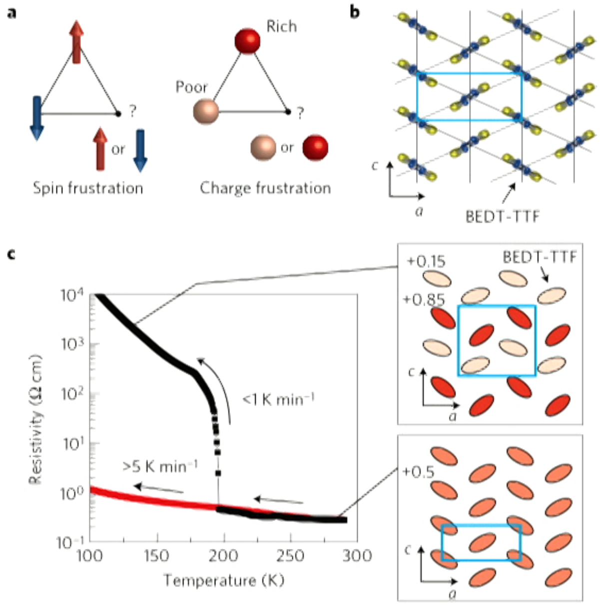

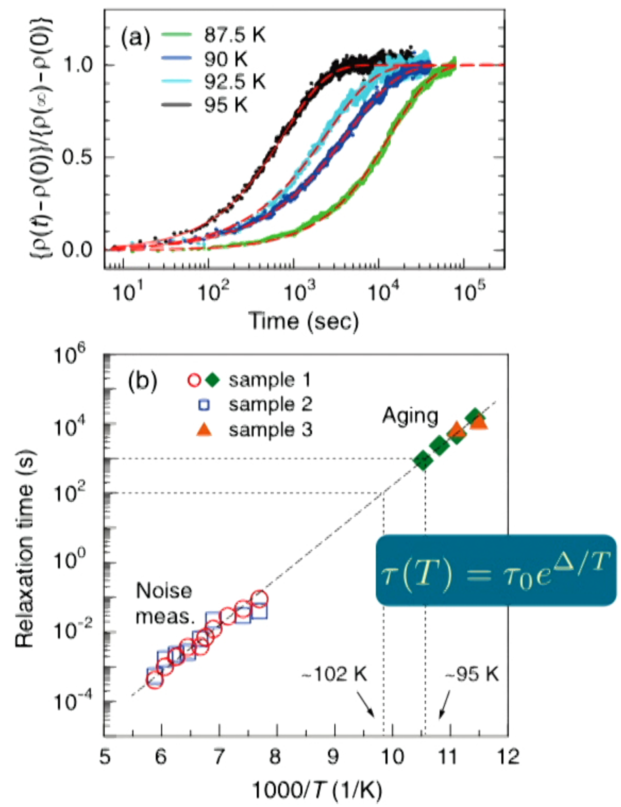

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Ising Model

Simplest interaction: **Nearest Neighbor repulsion** gives **Ising model** ($V \gg t$)

$$H = \sum_{\langle ij \rangle} V \left(n_i - \frac{1}{2} \right) \left(n_i - \frac{1}{2} \right)$$

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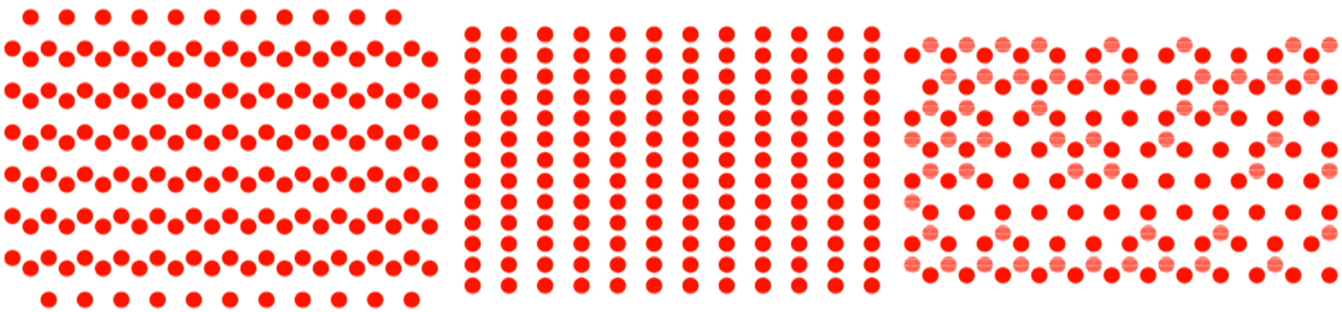

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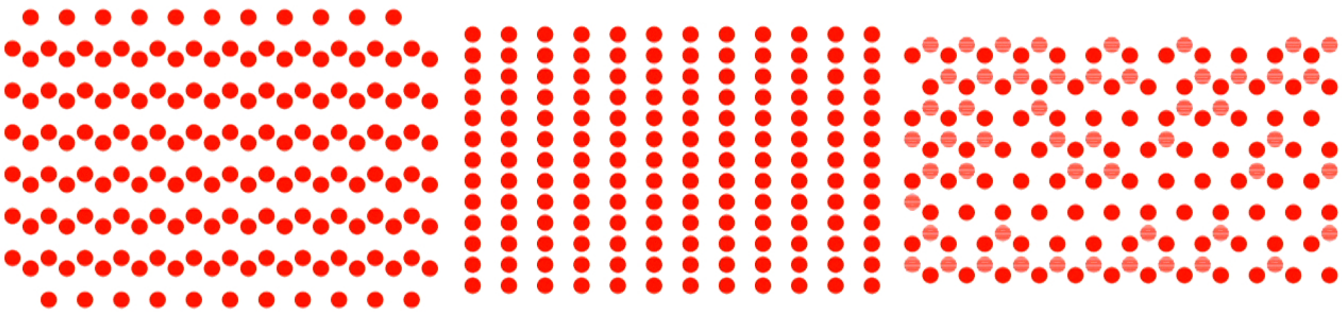
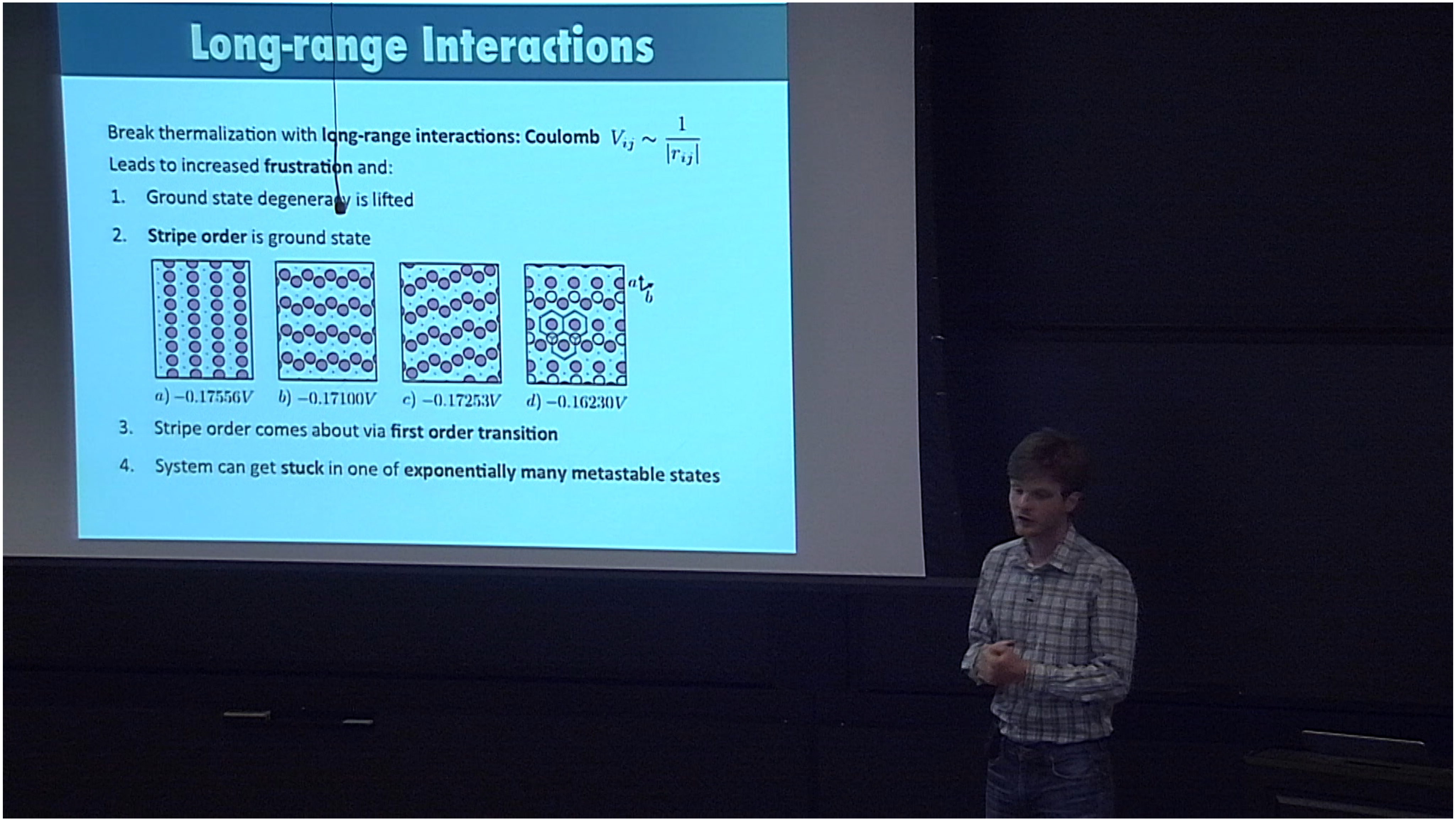


Upon inclusion of **hopping** leads to **Liquid-like state**

This cannot explain **slowing down!**


Long-range Interactions
Break thermalization with long-range interactions: Coulomb $V_{ij} \sim \frac{1}{|r_{ij}|}$
Leads to increased frustration and:
1. Ground state degeneracy is lifted
2. Stripe order is ground state
a) −0.17556V
b) −0.17100V
c) −0.17253V
d) −0.16230V
3. Stripe order comes about via first order transition
4. System can get stuck in one of exponentially many metastable states

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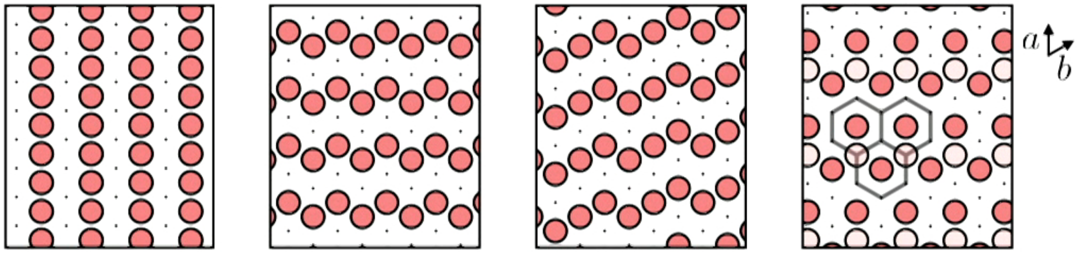

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Monte Carlo: Arrhenius-Law

Using **classic Monte Carlo**

with **Ewald summation**

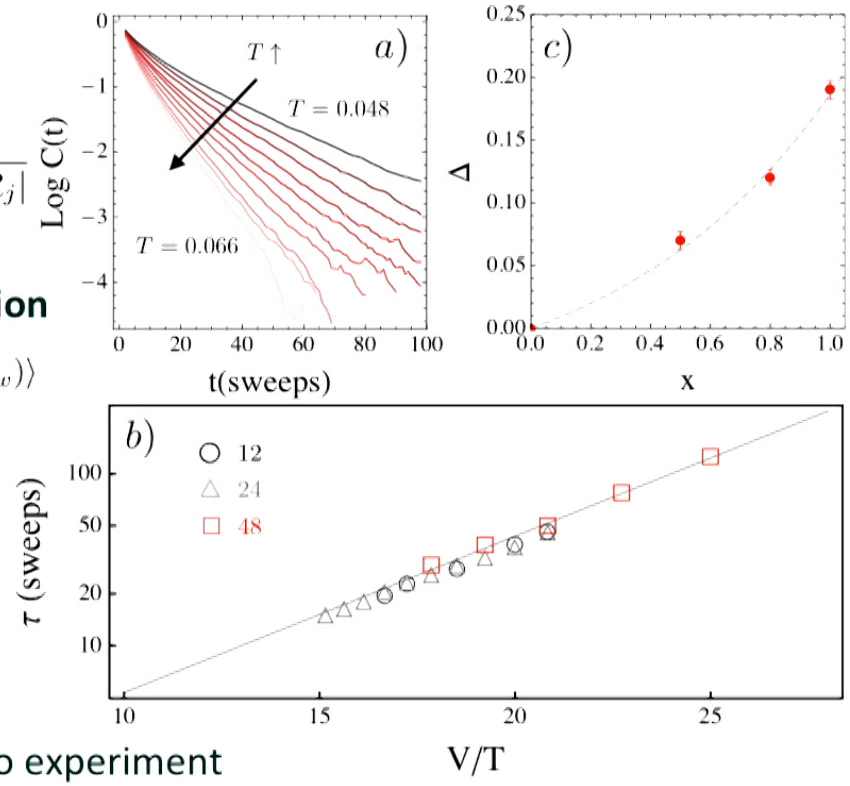
$$V_{ij} = (1-x)V\delta_{|R_i-R_j|=1} + x\frac{V}{|R_i-R_j|}$$

Measure **autocorrelation function**

$$C(t+t_w,t_w) = \frac{2}{N}\sum_i \langle \delta n_i(t+t_w)\delta n_i(t_w)\rangle$$

Find **Arrhenius Law**

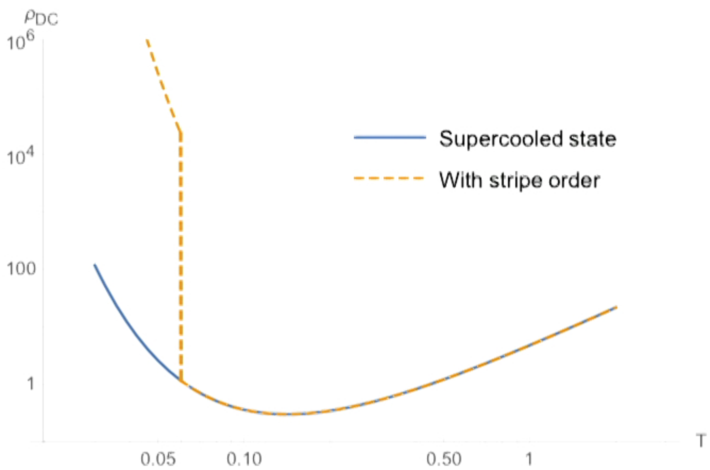
$$\tau(T) = \tau_0 e^{\Delta/T}$$



Gap $\Delta \sim 2300K$ corresponds to experiment

EDMFT: Conductivity

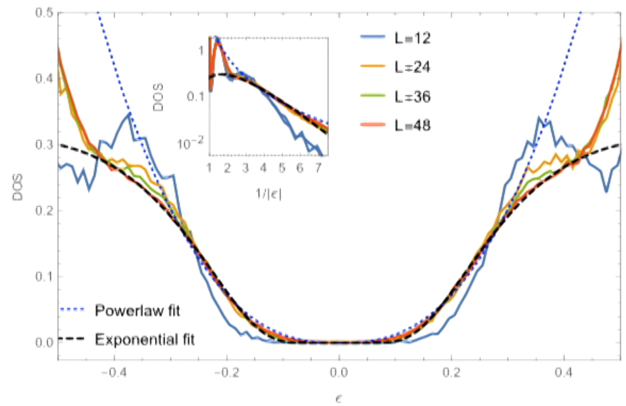
Semi-classical limit of **Extended Dynamical Mean Field Theory** yields qualitative results for **resistivity:**



$$\overline{n} - \overline{n}^2 = \sum_k \frac{1}{(\overline{n} - \overline{n}^2)^{-1} + \beta(\Delta + V_k)}$$

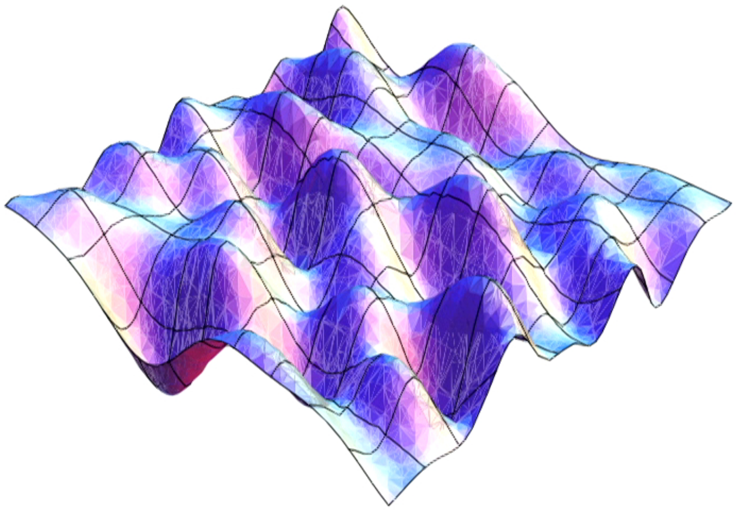
$$\sigma_{DC} \sim \int_{-\infty}^{\infty} d\omega \, \frac{\rho^2(\omega)}{4T\cosh^2\frac{\omega}{2T}} = \frac{\beta}{8}\sqrt{\frac{\beta}{\Delta\pi}}e^{-\frac{1}{4}\beta\Delta}$$

Electron glass - Outlook



1. How does the single-particle **density of states** look like?
2. What is the structure of the **manifold of metastable states**?
3. What is the relation to **ETH** and quantum **chaos**?
4. Is there a **'true' glass transition** at finite temperature?

Many-Body Localization



Quenched disorder leads to exponentially localized WF $|\Psi(r)| \sim e^{-r/\xi}$

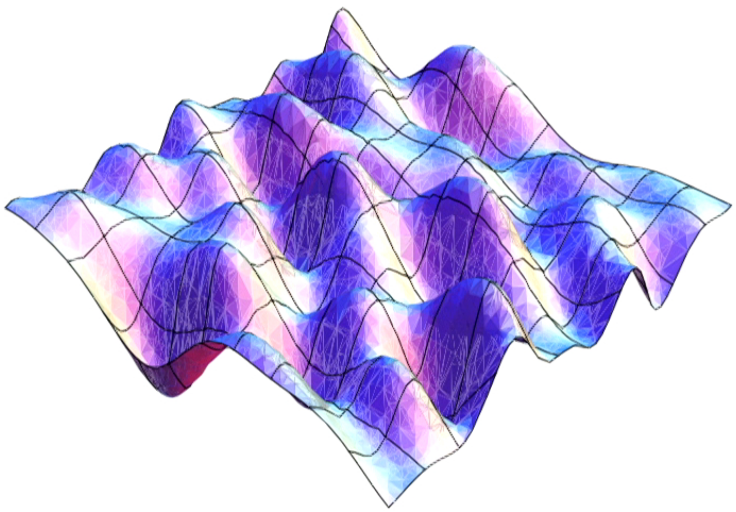
Anderson localization Hamiltonian

$$H = -t \sum_{\langle ij \rangle} (c_i^\dagger c_j + h.c.) + \sum_i \mu_i n_i$$

can be **diagonalized** $H = \epsilon_i \tilde{n}_i$

Anderson '58
Basko, Aleiner, Altshuler '06
Huse, Nandkishore, Oganesyan '14
Bardarson, Pollmann, Moore '12

Many-Body Localization



Quenched disorder leads to exponentially localized WF $|\Psi(r)| \sim e^{-r/\xi}$

Anderson localization Hamiltonian

$$H = -t \sum_{\langle ij \rangle} (c_i^\dagger c_j + h.c.) + \sum_i \mu_i n_i$$

can be **diagonalized** $H = \epsilon_i \tilde{n}_i$

Local Integrals of Motion (LIOMs)

Anderson '58
Basko, Aleiner, Altshuler '06
Huse, Nandkishore, Oganesyan '14
Bardarson, Pollmann, Moore '12

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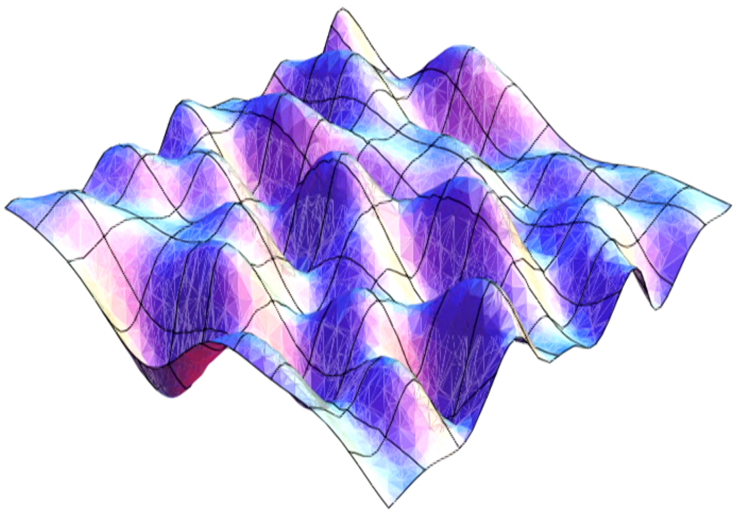

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Interactions '**dress**' Anderson integrals of motion

In **Many-Body Localized phase** LIOMs still exist that **prevent thermalization**

- **Logarithmically slow** growth of entanglement/entropy
- Vanishing **conductivity**

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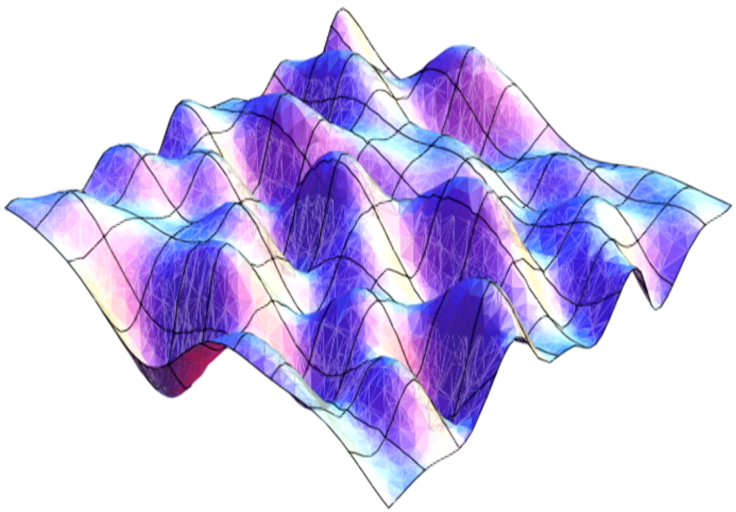

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Unitary Transformation

For every Hamiltonian, there exists a **unitary transformation** that brings it into the classical form $H = \sum_i \xi_i \tau_i^z + \sum_{ij} J_{ij} \tau_i^z \tau_j^z + \ldots$

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$X = c_\alpha^\dagger c_\beta^\dagger c_\gamma c_\delta \qquad \tan 2\lambda = -\frac{V_{\alpha\beta\gamma\delta}}{\xi_\alpha + \xi_\beta - \xi_\gamma - \xi_\delta}$

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$$H = \sum_i \xi_i \tau_i^z + \sum_{ij} J_{ij} \tau_i^z \tau_j^z$$

$$\tau_i^z = \hat{U} \hat{n}_i \hat{U}^\dagger = \hat{n}_i + \alpha_{i;jk} \hat{c}_j^\dagger \hat{c}_k + \alpha_{i;jklm} \hat{c}_j^\dagger \hat{c}_k^\dagger \hat{c}_l \hat{c}_m$$

Compute J_{ij} and $\alpha_{i;jklm}$!

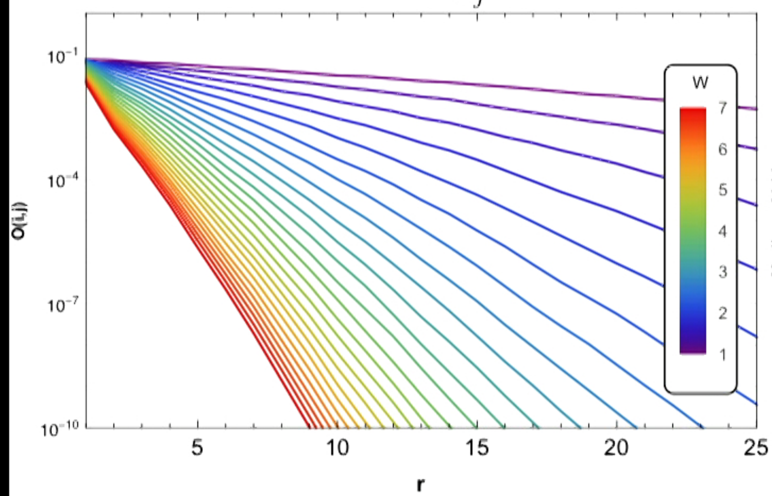
Typical Integrals of motion

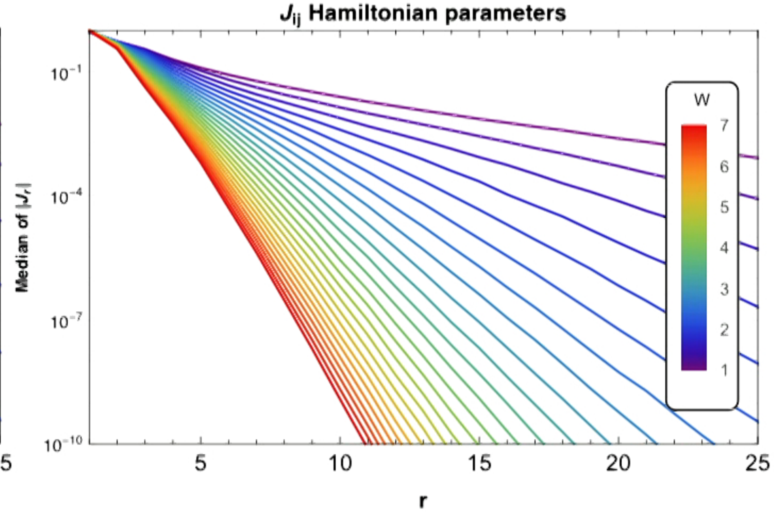
Our **model**: $H=\sum_{i=1}^{N}\epsilon_i n_i + t\sum_{i=1}^{N-1}(c_i^\dagger c_{i+1}+c_{i+1}^\dagger c_i) + V\sum_{i=1}^{N-1} n_i n_{i+1}$ $\quad \epsilon_i \in [-W/2, W/2]$

Take the **median** of all Integrals of Motion for many disorder realizations

As a function of **distance** and **disorder strength**

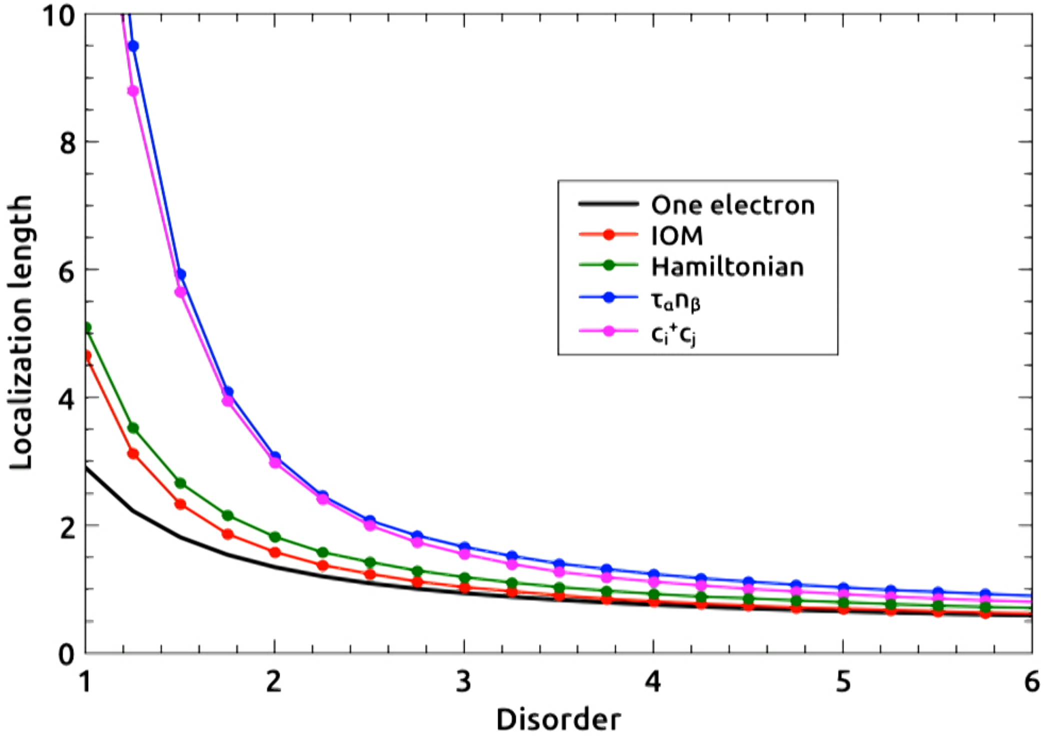
$$O(i,j)=\frac{\mathrm{Tr}\ \hat{\tau}_i^z \hat{n}_j}{\mathrm{Tr}\ \hat{n}_j}.$$





Typical Localization Length

Exponential decay can give us **localization length:**



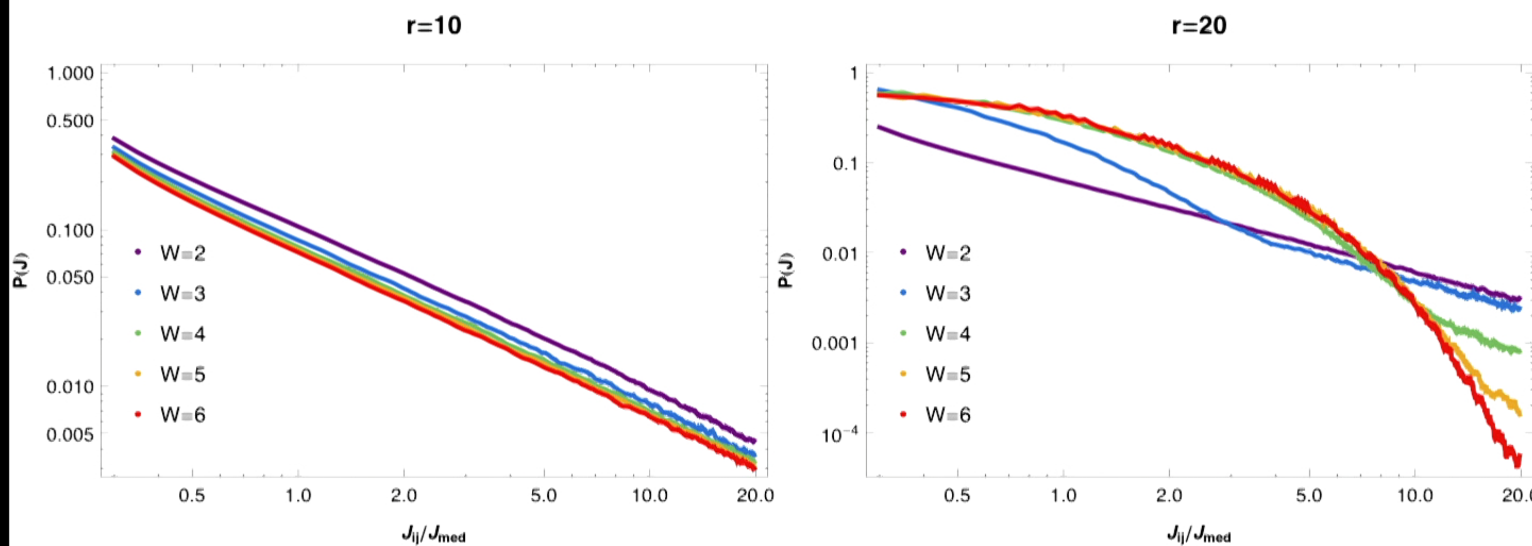
No **sign of transition**!

Rare fluctuations

Picture much less clear when looking at **Average values** instead of **Typical**

Delocalization can occur through only **few nonlocal terms**

Full distribution of J_{ij} is consistently $P(|J|) \sim 1/J$ for **weak disorder**



Many-Body Localization – Outlook

Shown that we can **compute Local Integrals of Motion**

1. How does **delocalization transition** act on integrals of motion?
   Role of rare fluctuations most likely the key factor

2. Can we compute IOMs for **other systems**?
   Heisenberg model, Hubbard model, Kondo lattice model

3. Systematic extension of **Hartree-Fock methods**?
   New class of trial wavefunctions of the form $e^{\mathcal{A}_{ij}{}^{kl} c_i^\dagger c_j^\dagger c_l c_k} c_{i_1}^\dagger \cdots c_{i_k}^\dagger |0\rangle$

Thanks to...

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Leon Balents (Santa Barbara, CA, USA)

Miguel Ortuno (Murcia, Spain)

Andres Somoza (Murcia, Spain)

Summary

Thermalization in Quantum Systems

In general: hot subsystem A in cold bath B thermalizes

Bosons have crossover from **ballistic** to **diffusive**

Reference: LR & Zaanen, soon on arXiv

Self-generated glasses

Frustration and **long-range** interactions prevent thermalization

Model & experiments show **Arrhenius law** slowing down

References: LR, Nussinov, Balents, Dobrosavljevic, arXiv:1605.01822; **LR**, Ralko, Fratini, Dobrosavljevic, arXiv:1508.03065; Mahmoudian, **LR**, Ralko, Fratini, Dobrosavljeci, PRL 115 (2015)

Many-Body Localization

Quenched disorder creates **local integrals of motion**

Computed **typical properties** of LIOMs, displays locality

MBL-to-ergodic transition requires study of **rare fluctuations**

References: LR, Ortuno, Somoza, arXiv: 1610.06238; **LR**, Ortuno, PRL 116 (2015)