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Flow Equation Methods for **Many-Body Localisation**

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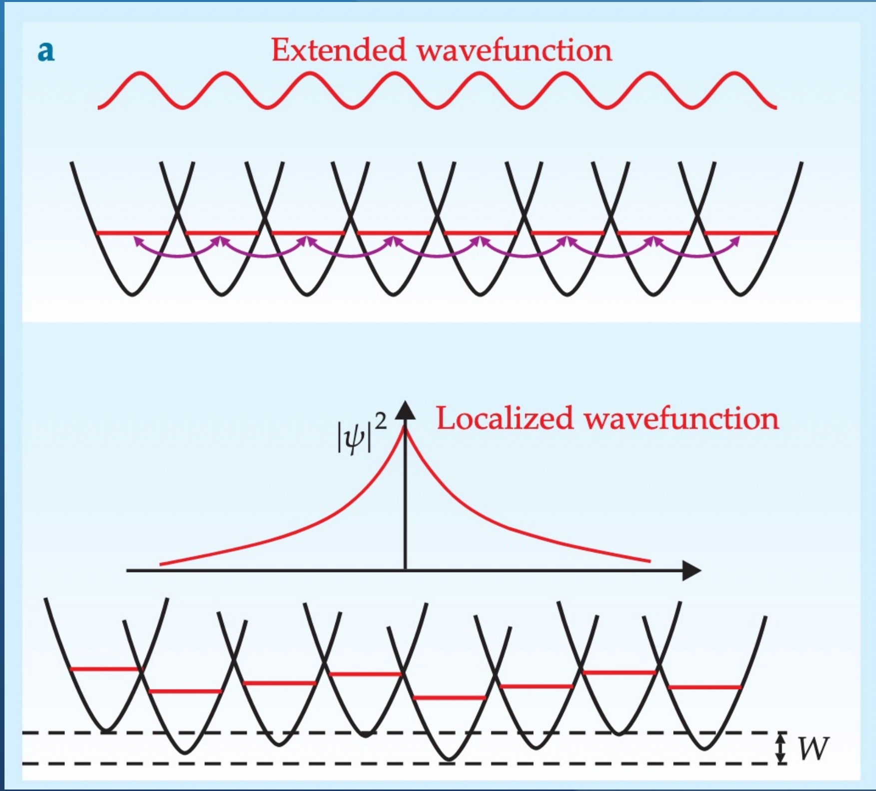
@PhysicsSteve
@EBQM_

What is (Single-Particle) Localisation?

- In a **disorder-free** system, wavefunctions are **extended**
- In a **disordered** system, wavefunctions are **localised**
  - **No thermalisation!**
- Localisation is an **interference effect**

  Anderson localisation



Aspect & Inguscio, *Physics Today* **35** (2009)

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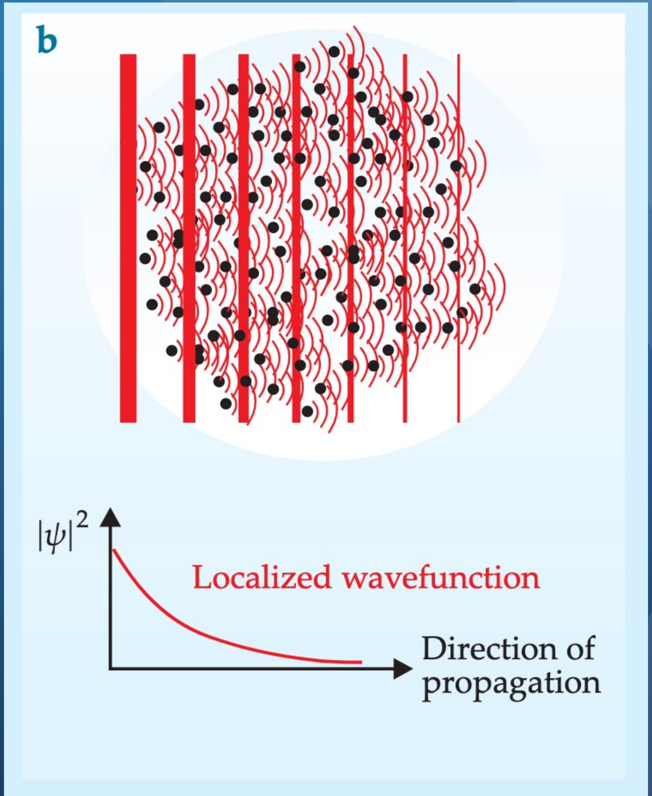
  Anderson localisation

  Fragile, easily destroyed!

  (e.g. by temperature, coupling to an environment, many-body interactions…?)

- Or is it…?



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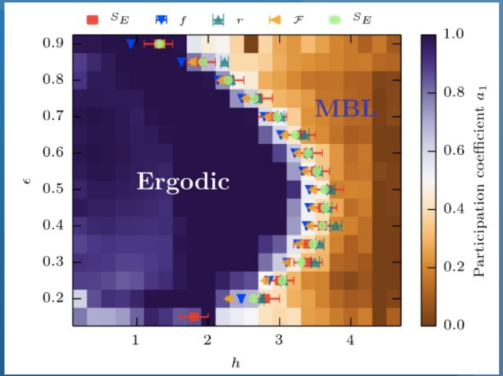
Many-Body Localisation (MBL)

- In a nutshell, MBL is Anderson localisation + interactions
- Not a ground state property: eigenstates at *any* energy density can be localised
- Most numerical work on MBL focuses on the disordered XXZ model in 1D:

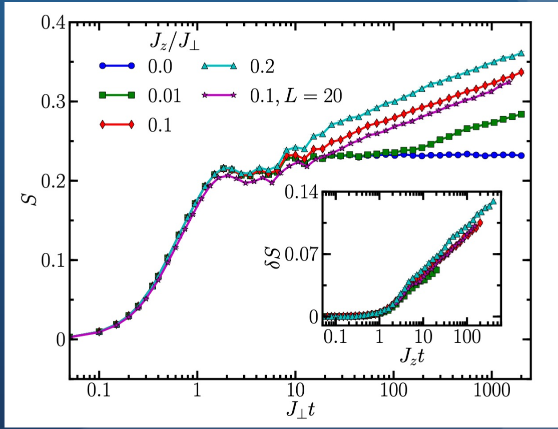
$$\mathcal{H} = \sum_i \left[J(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + J_z S_i^z S_{i+1}^z) + h_i S_i^z \right]$$

(with $h_i \in [-W, W]$)

- Many strange properties: logarithmic (slow) growth of entanglement entropy with time, long 'memory' of initial conditions…



PRB 91, 981103 (2015)



PRL 109, 017202 (2012)

Local Integrals of Motion

- Almost all observed features can be explained using the "l-bit" model
  ("l-bits" are *localised bits*, also known as Local Integrals of Motion or LIOMs)

$$\tilde{\mathcal{H}} = \sum_i h_i \tau_i^z + \sum_{ij} J_{ij} \tau_i^z \tau_j^z + \sum_{ijk} J_{ijk} \tau_i^z \tau_j^z \tau_k^z \ldots$$

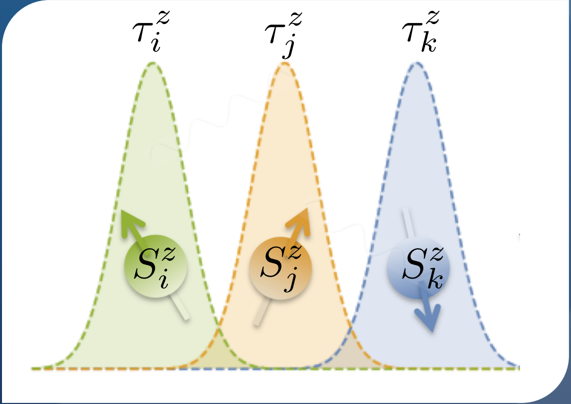
Huse *et al.*, PRB **90**, 174202 (2014), Serbyn *et al.*, PRB **90**, 174302 (2014), Ros *et al.*, Nuc. Phys. B **891**, 420 (2015)

where the coefficients $J_{ij\ldots}$ decay exponentially with distance $\sim \exp[|i-j|/\xi]$

- This 'toy model' is related to the microscopic XXZ model by a (quasi-local) unitary transform:

$$\tilde{\mathcal{H}} = U^\dagger \mathcal{H} U \qquad \tau_i^z = U S_i^z U^\dagger$$

- But how to compute this in practice?



Diagonalising a many-body problem

- Let's say we want to diagonalise a Hamiltonian $\mathcal{H} = \mathcal{H}_0 + V$ where H_0 contains the diagonal terms, and V contains the off-diagonal terms.
- We want to use a unitary transform to try to obtain the *l*-bit diagonal form.
- Try a Schrieffer-Wolff transform:

$$\boxed{\tilde{\mathcal{H}} = \mathrm{e}^{S}\mathcal{H}\mathrm{e}^{-S} = \mathcal{H} + [S, \mathcal{H}] + \ldots}$$

  - To leading order, can diagonalise H by choosing S such that [S,H] = -V
  - ...but higher-order terms complicate things and prevent this transform from being exact

- **Key idea**: instead of one 'large' unitary transform, let's make infinitely many infinitely small transforms.

The Flow Equation Method

- Build the full transform using a series of **infinitesimal unitary transforms**:
  - Parameterise transform by a fictitious *flow time* denoted l

$$\mathcal{H}(l=0) \longrightarrow \longrightarrow \longrightarrow \longrightarrow \mathcal{H}(l\to\infty) = \tilde{\mathcal{H}}$$

  - **l=0** is the initial microscopic basis, and **l → ∞** is the diagonal basis
  - Apply infinitesimal unitary transform:

$$\boxed{\begin{aligned}\mathcal{H}(l+\mathrm{d}l) &= \mathrm{e}^{\mathrm{d}l\,\eta(l)}\mathcal{H}(l)\mathrm{e}^{-\mathrm{d}l\,\eta(l)} \\ &= \mathcal{H}(l) + \mathrm{d}l[\eta(l),\mathcal{H}(l)]\end{aligned}}$$

(where $\eta(l)$ is a generator to be chosen later)

- Flow of Hamiltonian given by:

$$\boxed{\frac{\mathrm{d}\mathcal{H}}{\mathrm{d}l} = [\eta(l),\mathcal{H}(l)]}$$

A Toy Example

- For non-interacting spinless fermions in a disordered potential:

$$\boxed{\mathcal{H} = \mathcal{H}_0 + V = \sum_i h_i c_i^\dagger c_i + \frac{1}{2}\sum_i J_i (c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i)}$$

A Toy Example

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$$\mathcal{H}(l) = \mathcal{H}_0(l) + V(l) = \sum_i h_i(l) c_i^\dagger c_i + \frac{1}{2}\sum_{i \neq j} J_{ij}(l)(c_i^\dagger c_j + c_j^\dagger c_i)$$

- With Wegner's choice* of generator $\eta = [\mathcal{H}_0, V]$, the flow equations are:

$$\begin{aligned} \frac{\mathrm{d}\mathcal{H}}{\mathrm{d}l} &= [\eta, \mathcal{H}] = [[\mathcal{H}_0, V], \mathcal{H}] \\ &= -\frac{1}{2}\sum_{ij} \left(J_{ij}(h_i - h_j)^2 + \sum_k J_{ik} J_{kj} (2h_k - h_i - h_j) \right) (c_i^\dagger c_j + c_j^\dagger c_i) \end{aligned}$$

* See e.g. F. Wegner, Ann. Phys. **506**, 77 (1994), S. Kehrein, *The Flow Equation Approach to Many-Particle Systems* (2007)

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- With Wegner's choice* of generator $\eta = [\mathcal{H}_0, V]$, the flow equations are:

$$\frac{\mathrm{d}J_{ij}}{\mathrm{d}l} = -J_{ij}(h_i - h_j)^2 - \sum_k J_{ik} J_{kj} (2h_k - h_i - h_j)$$

$$\frac{\mathrm{d}h_i}{\mathrm{d}l} = 2J_{ij}^2 (h_i - h_j)$$

$$\boxed{J_{ij}(l) \sim \mathrm{e}^{-l(h_i - h_j)^2} J_{ij}(0)}$$

* See e.g. F. Wegner, Ann. Phys. **506**, 77 (1994), S. Kehrein, *The Flow Equation Approach to Many-Particle Systems* (2007)

Interacting Fermions

- Specify to a model of *interacting* fermions (equivalent to XXZ spin chain):

$$\mathcal{H} = \sum_i h_i c_i^\dagger c_i + \frac{1}{2} J_0 \sum_i (c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i) + \Delta_0 \sum_i n_i n_{i+1}$$

- Under the action of the flow equation method, the Hamiltonian becomes diagonal in the single-particle basis and takes the following form:

$$\tilde{\mathcal{H}} = \sum_i \tilde{h}_i \tilde{n}_i + \sum_{ij} \tilde{\Delta}_{ij} \tilde{n}_i \tilde{n}_j + \cancel{\sum_{ijk} \tilde{\Delta}_{ijk} \tilde{n}_i \tilde{n}_j \tilde{n}_k} + \ldots$$

  - Problem: generates (many…) new couplings

- Solution: **truncate** the running Hamiltonian
  - Restricts us to either the **strong disorder** or **weak interaction** limit
  - Expect to describe the MBL phase well

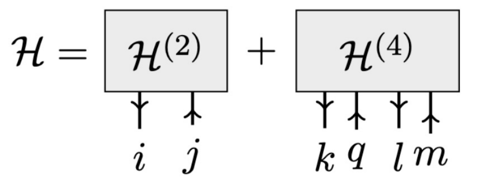
(Alternatively, implement exactly on small systems: PRL **119**, 075701 (2017))

The Flow Equation Method

arXiv:2110.02906

- Introduce graphical notation for a generic interacting (fermionic) Hamiltonian:

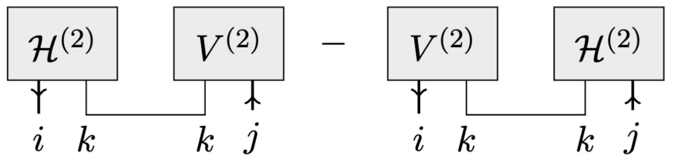
$$\mathcal{H} = \sum_{ij} \mathcal{H}^{(2)}_{ij} + \sum_{kqlm} \mathcal{H}^{(4)}_{kqlm}$$
$$= \sum_{ij} H^{(2)}_{ij} : c^\dagger_i c_j : + \sum_{kqlm} H^{(4)}_{kqlm} : c^\dagger_k c_q c^\dagger_l c_m :$$



$$\eta = [\mathcal{H}_0, V] = \left[\mathcal{H}^{(2)}, V^{(2)}\right] + \left[\mathcal{H}^{(4)}, V^{(2)}\right] + \left[\mathcal{H}^{(2)}, V^{(4)}\right] + \ldots$$

- Commutators can be computed by sum of all one-point contractions, e.g.:

$$\left[\mathcal{H}^{(2)}, V^{(2)}\right] = \sum_{ijk} \left(\mathcal{H}^{(2)}_{ik} V^{(2)}_{kj} - V^{(2)}_{ik} \mathcal{H}^{(2)}_{kj}\right)$$



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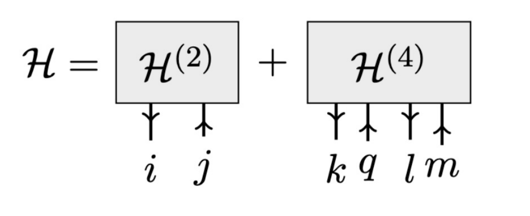
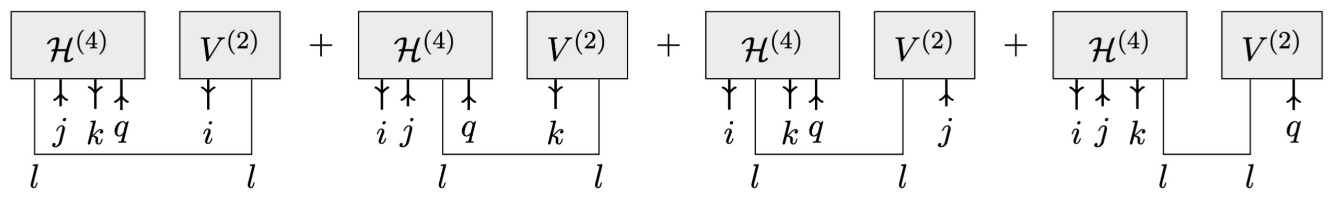
&= \sum_{ij} H^{(2)}_{ij} :c^\dagger_i c_j: + \sum_{kqlm} H^{(4)}_{kqlm} :c^\dagger_k c_q c^\dagger_l c_m:
\end{aligned}
$$



- The same goes for higher-order commutators:



- Why? Systematic extension to higher orders, efficient to compute using modern parallel processing techniques (GPUs!), friendlier 'tensor network'-like notation.

Aubry-André-Harper Model (1D)

$$\mathcal{H} = \sum_i h_i c_i^\dagger c_i + \frac{1}{2} J_0 \sum_i (c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i) + \Delta_0 \sum_i n_i n_{i+1}$$

- Instead of random disorder, use a quasiperiodic potential:

$$h_i = W \cos(2\pi i/\phi + \theta)$$

where ϕ is some irrational number and θ is a random global phase

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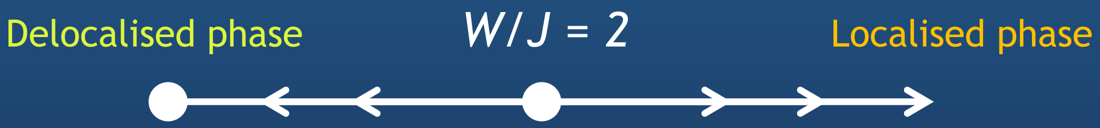
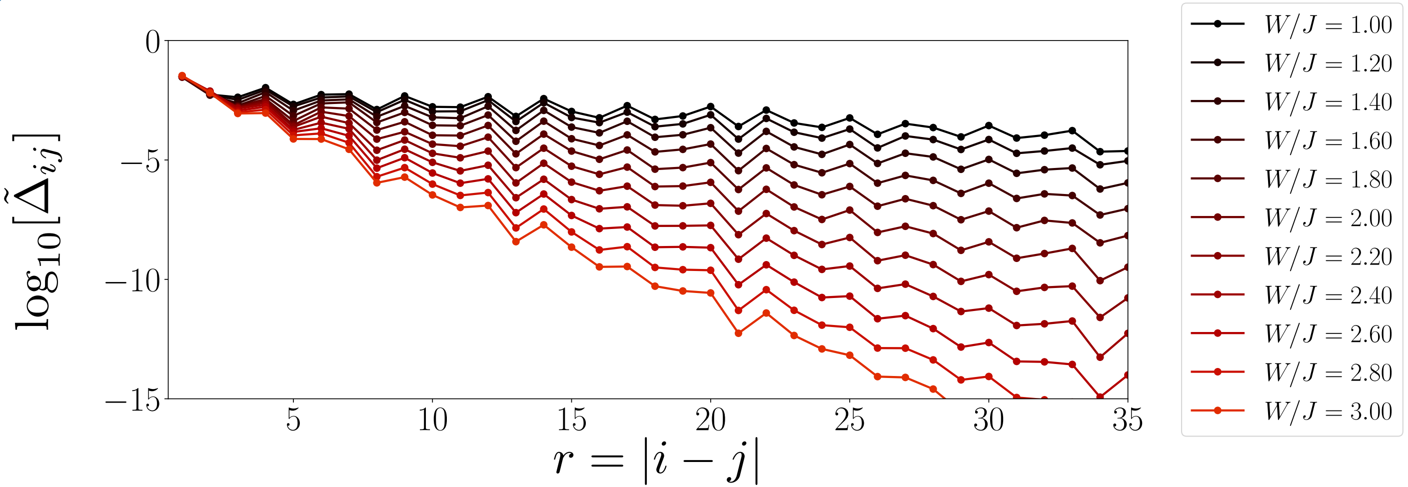
- Non-interacting system: phase transition at W/J=2



(At critical point, energy spectrum is a Cantor set - only example I know of a system exhibiting level *attraction*...!)

Interacting Aubry-André-Harper Model (1D)

- Compute the l-bit interactions: $\tilde{\mathcal{H}} = \sum_i \tilde{h}_i \tilde{n}_i + \sum_{ij} \tilde{\Delta}_{ij} \tilde{n}_i \tilde{n}_j$



$\Delta_0 = 0.1$

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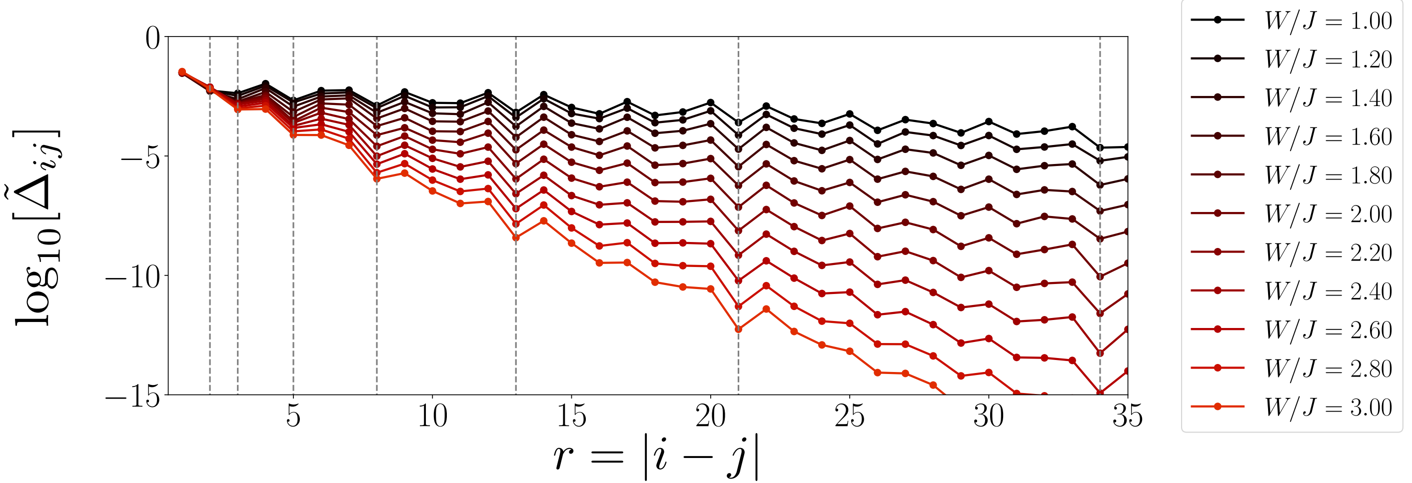

- Strange 'dips' at **j = 2, 3, 5, 8, 13, 21, 34…?**
  - Fibonacci numbers!
  - Comes from choice of incommensurate potential: here the golden ratio
  - Physical reason: resonances for all p, q where $p/q \approx \phi$

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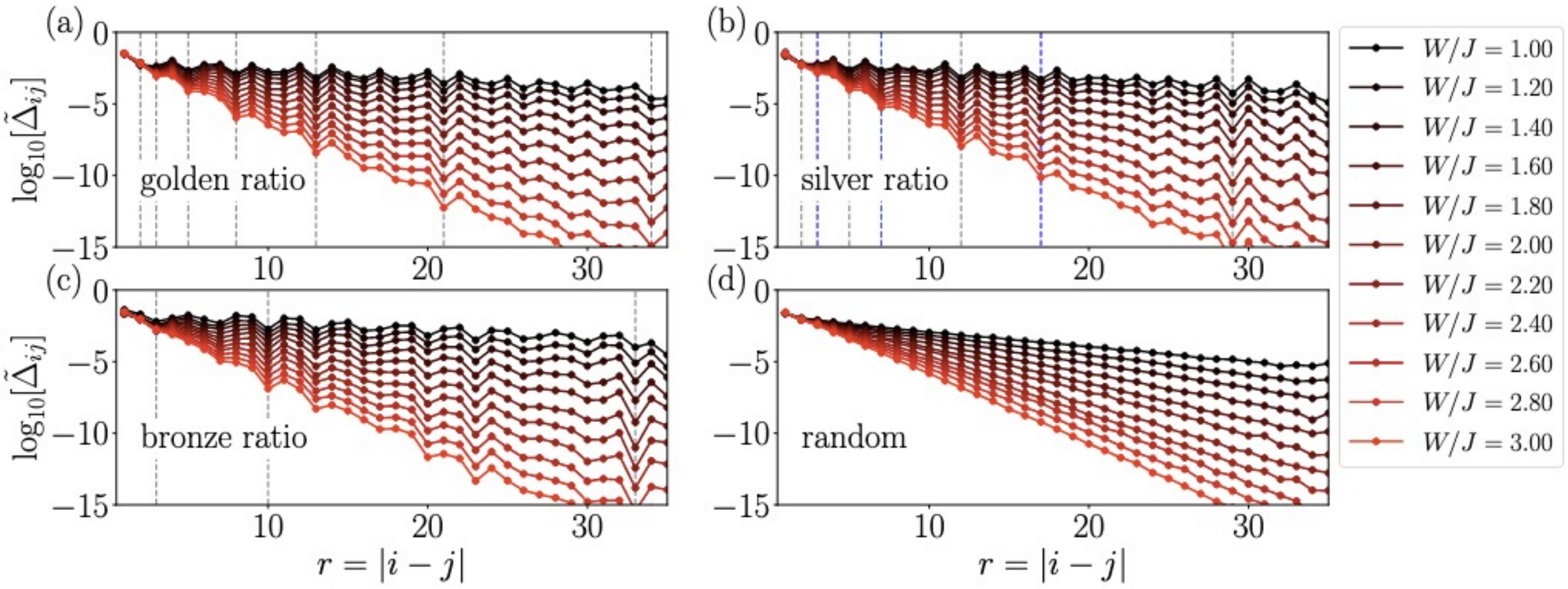
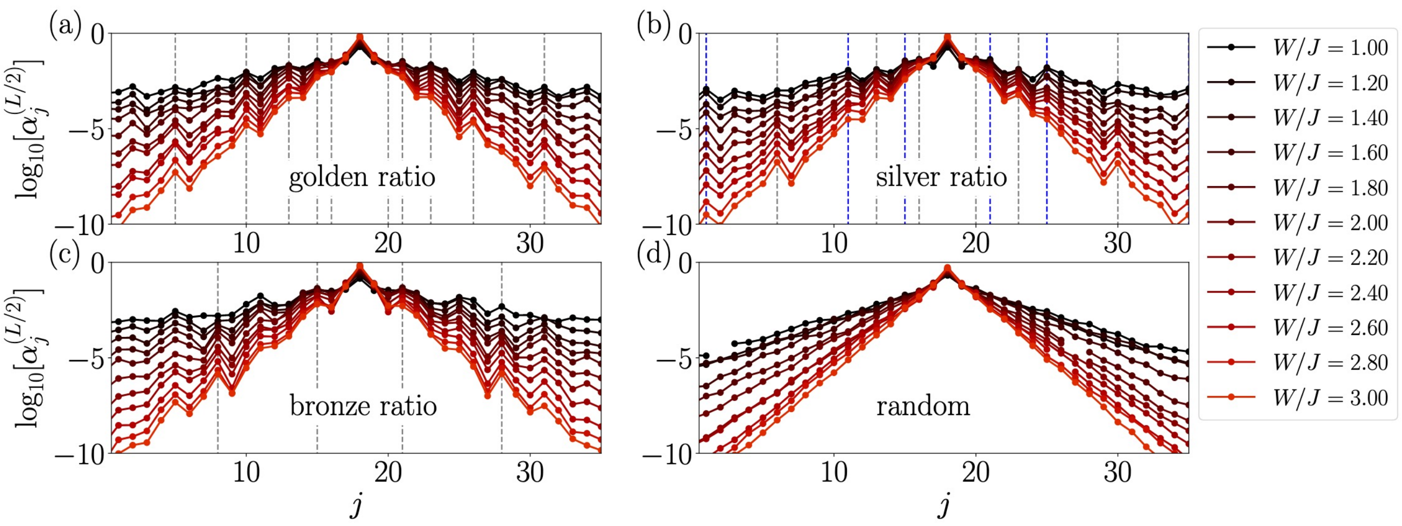


Evidence for a phase transition

- We can also directly compute the *l*-bits:

$$\tilde{n}_i = \sum_j \alpha_j^{(i)} : n_j : + \sum_{j\neq k} \beta_{jk}^{(i)} : c_j^\dagger c_k : + \sum_{j\neq k} \gamma_{jk}^{(i)} : n_j n_k : + \sum_{j\neq k \vee l \neq m} \xi_{jklm}^{(i)} : c_j^\dagger c_k c_l^\dagger c_m : \ldots$$



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- Define two ratios which measure the quadratic and quartic 'weights' respectively:

$$f_2 = \frac{\sum_j |\alpha_j^{(i)}|^2 + \sum_{jk} |\beta_{jk}^{(i)}|^2}{||n||^2}$$

$$f_4 = \frac{\sum_{jk} |\Delta_{jk}^{(i)}|^2 + \sum_{jkpq} |\xi_{jkpq}^{(i)}|^2}{||n||^2}$$

- Delocalised phase: $f_2/f_4 \rightarrow 0$
- Localized phase: $f_4/f_2 \rightarrow 0$

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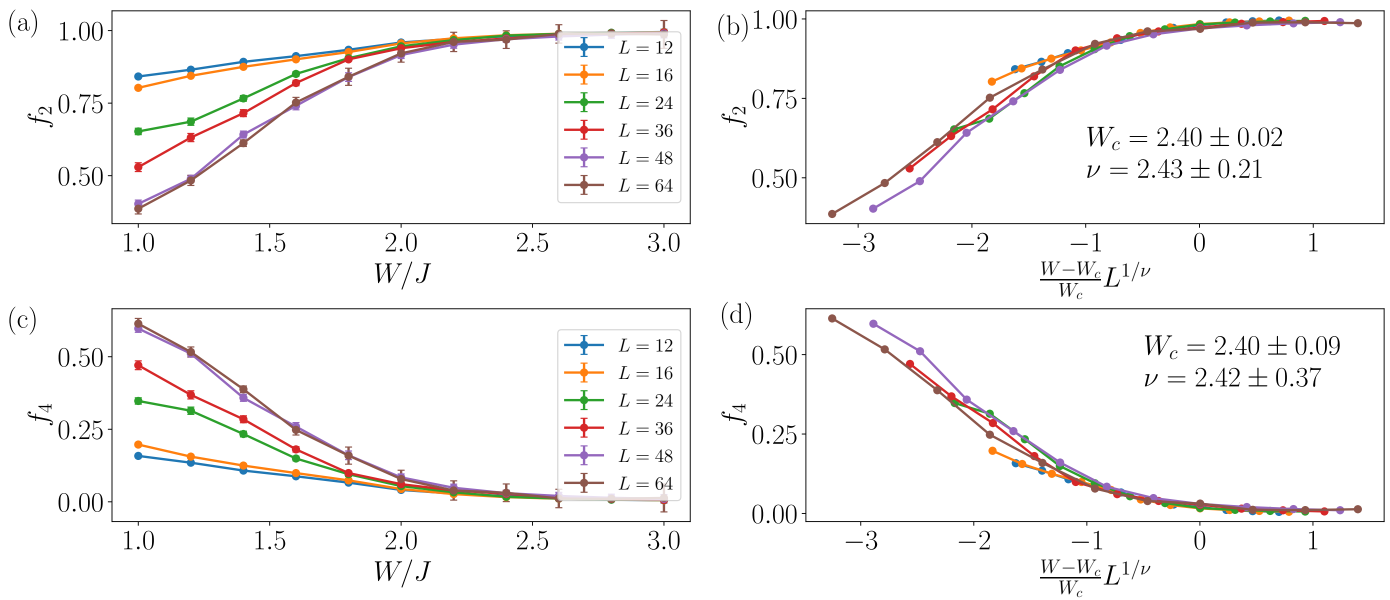
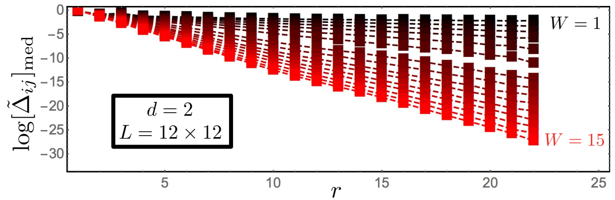


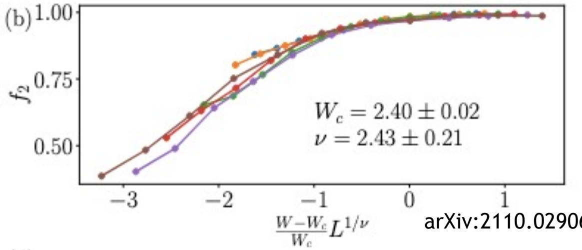
Summary

- **Local Integrals of Motion**:
  - Numerically construct LIOMs in d=1,2,3
  - Evidence for phase transition
- **Dynamics**:
  - Method can be used to compute quench dynamics
  - Imbalance, correlation functions, etc… Eur. Phys. J. B 93 (22)
- **Periodic drive**:
  - Extension to Floquet systems
  - Periodic drive = **synthetic extra dimension**
  - Floquet LIOMs!

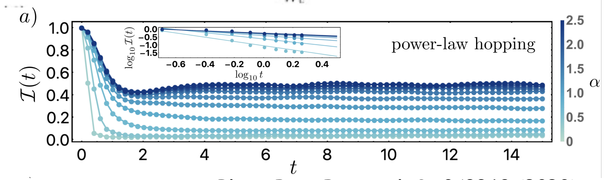
- **Future directions:**
  - ○ Hubbard model *(in progress…!)*
  - ○ Wannier-Stark localisation *(in progress…!)*
  - ○ Drive + disorder = time crystals…?
  - ○ Unitary transforms for MPOs



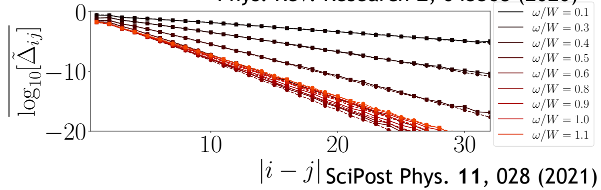
Phys. Rev. B 97, 060201 (2018)



arXiv:2110.02906



Phys. Rev. Research **2**, 043368 (2020)

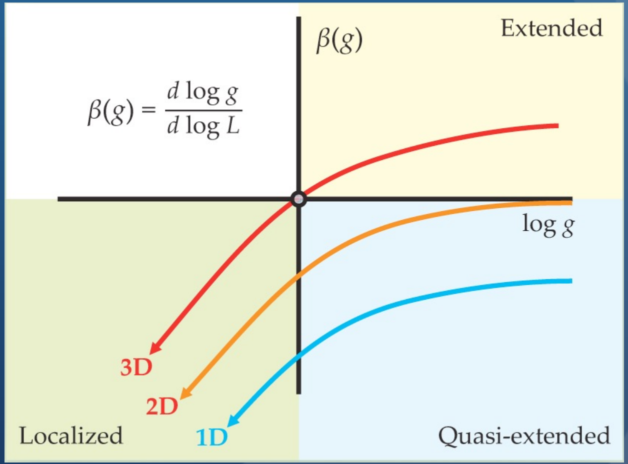


SciPost Phys. **11**, 028 (2021)

When does ETH fail?

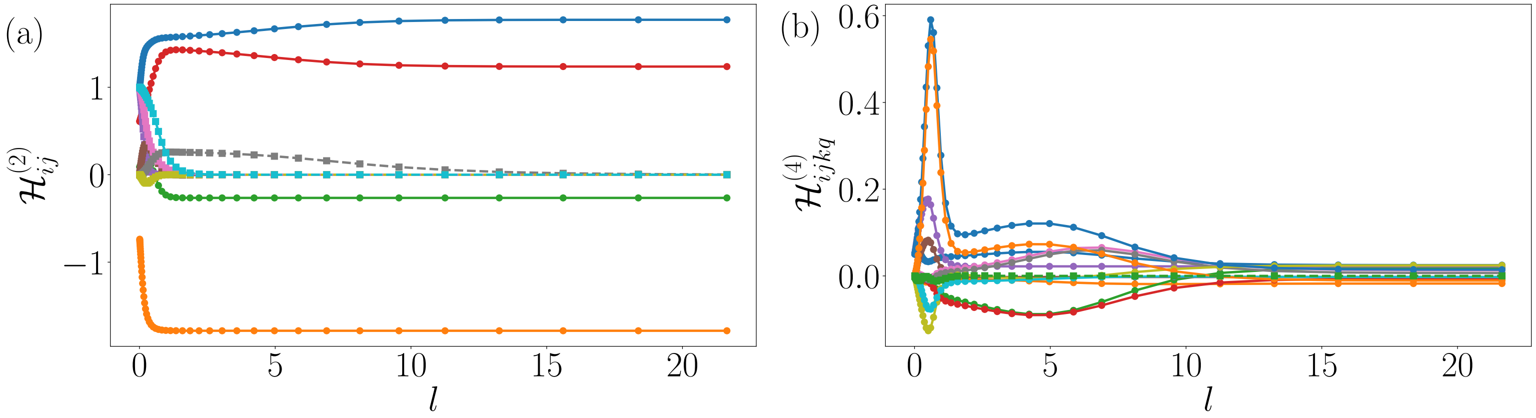
- The Eigenstate Thermalisation Hypothesis fails in certain cases:
  - *Integrable systems* have an extensive number of conserved quantities which prevent the system from thermalising
  - *Disordered systems* can spontaneously fail to thermalise, even if they are non-integrable

- A case which is both *disordered* and *integrable*:
  - Anderson Localisation
  - Non-interacting quantum systems in d<3 are localised by any finite concentration of disorder (in d=3 there is a transition)

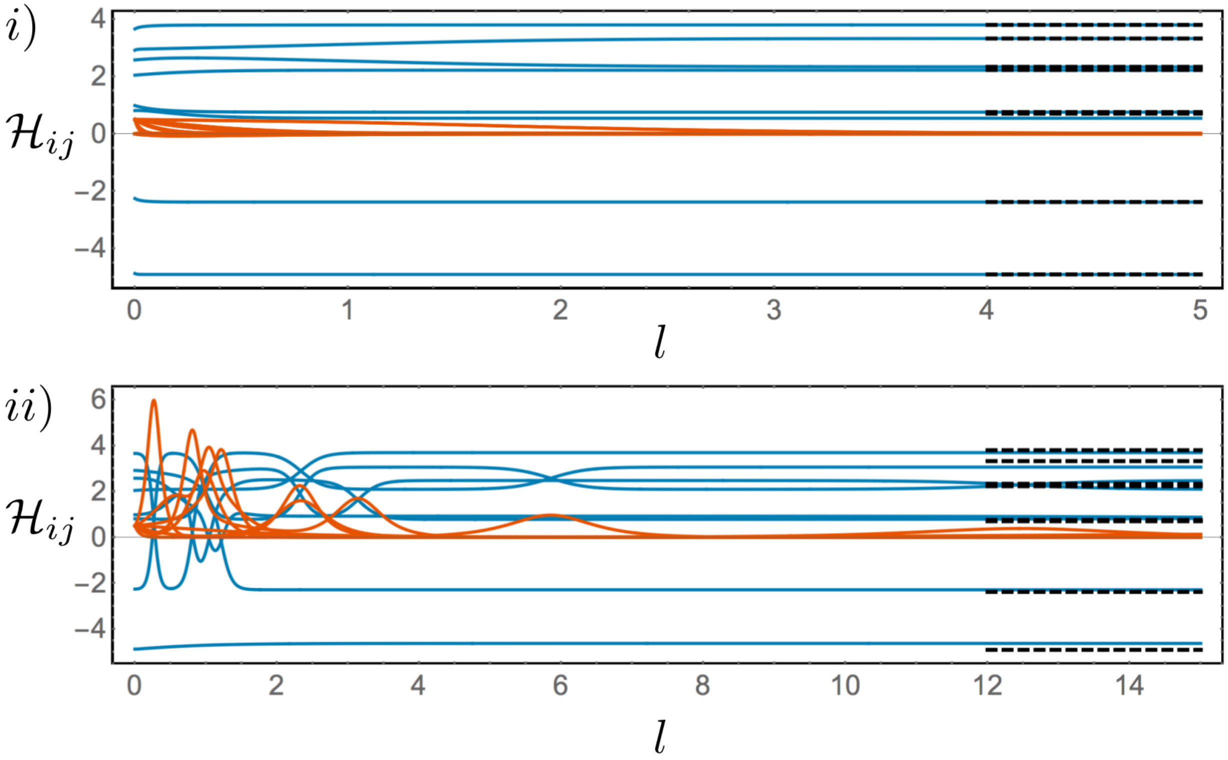


Physics Today **62**, 8, 24 (2009)

Flow of the coefficients



A Toy Example

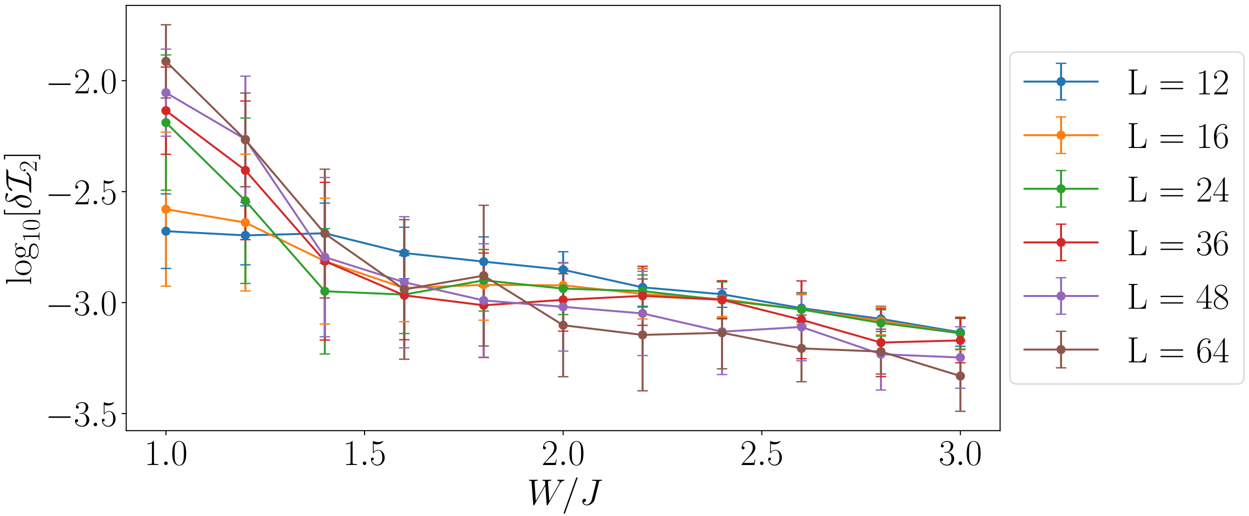


Wegner

Toda

Flow Invariant

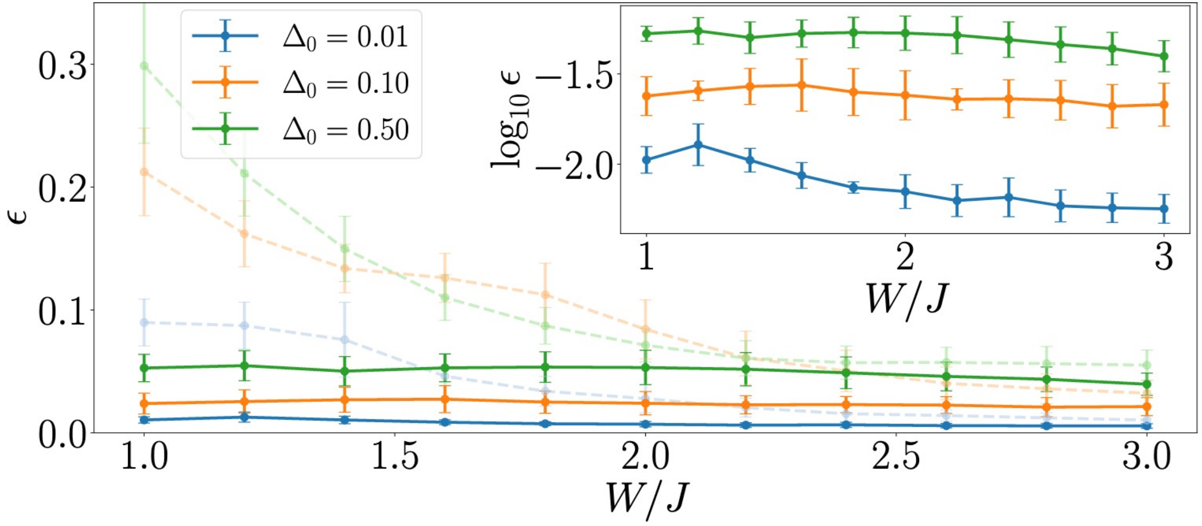
$$I_2 = \mathrm{Tr}[\mathcal{H}^2]$$



Relative error

arXiv:2110.02906v1

$$\varepsilon = \frac{1}{2^L} \sum_n \left| \frac{E_n^{ED} - E_n^{FE}}{E_n^{ED}} \right|$$



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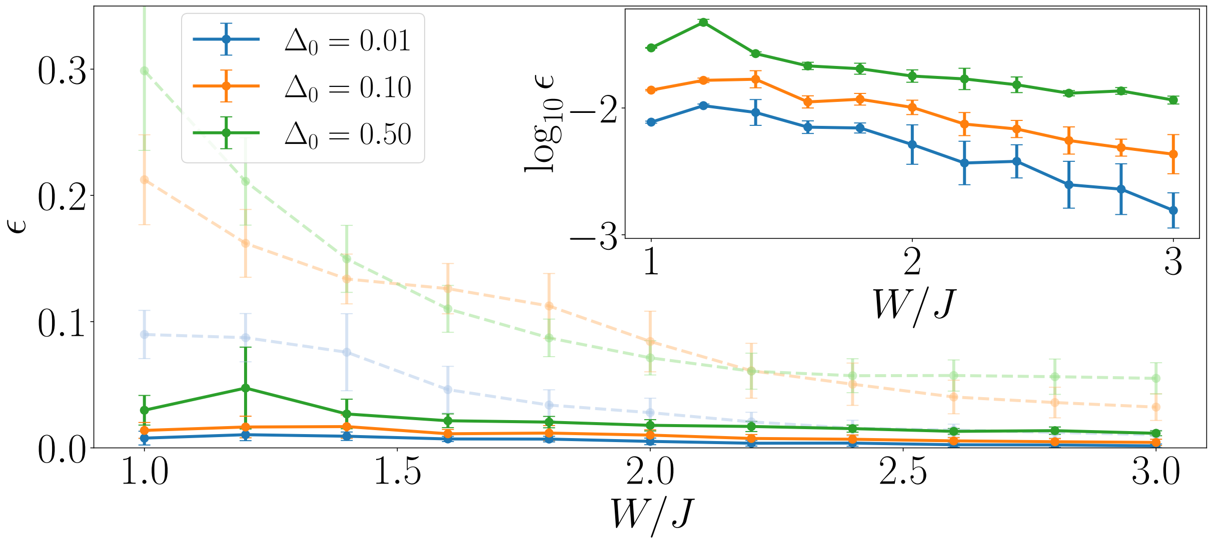
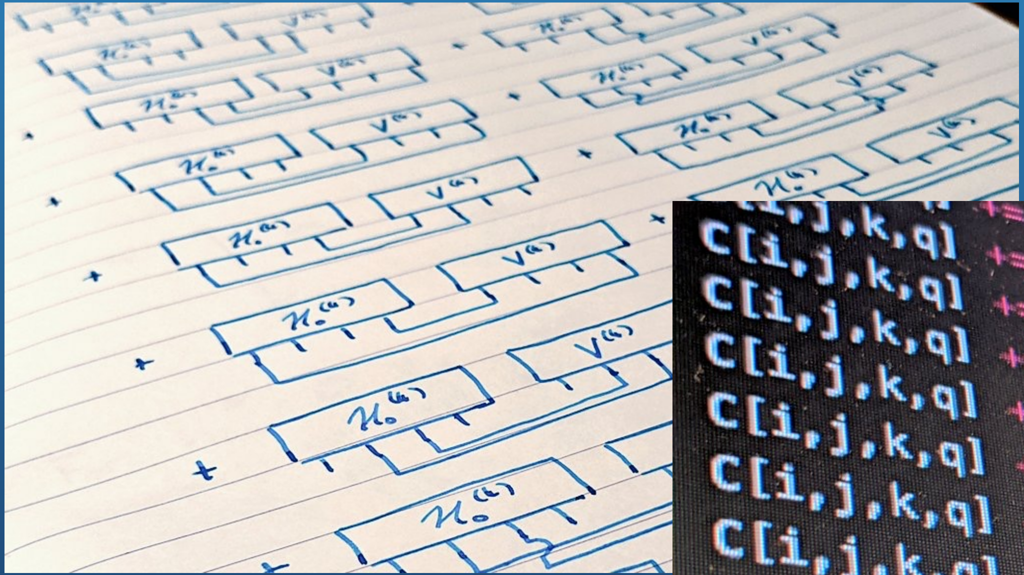
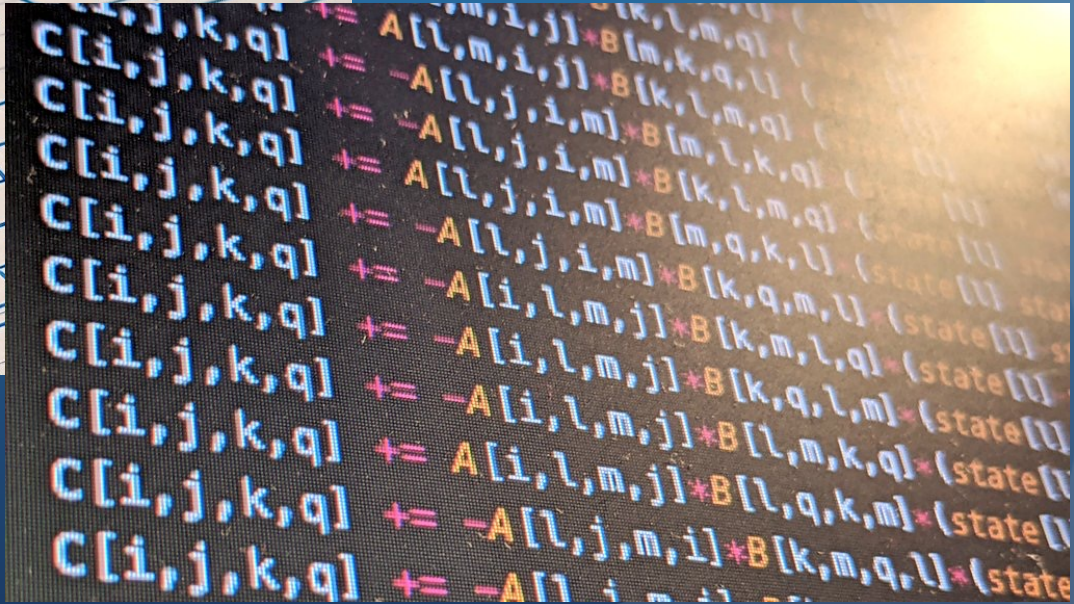
arXiv:2110.02906v2, coming soon!
(Preliminary result, more data to come)
Improved convergence
Better accuracy



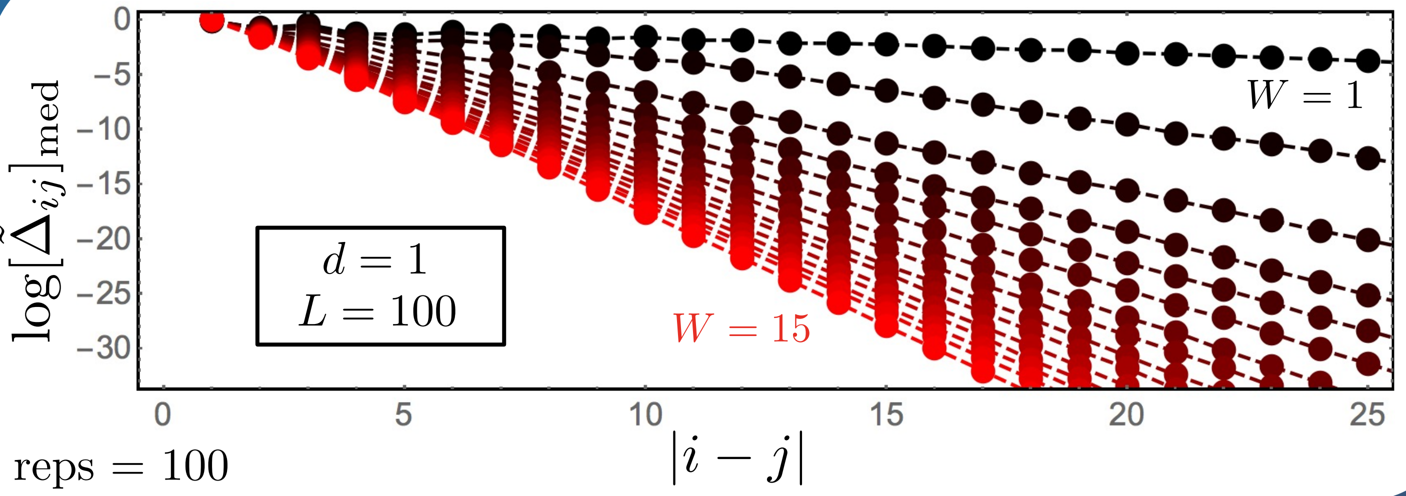
What about 2-point contractions?





Decay of *l*-bit couplings in 1D

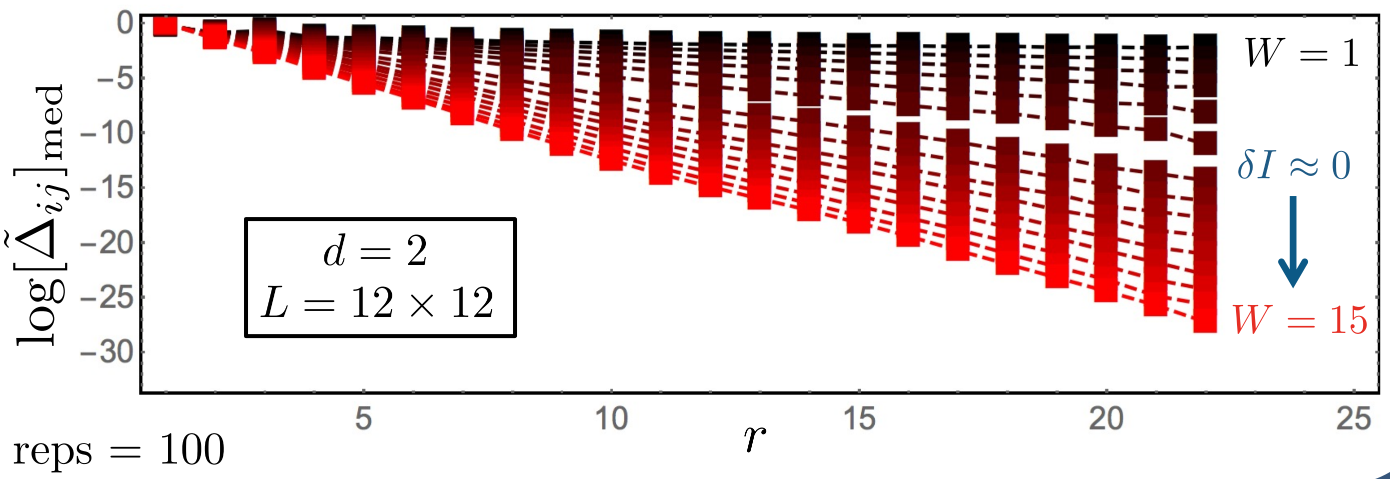
$$\tilde{\mathcal{H}} = \sum_i \tilde{h}_i \tilde{n}_i + \frac{1}{2}\sum_{ij} \tilde{\Delta}_{ij} \tilde{n}_i \tilde{n}_j$$



SJT & M. Schiró, PRB **97**, 060201(R) (2018)
[*cf. L. Rademaker et al.* Ann. Phys. **529**, 1600322 (2017)]

Decay of *l*-bit couplings in 2D

$$\tilde{\mathcal{H}} = \sum_i \tilde{h}_i \tilde{n}_i + \frac{1}{2} \sum_{ij} \tilde{\Delta}_{ij} \tilde{n}_i \tilde{n}_j$$



$r = |x_i - x_j| + |y_i - y_j|$

SJT & M. Schiró, PRB **97**, 060201(R) (2018)
[*cf. T. Wahl et al.*, Nature Physics **15**, 164 (2019)]

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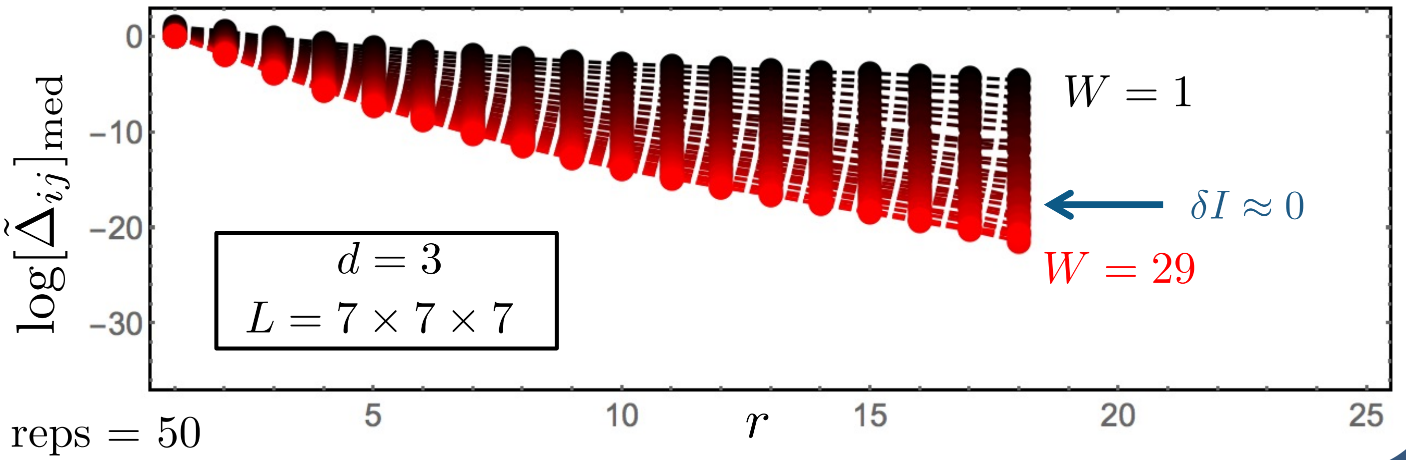
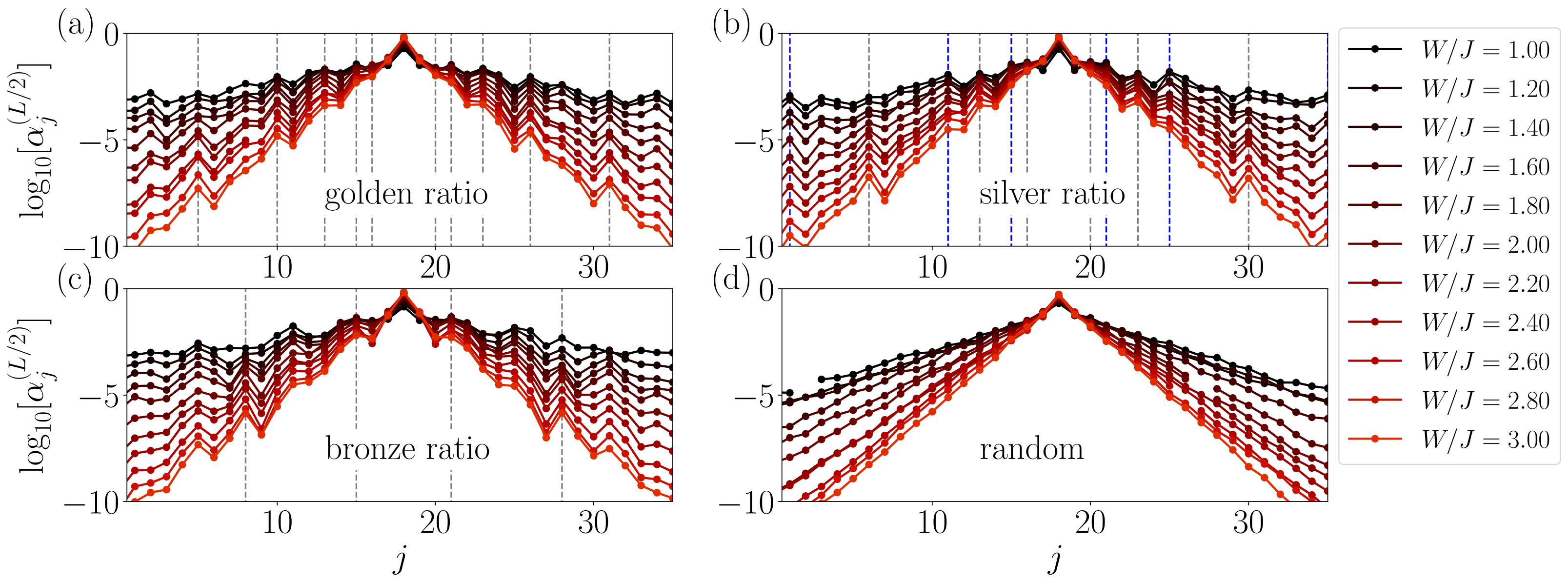
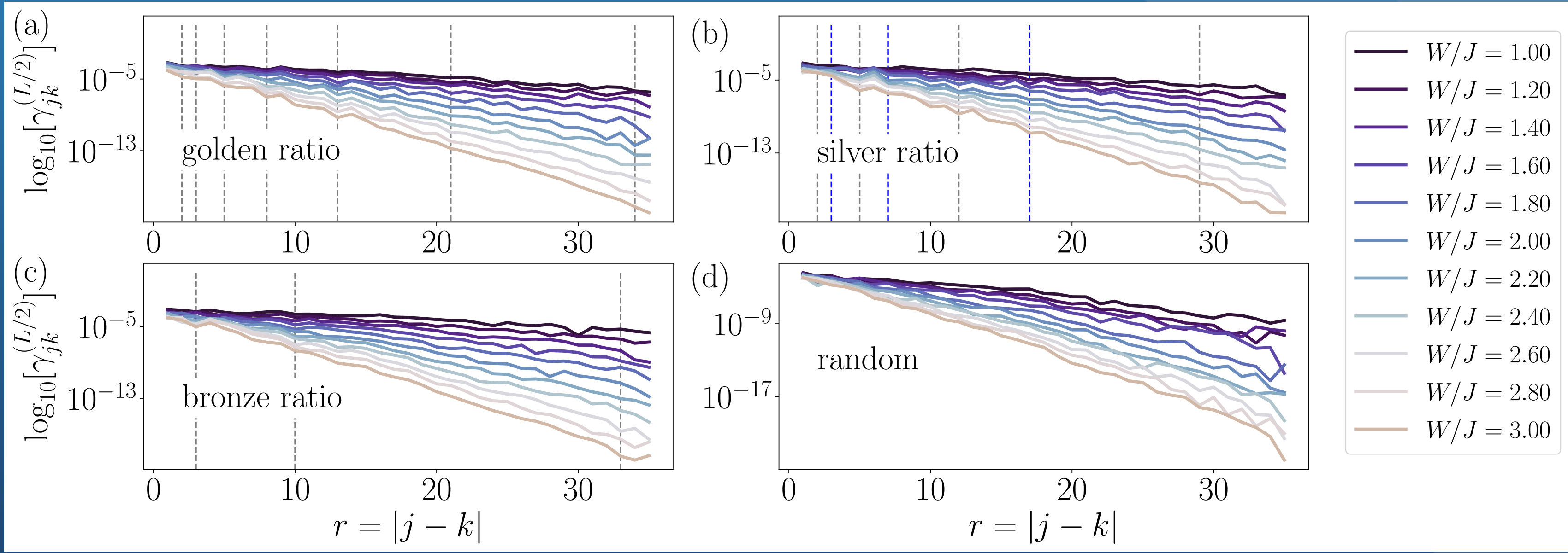


$$r = |x_i - x_j| + |y_i - y_j| + |z_i - z_j|$$

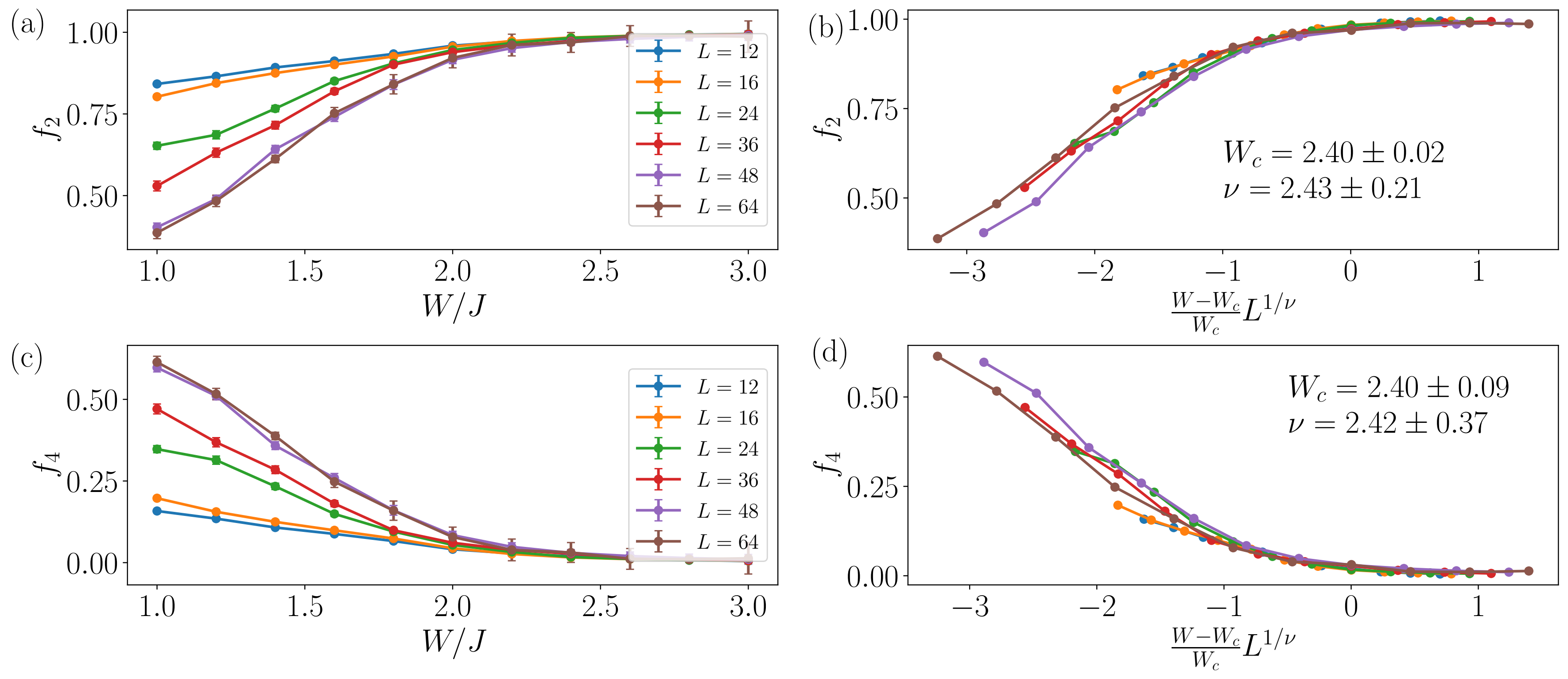
Real Space Support of the l-bits



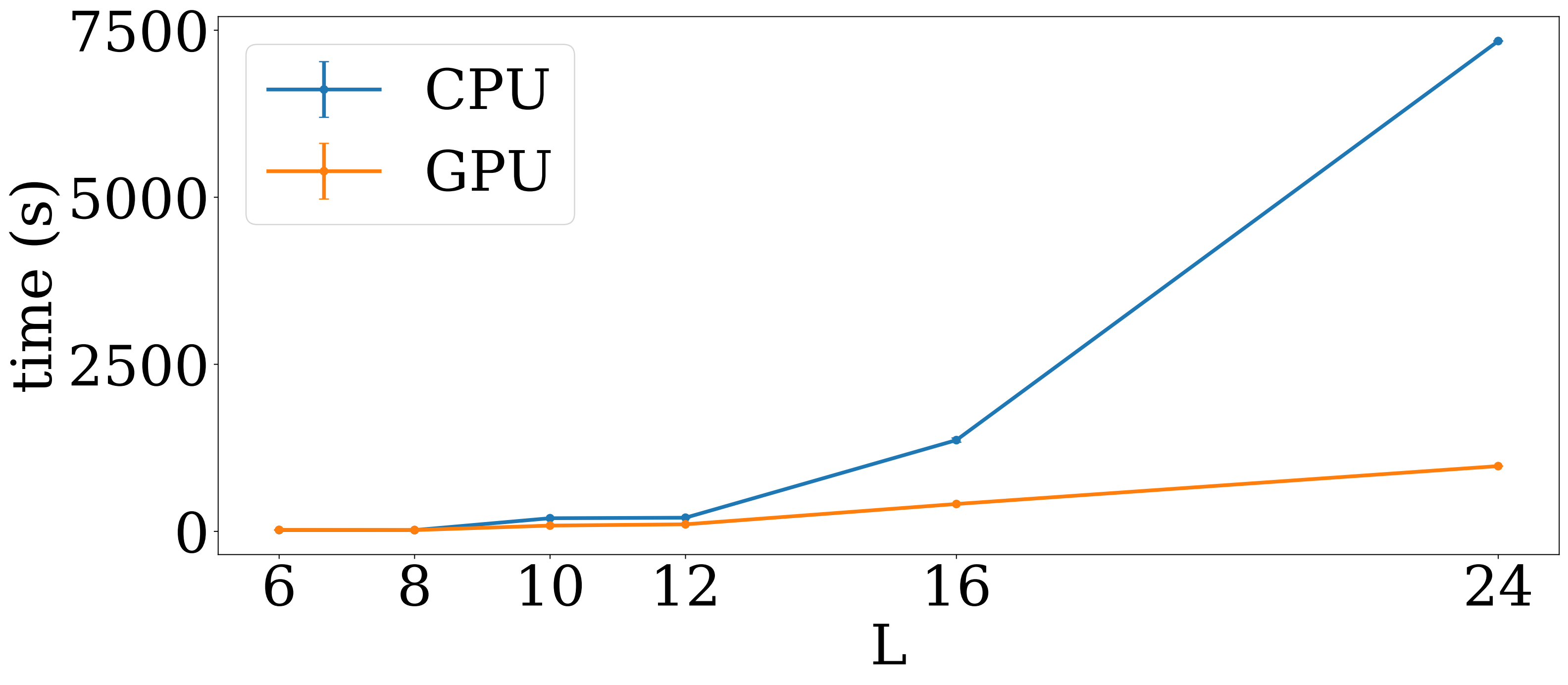
Real Space Support of the l-bits



Finite-size Scaling for Phase Transition



CPU-GPU Speed Comparisons



Long-Range Couplings

- Let's make things a bit more interesting:
  - We start again from an interacting model, this time with long-range couplings

$$\boxed{\mathcal{H} = \sum_i h_i c_i^\dagger c_i + \sum_{ij} J_{ij} c_i^\dagger c_j + \frac{1}{2} \sum_{ij} \Delta_{ij} n_i n_j}$$

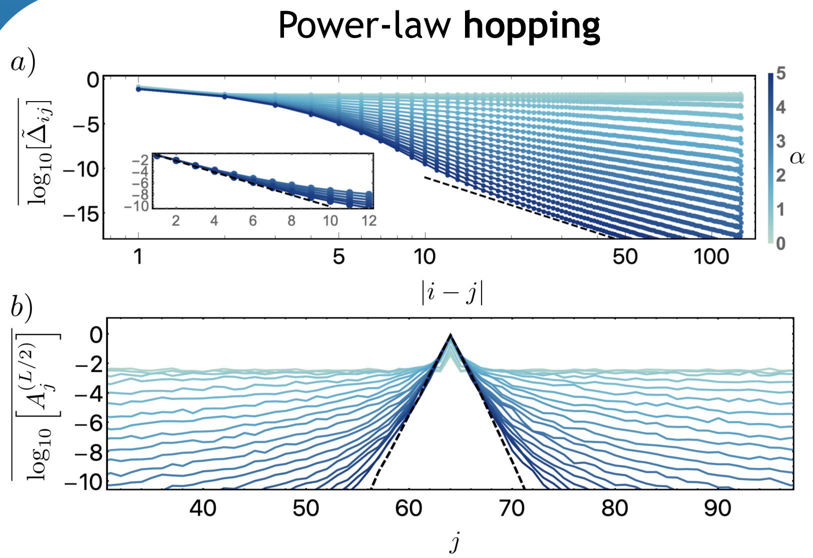
  - We draw the couplings randomly from distributions with standard deviations:

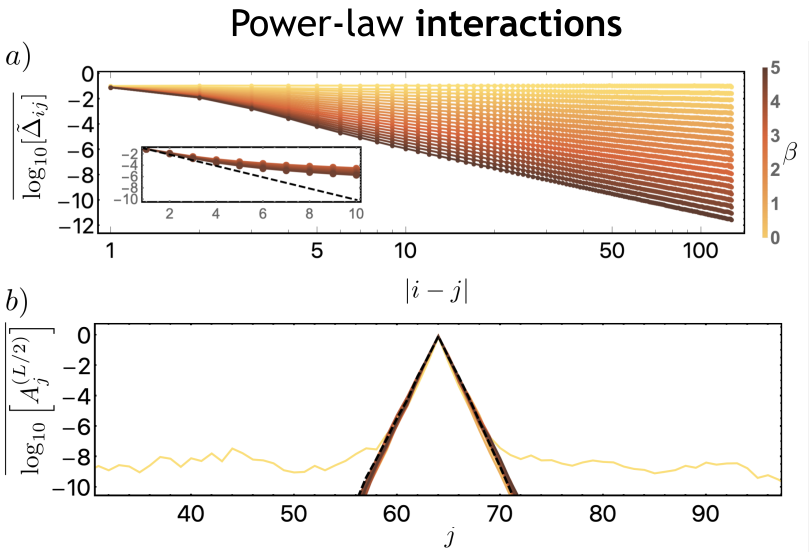
$$\sigma_J = \frac{J_0}{|i-j|^\alpha} \qquad \sigma_\Delta = \frac{\Delta_0}{|i-j|^\beta}$$

- In the non-interacting case, this is known as the **Power-Law Random Banded Matrix** model, and has an Anderson localisation transition at $\alpha = d$
  - With short-range interactions in d=1, transition at $\alpha \approx 1.2$ PRE **85**, 050102 (2012)
  - When $\alpha, \beta \to \infty$ this model is many-body localised.
- Do long-range couplings **destroy MBL**?

Long-Range Couplings

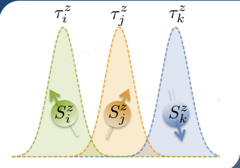
Phys. Rev. Research **2**, 043368 (2020)





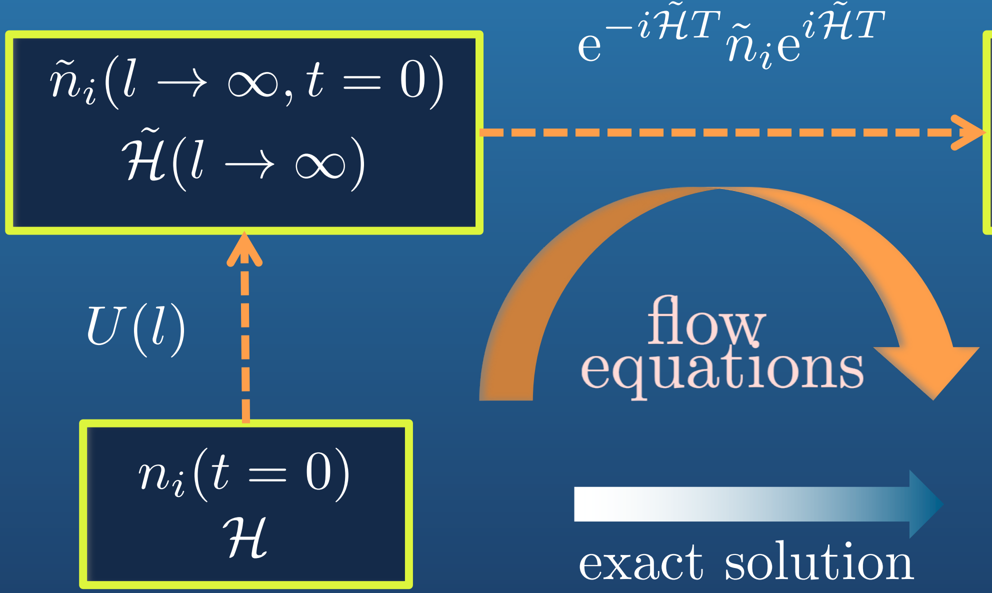
Upper panels: *l*-bit interactions in the diagonal basis

Lower panels: real-space support of *l*-bits in the microscopic (physical) basis



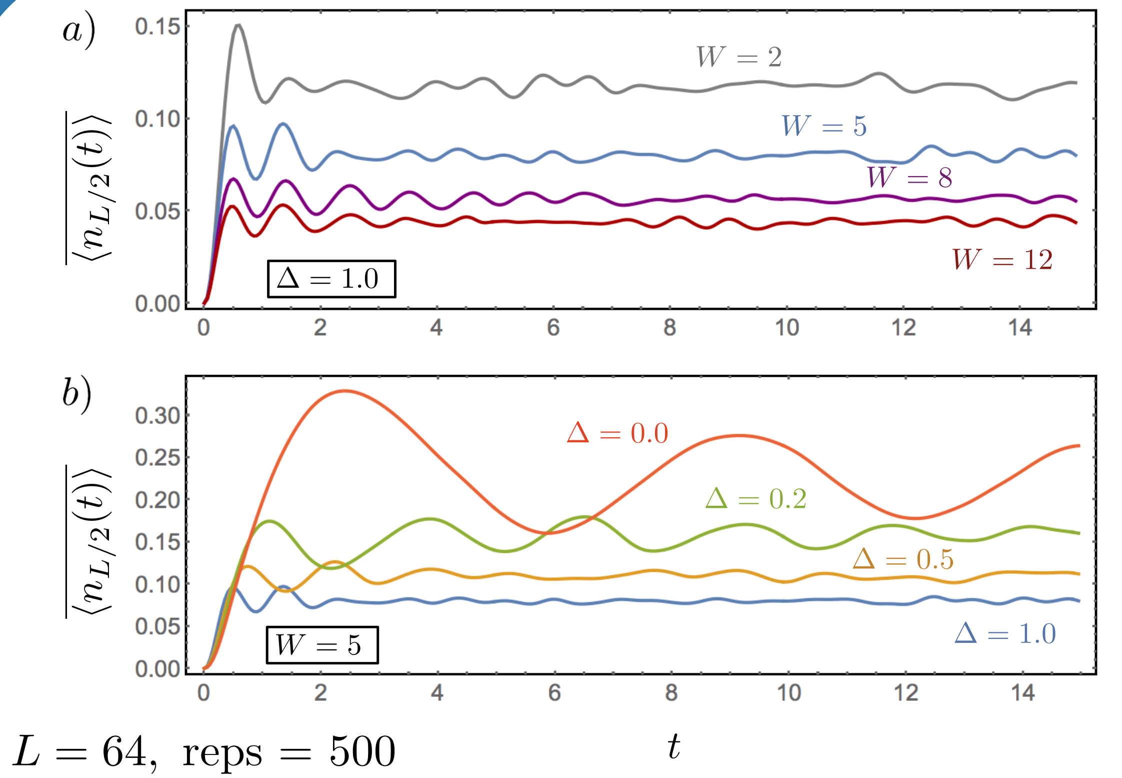
Non-equilibrium Dynamics

- Transform the operator into the same basis as the Hamiltonian, time-evolve, then transform back again.



see, e.g., Hackl & Kehrein, J. Phys: Cond Mat 21, 1 (2008)

Quench Dynamics

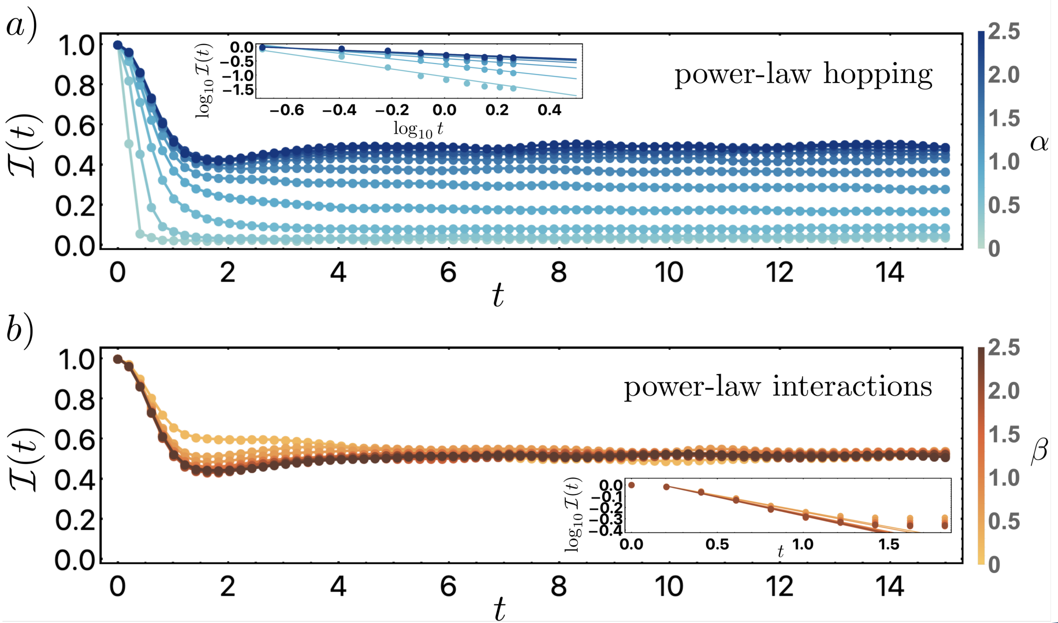


SJT & M. Schiró, PRB **97**, 060201(R) (2018)

Quench Dynamics

- Starting from a charge density wave state (010101…) we can time-evolve the system and compute the imbalance: $\mathcal{I}(t) = \frac{2}{L}\sum_i (-1)^i \langle n_i(t)\rangle$

Phys. Rev. Research 2, 043368 (2020)



$L = 64$

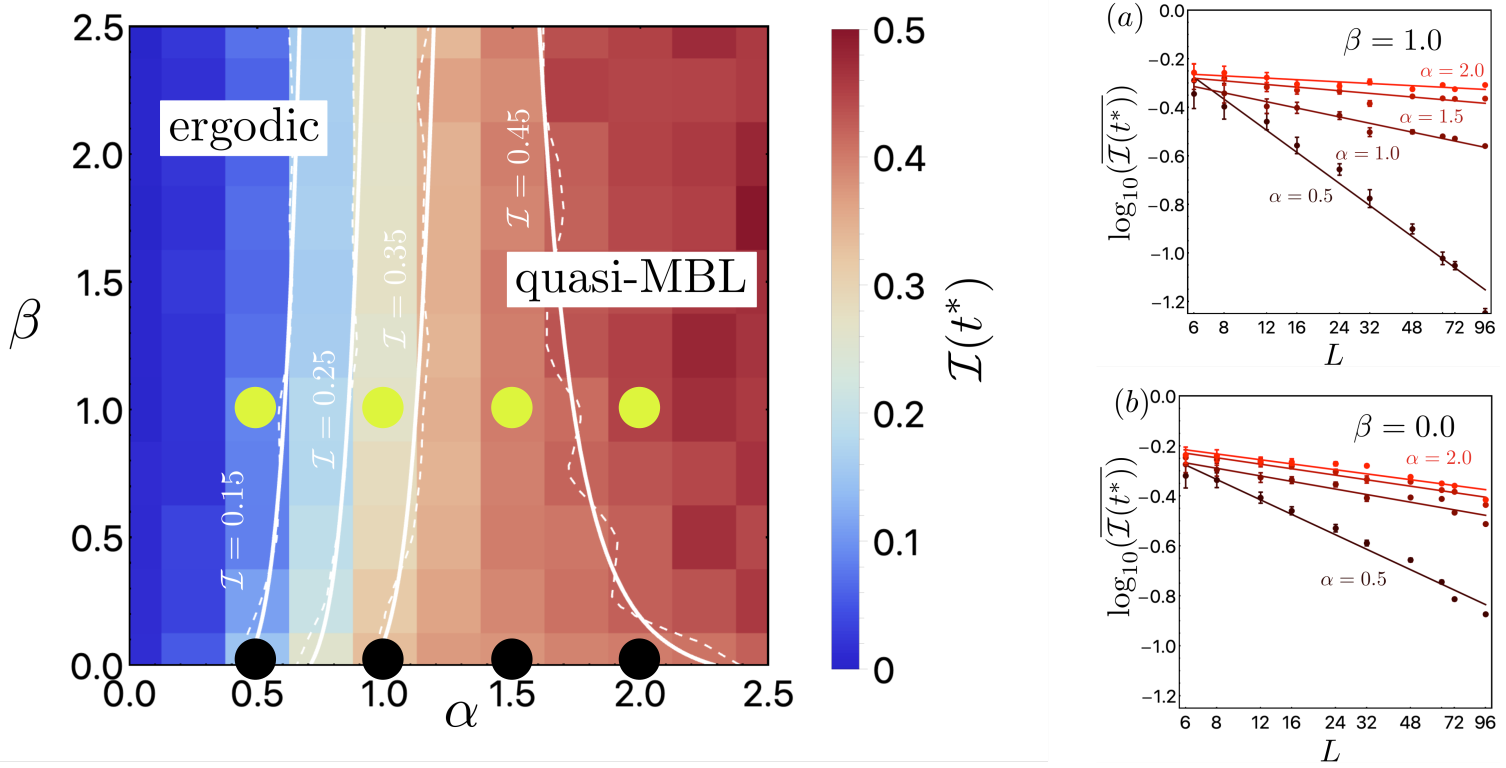
$\Delta_0 = 0.1$

$J_0 = 0.5$

$N_s = 256$

➢ MBL survives the presence of long-range interactions!

Dynamical Phase Diagram



Phys. Rev. Research 2, 043368 (2020)

Time-Dependent Hamiltonians

- The flow equation method can be formally extended to time-dependent Hamiltonians by using a **time-dependent** unitary transform to simplify the Schrodinger equation $i\partial_t|\psi(t)\rangle = H(t)|\psi(t)\rangle$:

$$\boxed{\begin{aligned} |\tilde{\psi}(t)\rangle &= U(t)|\psi(t)\rangle \\ i\partial_t|\tilde{\psi}(t)\rangle &= \underbrace{U(t)\left[H(t) - i\partial_t\right]U^\dagger(t)}_{\tilde{\mathcal{H}}(t)}|\tilde{\psi}(t)\rangle \end{aligned}}$$

- End up with a partial differential equation in 2 variables – difficult!

$$\boxed{\partial_l H(l,t) = [\eta(l,t), H(l,t)] + i\partial_t \eta(l,t)}$$

A Very Brief Introduction to Floquet Theory

- Periodically driven system have *time-dependent* Hamiltonians which satisfy $H(t) = H(t+T)$ where T is the drive period
- Floquet's theorem, analagous to Bloch's theorem in solid-state, says that there is a complete set of solutions of the time-dependent Schrodinger equation known as 'Floquet eigenstates'

$$\boxed{|\Psi_\alpha(t)\rangle = \mathrm{e}^{-i\varepsilon_\alpha t/\hbar}|\psi_\alpha(t)\rangle}$$

- These states satisfy:

$$\boxed{|\psi_\alpha(t+T)\rangle = |\psi_\alpha(t)\rangle \qquad \text{and} \qquad (H(t) - i\partial_t)\,|\psi_\alpha(t)\rangle = \varepsilon_\alpha|\psi_\alpha(t)\rangle}$$

- The main object of interest is no longer the Hamiltonian, but the Floquet evolution operator:

$$\boxed{K = (H(t) - i\partial_t)}$$

Extended Floquet Hilbert Space

- Since the Floquet modes are periodic, we can expand them in terms of Fourier harmonics at integer multiples of their fundamental frequency:

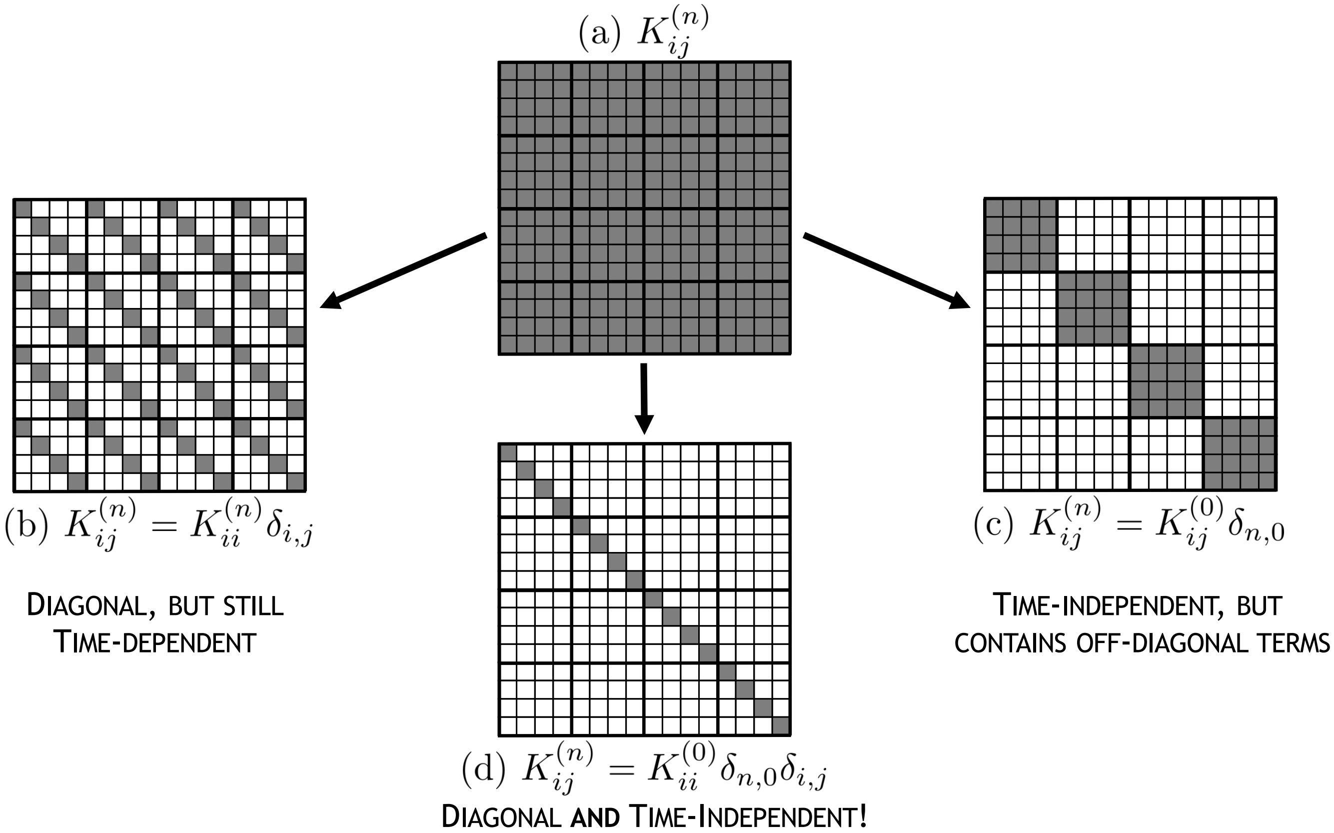
$$\boxed{|\psi_\alpha(t)\rangle = \sum_n |\psi_\alpha^n\rangle \mathrm{e}^{in\omega t} = \sum_n |\psi_\alpha^n\rangle \otimes \sigma_n}$$

where σ_n is a creation operator in 'frequency space'

- This allows us to rewrite the problem of finding the Floquet modes into a conventional eigenvalue problem in a higher-dimensional space, where we want to diagonalise the following object:

$$\boxed{K = H(t) - i\partial_t = \sum_n H^{(n)} \otimes \sigma_n + 1 \otimes \omega\hat{n}}$$

Periodically Driven Systems



Example: The Driven Anderson Model

- As an example, let's take the Anderson model with periodic drive:

$$H(t) = F(t)\sum_{i=1}^{L} h_i c_i^\dagger c_i + G(t)\sum_{i=1}^{L-1} J_0\left(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i\right)$$

- The Floquet evolution operator becomes:

$$K(l) = \sum_n \left(\sum_i h_i^{(n)} c_i^\dagger c_i + \sum_{ij} J_{ij}^{(n)} c_i^\dagger c_j\right) \otimes \sigma_n + 1 \otimes \omega\hat{n}$$

$$h_i F(t) = \sum_n h_i^{(n)} e^{in\omega t} = \sum_n h_i^{(n)} \otimes \sigma_n$$

$$J_{ij} G(t) = \sum_n J_{ij}^{(n)} e^{in\omega t} = \sum_n J_{ij}^{(n)} \otimes \sigma_n$$

Example: The Driven Anderson Model

- As an example, let's take the Anderson model with periodic drive:

$$H(t) = F(t)\sum_{i=1}^{L} h_i c_i^\dagger c_i + G(t)\sum_{i=1}^{L-1} J_0\left(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i\right)$$

- The Floquet evolution operator becomes:

$$K_0 = \left[\sum_i h_i^{(0)} c_i^\dagger c_i\right] \otimes 1 + 1 \otimes \omega\hat{n}$$

$$K_{\mathrm{off}} = \sum_{n\neq 0}\sum_i h_i^{(n)} c_i^\dagger c_i \otimes \sigma_n + \sum_n \sum_{ij} J_{ij}^{(n)} c_i^\dagger c_j \otimes \sigma_n$$

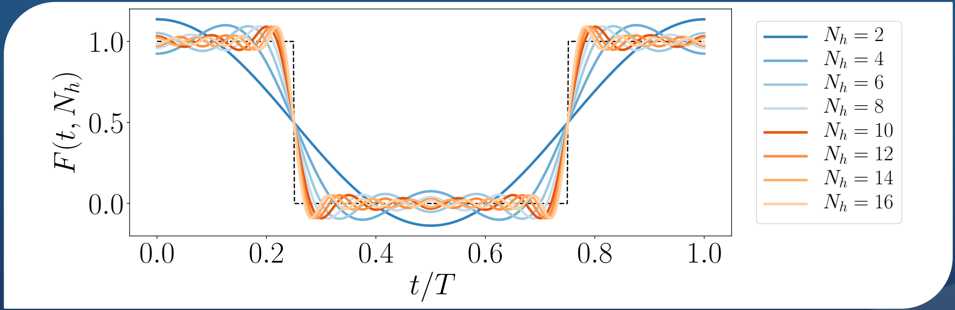
arXiv:2009.03186

Example: The Driven Anderson Model

- Choose the most challenging form of drive we can find:

$$H(t) = \begin{cases} \sum_{i=1}^{L} h_i c_i^\dagger c_i, & \text{if } T/4 \le t < 3T/4 \\ \sum_{i=1}^{L-1} J_0 \left(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i \right), & \text{otherwise} \end{cases}$$

  - discontinuous drive: infinitely many Fourier components!
  - have to **truncate** the expansion in terms of harmonics
  - only keep N_h harmonics of the drive



$$G(t) = 1 - F(t)$$

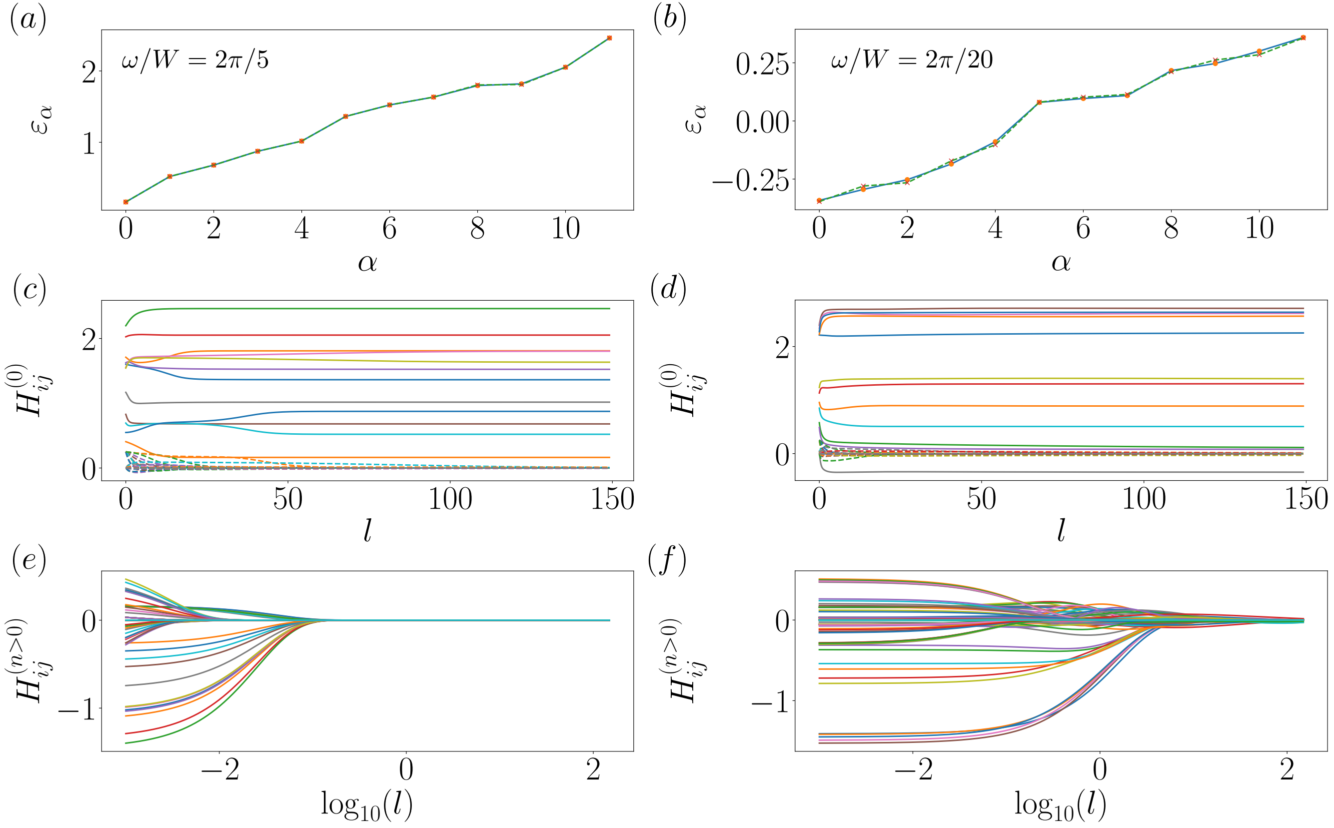
Periodically Driven Systems

$L = 12$

$W = 5$

$J_0 = 0.5$

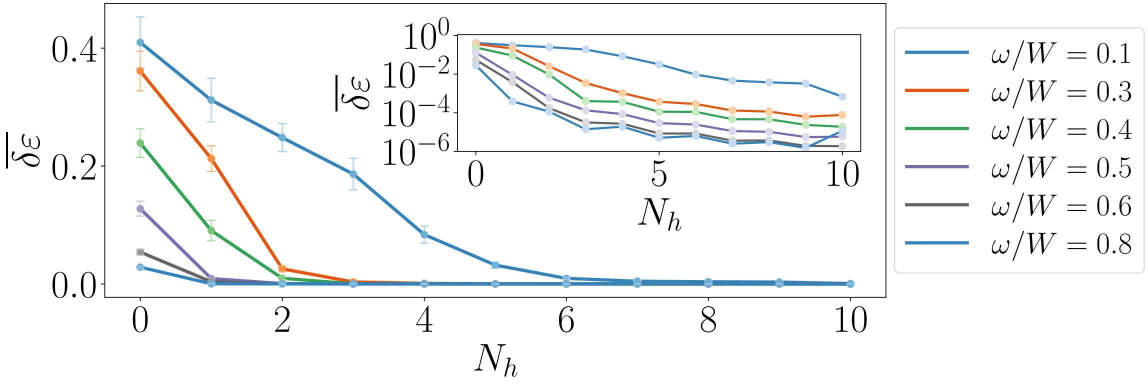
$N_h = 5$



Accuracy Check: Quasienergies

- We can quantify the accuracy versus both frequency and number of harmonics by computing the relative error:

$$\delta\varepsilon = \frac{1}{L}\sum_{\alpha}\left|\frac{\varepsilon_{\alpha}^{ED} - \varepsilon_{\alpha}^{FE}}{\varepsilon_{\alpha}^{ED}}\right|$$



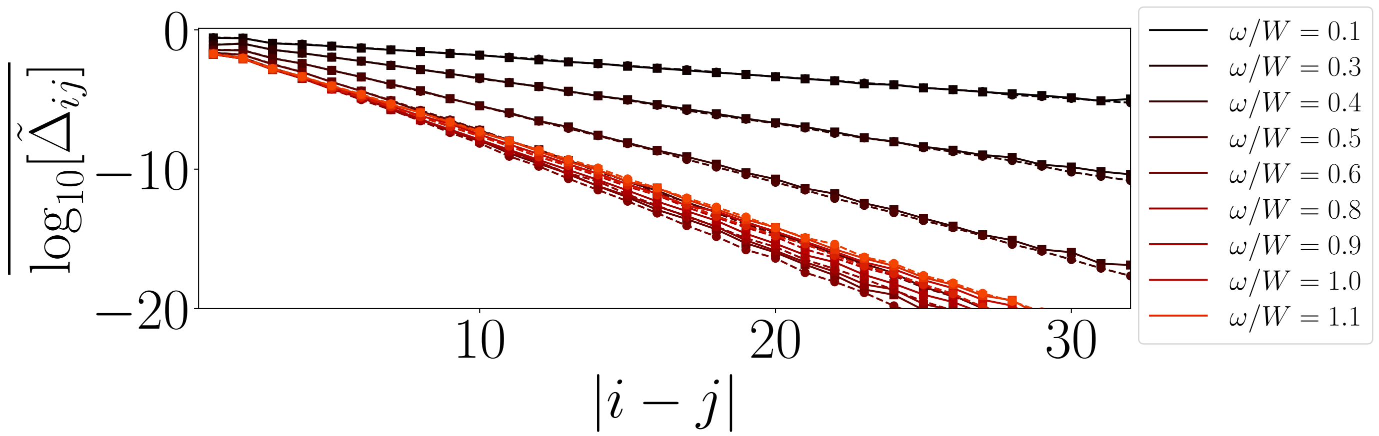
- High accuracy at all frequencies if enough harmonics retained!

Floquet l-bits

- We can put together everything we've seen so far and compute the **Floquet integrals of motion** for a weakly interacting driven system:

$$\tilde{K} = \tilde{H}_F \otimes 1 + 1 \otimes \omega \hat{n}$$

$$\tilde{H}_F = \sum_i \tilde{h}_i n_i + \frac{1}{2} \sum_{ij} \tilde{\Delta}_{ij} n_i n_j$$



Dissipative Flow Equations

Lorenzo Rosso, Fernando Iemini, Marco Schirò, Leonardo Mazza, SciPost Phys. 9, 091 (2020)

- Start from a Markovian Lindblad Master equation:

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = \mathcal{L}[\rho(t)] = -\frac{i}{\hbar}[H, \rho(t)] + \sum_{\alpha} L_{\alpha}\rho(t)L_{\alpha}^{\dagger} - \frac{1}{2}\left\{L_{\alpha}^{\dagger}L_{\alpha}, \rho(t)\right\}$$

- Goal is to diagonalize the Lindbladian with a transform given by:

$$\mathcal{L}(\ell) = \mathcal{S}(\ell)\,\mathcal{L}\,\mathcal{S}(\ell)^{-1} \qquad \mathcal{S}(\ell) = \mathcal{T}_{\ell}\exp\left[\int_0^{\ell}\eta(\ell')\mathrm{d}\ell'\right]$$

- Results in flow equation of the form:

$$\frac{\mathrm{d}\mathcal{L}(\ell)}{\mathrm{d}\ell} = [\eta(\ell), \mathcal{L}(\ell)]$$