

# *Non-equilibrium and periodically driven quantum systems*

## Tutorial

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## *Outline*

- I. Eigenvalue statistics
- II. Forward scattering approximation.

# I. Eigenvalue statistics

## Preliminaries : Symmetries of a Hamiltonian

Consider a 1 d spin-1/2 interacting system of  $N$  sites described by a Hamiltonian like

$$H = \sum_{i=1}^{L-1} (J_x S_i^x S_{i+1}^x + J_y S_i^y S_{i+1}^y + J_z S_i^z S_{i+1}^z) + h \sum_{i=1}^L S_i^z$$

the symmetry of such Hamiltonian includes translation, inversion, magnetization ( $M_z = \sum_{i=1}^L S_i^z$ ) etc.

- **Translation** : The action of translation operator ( $T$ ) is

$$T|S_0^z, S_1^z, S_2^z, \dots, S_{N-1}^z\rangle = |S_{N-1}^z, S_1^z, S_2^z, \dots, S_{N-2}^z\rangle \quad ; \quad T^N = I$$

- The eigenstates of  $T$  can be chosen as  $T|\Psi(k)\rangle = e^{ik}|\Psi(k)\rangle$  where  $k = \frac{2n\pi}{N}$ ,  $n = 0, \dots, N-1$ .
- If, the system has translation symmetry :  $[H, T] = 0$ .
- $H$  is block diagonalized in momentum basis as  $\langle\Psi(k)|H|\Psi(k')\rangle = 0$  if  $k \neq k'$ .

- How to construct the  $|\Psi(k)\rangle$  s ?

$$|\Psi^a(k)\rangle = \frac{1}{\sqrt{N_a}} \sum_{r=0}^{N-1} e^{-ikr} T^r |a\rangle$$

- Example : for  $N = 6$  and  $k = 0$

$$|\Psi^0(0)\rangle = |000000\rangle$$

$$|\Psi^1(0)\rangle = \frac{1}{\sqrt{6}}(|100000\rangle + |010000\rangle + \dots + |000001\rangle)$$

$$|\Psi^3(0)\rangle = \frac{1}{\sqrt{6}}(|110000\rangle + |011000\rangle + \dots + |100001\rangle)$$

...

$$|\Psi^9(0)\rangle = \frac{1}{\sqrt{3}}(|100100\rangle + |010010\rangle + |001001\rangle)$$

...

$$|\Psi^{21}(0)\rangle = \frac{1}{\sqrt{2}}(|101010\rangle + |010101\rangle)$$

- $k = 0$  sector is the largest one.

- **Inversion** : Inversion operator ( $P$ ) acts as

$$P|S_0^z, S_1^z, S_2^z, \dots, S_{N-1}^z\rangle = |S_{N-1}^z, \dots, S_2^z, S_1^z, S_0^z\rangle \quad P^2 = I$$

- The eigenstates of  $P$  can be chosen as  $P|\Phi(p)\rangle = p|\Phi(p)\rangle$  where  $p = \pm 1$ .
- In general  $[T, P] \neq 0$  but for  $k = 0, \pi$  they commute. So,  $k = 0$  and  $\pi$  sector can be further block diagonalized into two part using inversion symmetry.
- **Example** : Consider the following two states

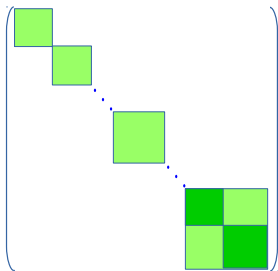
$$|\psi^{11}(0)\rangle = \frac{1}{\sqrt{6}}(|110100\rangle + |011010\rangle + \dots + |101001\rangle)$$
$$|\psi^{19}(0)\rangle = \frac{1}{\sqrt{6}}(|001011\rangle + |100101\rangle + \dots + |010110\rangle)$$

- We can construct

$$|\Theta(k=0, p=+1)\rangle = \frac{1}{\sqrt{2}}(|\Psi^{11}(0)\rangle + |\Psi^{19}(0)\rangle)$$

$$|\Theta(k=0, p=-1)\rangle = \frac{1}{\sqrt{2}}(|\Psi^{11}(0)\rangle - |\Psi^{19}(0)\rangle)$$

- One can check  $\langle \Theta(k=0, p=+1) | H | \Theta(k=0, p=-1) \rangle = 0$ . This means we can further reduce the number of states in  $k=0$  sector by working in a particular inversion symmetry sector.



- Some numbers : In a 2D spin-1/2 Heisenberg model, one can deal with  $6 \times 6$  ( $\text{HSD}=2^{36}$ ) systems by using 7 such conserved quantities ( $M_z, Z, k_x, k_y, p_x, p_y, p_d$ ). The size of ( $M_z = 0, Z = +1, k_x = 0, k_y = 0, p_x = +1, p_y = +1, p_d = +1$ ) sector is 15804955 ( $\approx 4348$  times reduction).
- Ref : “Computational Studies of Quantum Spin Systems”, A. W. Sandvik, AIP Conf.Proc.1297:135,2010.

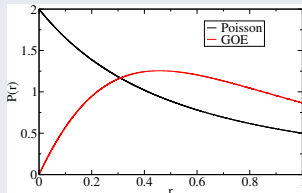


## I. Eigenvalue Statistics : Measure of quantum chaos

- Store the eigenvalues ( $e$ ) in increasing order and calculate the gaps ( $\Delta$ ) :  $\Delta(i) = e(i+1) - e(i)$ . Then, study (average, distribution etc) the following quantity

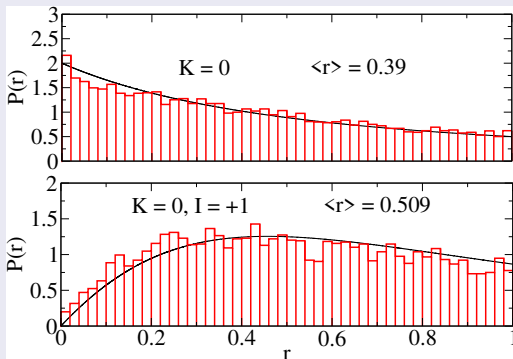
$$r = \frac{\min(\Delta(i), \Delta(i+1))}{\max(\Delta(i), \Delta(i+1))}$$

- For integrable systems,  $r$  shows Poissonian distribution with  $P(r) = \frac{2}{(1+r)^2}$  and  $\langle r \rangle \approx 0.386$ . No, level repulsion.
- Non-integrable systems shows level repulsion,  $r$  shows *GOE* distribution ( $P(r) = \frac{27}{4} \frac{r+r^2}{(1+r+r^2)^{2.5}}$ ) and  $\langle r \rangle \approx 0.536$ .



## one subtle issue

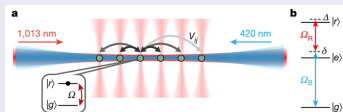
- One needs to resolve all the conserved quantities present in the system, otherwise you will get wrong result.



- Ref : "Quantum Signatures of Chaos ", Fritz Haake.

# I. Forward scattering approximation

# Introduction : Experiment



Array of 51  $^{87}\text{Rb}$  atom described by

$$\frac{\mathcal{H}}{\hbar} = \sum_i \frac{\Omega_i}{2} \sigma_x^i - \sum_i \Delta_i n_i + \sum_{i < j} V_{ij} n_i n_j$$

$$|r\rangle = |70S_{1/2}, J = 1/2, m_J = -1/2\rangle$$

$$|g\rangle = |5S_{1/2}, F = 2, m_F = -2\rangle$$

## Quantum many body scars

Turner et al, *Nature Physics* **14**, 745-749 (2018).

$$\begin{aligned} HSD_L &= \#| \underbrace{r, g, \dots, g}_{L-1 \text{ sites}} \rangle + \#| \underbrace{r, g, \dots, g, r}_{L-2 \text{ sites}} \rangle \\ &= HSD_{L-1} + HSD_{L-2} \end{aligned}$$

with  $HSD_1 = 2$  and  $HSD_2 = 3$  we get  $HSD_L^{OBC} = F_{L+2}$

similarly we get  $HSD_L^{PBC} = F_{L-1} + F_{L+1} \sim \tau^L$  in large  $L$  limit.

$\tau$  is the golden ratio  $\sim 1.62$

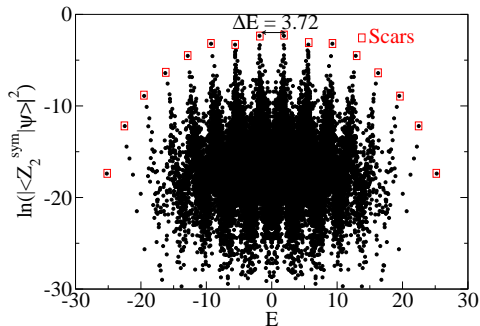
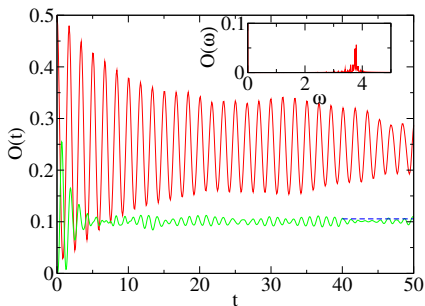
## The effective Hamiltonian

$$H = - \sum_i (\tilde{\sigma}_i^x + \lambda \sigma_i^z)$$

where  $\tilde{\sigma}_i^x = P_{i-1} \sigma_i^x P_{i+1}$  and  $P_i = \frac{1 - \sigma_i^z}{2}$ .

$$\psi(t=0) = \mathbb{Z}_2^{\text{sym}} = \frac{|0,1,0,1,\dots\rangle + |1,0,1,0,\dots\rangle}{\sqrt{2}}$$

$$N = 30, HSD = 1860498, HSD(K=0, P=+1) = 31836$$



## II A. Forward scattering approximation (from $|\mathbb{Z}_2\rangle$ )

## Preliminaries 1 : Gram-Schmidt orthogonalization

- Let,  $Z = \{z_1, z_2, z_3 \cdots, z_n\}$  is a set of linearly independent vectors (non-orthogonal in general).
- Gram-Schmidt process generates a corresponding orthogonal set of vectors  $Q = \{q_1, q_2, \cdots, q_n\}$  such that  $sp\{Q\} = sp\{Z\}$ .
- $Q$  is given by

$$q_1 = z_1$$

$$q_2 = z_2 - \text{proj}_{q_1}(z_2)$$

$$q_3 = z_3 - \text{proj}_{q_1}(z_3) - \text{proj}_{q_2}(z_3)$$

$$\vdots$$

$$q_k = z_k - \sum_{i=1}^{k-1} \text{proj}_{q_i} z_k$$

where  $\text{proj}_q(z) = \frac{\langle q|z \rangle}{\langle q|q \rangle} q$ .

- You can orthonormalize  $Q$  if you wish.



## Preliminaries 2: Lanczos algorithm

- **Motivation** : Calculation of ground and a few low lying excited states of large (Hilbert space dimension  $D$ ) quantum systems described by a Hamiltonian  $H$ .
- **Krylov subspace** :  $\mathcal{H}_k \equiv \{v_0, H v_0, H^2 v_0, H^3 v_0, \dots, H^{k-1} v_0\}$  where  $v_0$  is a initial choice which should have nonzero overlap with the ground state. In many cases ( $k \ll D$ ).
- orthonormalize the Krylov subspace by the following iteration

$$\beta_1 v_1 = w_0 = H v_0 - \alpha_0 v_0$$

$$\beta_2 v_2 = w_1 = H v_1 - \alpha_1 v_1 - \beta_1 v_0$$

$$\vdots$$

$$\beta_{i+1} v_{i+1} = w_i = H v_i - \alpha_i v_i - \beta_i v_{i-1}$$

where  $\alpha_i = v_i^T H v_i$  and  $\beta_i = \|w_{i-1}\| = v_{i-1}^T H v_i$ .

## Preliminaries 2: Lanczos algorithm

- $V = \{v_1, v_2, \dots, v_n\}$  are known as Lanczos vectors each of size  $(D \times 1)$ .
- Note that we do orthogonalization w.r.t only previous two vectors. But, the beauty of Lanczos algorithm is that this guarantees global orthonormality (in exact arithmetic). Therefore,  $V^T V = I$ .
- This gives the following tridiagonal matrix

$$H^{Lanczos} = V^T H V = \begin{pmatrix} \alpha_0 & \beta_1 & & & \\ \beta_1 & \alpha_1 & \beta_2 & & \\ & \beta_2 & \alpha_2 & \ddots & \\ & & \ddots & \ddots & \beta_{k-1} \\ & & & \beta_{k-1} & \alpha_{k-1} \end{pmatrix}_{(k \times k)}$$

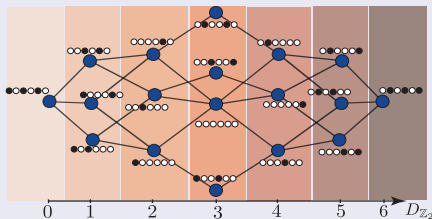
- Diagonalization of  $H_{Lanczos} \implies$  low lying eigenvalues of  $H$ .

## Preliminaries 2: Lanczos algorithm

- Eigenvectors : one need to store all the Lanczos vectors i.e the matrix  $V$ .
- If  $H_{Lanczos}\psi^0 = E_0\psi^0$  then  $\Psi = V_{D\times k}\psi_{k\times 1}^0$  gives an approximate eigenstate of  $H$  of eigenvalue  $E_0$ .
- **Stability** : very prone to numerical instability. Loss of orthogonality is the main issue. Reorthogonalization should be done whenever necessary.
- some numbers : Ground and low lying excited states of systems with Hilbert space dimension ( $D \sim 30000000$ ) can be obtained with  $k$  as small as 1000.
- Ref : "Lanczos Algorithms for Large Symmetric Eigenvalue Computation " by Cullum & Willoughby.

## FSA (from $\mathbb{Z}_2$ )

- Lanczos calculation starting from  $|v_0\rangle = \mathbb{Z}_2$  with Krylov space dimension  $(k) L + 1$  is sufficient to capture the scars in  $PXP$  model.



- Lets do the following decomposition of  $PXP$  model

$$H = - \sum_i \tilde{\sigma}_i^x = H^+ + H^- \quad \text{where} \quad H^\pm = - \sum_{i \in \text{even}} \tilde{\sigma}_i^\pm - \sum_{i \in \text{odd}} \tilde{\sigma}_i^\mp$$

- Note that  $H^- \mathbb{Z}_2 = 0$  and  $H^+ \bar{\mathbb{Z}}_2 = 0$ . So, if we take  $v_0 = \mathbb{Z}_2$ , then from Lanczos algorithm

## FSA (from $\mathbb{Z}_2$ )

$$\beta_1 v_1 = H v_0 - \alpha_0 v_0 = H^+ v_0 \quad \text{as } \alpha_0 = v_0^T H v_0 = 0$$

$$\beta_2 v_2 = H v_1 - \alpha_1 v_1 - \beta_1 v_0 = H^+ v_1 + (H^- v_1 - \beta_1 v_0) \quad \text{as } \alpha_1 = 0$$

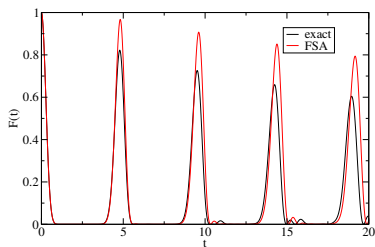
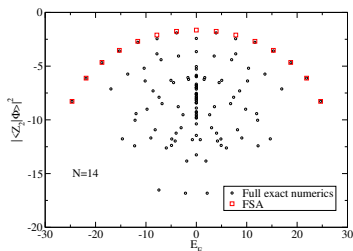
- $\alpha_i = 0, \forall i$ .
- note that  $H^+ v_0 = -\sum_{i \in \text{odd}} |0_i 0 1 0 1 0 \dots\rangle$ . So,  $\beta_1 = \|H^+ v_0\| = \sqrt{\frac{L}{2}}$ .
- $H^- v_1 = \frac{L}{2} \sqrt{\frac{2}{L}} |1 0 1 0 \dots\rangle = \beta_1 v_0$ .  $\therefore (H^- v_1 - \beta_1 v_0) = 0$ .
- Similarly,  $H^- v_2 - \beta_2 v_1 = 0$ .
- Let's write (though not true in general)

$$H^+ v_i = \beta_{i+1} v_{i+1} \quad \textbf{forward scattering}$$

$$H^- v_i = \beta_i v_{i-1} \quad \textbf{backward scattering}$$

- Exact at all  $j$ , only for free paramagnet ( $H = -\sum_i \sigma_i^x$ ).

$$H_{FSA}^{PXP} = V^T H V = \begin{pmatrix} 0 & \beta_1 & & & \\ \beta_1 & 0 & \beta_2 & & \\ & \beta_2 & 0 & \ddots & \\ & & \ddots & \ddots & \beta_{k-1} \\ & & & \beta_{k-1} & 0 \end{pmatrix}_{((L+1) \times (L+1))}$$



- FSA gives good results at very small ( $\sim L$ ) computational cost.
- To calculate observables  $\Rightarrow$  store FSA vectors ( $\sim L\phi^L$ ).

## Perfect scars and perfect oscillations

- Why the oscillations decay ? System leak outside the FSA manifold.
- Quantify the FSA errors :

$$\delta_j = ||H^-|v_j\rangle - \beta_j|v_{j-1}\rangle||$$

- $\delta_j \neq 0$  for  $j > 2$  in *PXP* model.
- Can the oscillation be enhanced and made nearly perfect ?
- Note that, FSA errors  $\equiv$  **damping force**. Therefore,  

reduction of FSA errors  $\Rightarrow$  enhancement of oscillations.
- What term can be added to *PXP* model to fulfill this dream ??

$$H_{\text{perturb}} = -h_{xz} \sum_i \tilde{\sigma}_i^x (\sigma_{i-2}^z + \sigma_{i+2}^z)$$

FSA with  $H_B = H^{PXP} + H_{\text{perturb}}$

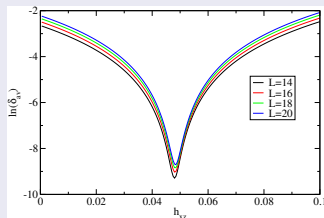
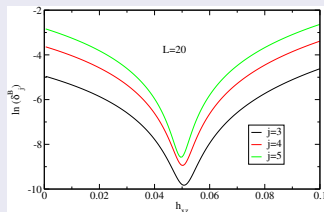
Redefine the decomposition  $\Rightarrow H_B = H_B^+ + H_B^-$  with

$$H_B^\pm = - \sum_{i \in \text{even}} \tilde{\sigma}_i^\pm W_i - \sum_{i \in \text{odd}} \tilde{\sigma}_i^\mp W_i$$

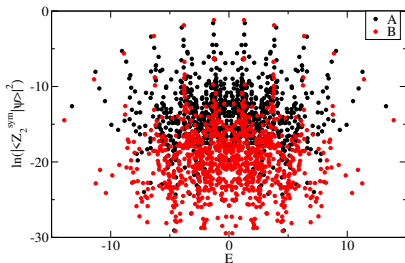
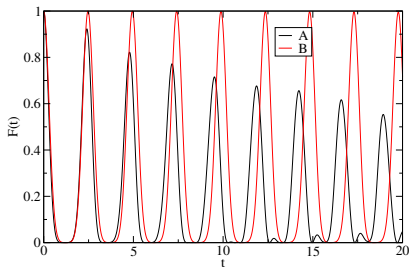
where  $W_i = \mathbb{I} + h_{xz}(\sigma_{i-2}^z + \sigma_{i+2}^z)$ .

the new FSA errors :  $\delta_j^B = ||H_B^- |v_j^B\rangle - \beta_j^B |v_{j-1}^B\rangle||$ .

Again,  $\delta_1^B = \delta_2^B = 0$ .







further

$$\delta H_R = \sum_i \sum_{d=2}^R h_d (\sigma_{i-d}^z + \sigma_{i+d}^z)$$

with

$$h_d = h_0 (\tau^{d-1} - \tau^{-(d-1)})^{-2}$$

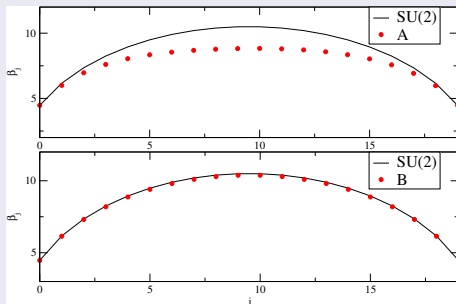
gives 99.9999% revival for N=32 !!!

- Rest of the spectrum becomes strongly ergodic.

## Emergent $SU(2)$ algebra

- When all FSA errors are cancelled, FSA vectors become eigenstate of  $H_B^z = [H_B^+, H_B^-]$ .
- $\{H_B^+, H_B^-, H_B^z\}$  plays the role of  $\{S^+, S^-, S^z\}$  within  $\mathcal{K}_{L+1}$  and forms an  $s = L/2$  representation of  $SU(2)$  algebra.

$$\begin{aligned} S^- |s, j\rangle &= \sqrt{(s+j)(s-j+1)} |s, j-1\rangle \\ H_B^- |v_j^B\rangle &= \beta_j |v_{j-1}^B\rangle \end{aligned}$$



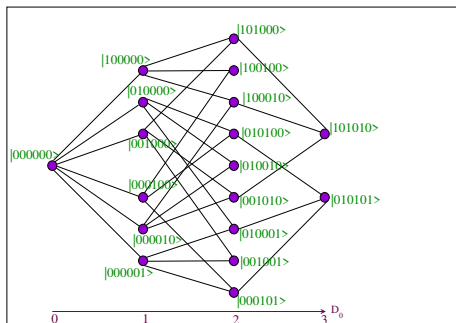
## II B. Forward scattering approximation (from $|0\rangle$ ).

## Decompose the PXP Hamiltonian

$$H = - \sum_i \tilde{\sigma}_i^x = H^+ + H^-$$

where

$$H^\pm = - \sum_i \tilde{\sigma}_i^\pm$$



- # FSA vectors =  $\frac{L}{2} + 1$ .

- We find, in this case also, the first two step is exact i.e  $\delta_1 = \delta_2 = 0$  and  $\delta_i \neq 0$  for  $i \geq 3$ .

- We find  $\sum_{i=3}^{L/2+1} \delta_i = 17.54$  for  $|0\rangle$  where as  $\sum_{i=3}^{L+1} \delta_i = 1.85$  for  $\mathbb{Z}_2$  in bare PXP model (Model-A) at  $L=20$ . This causes rapid thermalization from  $|0\rangle$ .

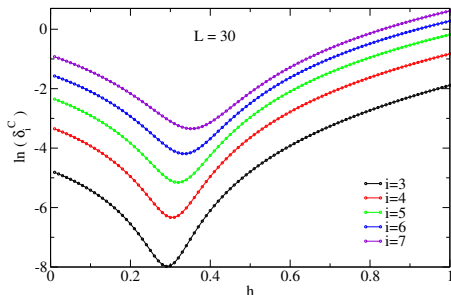
- Can we come up with terms that reduces the FSA errors for  $|0\rangle$  ??  
(Again the most challenging part).

$$\textbf{Model-C : } H_C = - \sum_i \tilde{\sigma}_i^x - (h \sum_i \tilde{\sigma}_i^+ \tilde{\sigma}_{i-1}^- \tilde{\sigma}_{i+1}^- + h.c)$$

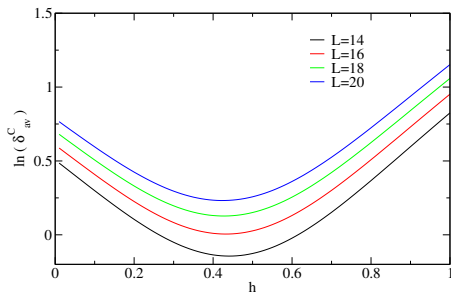
the additional term connects  $|\cdots 01010 \cdots\rangle$  to  $|\cdots 00100 \cdots\rangle$ .

- Again we find  $\delta_1^C = \delta_2^C = 0$  though the FSA vector changes.

- Higher order FSA errors must also be minimized. But unlike  $\mathbb{Z}_2$ , both  $\delta_j^C$  and corresponding  $h^{min}$  increases steadily with  $i$ .



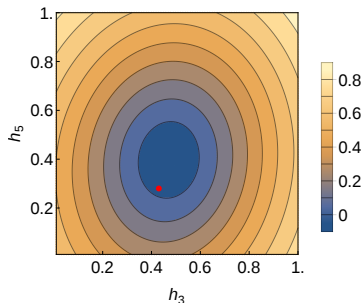
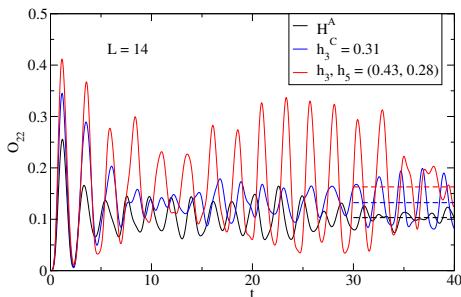
- Average error per step increases with  $L$ , much more rapidly compared to  $\mathbb{Z}_2$ .



- **Solution :** Just like the  $\mathbb{Z}_2$  case, add longer range term of similar nature.

$$H = H^C + h_5 \sum_i (\tilde{\sigma}_{i-1}^+ \tilde{\sigma}_{i+1}^+ \tilde{\sigma}_{i+2}^- \tilde{\sigma}_i^- \tilde{\sigma}_{i-2}^- + h.c.)$$

- these parameters must be optimized together.



## Physical realization

- Periodic dynamics of vacuum state ( $|0\rangle$ ).

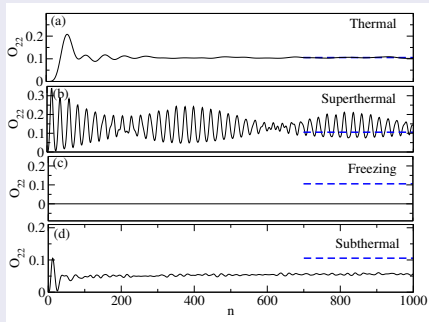
- Protocol :

$$\begin{aligned}\lambda(t) &= +\lambda ; 0 < t \leq T/2 \\ &= -\lambda ; T/2 < t \leq T.\end{aligned}$$

$$\begin{aligned}U(T, 0) &= e^{-iH[\lambda]T/2\hbar} e^{-iH[-\lambda]T/2\hbar} \\ &= e^{-iH_F T}\end{aligned}$$

- Variety of non-thermal phases.

- Superthermal.  $\implies$  FSA
- Freezing of wavefunction.
- Subthermal.



$$H_F^{eff} = \sum_i (C_1(\lambda, T) \tilde{\sigma}_i^x + C_2(\lambda, T) \tilde{\sigma}_i^y) + C_3(\lambda, T) \sum_i (\tilde{\sigma}_i^+ \tilde{\sigma}_{i-1}^- \tilde{\sigma}_{i+1}^- + h.c)$$

$$\left. \frac{|C_3|}{\sqrt{|C_1|^2 + |C_2|^2}} \right|_{\lambda^{super}, T^{super}} = 0.35$$

**Mukherjee et al, Phys. Rev. B 102, 075123 (2020)**



