

Effective low energy Hamiltonians through the variational Schrieffer-Wolff transformation

Anatoli Polkovnikov, Boston University

M. Bukov	Berkeley
E. Boyers	BU
P. Claeys	Cambridge
A. Chandran	BU
A. Dymarsky	UKY, SkolTech
O. Howell	BU
V. Gritsev	U Amsterdam
M. Kolodrubetz	UT Dallas
P. Mehta	BU
M. Pandey	BU
T. Renzo	BU
D. Sels	Harvard
S. Sugiura	Harvard
A. Sushkov	BU
J. Wurtz	BU

Jonathan



Pieter



Dries



Sho



Tamiro



Owen



Mohit



Non-equilibrium superconductivity, Flatiron Institute,
01/2020

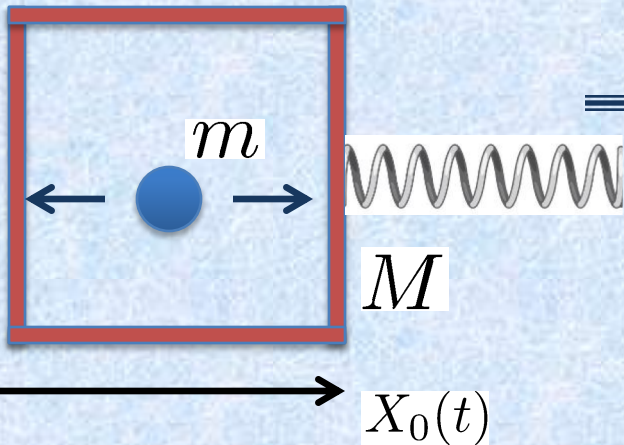
Main themes

- Intro: adiabatic gauge potential. Counter-diabatic (CD) and Fast-Forward (FF) driving in classical and quantum systems.
- **(Quantum) Curling.** Floquet realization of CD/FF driving. Adiabatic/isothermal state preparation. **Experiments**
- **(Quantum) dressing.** Variational Schrieffer-Wolff transformation. Effective Hamiltonians. **Numerical Simulations**
- Highly directional adiabatic landscapes.
- Efficient heat engines.



Moving frame transformations in classical systems.

Galilean transformation. Particle in a moving potential



$$H = \frac{p^2}{2m} + V(x - X_0(t))$$

Solving the problem in the Lab frame is difficult
– time dependent potential, moving boundary conditions, ...

Can go instead to the moving frame, define a new coordinate

$$\xi(t) = x(t) - X_0(t)$$

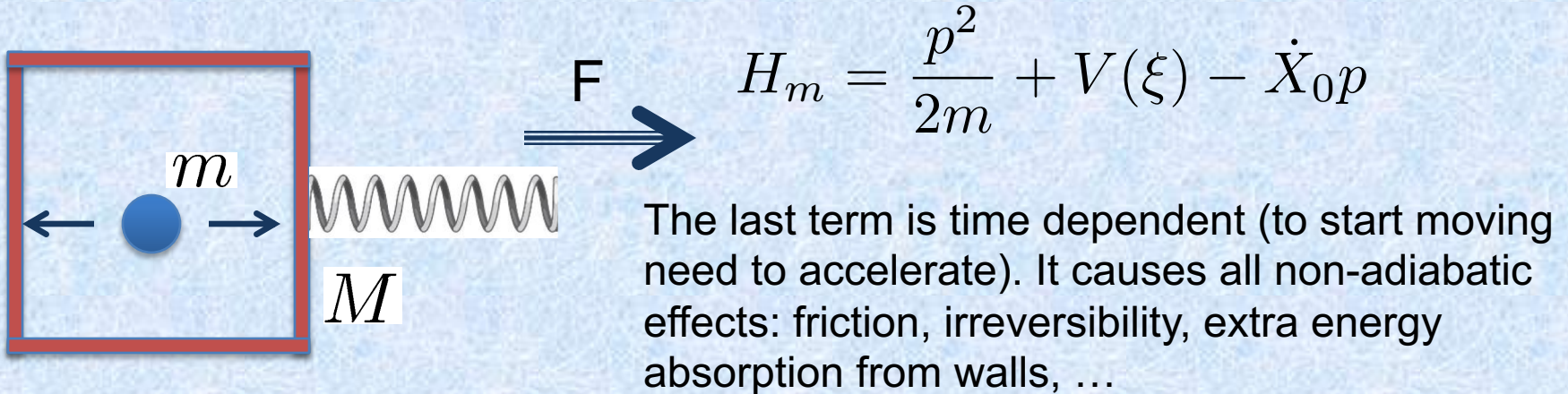
New effective moving Hamiltonian with a static potential and an extra Galilean term

$$H_m = \frac{p^2}{2m} + V(\xi) - \dot{X}_0 p$$

The problem is much simpler in the new frame.
The Galilean term vanishes in the slow limit;
recover the classical adiabatic theorem.

Counterdiabatic (transitionless) driving.

(M. Demirplak, S. A. Rice (2003), M. Berry (2009), S. Deffner, A. Del Campo, C. Jarzynski,.. (2010+), A. Clerk (2016+), vast literature in NMR).



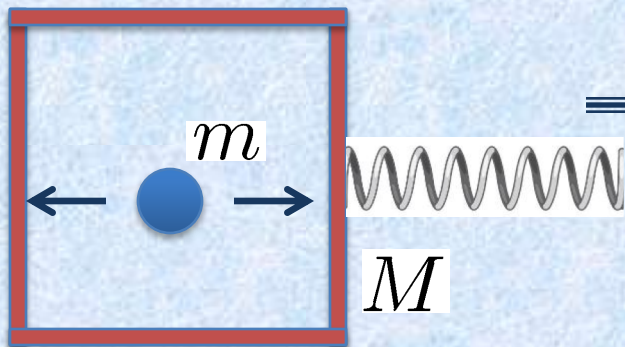
Idea: introduce a new counter term to the original (Lab frame) Hamiltonian

$$H \rightarrow H_{\text{CD}} = H + \dot{X}_0 p$$

In the moving frame we get
$$H_{\text{CD},m} = H_{\text{CD}} - \dot{X}_0 p = \frac{p^2}{2m} + V(\xi)$$

The moving CD Hamiltonian is static for **any** $X_0(t)$. Dynamics is completely adiabatic!

Fast-forward driving (many existing applications)



Need to realize:

$$H_{\text{CD}} = \frac{p^2}{2m} + V(x - X_0) + \dot{X}_0 p$$

Not always easy unless we are dealing with charged particles. Need to couple to the momentum

Do another (time-dependent) canonical transformation (recall electromagnetism)

$$p + m\dot{X}_0 = \eta \quad \text{This is simply a change of variables}$$

Obtain an equivalent CD Hamiltonian with a counter-gravitational force.

$$H_{\text{CD}} = \frac{\eta^2}{2m} - \cancel{\frac{m\dot{X}_0^2}{2}} + V(x - X_0) - m\ddot{X}_0 x$$

Define a *different* fast forward Hamiltonian to realize in the lab

$$H_{\text{FF}} = \frac{p^2}{2m} + V(x - X_0) - m\ddot{X}_0 x$$

This Hamiltonian has a shifted momentum of the particle, but it coincides with the correct momentum in the beginning and the end of the protocol if $\dot{X}_0(t) = 0$. Same initial and final states.

A waiter implementing a FF driving protocol to avoid food spillage in a complex system

Without counter term



With counter term



General approach: Need to find a canonical transformation where the Hamiltonian is time independent (up to possible energy shifts)

Gauge potential, a generator of continuous canonical transformations

$$\frac{\partial x}{\partial \lambda} = -\frac{\partial \mathcal{A}_\lambda}{\partial p}, \quad \frac{\partial p}{\partial \lambda} = \frac{\partial \mathcal{A}_\lambda}{\partial x} \quad \text{Easy to check that in this way we preserve the Poisson brackets.}$$

Equations of motion

$$\frac{dx}{dt} = \frac{\partial x}{\partial t} + \dot{\lambda} \frac{\partial x}{\partial \lambda} = \frac{\partial H}{\partial p} - \dot{\lambda} \frac{\partial \mathcal{A}_\lambda}{\partial p} = \frac{\partial H_m}{\partial p}, \quad \frac{dp}{dt} = -\frac{\partial H_m}{\partial x}$$

$$H_m = H - \dot{\lambda} \mathcal{A}_\lambda$$

The final ingredient. Need to find the canonical transformation, which leave the Hamiltonian invariant (stationary)

$$\{H(x(\lambda + \delta\lambda), p(\lambda + \delta\lambda), \lambda + \delta\lambda), H(x(\lambda), p(\lambda), \lambda)\} = 0 \\ \Leftrightarrow \{d_\lambda H, H\} = 0$$

$$d_\lambda H = \partial_\lambda H + \frac{\partial H}{\partial x} \frac{\partial x}{\partial \lambda} + \frac{\partial H}{\partial p} \frac{\partial p}{\partial \lambda} = \partial_\lambda H + \{\mathcal{A}_\lambda, H\}$$

We “simply” need to solve the equation

$$\{\partial_\lambda H + \{\mathcal{A}_\lambda, H\}, H\} = 0$$

Then we find the Adiabatic Gauge Potential (AGP). Implement the CD driving and solve (nearly) all the problems in the world: efficient heat machines – **energy problem**, perfect and fast analogue computers (will beat any quantum algorithm) – **technology**, eliminate dissipation – **no pollution**, quantum systems: infinitely fast adiabatic quantum computation – **cryptography, quantum phases...**

One caveat: in generic chaotic systems this equation does not have a solution. C. Jarzynski (1995).

There are no exact adiabatic transformations between chaotic energy shells.

Quantum systems.

Same story. Replace canonical transformations with unitary basis rotations

$$|\psi\rangle \rightarrow |\tilde{\psi}\rangle = U(\lambda(t))|\psi\rangle, \quad H \rightarrow \tilde{H} = U^\dagger H U$$

$$i\hbar d_t |\tilde{\psi}\rangle = U^\dagger (H - \dot{\lambda} \mathcal{A}_\lambda) U |\tilde{\psi}\rangle = (\tilde{H} - \dot{\lambda} \tilde{\mathcal{A}}_\lambda) |\tilde{\psi}\rangle, \quad \mathcal{A}_\lambda = i\hbar (\partial_\lambda U) U^\dagger$$

Define the moving (CD) Hamiltonian like in the classical case

$$H_m = H - \dot{\lambda} \mathcal{A}_\lambda \qquad H_{\text{CD}} = H + \dot{\lambda} \mathcal{A}_\lambda$$

Find the particular Adiabatic Gauge Potential (AGP)

$$[d_\lambda \tilde{H}, \tilde{H}] = 0 \Rightarrow \left[\partial_\lambda H + \frac{i}{\hbar} [\mathcal{A}_\lambda, H], H \right] = 0$$

Essentially need to solve the same equation. For any finite system it exists (because there is always U diagonalizing H) but the solution can become (exponentially) unstable, nonlocal, nonrealizable in chaotic systems.

Finding the AGP

Need to solve

$$[\partial_\lambda H + \frac{i}{\hbar}[\mathcal{A}_\lambda, H], H] = 0 \quad \leftrightarrow \quad \mathcal{A}_{\lambda, nm} = i\hbar \frac{\langle n | \partial_\lambda H | m \rangle}{E_m - E_n}$$

Finding the AGP is equivalent to the minimization problem

$$[\partial_\lambda H + \frac{i}{\hbar}[\mathcal{A}_\lambda, H], H] = 0 \quad \leftrightarrow \quad \frac{\delta \text{Tr} [(\partial_\lambda H + \frac{i}{\hbar}[\mathcal{A}_\lambda, H])^2]}{\delta \mathcal{A}_\lambda} = 0$$

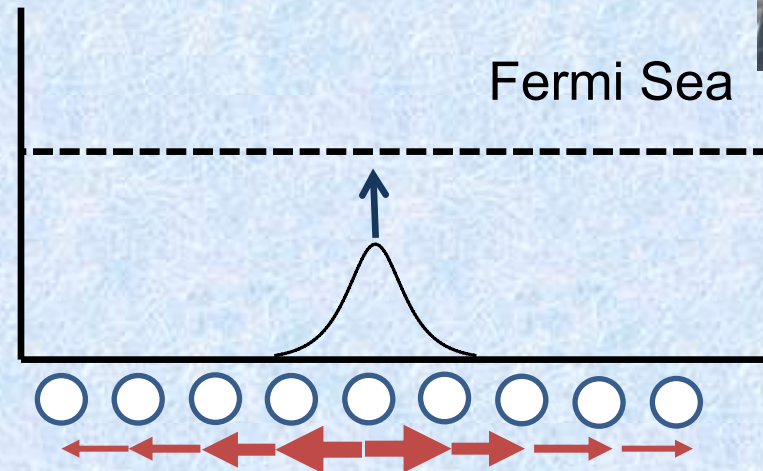
Can develop a variational procedure for finding gauge potentials (D. Sels, A.P., PNAS 2016).

$$G_\lambda \equiv \partial_\lambda H + \frac{i}{\hbar}[\mathcal{A}_\lambda, H]$$

the slowest locally dressed operator adiabatically connected to $\partial_\lambda H$. H. Kim, D. Huse 2015; M. Mierzejewski, P. Prelovšek, and T. Prosen 2015

Finding slow (almost conserved) operators $\sim$ finding local adiabatic transformations. Existence of local adiabatic transformations implies local conservation laws.

Example: quantum jumper of fighting the Anderson Orthogonality Catastrophe (semi-open system)



$$H = H_0 + \sum_j \lambda v_j c_j^\dagger c_j, \quad \mathcal{A}_\lambda^* = i \sum_j \alpha_j(\lambda) (c_j^\dagger c_{j+1} - c_{j+1}^\dagger c_j)$$

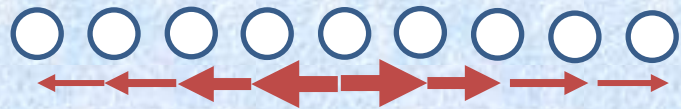
The exact AGP contains arbitrary range hoping terms

Result of the minimization: solution of the Laplace equation

$$-3\Delta\alpha + \lambda^2(\nabla_j v)^2\alpha = \lambda\nabla_j v_j$$

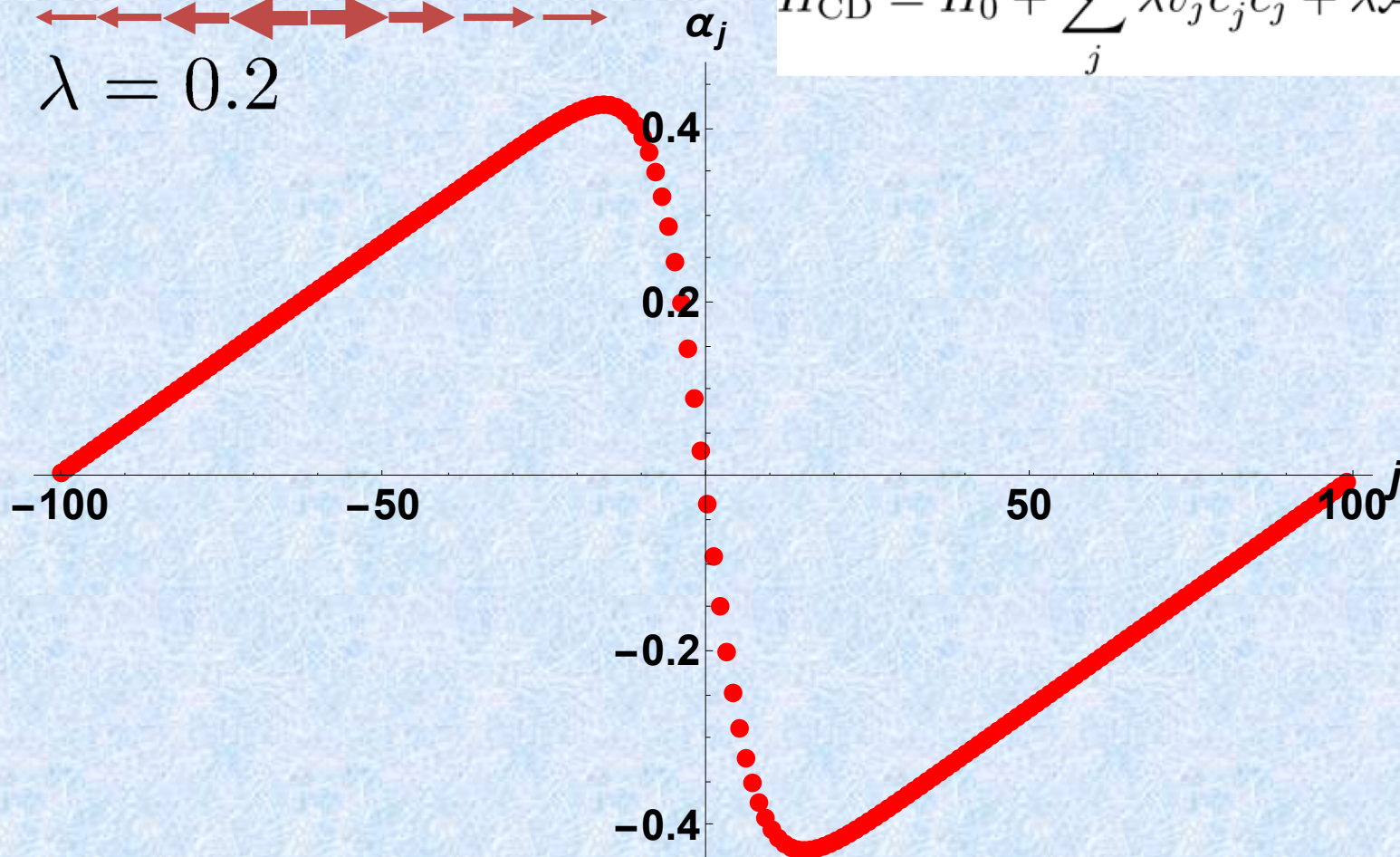
$$V(j, \lambda) = \frac{\lambda}{\cosh^2(j/8)}$$

$$\mathcal{A}_\lambda^* = i \sum_j \alpha_j(\lambda) (c_j^\dagger c_{j+1} - c_{j+1}^\dagger c_j)$$



$$\lambda = 0.2$$

$$H_{\text{CD}} = H_0 + \sum_j \lambda v_j c_j^\dagger c_j + \dot{\lambda} \mathcal{A}_\lambda^*$$



Like with a waiter: doable but difficult. Can map to FF protocol using the Peierls transformation.

Fast forward protocol

Perform a phase (Peierls) transformation: $c_j \rightarrow c_j e^{-i\varphi_j}$

$$H_{\text{FF}} = - \sum_j J_{\text{eff}}(j) \left(c_{j+1}^\dagger c_j + c_j^\dagger c_{j+1} \right) + \sum_j V_{\text{eff}}(j) c_j^\dagger c_j,$$

$$V_{\text{eff}}(j) = V(\lambda, j) - \ddot{\lambda} \sum_{k=-L}^j \frac{\alpha(k)}{1 + \dot{\lambda}^2 (\alpha(k))^2}, \quad J_{\text{eff}}(j) = \sqrt{1 + \dot{\lambda}^2 (\alpha(j))^2},$$

The CD protocol is only sensitive to the velocity. The FF protocol also knows about acceleration

Small velocity: potential renormalization (slowing particles in front)

Large velocity: need to locally renormalize the hopping = local time rescaling or the local refraction index (creating a kind of black hole)

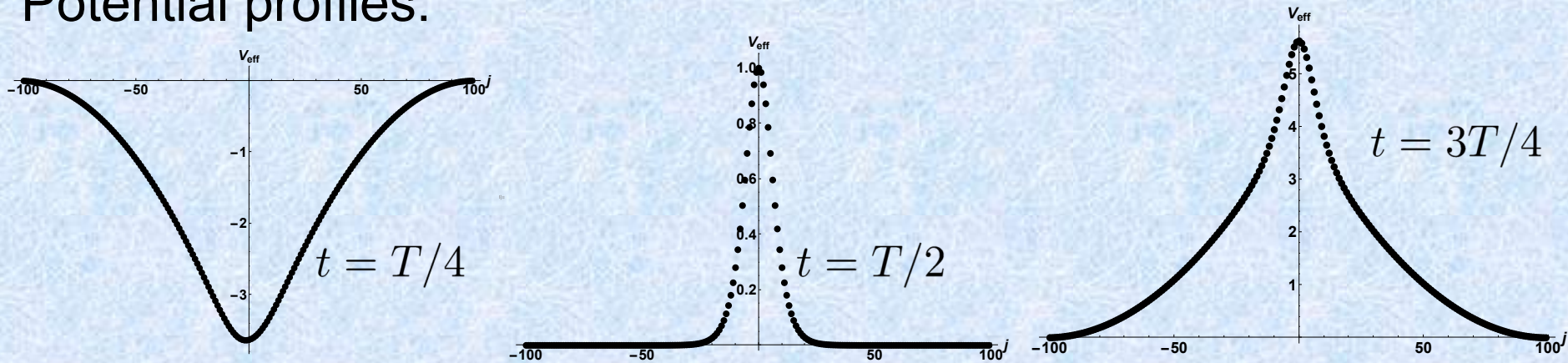
Can realize using the Floquet engineering – a general statement.

Snapshots of an effective potential and tunneling in FF protocol

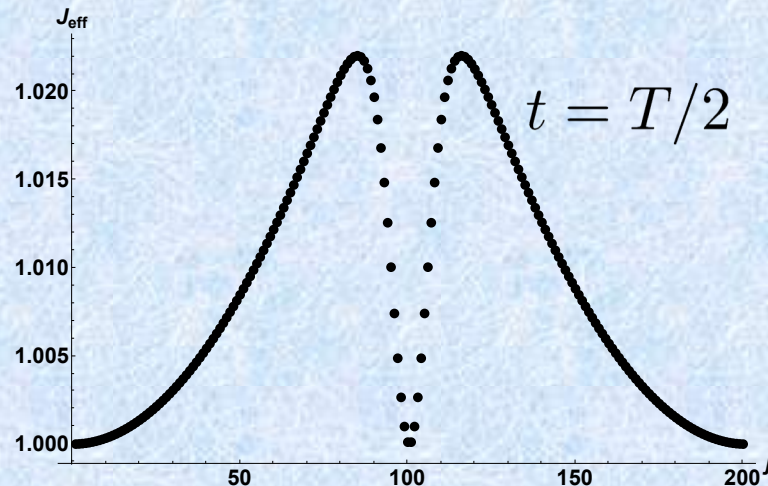
$$V(j, \lambda) = \frac{\lambda}{\cosh^2(j/8)}$$

$$\lambda(t) = 2 \sin^2 \left(\frac{\pi}{2} \sin^2(\pi t/2T) \right), \quad T = 10;$$

Potential profiles:



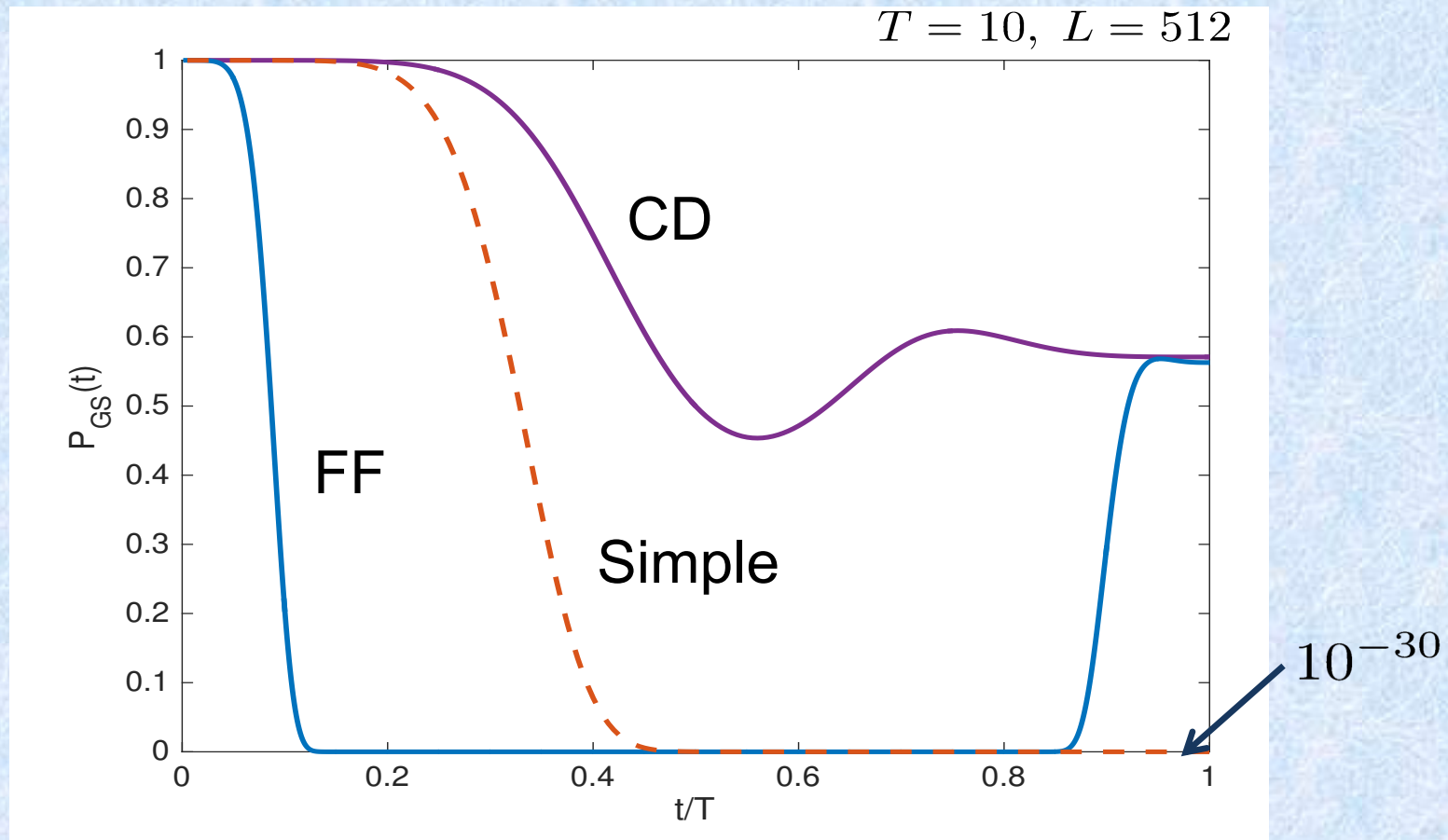
Tunneling profile
(less sensitive to time).



Numerics: half filling, 512 sites

$$V(j, \lambda) = \frac{\lambda(t)}{\cosh^2(j/\xi)}$$

$$\lambda(t) = 2 \sin^2 \left(\frac{\pi}{2} \sin^2(\pi t/2T) \right)$$



Beat Anderson Orthogonality Catastrophe.

Infinite temperature minimization (easy) works very well for the ground states.

Need a good general variational ansatz

$$\mathcal{A}_\lambda = i \sum_{k=1}^{k_{\max}} \alpha_k \underbrace{[H, [H, \dots [H, \partial_\lambda H]]]_{2k-1}},$$

P. Claeys et. al. PRL 2019. Becomes exact if $k_{\max} \rightarrow \infty$.

Treat the coefficients α_k as the variational parameters.

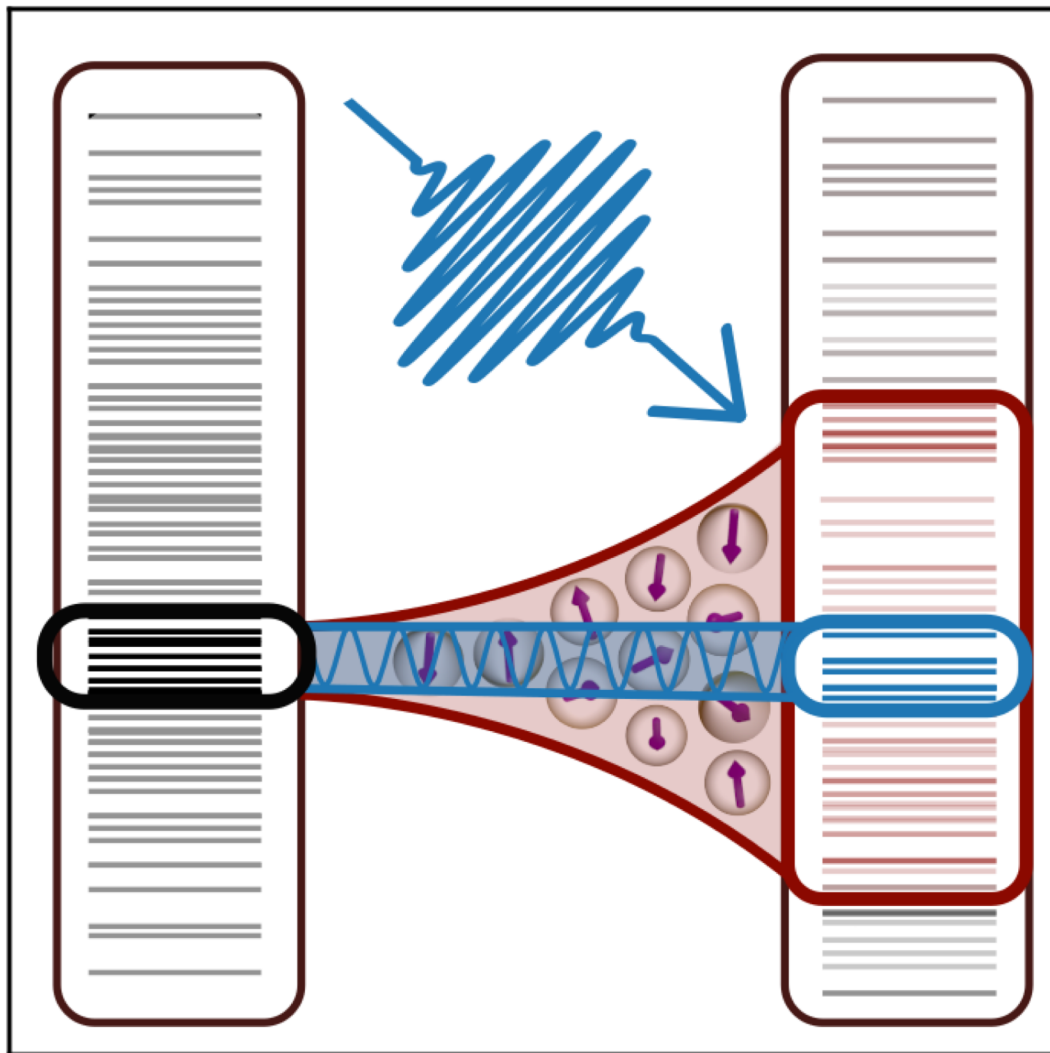
A simple quadratic minimization problem

$$\text{Tr} \left[(\partial_\lambda H + i[\mathcal{A}_\lambda, H])^2 \right] = \min$$

Find an approximate AGP.

Can realize this AGP using Floquet protocol. P. Claeys, M. Pandey, D. Sels, A.P. PRL 2019. Experiments in NV centers, stability to noise E. Boyers et. al. PRA 2019.

Floquet Realization of the CD driving

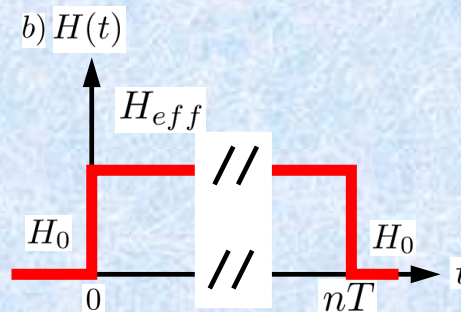
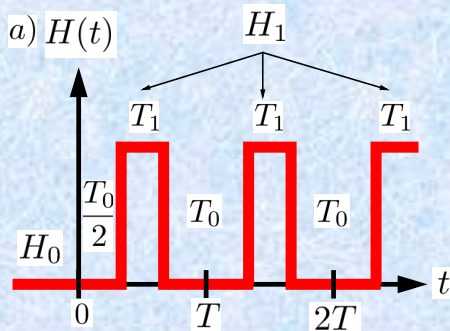


Use Floquet driving to suppress dissipation.

Fast state preparation,
reduced heating,
quantum simulations,

...

Floquet realization of CD Hamiltonians



$$U(T) = e^{-iH_1T_1} e^{-iH_2T_2} = e^{-iH_F T}$$

$$H_F = \frac{T_1 H_1 + T_2 H_2}{T} - i \frac{T_1 T_2}{2T} [H_1, H_2] + \dots$$

Need to match the CD protocol and the Floquet expansion (Floquet engineering)

$$H_{\text{CD}} = H + \dot{\lambda} \mathcal{A}_\lambda \quad \mathcal{A}_\lambda = i\alpha_1 [H, \partial_\lambda H] + i\alpha_3 [H, [H, [H, \partial_\lambda H]]]$$

One possibility

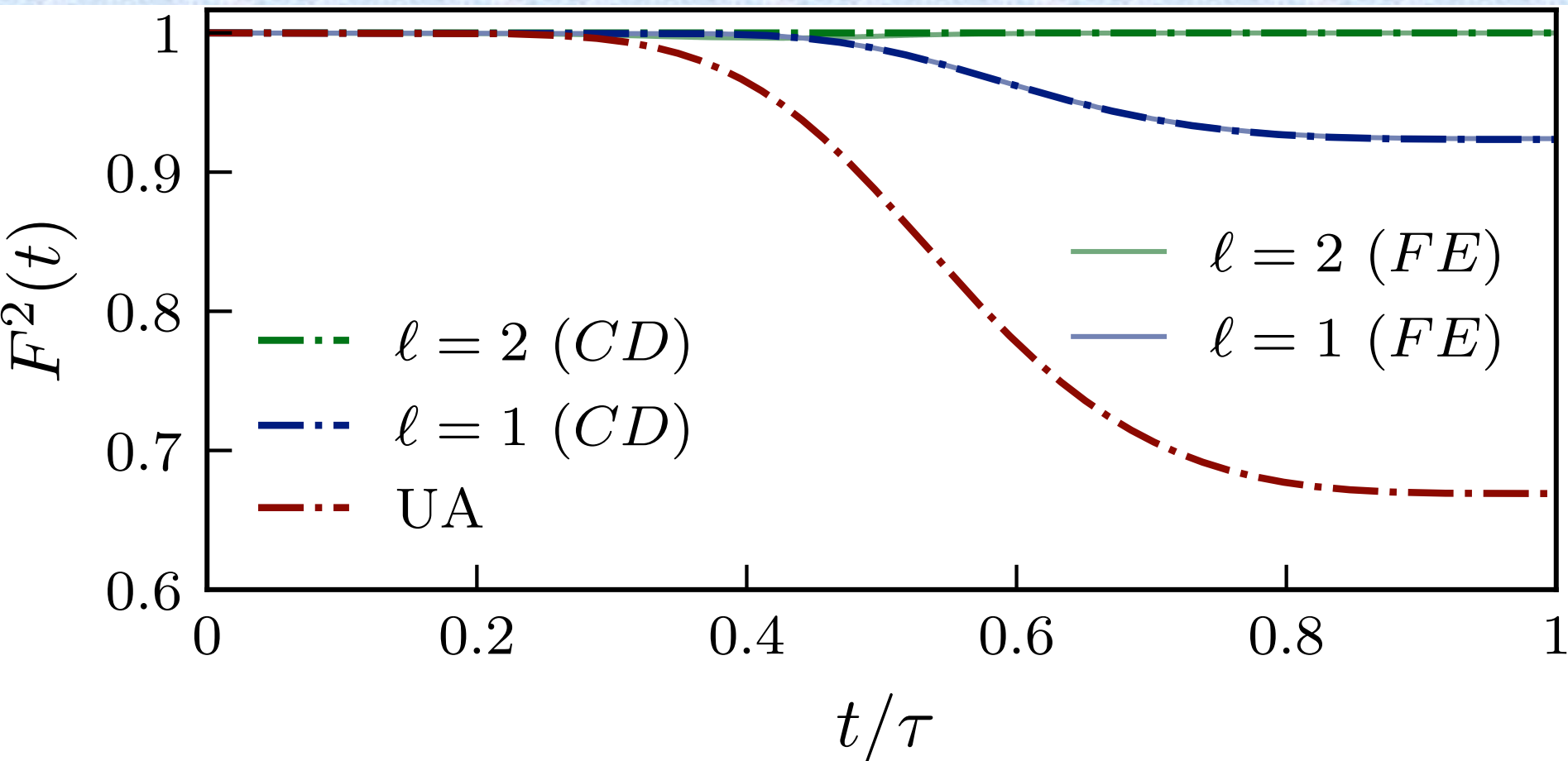
$$H_{FF}(t) = \left(1 + \frac{\omega}{\omega_0} \cos(\omega t) \right) H(\lambda) + \dot{\lambda} \sum_{k=1}^{k_{\max}} \beta_k \sin((2k-1)\omega t) \partial_\lambda H$$

$$H_F^{\text{rot}}(t) \approx H + i\dot{\lambda} \left[\frac{\beta_1}{\omega_0} [H, \partial_\lambda H] + \frac{1}{12} \frac{\beta_3 - 3\beta_1}{\omega_0^3} [H, [H, [H, \partial_\lambda H]]] + \dots \right]$$

Match the coefficients to find β_j through α_j . Realize the Floquet FF protocol

Example: adiabatic manipulation of a two-qubit gate

$$H = -2J\sigma_1^z\sigma_2^z - h(\sigma_1^z + \sigma_2^z) + 2h\lambda(\sigma_1^x + \sigma_2^x)$$

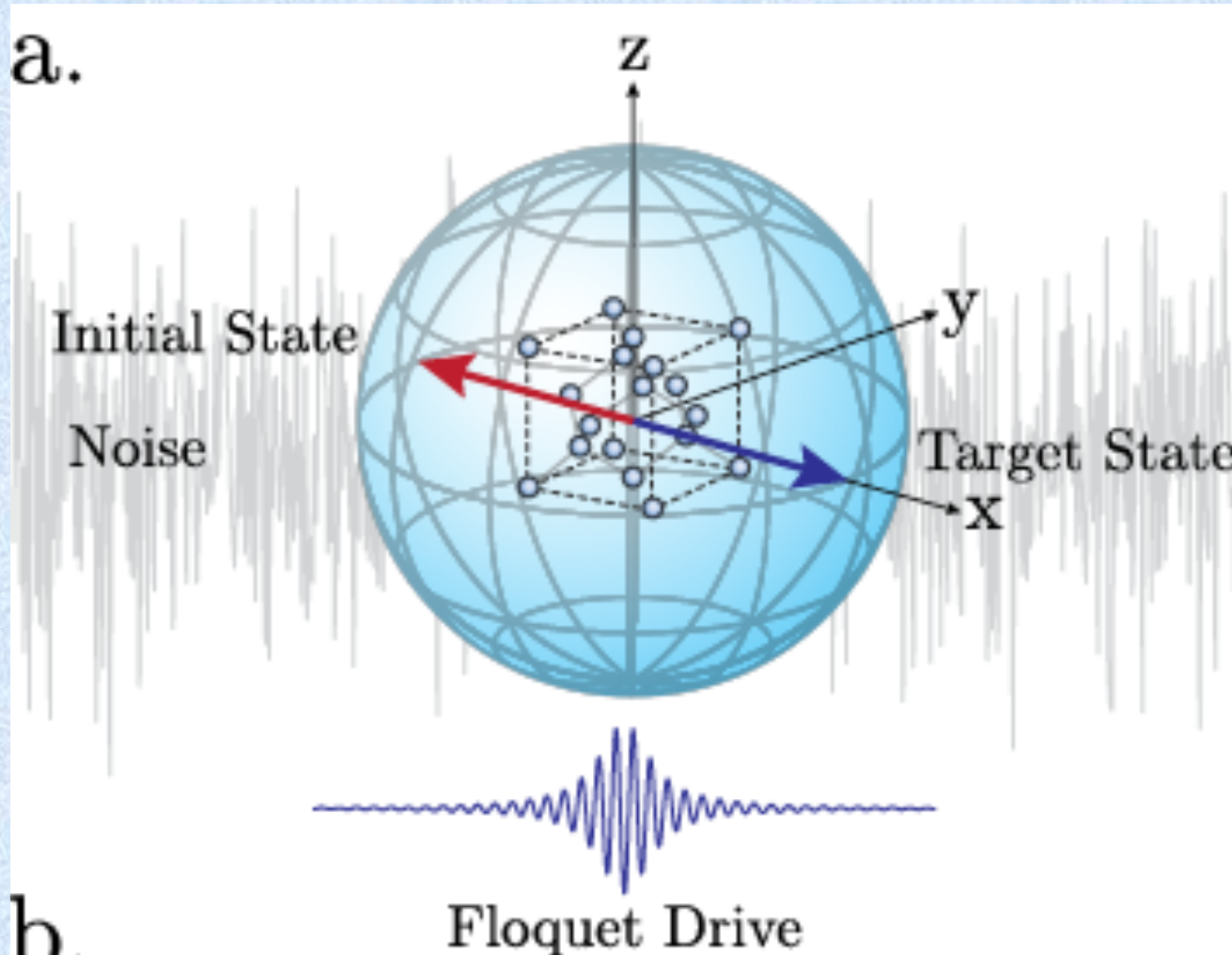


Experiments with NV centers in diamonds

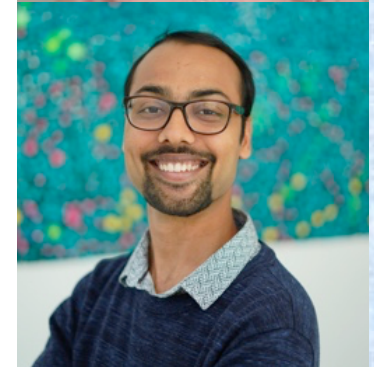
(E. Boyers, , , A. Sushkov, arXiv1811.09762)

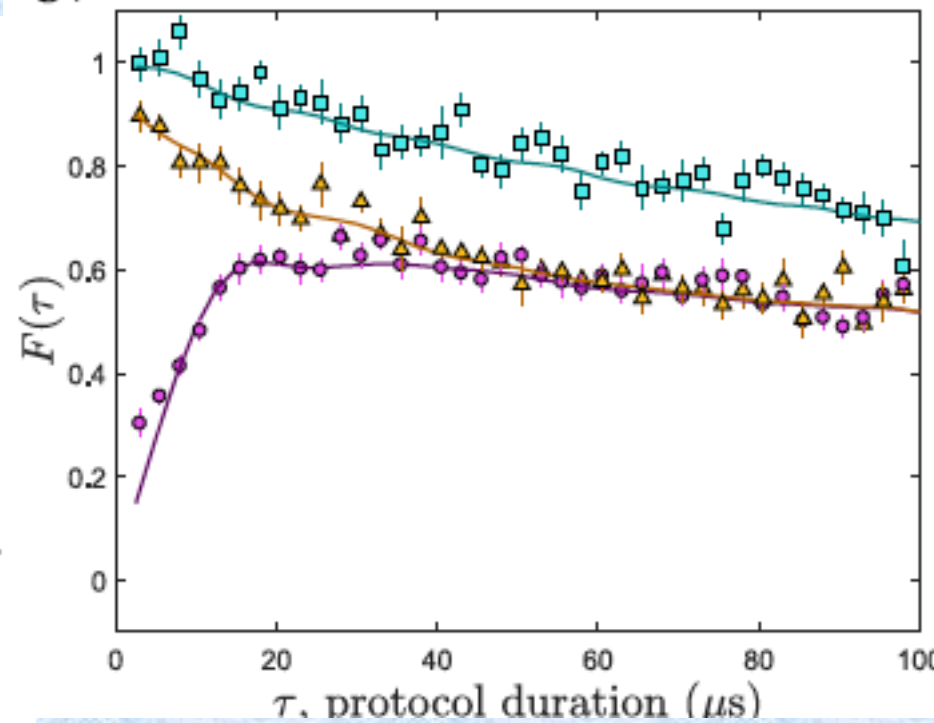
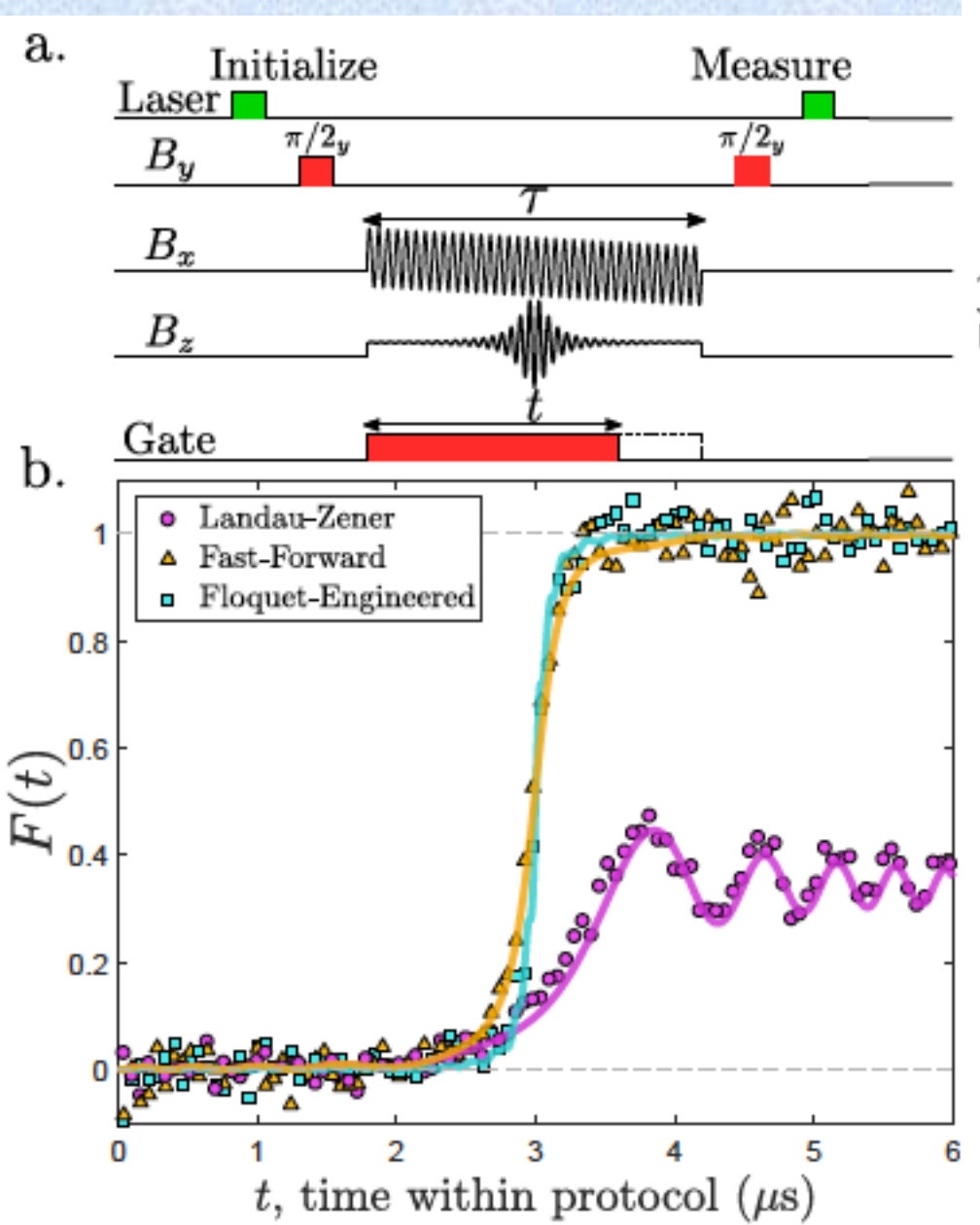
Goal: prepare quickly target state in the presence of noise

a.



b.





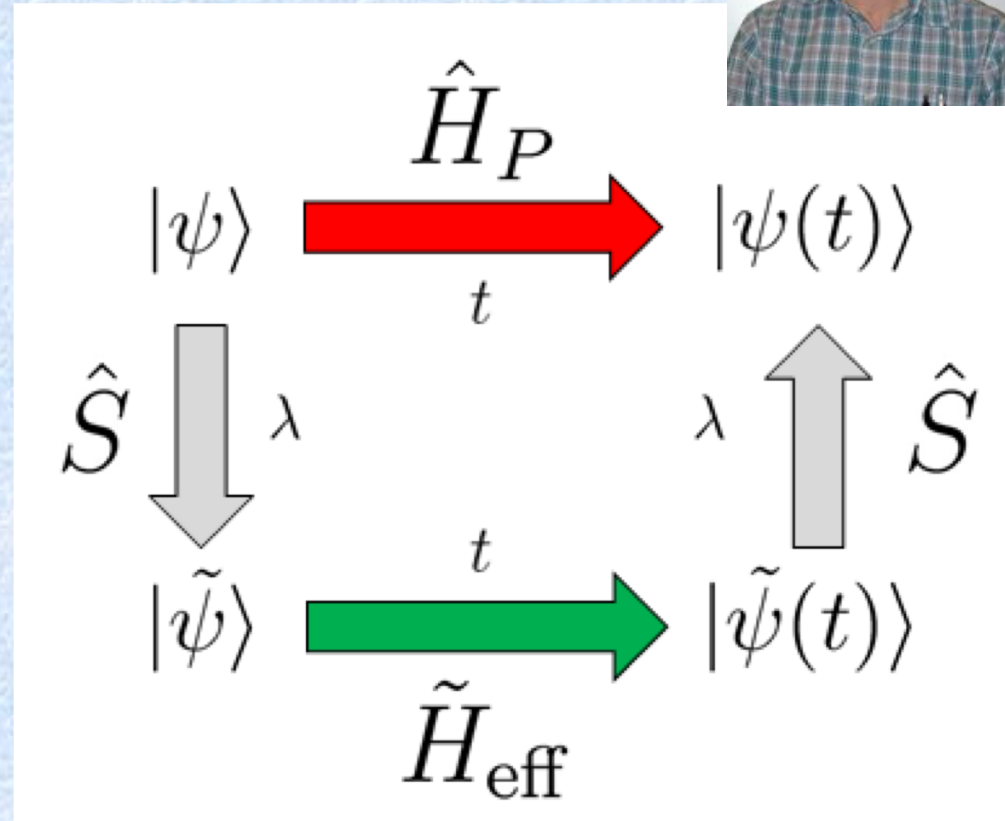
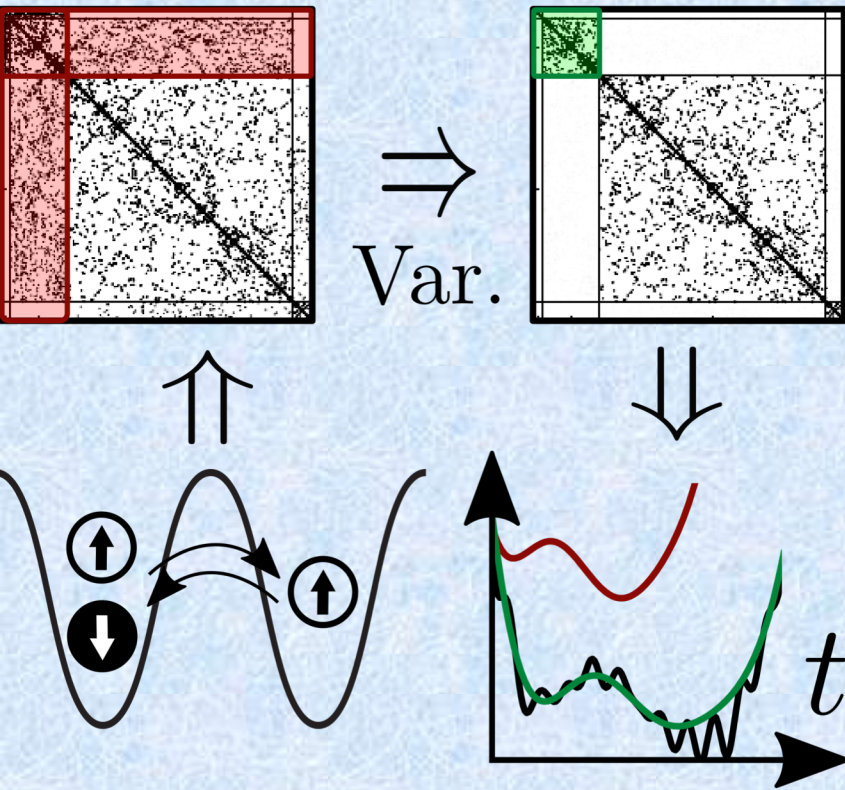
Noise dependence

Floquet protocol offers stability with respect to noise.

Performance of different protocols

Finding effective Hamiltonians

(with J. Wurtz and P. Claeys)



Use the variational minimization to find a non-perturbative Schrieffer-Wolff transformation and a low-energy effective theory.

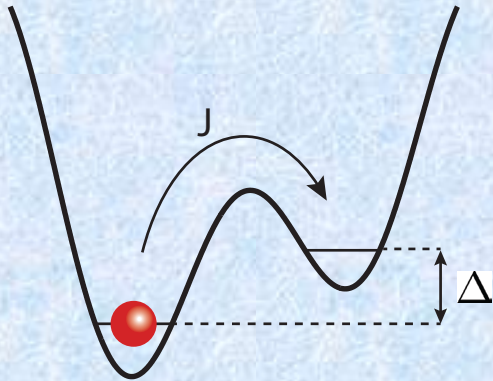
Perturbative SW transformation: rotating frame + high frequency (van Vleck) expansion (M. Bukov, M. Kolodrubetz, A.P. 2016).



A tilted two level system

$$H = \Delta a_2^\dagger a_2 - J(a_1^\dagger a_2 + a_2^\dagger a_1)$$

Assume $\Delta \gg J$



Go to the rotating frame $a_1 \rightarrow a_1, a_1^\dagger \rightarrow a_1^\dagger, a_2 \rightarrow a_2 e^{i\Delta t}, a_2^\dagger \rightarrow a_2^\dagger e^{-i\Delta t},$

$$H_{\text{rot}} = H - \Delta a_2^\dagger a_2 = -J \left(a_1^\dagger a_2 e^{-i\Delta t} + a_2^\dagger a_1 e^{i\Delta t} \right)$$

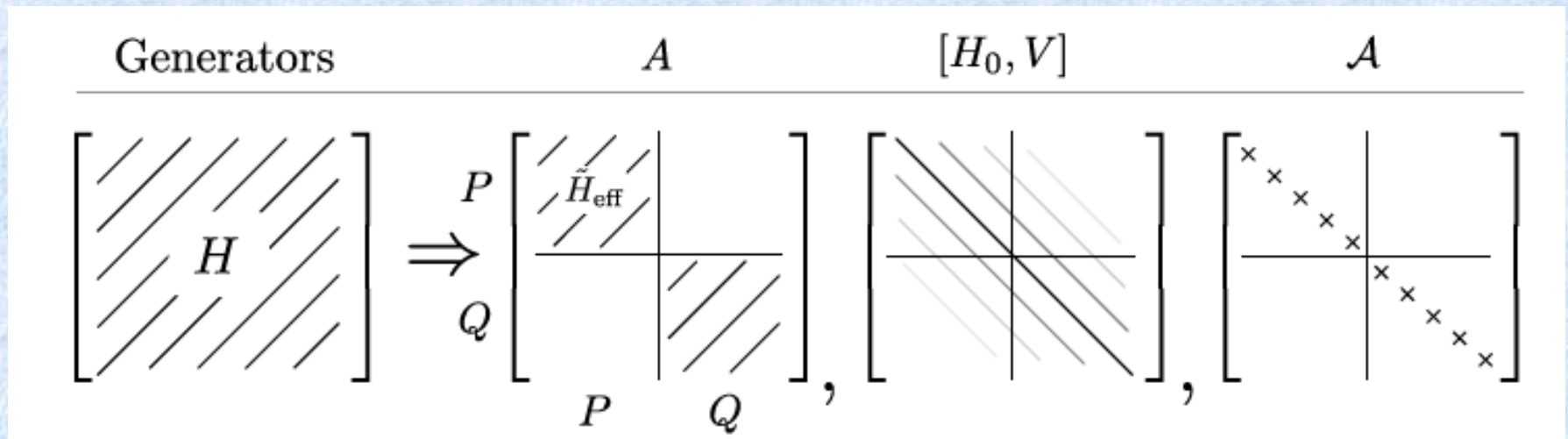
Apply high frequency expansion, get a block-diagonal Hamiltonian

$$H_F^{(0)} = 0, \quad H_F^{(1)} = \frac{1}{\Delta} [H_1, H_{-1}] = \frac{J^2}{\Delta} [a_2^\dagger a_2 - a_1^\dagger a_1]$$

(Anderson $\rightarrow$ Kondo, Hubbard $\rightarrow$ tJ, ...)

Main problem: this is an asymptotic uncontrolled expansion, especially when scales are comparable.

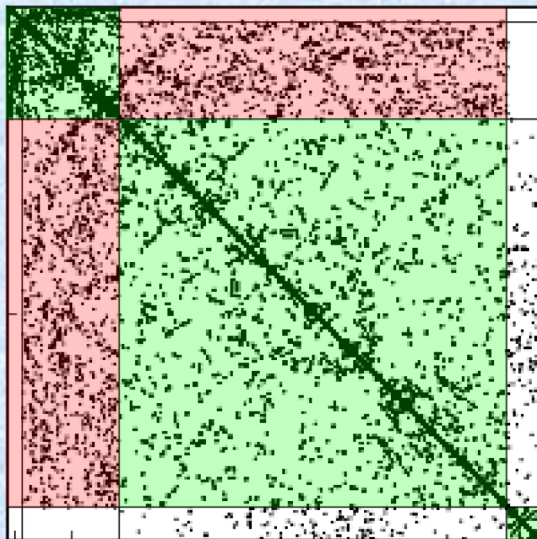
Schematic representation of different methods



SW

Flow Equations

AGP

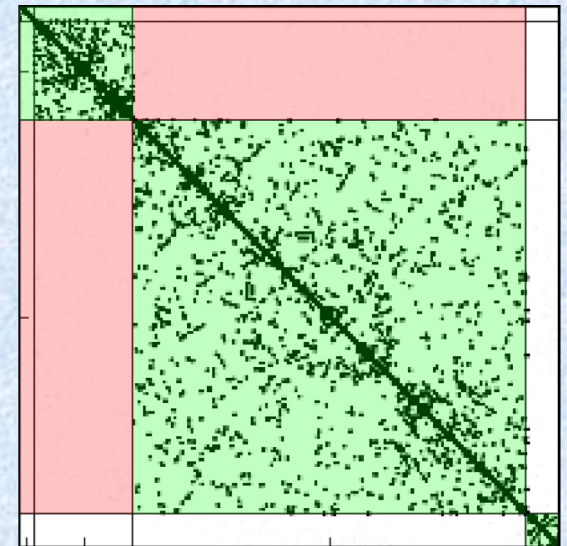


Variational AGP



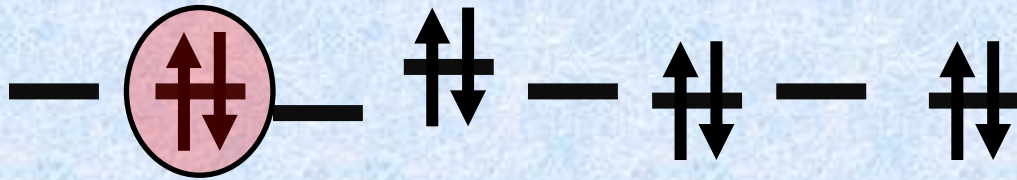
Almost ideal SW

$$i\partial_\lambda |\psi_n\rangle = \mathcal{A}_n |\psi_n\rangle$$

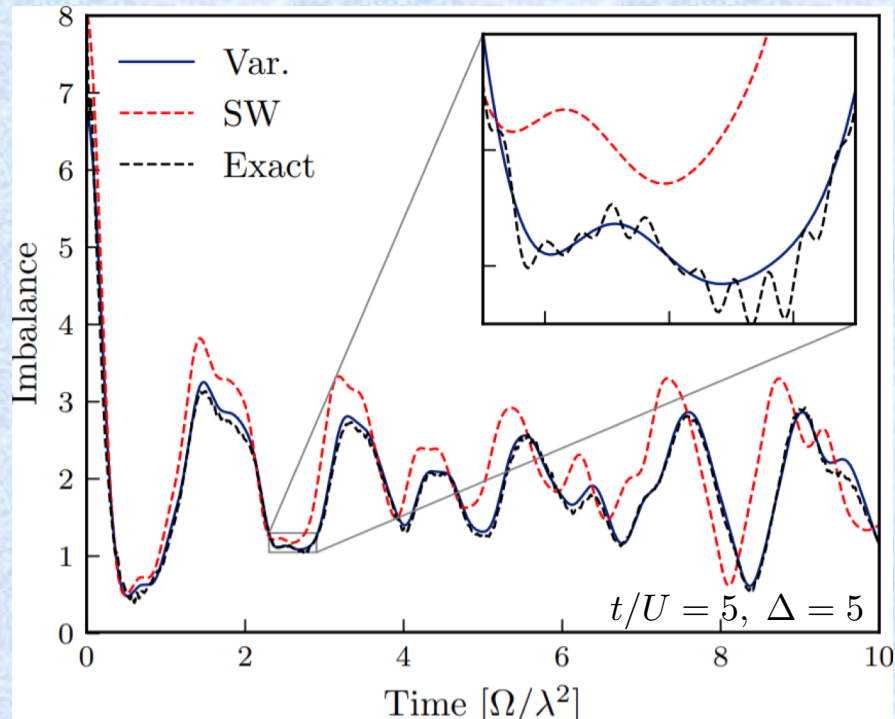


Results

Disordered attractive Hubbard model



The low energy manifold maps to an effective spin model (standard SW). Numerically MBL transition at $\delta_i \sim \pm t^2/U \sim \pm J$



Small oscillations due to projections to other sectors with one or more spinons.
Can be added to simulations.

8 site model.

Heisenberg: MBL ✓

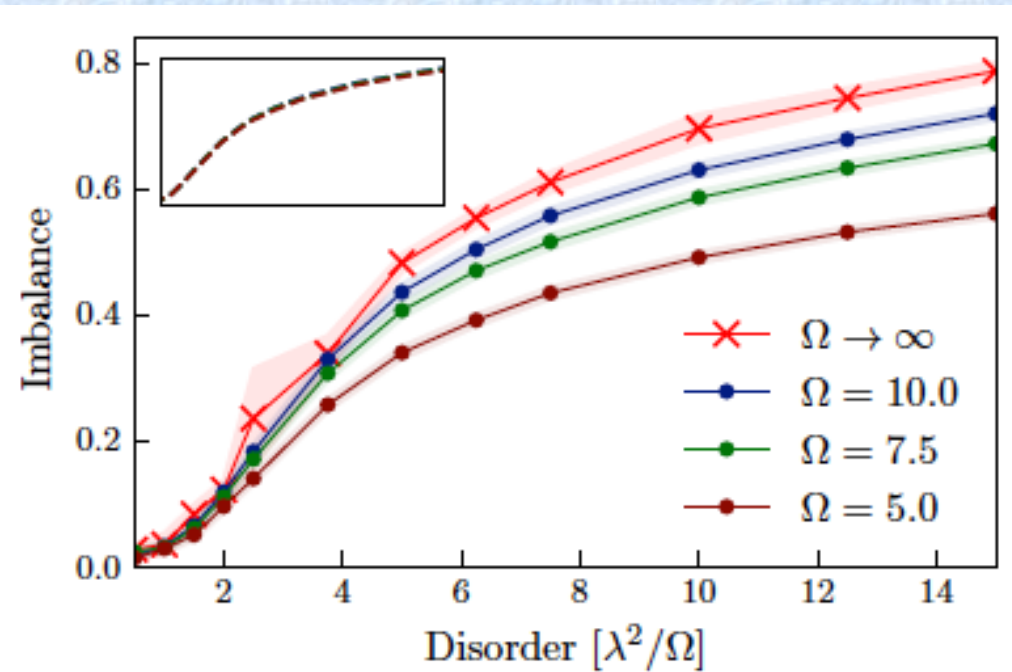
0 — $\uparrow\downarrow$ — $\uparrow\downarrow$ — $\uparrow\downarrow$ — $\uparrow\downarrow$

2 — $\uparrow\downarrow$ $\uparrow\downarrow$ $\uparrow\downarrow$ — $\uparrow\downarrow$ — $\uparrow\downarrow$

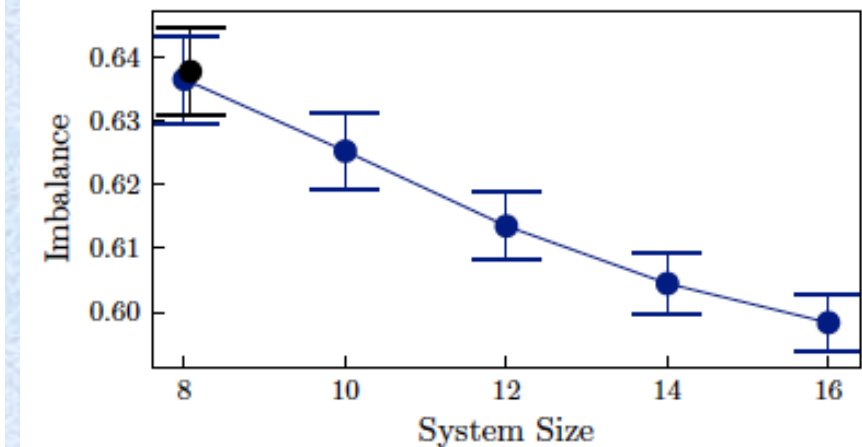
Easy to see pictorially, even a single spinon destroys MBL (also U. Krause, T. Pellegrin, P. W. Brouwer, D. A. Abanin, M. Filippone, 2019)

tJ Model: MBL ✗

18 site model



$\Delta = 10, U/t \equiv \Omega/\lambda = 7.5$



Can accurately extract spinon distribution in the TD limit.

Weakly nonintegrable XY Model

$$H = \sum_i \underbrace{\sigma_x^i \sigma_x^{i+1} + \sigma_y^i \sigma_y^{i+1} + 3\sigma_z^i}_{\text{Free fermions}} + \underbrace{1.25\sigma_x^i}_{\text{Does not conserve \#}}$$

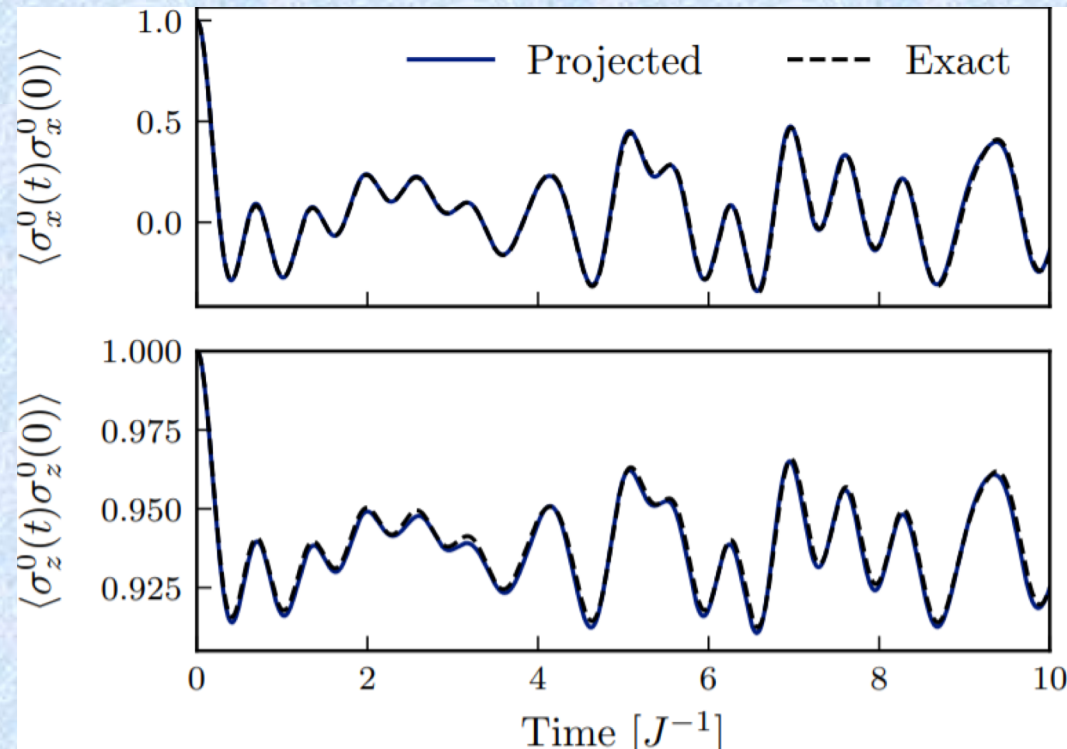
Free fermions

Does not conserve #

Time correlation functions of GS

Ground state response function, 16 sites

Exact: 65,536 states, Projected: 137 states



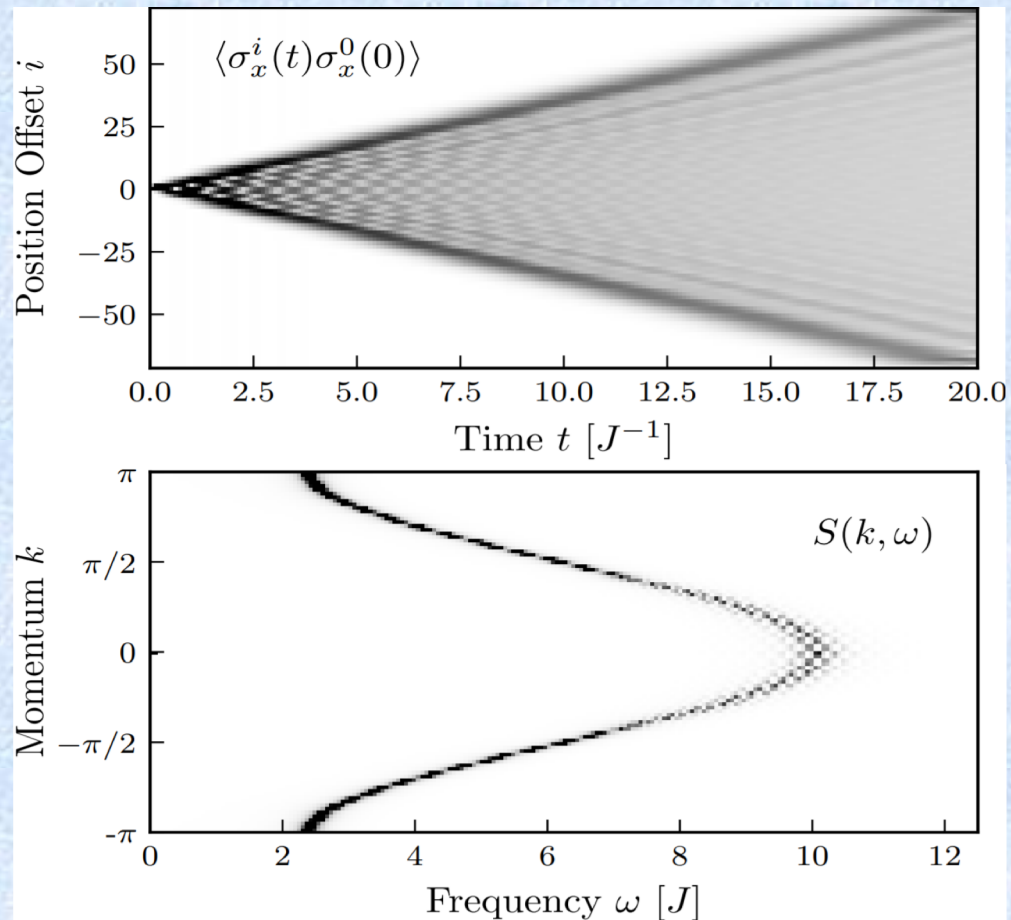
Larger System Size.

Local rotation $\Leftrightarrow$ Restore particle conservation by dressing them.

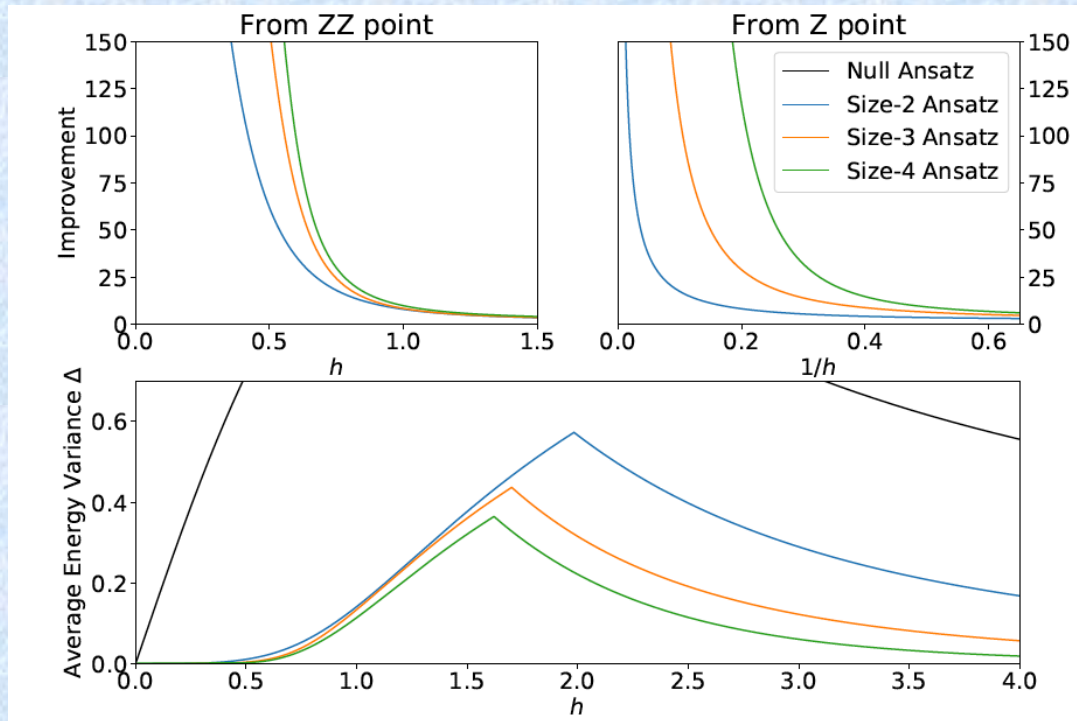
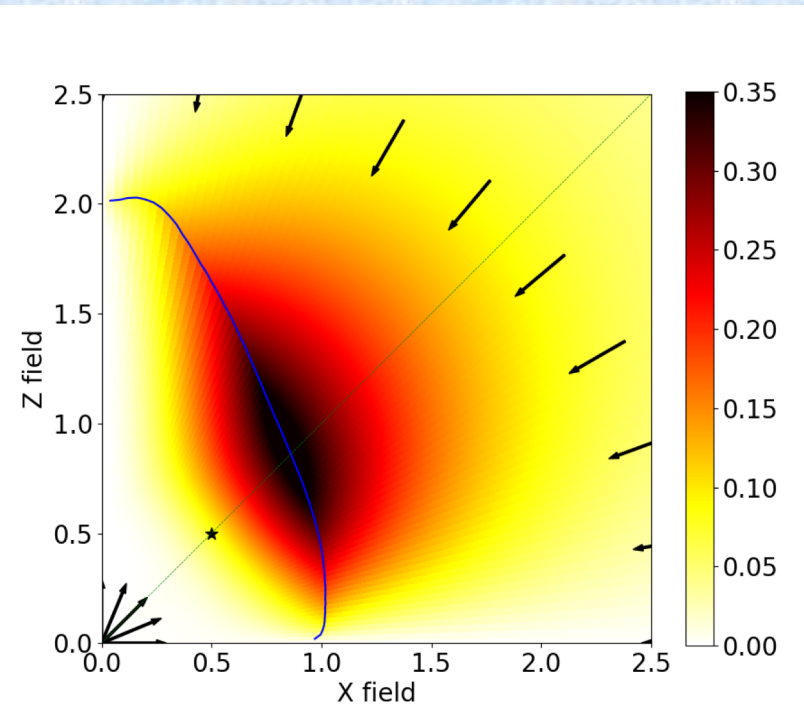
Response function for 128 sites

Can see overlapping particle sectors, broadening, life time

Properly dressed quasi-particles are very stable even at infinite temperatures.



Work in progress: optimal dressing, directional SW TFI model with longitudinal field. 2-particle sector. 14 sites



Can reach machine precision with a moderate ansatz if follow optimal directions

Very rich landscape of the Hilbert space even at infinite temperature

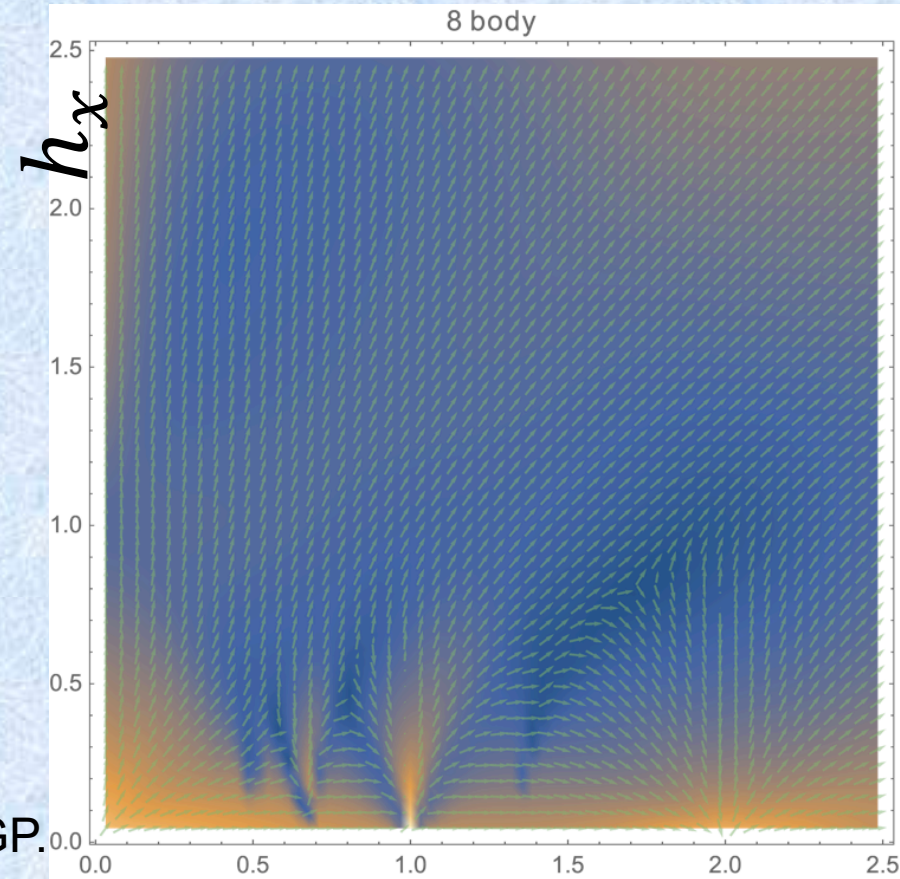
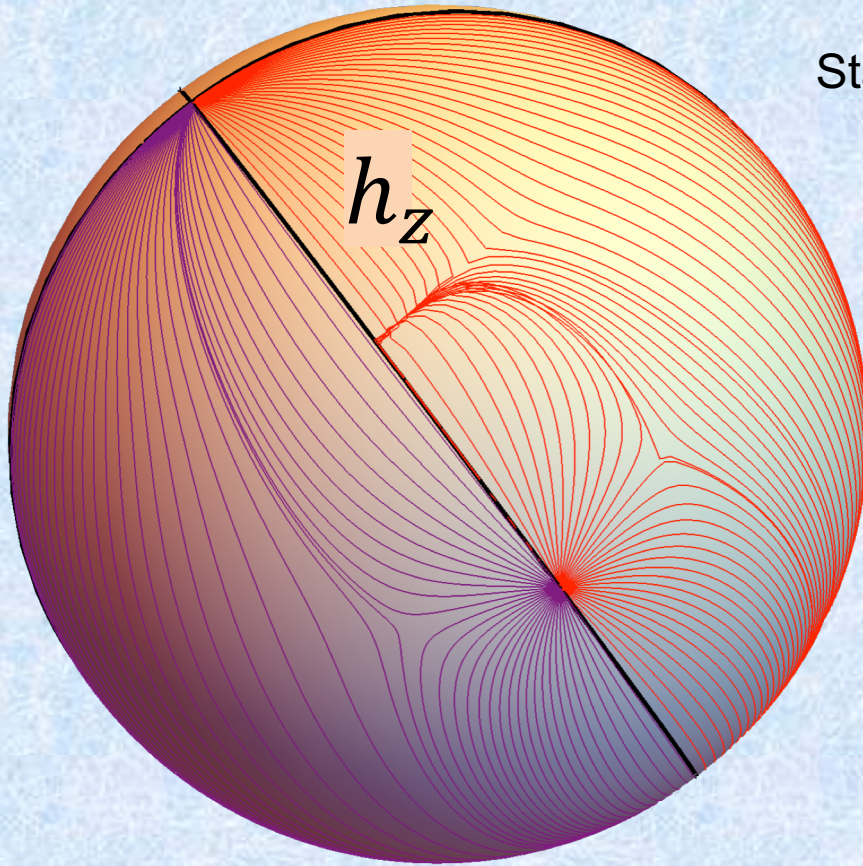


S. Sugiura P. Claeys, A. Dymarsky, A.P. in progress

Infinite temperature adiabatic flows

Adiabatic flows like RG flows – connect different Hamiltonians.

Starting at highly degenerate points is optimal.



Many body dark states (scars) emerge near singular points. They cancel singularities of AGP.

Orthogonal (bad) directions, very poor to no convergence of adiabatic transformations.

h_z

CD driving of open systems: engineering fast dissipative thermalization

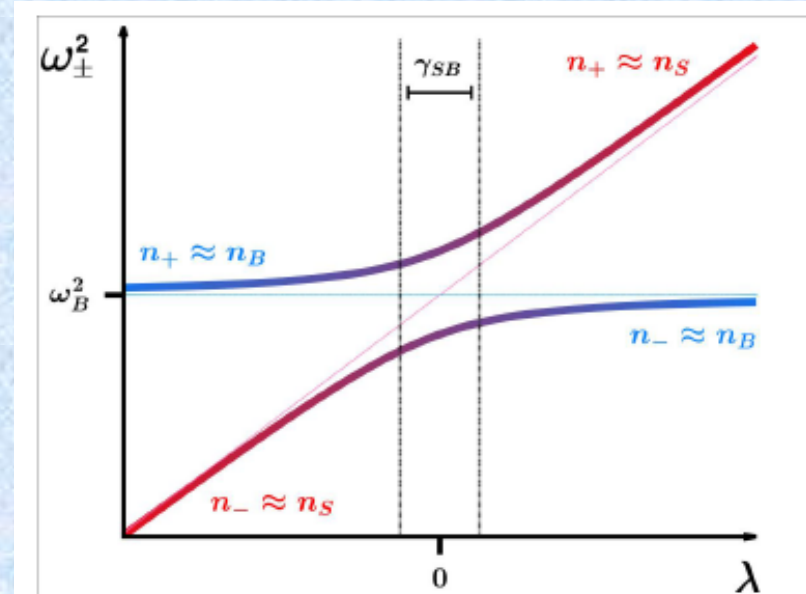
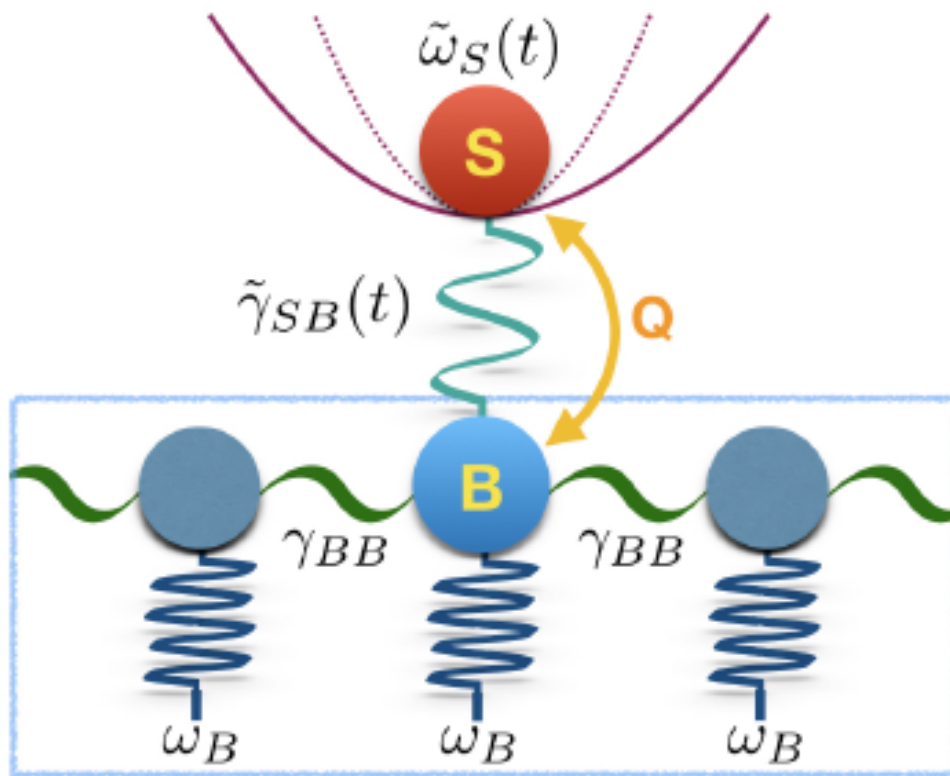
(T. Renzo, A. Chandran, A.P., PRB 2018)



$$H_{bath} = \sum_{j=1}^N \left[\frac{1}{2} p_j^2 + \frac{1}{2} \omega_B^2 x_j^2 - \gamma_{BB} \omega_B^2 x_j x_{j+1} \right]$$

$$H_S(t) = \frac{P^2}{2} + \frac{\omega_S^2}{2} X^2$$

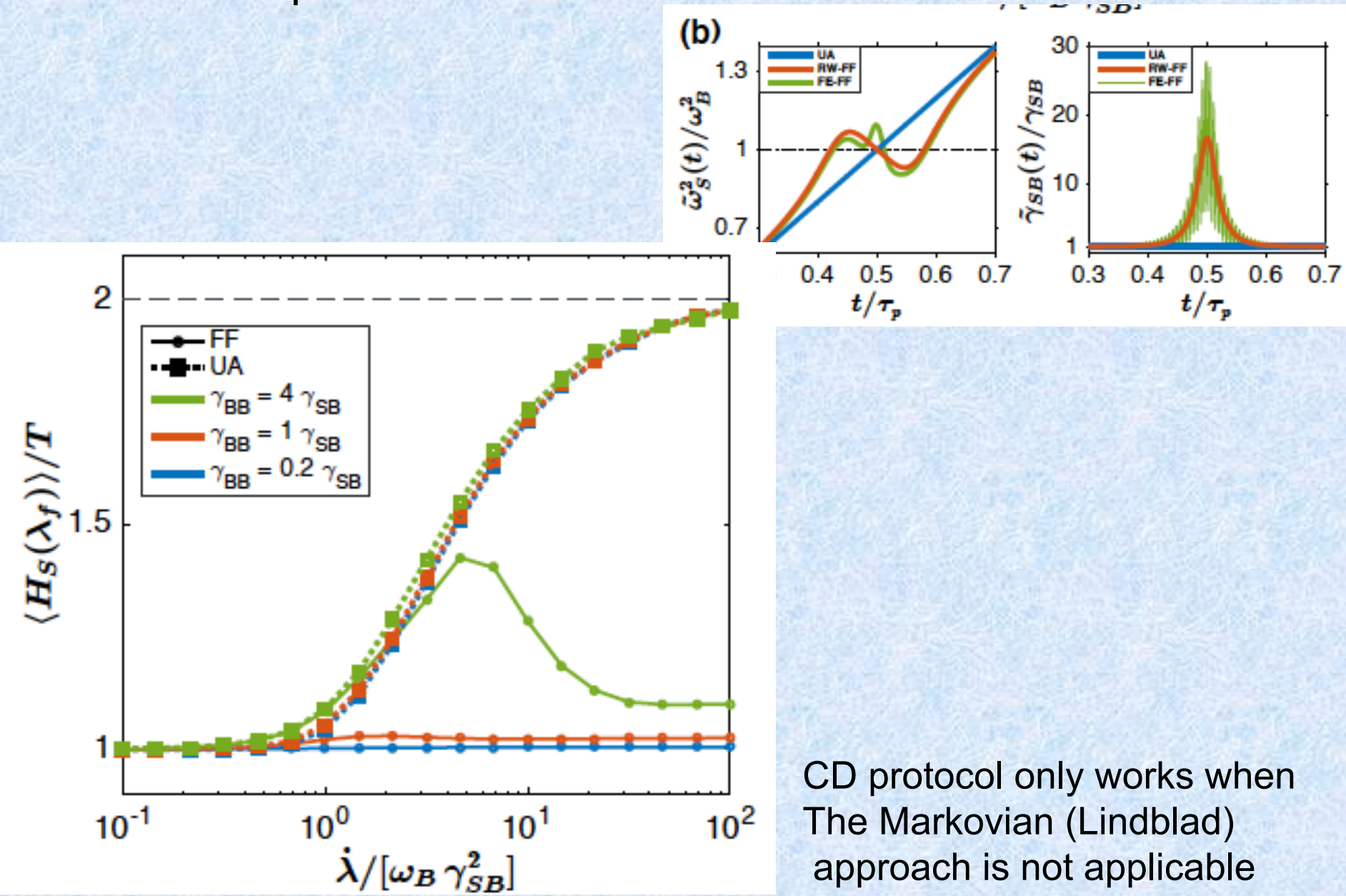
$$H_{SB} = -\tilde{\gamma}_{SB}(t) \omega_B^2 x_B X$$



$$\lambda(t) = \frac{\omega_S^2(t) - \omega_B^2}{\omega_B^2}$$

Drive an oscillator through a resonance with an optical phonon bath. Slow limit – isothermal process.

Different constraints: can not access bath. Can develop Floquet fast-forward protocol with some efforts



CD protocol only works when
The Markovian (Lindblad)
approach is not applicable

Summary

- Local driving can be very powerful for suppressing dissipation, state preparation (recent works by several groups on glasses).
- Floquet engineering of CD protocols is possible without extra controls.
- Very efficient variational SW transformation for getting effective Hamiltonians, states.
- Wide range of applications: Infinite temperature phase diagrams, geometry, new types of singularities, many-body dark states (scars), sensitive probes of quantum chaos, finding hidden integrability, non-perturbative Floquet Hamiltonians, optimal directions for annealing and state preparation, efficient fast heat engines, ...