[17pS101-5] 動的モード分解による量子多体系の長時間ダイナミクス予測

Forecasting long-time dynamics of quantum many-body systems by dynamic mode decomposition

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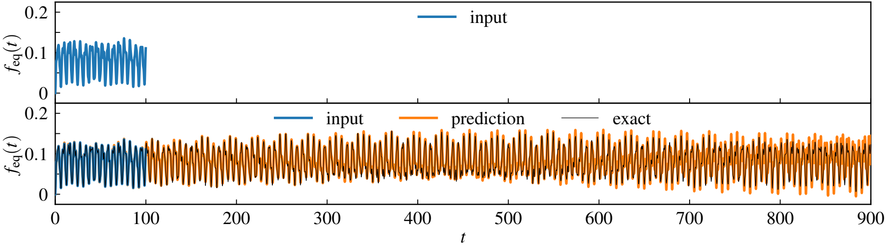
支援：学術変革領域研究 (A) 学習物理学の創成



R. Kaneko, M. Imada, Y. Kabashima, and T. Ohtsuki, arXiv:2403.19947.

Outline

- Introduction
  Numerical simulations of long-time dynamics are difficult
- Data-driven method
  Dynamic mode decomposition (DMD)
- Examine applicability to several quantum dynamics
  - Time evolution with oscillations
  - Time evolution with power-law decay
- Conclusions

Experimental advances in observing dynamics of quantum many-body systems

pump probe measurements
in copper oxides

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[S.Kaiser et al., PRB.89.184516('14)]

microscope measurement
of ultracold atom systems

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[M.Cheneau et al., Nature.481.484('12)]

- It is important to compare them with numerical simulations

Numerical simulations of long-time dynamics are challenging

- Solve time-dependent Schrödinger equation to get the wave function at each time step $|\psi(t)\rangle = e^{-iHt/\hbar}|\psi(0)\rangle$
  - Exact diagonalization methods are feasible only for small systems

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  - Negative-sign problem in real-time path integral simulations
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  - Calculable for a very shot time: $t \sim \dfrac{\hbar}{\text{(energy scale)}}$
  - Due to the high entanglement after long time evolutions

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Figure is removed for copyright reasons.

Sudden quench in the 2D transverse-field Ising model [M.Schmitt, M.Heyl, PRL.125.100503('20)]

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2D Bose-Hubbard model

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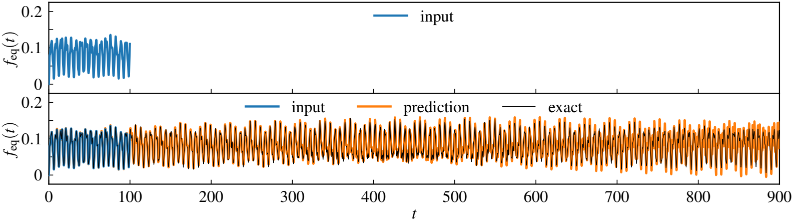
2D Transverse-field Ising model

[R.Kaneko and I.Danshita, CommunPhys.5.65('22); R.Kaneko and I.Danshita, PRA.108.023301('23)]

Motivation: Is there any easier data-driven methods?

- Yes!



- Only require numerical or experimental short-time data as an input
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- Accurate forecasts at time as long as nearly an order of magnitude longer than that of the short-time training data

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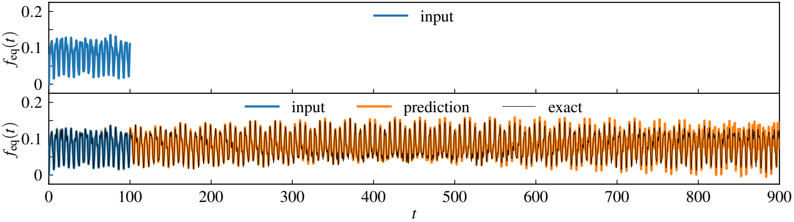

- Only require numerical or experimental short-time data as an input
  (We do not need to calculate the time-evolved wave function)
- Accurate forecasts at time as long as nearly an order of magnitude longer than that of the short-time training data
- Useful when combined with state-of-the-art time-dependent VMC, which can calculate up to $t \sim \mathbf{100}\hbar/$(energy scale)
  [K.Ido et al., PRB.92.245106('15); K.Ido et al., Sci.Adv.3.e1700718('17)]

Dynamic mode decomposition (DMD)

[J.N.Kutz et al., Dynamic Mode Decomposition: Data-Driven Modeling of Complex Systems ('16)]

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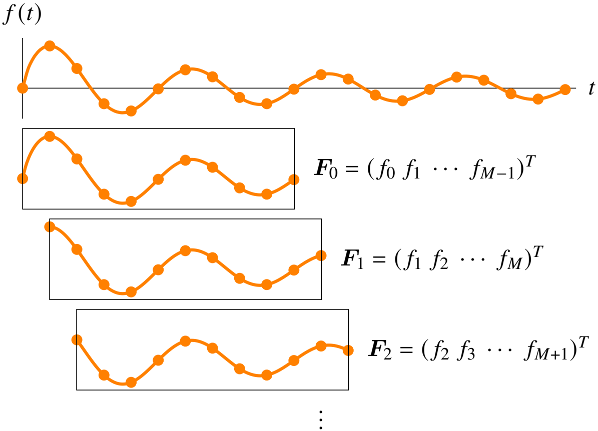
- Originally developed in fluid dynamics
- Not so many applications to quantum-many body systems so far
- Case studies of spin correlation functions in the transverse-field Ising model
  1. Oscillatory behavior: Quench dynamics in 2D
  2. Critical power-law decay: Unequal-time (time-displaced) correlation in 1D

Details of DMD 1

[J.N.Kutz, S.L.Brunton, B.W.Brunton, J.L.Proctor,
Dynamic Mode Decomposition: Data-Driven Modeling of Complex Systems ('16)]



- Interval of time step $\boldsymbol{\Delta t}$ is the same for all points
- Divide time-series data $\boldsymbol{f_n = f(n \cdot dt)}$ $\boldsymbol{(n = 0, 1, 2, \ldots, N-1)}$ into short-interval sequences (snapshots)

Details of DMD 2

[J.N.Kutz, S.L.Brunton, B.W.Brunton, J.L.Proctor, Dynamic Mode Decomposition: Data-Driven Modeling of Complex Systems ('16)]

- Generate matrices from time-series data $f_n = f(n \cdot dt)$ $(n = 0, 1, 2, \ldots, N-1)$

$$X_0 = \begin{pmatrix} f_0 & f_1 & f_2 & \cdots & f_{N-M-1} \\ f_1 & f_2 & f_3 & \cdots & f_{N-M} \\ f_2 & f_3 & f_4 & \cdots & f_{N-M+1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ f_{M-1} & f_M & f_{M+1} & \cdots & f_{N-2} \end{pmatrix}$$

$$X_1 = \begin{pmatrix} f_1 & f_2 & f_3 & \cdots & f_{N-M} \\ f_2 & f_3 & f_4 & \cdots & f_{N-M+1} \\ f_3 & f_4 & f_5 & \cdots & f_{N-M+2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ f_M & f_{M+1} & f_{M+2} & \cdots & f_{N-1} \end{pmatrix}$$

- Assume the presence of linear transformation A satisfying $X_1 \approx AX_0$
  - A is obtained by applying Moore-Penrose pseudoinverse $X_0^{-1} = X_0^\dagger (X_0 X_0^\dagger)^{-1}$ or $X_0^{-1} = (X_0^\dagger X_0)^{-1} X_0^\dagger$ to $X_1 \approx AX_0$ from right
- Eigenmodes of A give the information of the long-time dynamics
  - AX_1 gives f_N, A^2X_1 gives f_{N+1}, A^3X_1 gives f_{N+2}, ...

Details of DMD 3

When the matrix size gets larger, diagonalization becomes harder
We also want to remove unstable modes

1. Apply singular value decomposition (SVD) to $\boldsymbol{X_0}$ for low-rank approximation

$$\boldsymbol{X_0 = U\Sigma V^\dagger \approx U_R \Sigma_R V_R^\dagger}$$

2. $\boldsymbol{R} \times \boldsymbol{R}$ projection of $\boldsymbol{A = X_1 X_0^{-1} \approx X_1 V_R \Sigma_R^{-1} U_R^\dagger}$

$$\boldsymbol{U_R^\dagger A U_R \approx U_R^\dagger X_1 V_R \Sigma_R^{-1} =: \tilde{A}}$$

3. Diagonalize $\boldsymbol{\tilde{A}}$: $\{$Eigenvalues of $\boldsymbol{A}\} \supset \{$Eigenvalues of $\boldsymbol{\tilde{A}}\}$

$$\boldsymbol{\tilde{A} W = W \Lambda}$$

4. Eigenvectors of $\boldsymbol{A}$ satisfying $\boldsymbol{A\Phi \approx \Phi\Lambda}$

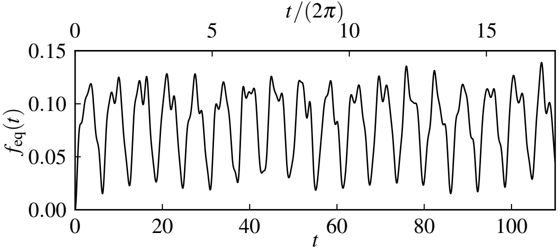
$$\boldsymbol{\Phi = X_1 V_R \Sigma_R^{-1} W}$$

5. Time evolution

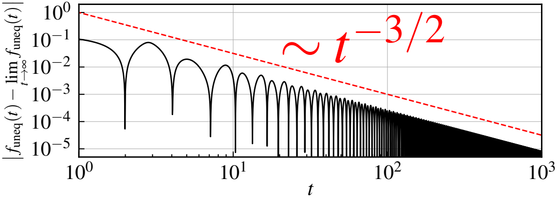
$$\boldsymbol{F_n \approx A^n F_0 = A^n \Phi\Phi^{-1} F_0 \approx \Phi\Lambda^n\Phi^{-1} F_0}$$

Hereafter, we will focus on ...

- Case 1: time evolution without damping



- Case 2: time evolution with power-law decay



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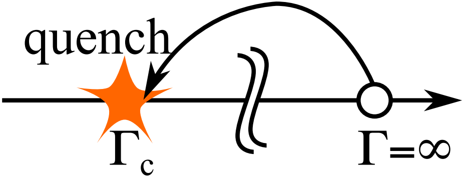
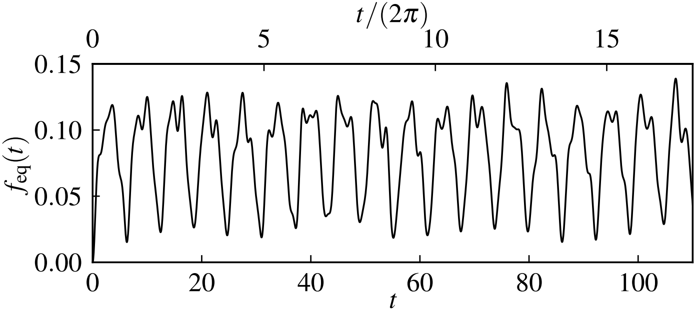


Square transverse-field Ising model
(4×4 sites)

$$H = -J \sum_{\langle ij \rangle} S_i^z S_j^z - \Gamma \sum_i S_i^x$$

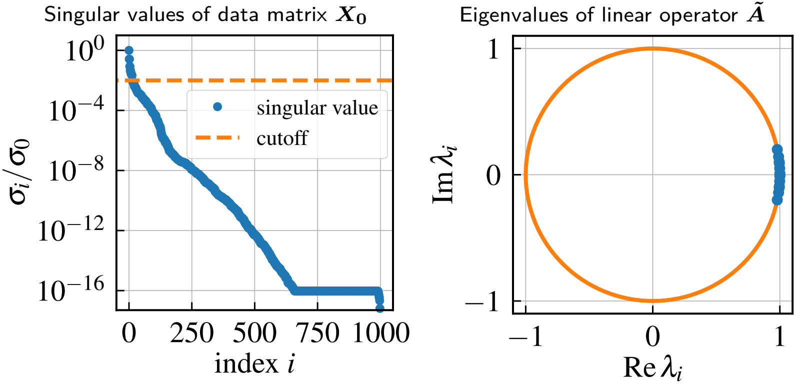
$$|\psi(t)\rangle = e^{-iHt/\hbar} | \rightarrow\rightarrow \cdots \rightarrow \rangle$$

$$f_{\mathrm{eq}}(t) := \langle \psi(t) | S_1^z S_0^z | \psi(t) \rangle$$



- Equal-time correlation functions after a sudden quench (obtained by exact diag.)
- Oscillatory behavior for finite systems (although nonintegrable)

Results: Learning $t \leq 100$, predicting $t \leq 1000$



- Parameters $\boldsymbol{M = 1000}$, $\boldsymbol{N = 2M}$, $\boldsymbol{\Delta t = 0.05}$
  $\boldsymbol{(t_{\text{snap}} = M \cdot \Delta t = 50}$, $\boldsymbol{t_{\text{input}} = N \cdot \Delta t = 100)}$
- Singular values decay exponentially
- Keep eigenmodes as many as possible unless time-series diverge
  cutoff $\boldsymbol{\epsilon = 0.01}$ $\rightarrow$ rank $\boldsymbol{R = 13}$
- $|$Eigenvalues$|$ $\leq \boldsymbol{1}$ $\rightarrow$ dynamics is stable

Details of DMD 2

[J.N.Kutz, S.L.Brunton, B.W.Brunton, J.L.Proctor, Dynamic Mode Decomposition: Data-Driven Modeling of Complex Systems ('16)]

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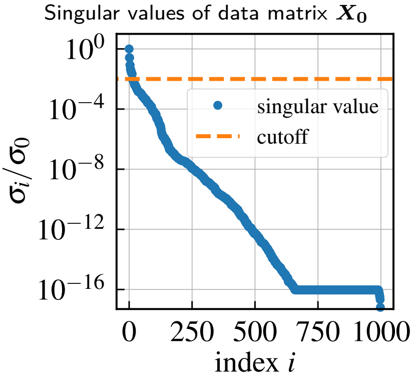

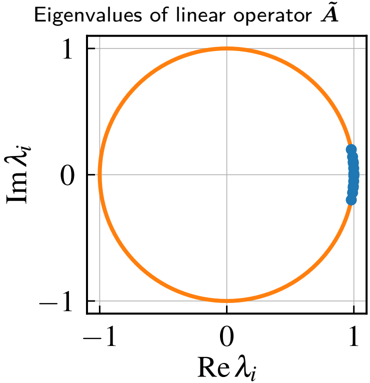

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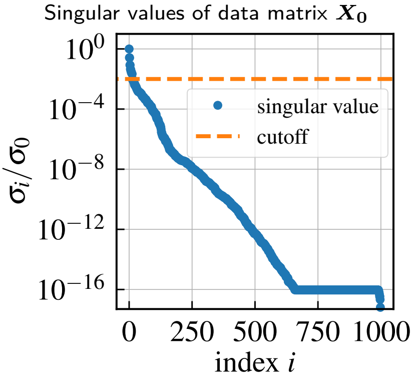

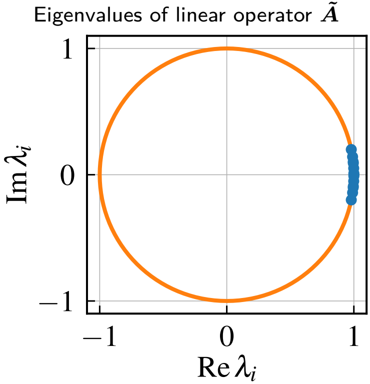

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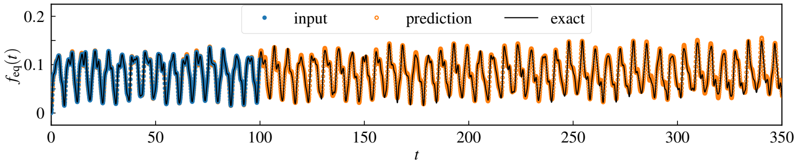
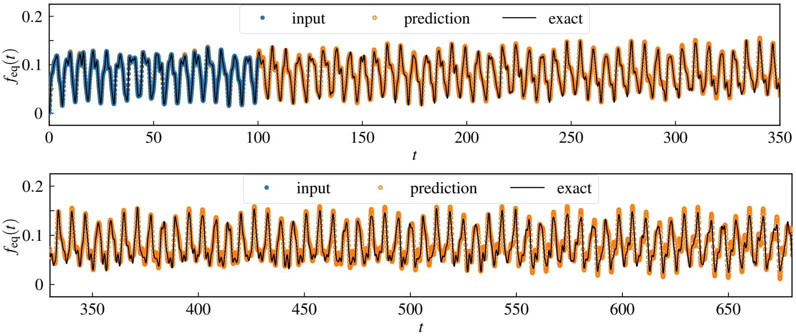


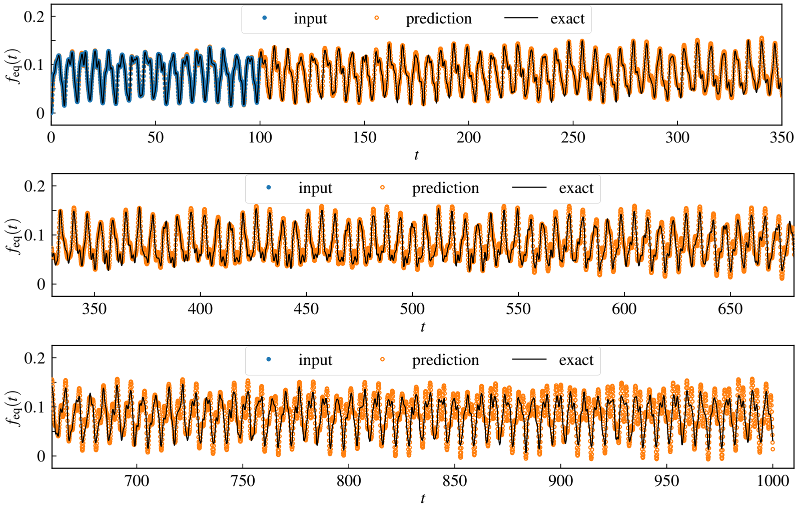
- Good agreement for $\boldsymbol{t \leq 350}$

Results: Learning $t \leq 100$, predicting $t \leq 1000$



- Good agreement for $t \leq 700$

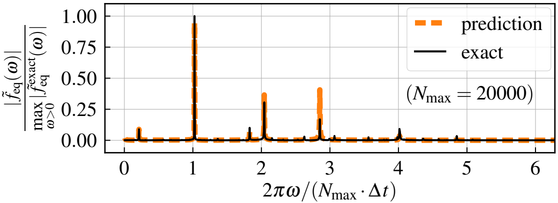
Results: Learning $t \leq 100$, predicting $t \leq 1000$

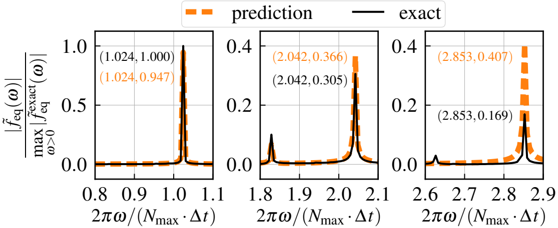


- Good agreement for $t \leq 1000$ ($= 10$ times the duration of input)

Results: Correlation function in Fourier space

$$\tilde{f}(\omega) = \sum_{n=0}^{N_{\max}-1} f_n \exp\left(-\frac{2\pi i \omega n}{N_{\max}}\right) \quad (\omega = 0, 1, \ldots, N_{\max}-1)$$





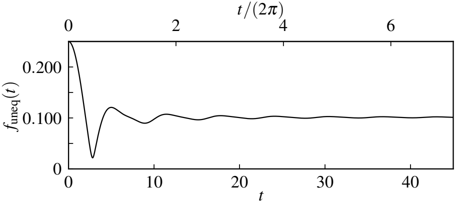
- Reproduce peak positions having intensity more than 10% of max peak

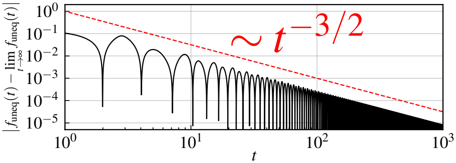
Case 2: time evolution with power-law decay

- Ground state of the 1D transverse-field Ising model at the critical point
- Exact unequal-time correlation (time-displaced) function described by Bessel and Anger-Weber functions
  [T.N.Tommet and D.L.Huber, PRB.11.450('75); G.Müller and R.E.Shrock, PRB.29.288('84)]

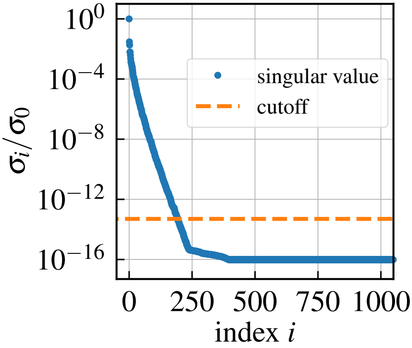
$$\begin{aligned} C^{xx}_{\mathrm{uneq}}(r,t) &= \langle \psi_0' | S^x_0(0) S^x_r(t) | \psi_0' \rangle \\ &= \frac{1}{\pi^2} + \frac{1}{4}\left[J_{2r}(2\Gamma t) + iE_{2r}(2\Gamma t)\right]^2 \\ &\quad - \frac{1}{4}\left[J_{2r-1}(2\Gamma t) + iE_{2r-1}(2\Gamma t)\right] \times \left[J_{2r+1}(2\Gamma t) + iE_{2r+1}(2\Gamma t)\right] \end{aligned}$$

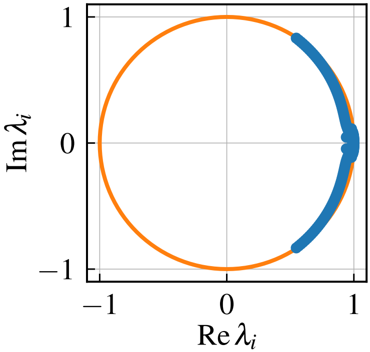
- Predict absolute values of the correlations: $f_{\mathrm{uneq}}(t) = |C^{xx}_{\mathrm{uneq}}(r=0,t)|$





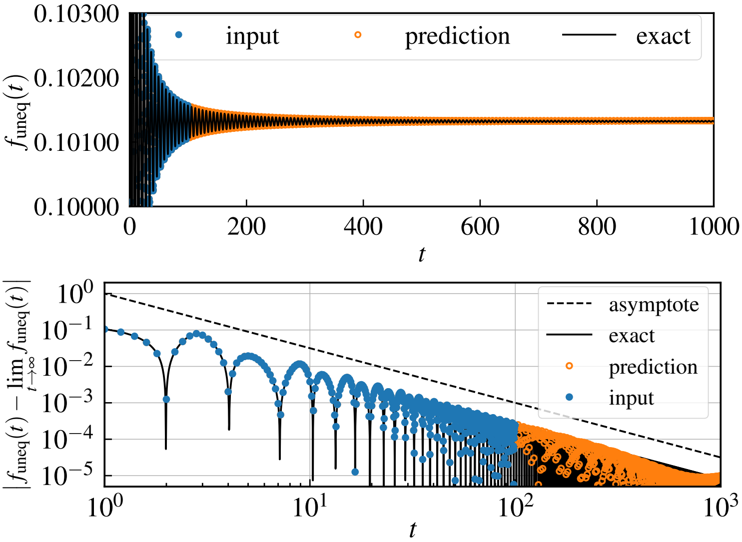
Results: Learning $t \leq 100$, predicting $t \leq 1000$





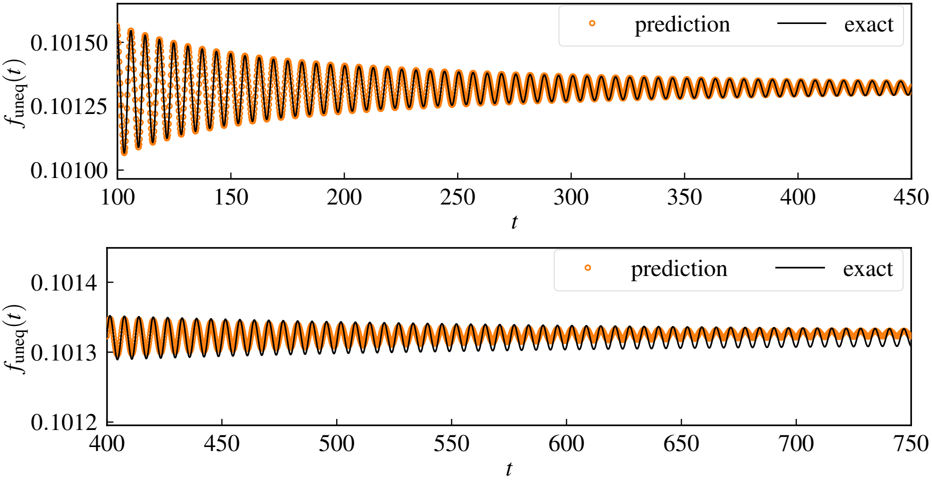
- Parameters $\boldsymbol{M = 5000}$, $\boldsymbol{N = 2M}$, $\boldsymbol{\Delta t = 0.01}$ $(\boldsymbol{t_{\mathrm{snap}} = M \cdot \Delta t = 50}$, $\boldsymbol{t_{\mathrm{input}} = N \cdot \Delta t = 100})$
- Singular values decay exponentially
- Keep eigenmodes as many as possible unless time-series diverge cutoff $\boldsymbol{\epsilon = 5 \times 10^{-14}} \rightarrow$ rank $\boldsymbol{R = 193}$
- $|$Eigenvalues$|$ $\boldsymbol{\leq 1} \rightarrow$ dynamics is stable

Results: Learning $t \leq 100$, predicting $t \leq 1000$



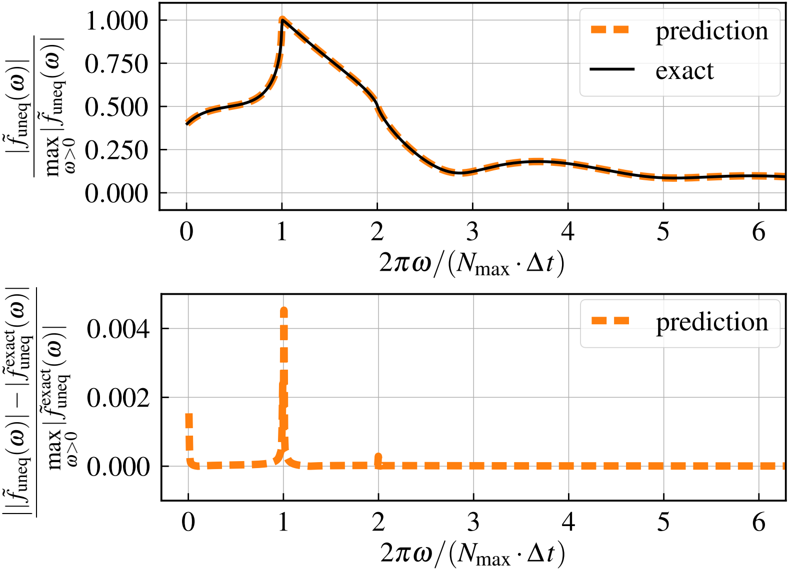
- Reproduce convergence to a nonzero value: $\mathbf{1/\pi^2 \approx 0.10132}$
- Reproduce power-law decay: $\boldsymbol{t^{-3/2}}$

Results: Learning $t \leq 100$, predicting $t \leq 1000$



- Good agreement for $t \leq 400$
- Slightly underestimate amplitude of oscillations as t increases, although period and center of oscillations are well reproduced

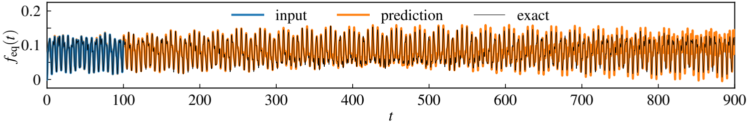
Results: Correlation function in Fourier space



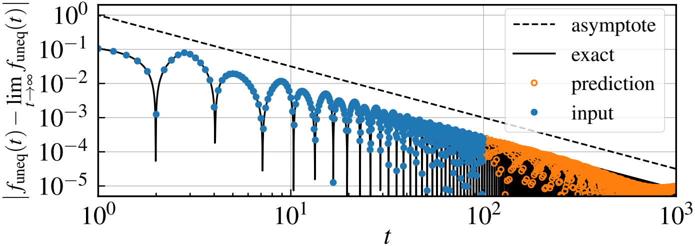
- Error $\lesssim \mathbf{0.4\%}$

Conclusions

- Data-driven method (Dynamic Mode Decomposition, DMD) for predicting long-time dynamics quantum many-body systems
- Examine data with and without damping
  - Accurate prediction up to nearly 10 times the duration of input time



  - Reproduce power-law decay including its exponent



- Outlook: Apply DMD to experimental data

R. Kaneko, M. Imada, Y. Kabashima, and T. Ohtsuki, arXiv:2403.19947.