

Machine-Learning-Assisted Construction of Appropriate Rotating Frame

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Outline

- **Introduction**
- **Propose methods & Demonstration**
- **Summary**

Recent application of ML to physics

● Physics and Machine Learning(ML)

➤ Apply ML to Physics

- detect/classify phase (transitions)
(can be applied only to the known phase)
- describe the equilibrium/steady state
(just numerical, other sophisticated methods)
- Material Informatics
(need more data)
- remove noise and improve the accuracy of measurement



These directions will not directly give progress in analytical methods.

Can we develop analytical methods with the aid of machine learning?

How did we physicists develop analytical methods?

● Scale separation

- Nonlinear system \Rightarrow reduction
- The Hubbard model \Rightarrow Heisenberg model
- Open quantum system \Rightarrow Markov app., GKSL equation
- Periodically-driven system \Rightarrow high-frequency expansion
- (Renormalization Group \Rightarrow cutoff scale)
- (DMRG, Tensor network \Rightarrow SVD & reduction)

How did we physicists develop analytical methods?

● Scale separation

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- (Renormalization Group \Rightarrow cutoff scale)
- (DMRG, Tensor network \Rightarrow SVD & reduction)

We find these approaches in systems which have apparent scale separation.

Scale separation & Appropriate Unitary tr.

- **Appropriate Frame gives a perturbative approach**

- Periodically-driven system : Rotating Frame (high-frequency expansion)

$$U_{t,t_0} = e^{-iK(t)} e^{-iH_F(t-t_0)/\hbar} e^{iK(t_0)} \quad H_F = e^{iK(t)} \left[H(t) - i\hbar \frac{d}{dt} \right] e^{-iK(t)}$$

▷ $e^{-iK^{(n)}(t)} \left[H(t) - i\hbar \frac{d}{dt} \right] e^{iK^{(n)}t} \simeq \tilde{H}^{(n)}(t) \quad \tilde{H}^{(n)}(t) = H_F^{(n)} + V^{(n)}(t).$

- Cavity QED system : Asymptotically-Decoupled Frame

(a kind of quantum version of the High-Frequency expansion)

$$\hat{H}_C = \int dx \hat{\psi}_x^\dagger \left[\frac{(-i\hbar\partial_x - q\hat{A})^2}{2m} + V(x) \right] \hat{\psi}_x + \hbar\omega_c \hat{a}^\dagger \hat{a} + \hat{H}_\parallel$$

▷ $\hat{U} = \exp \left[-i\xi_g \int_{-\infty}^{\infty} dx \hat{\psi}_x^\dagger (-i\partial_x) \hat{\psi}_x \hat{\pi} \right] \quad \hat{H}_U = \frac{\hat{p}^2}{2m_{\text{eff}}} + V(x + \xi_g \hat{\pi}) + \hbar\Omega \hat{b}^\dagger \hat{b},$

By using the scale separation, we can construct the frame/projection in which the dressed/projected Hamiltonian has desirable properties.

Scale separation & Appropriate Unitary tr.

Can we develop analytical methods with the aid of machine learning?



Can we find appropriate unitary tr. or projection with the aid of machine learning?



Can we find “implicit” scale separation with the aid of machine learning?

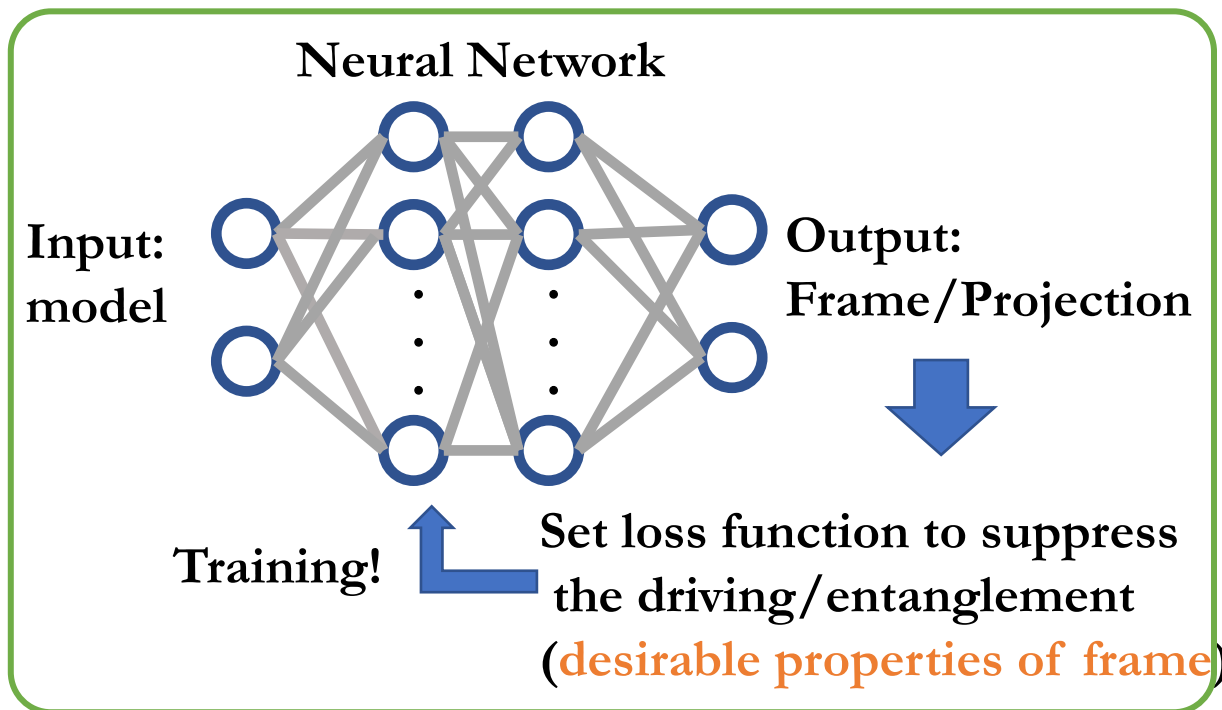
Outline

- Introduction
- **Propose methods & Demonstration**
- Summary

What I want to do with machine learning

- Find an appropriate frame with the aid of ML and “implicit” scale separation

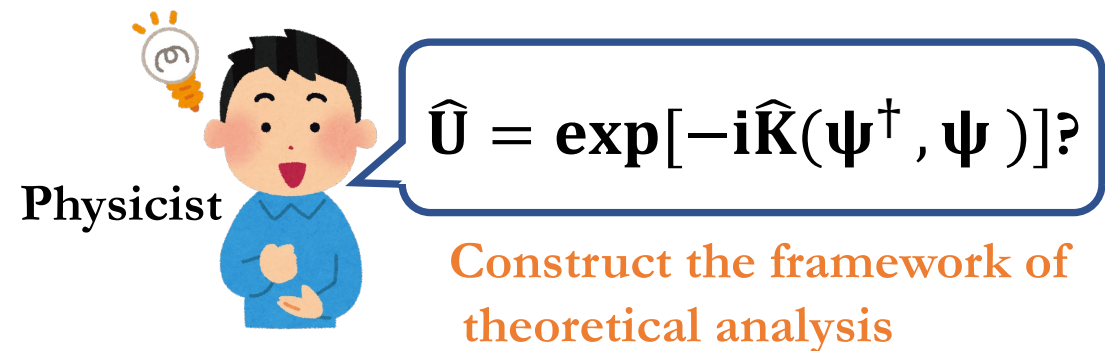
Step1: Numerically derive the unitary tr.



Step2: Convert the results into operators

We get (Rotating) frame numerically
 $\{U(t) = \exp[iK(t)]\}$

We can also calculate the parameter dependence



If it is not valid, we get the frame numerically in another model and construct another candidate

Check the validity by hand

Quick review of Floquet theory & RF

$$\begin{aligned}\hat{H}(t) &= \hat{H}_0 + \hat{V}(t) & i \frac{d}{dt} |\psi(t)\rangle &= \hat{H}(t) |\psi(t)\rangle & \hat{U}(t) &= \exp[i\hat{K}(t)] \\ i \frac{d}{dt} |\tilde{\psi}(t)\rangle &= i \frac{d}{dt} \hat{U}(t) |\psi(t)\rangle & \hat{K}'(t) &= \frac{d}{dt} \hat{K}(t) \\ &= \hat{U}(t) (\hat{H}(t) - \hat{K}'(t)) \hat{U}^\dagger(t) |\tilde{\psi}(t)\rangle & \hat{H}_r(t) &= \hat{U}(t) (\hat{H}(t) - \hat{K}'(t)) \hat{U}^\dagger(t)\end{aligned}$$

When focusing on periodically-driven systems ($\hat{H}(t) = \hat{H}(t + T)$),

there is the time-periodic unitary transformation $\hat{U}_F(t) = \hat{U}_F(t + T)$, $\hat{H}_r(t) = \hat{H}_F$

It is usually difficult to calculate the exact RF ($\hat{U}_F(t)$) and we often calculate it perturbatively by using the high-frequency expansion such as the Floquet-Magnus exp. or Van-Vleck exp.

Perturbatively calculated RF ($\hat{U}_A(t)$) is often appropriate, because we can calculate the heating rate.

Demonstration

● Model

- Interacting quantum Two-Spin model under driving

$$\hat{H}(t) = \hat{H}_0 + \hat{V}(t)$$

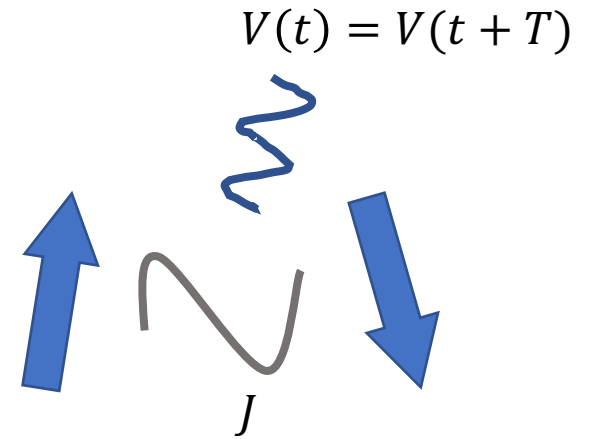
$$\hat{H}_0 = - \sum_{\alpha} (J_{\alpha} \hat{S}_1^{\alpha} \otimes \hat{S}_2^{\alpha} + h_{\alpha} \sum_i \hat{S}_i^{\alpha})$$

$$\hat{V}(t) = - \sum_{\alpha} \xi_{\alpha} \sin(\Omega t) \sum_i \hat{S}_i^{\alpha}$$

$$\vec{J} = (J_x, J_y = 0, J_z), \quad \vec{h} = (h_x = 0, h_y = 0, h_z), \quad \vec{\xi} = (\xi, 0, 0)$$

$$H_0 = -J_x(\tau^x \otimes \sigma^x) - J_z(\tau^z \otimes \sigma^z) - h_z(\tau^0 \otimes \sigma^z + \tau^z \otimes \sigma^0)$$

$$V(t) = -\xi \sin(\Omega t) (\tau^0 \otimes \sigma^x + \tau^x \otimes \sigma^0)$$

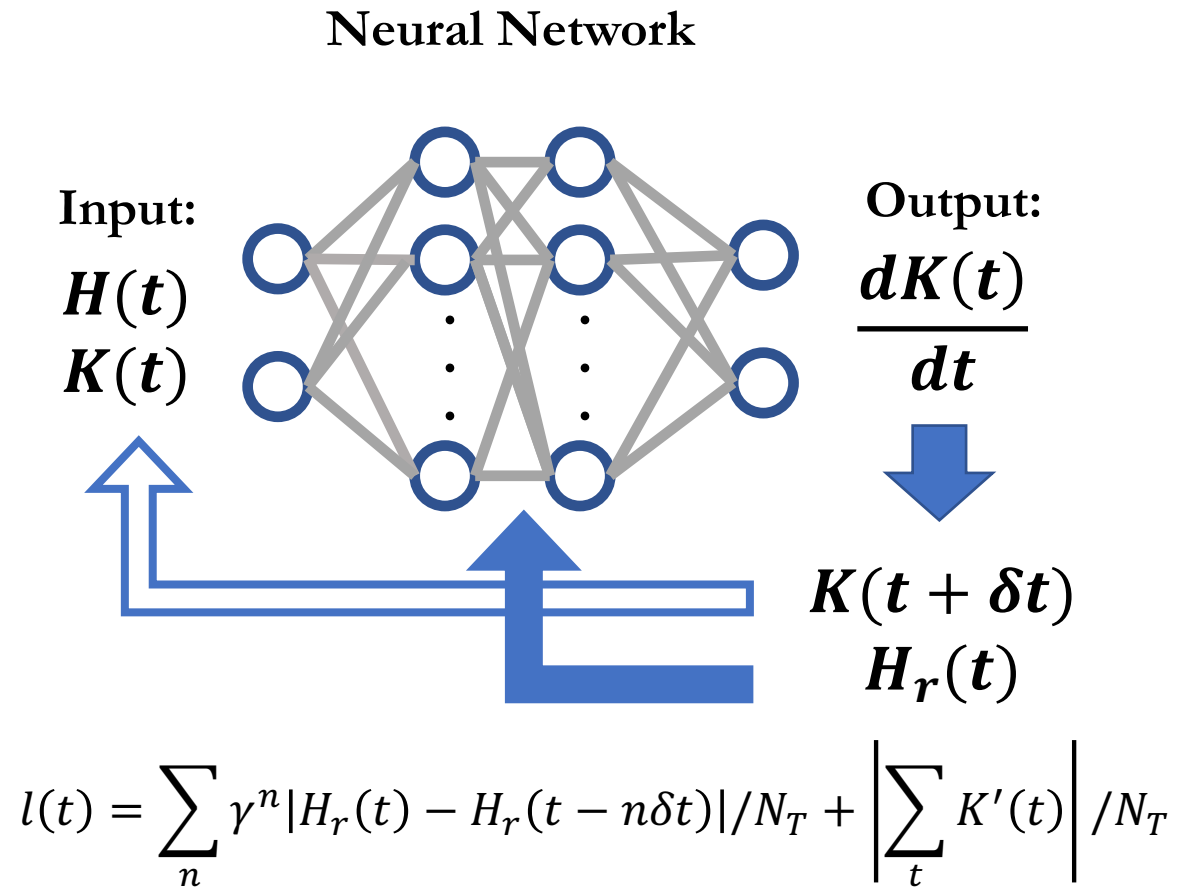


$$\begin{pmatrix} |\uparrow\uparrow\rangle \\ |\uparrow\downarrow\rangle \\ |\downarrow\uparrow\rangle \\ |\downarrow\downarrow\rangle \end{pmatrix}$$

Setup

● Model of Machine Learning

- Recurrent Neural Network



Remarks:

Model:

$$\widehat{H}(t) = \widehat{H}_0 + \widehat{V}(t)$$

$$\widehat{H}_0 = \sum_{\alpha} (J_{\alpha} \widehat{S}_1^{\alpha} \otimes \widehat{S}_2^{\alpha} + h_{\alpha} \sum_i \widehat{S}_1^{\alpha})$$

$$\widehat{V}(t) = - \sum_{\alpha} \xi_{\alpha} \sin(\Omega t) \sum_i \widehat{S}_i^{\alpha}$$

Formalism:

$$\widehat{H}_r(t) = \widehat{U}(t)(\widehat{H}(t) - \widehat{K}'(t))\widehat{U}^+(t)$$

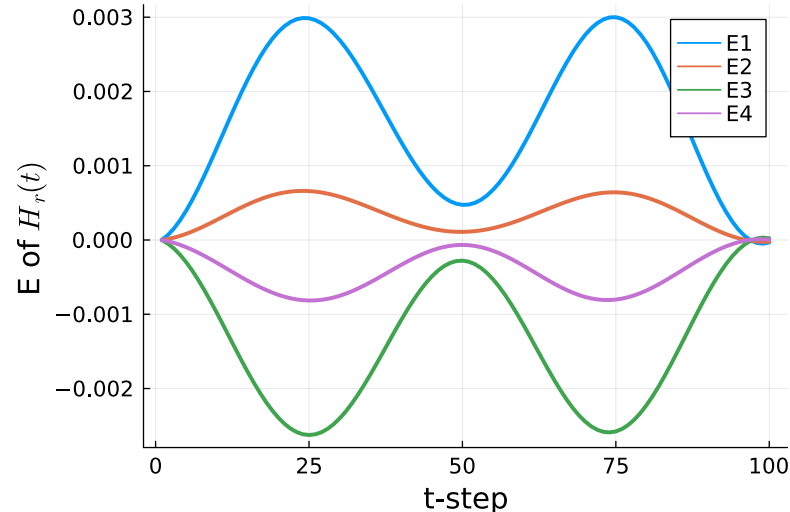
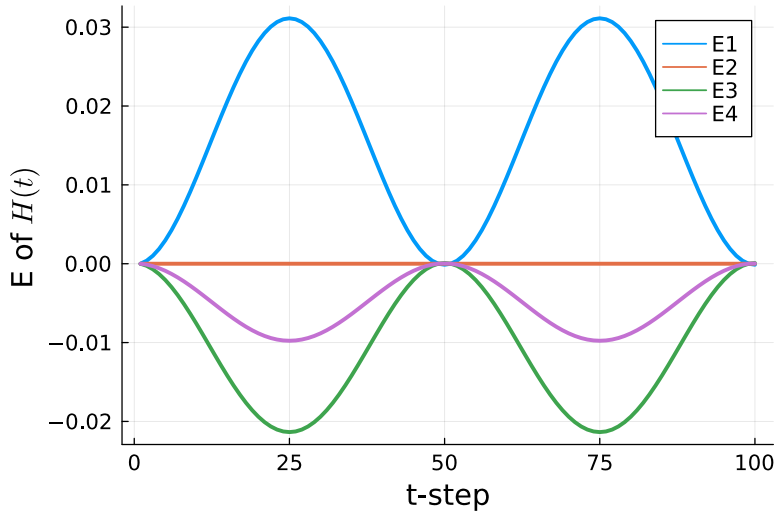
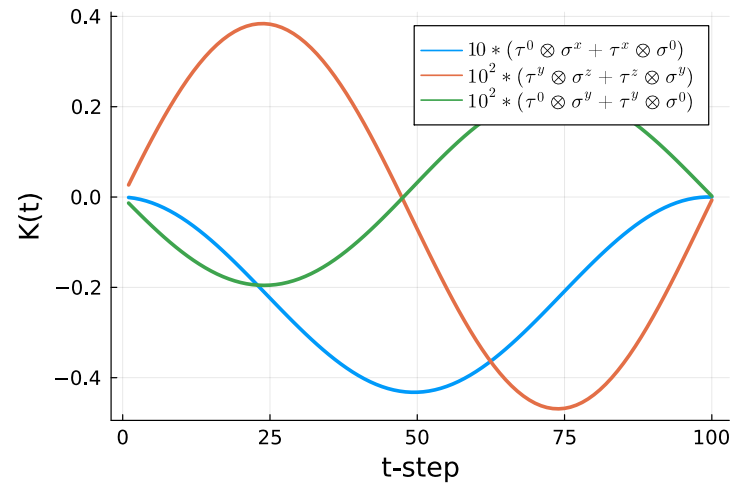
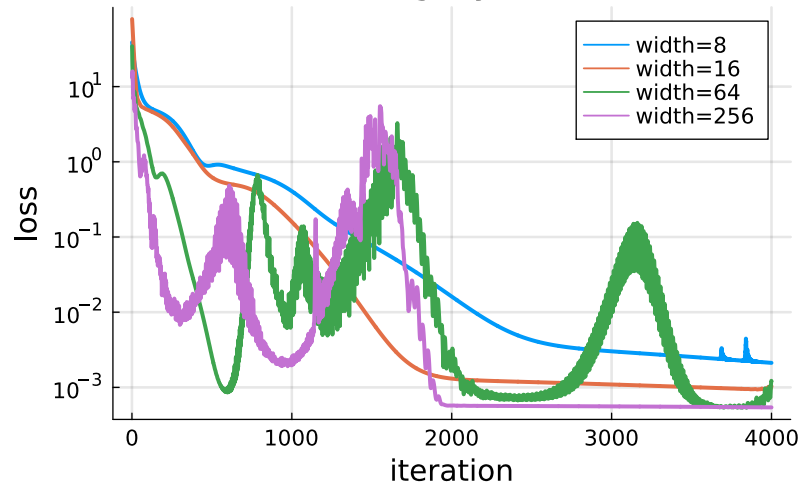
$$\widehat{U}(t) = \exp[i\widehat{K}(t)]$$

$$\widehat{K}'(t) = \frac{d}{dt} \widehat{K}(t)$$

Step 1: Numerically derive the RF with ML

High-Frequency regime

Learning dynamics



Remarks:

Model:

$$\hat{H}(t) = \hat{H}_0 + \hat{V}(t)$$

$$\hat{H}_0 = \sum_{\alpha} (J_{\alpha} \hat{S}_1^{\alpha} \otimes \hat{S}_2^{\alpha} + h_{\alpha} \sum_i \hat{S}_1^{\alpha})$$

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Formalism:

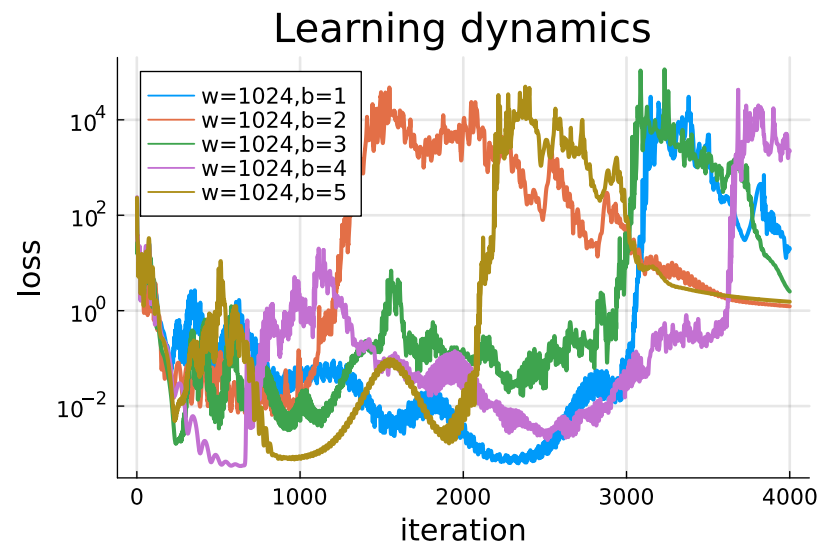
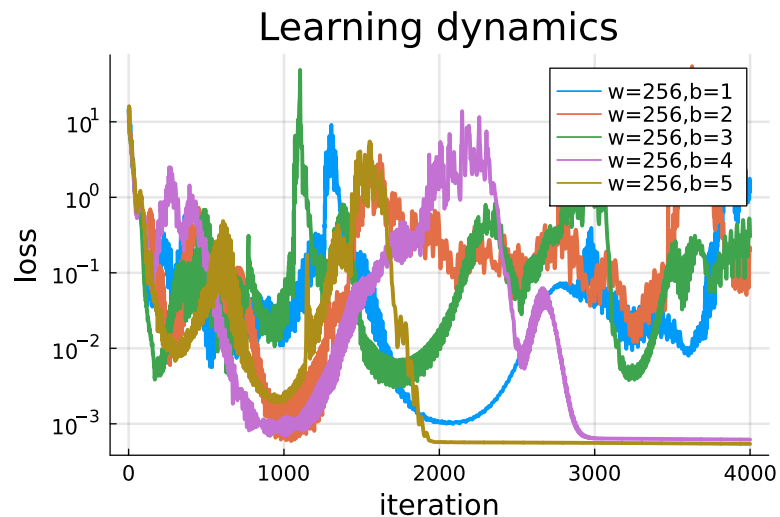
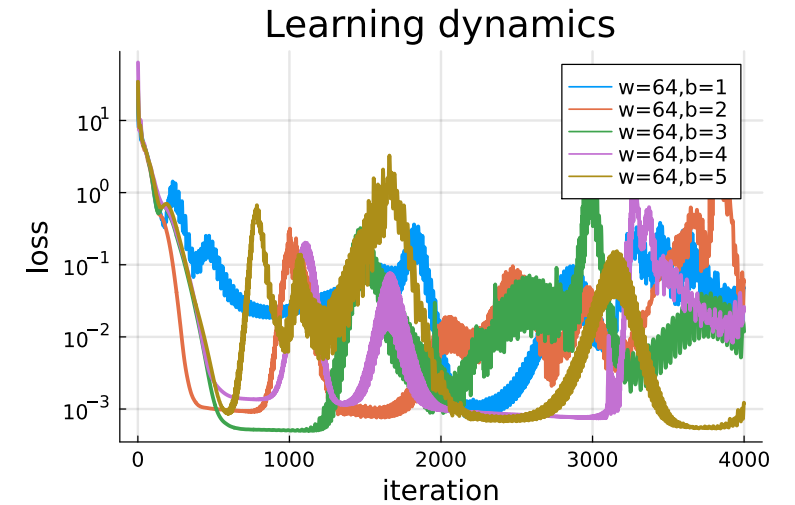
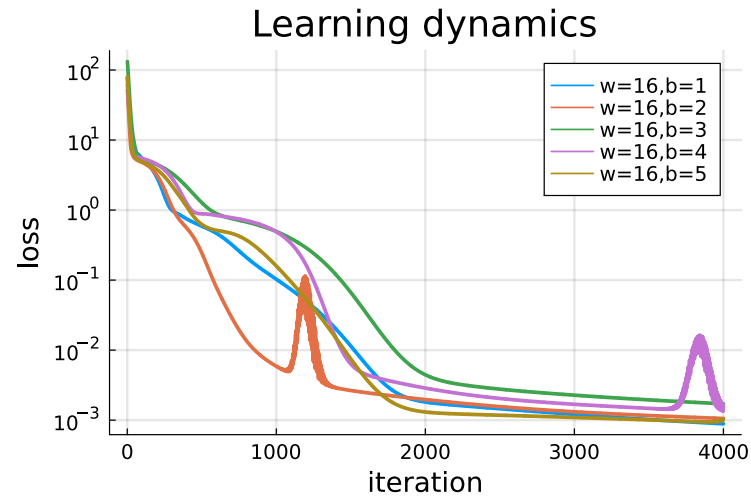
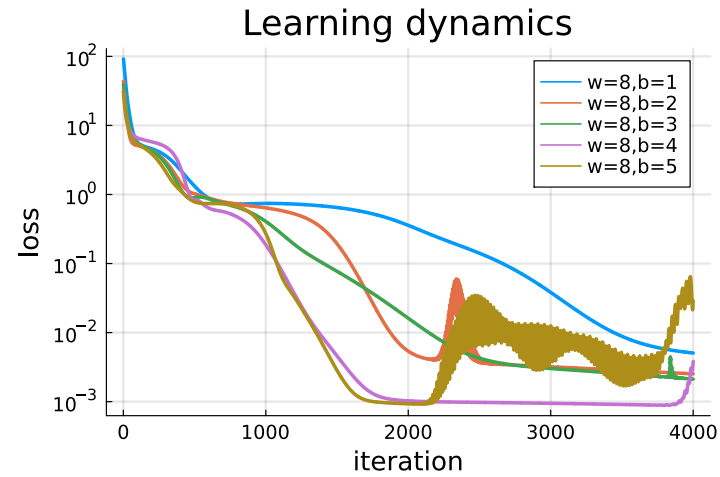
$$\hat{H}_r(t) = \hat{U}(t)(\hat{H}(t) - \hat{K}'(t))\hat{U}^+(t)$$

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Step 1: Numerically derive the RF with ML

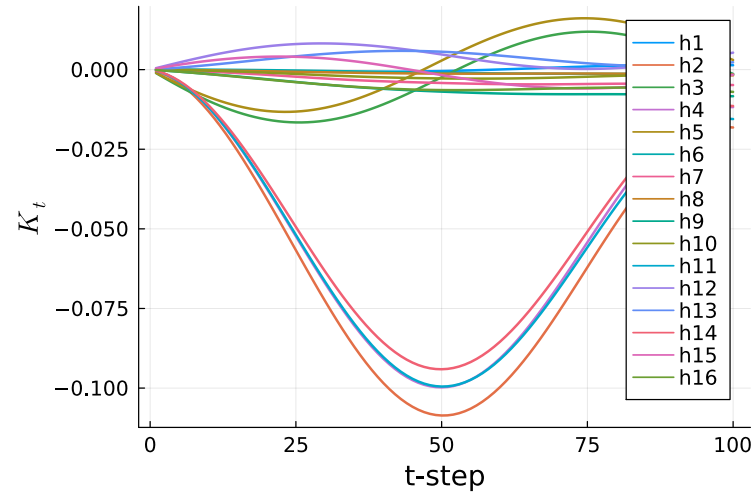
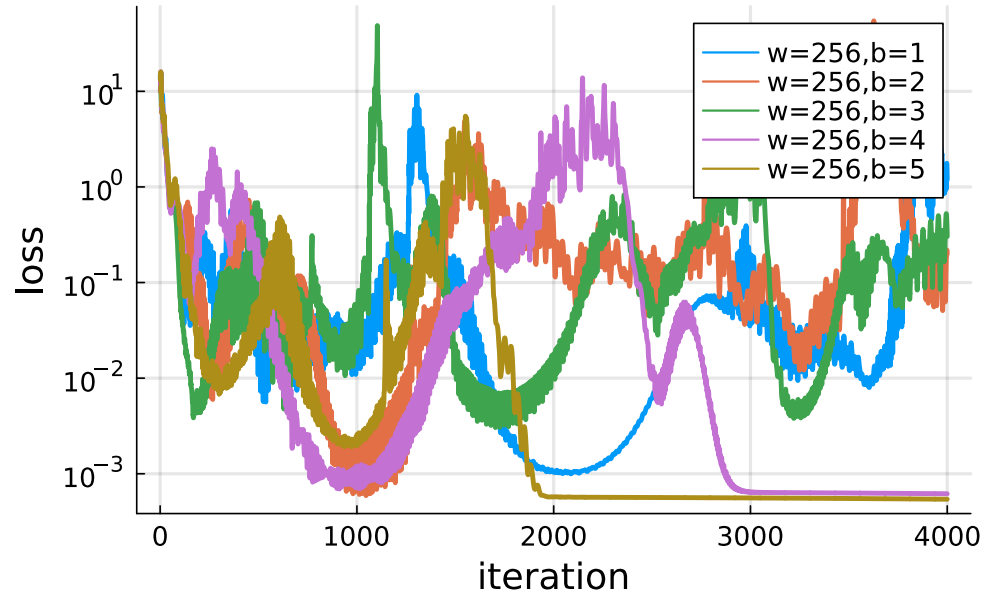
- hidden layer width dependence of learning dynamics



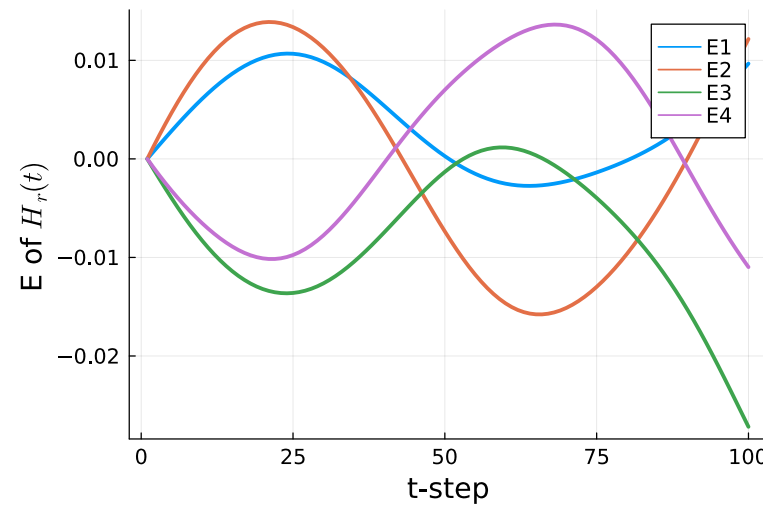
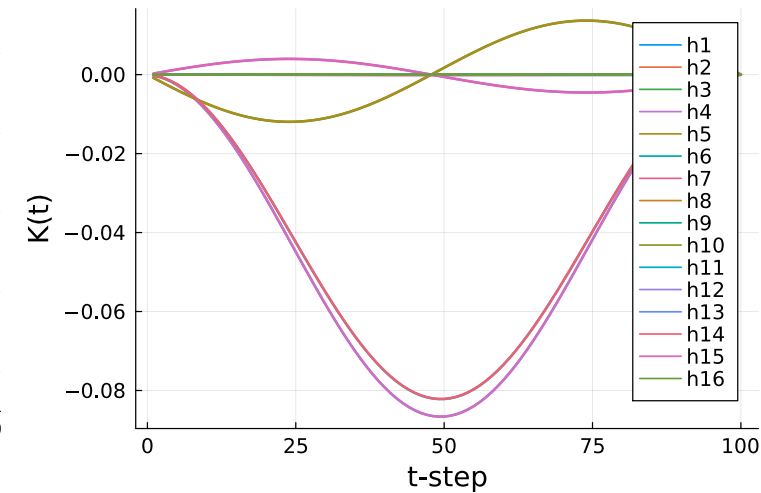
Step 1: Numerically derive the RF with ML

- If learning doesn't work well,

Learning dynamics



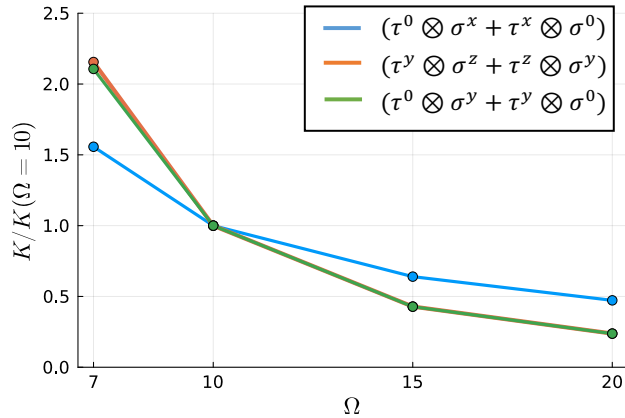
Success case



Step 2: Convert the result to operator form

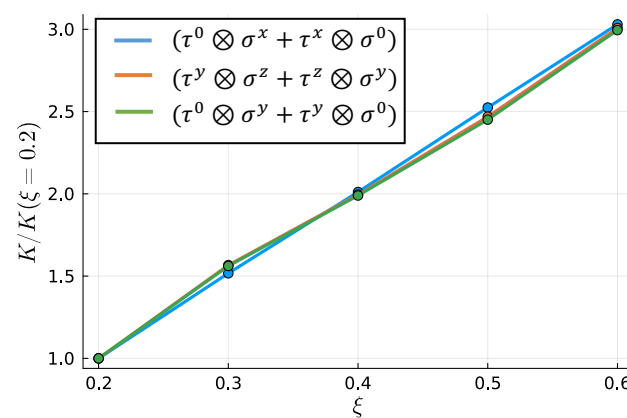
Parameter dependence & translate it to operator form

(c) $(\xi, J_z, J_x, h_z) = (0.2, 1.0, 0.7, 0.5)$



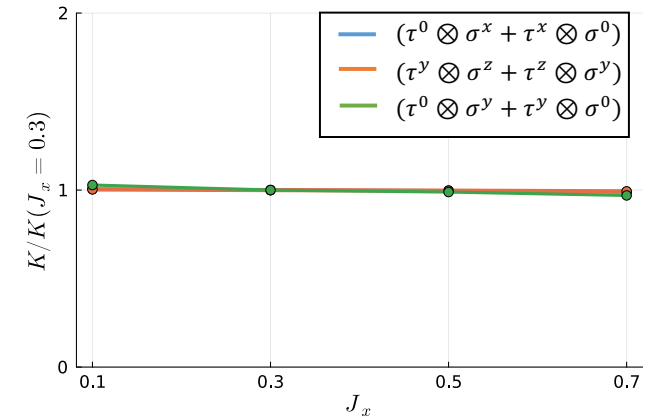
bl $\propto \Omega^{-1}$, or, gr $\propto \Omega^{-2}$

(b) $(J_z, J_x, h_z, \Omega) = (1.0, 0.7, 0.5, 10)$



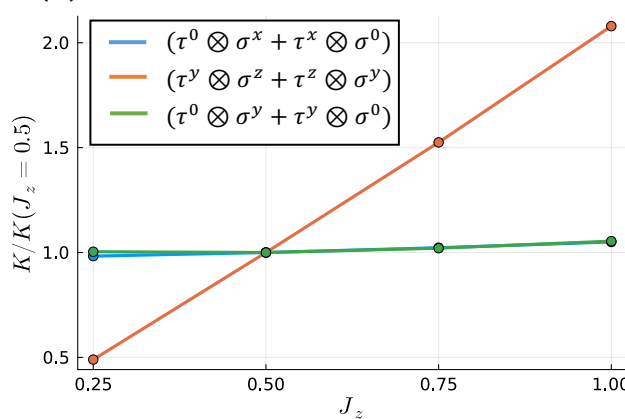
bl, or, gr $\propto \xi^{-1}$

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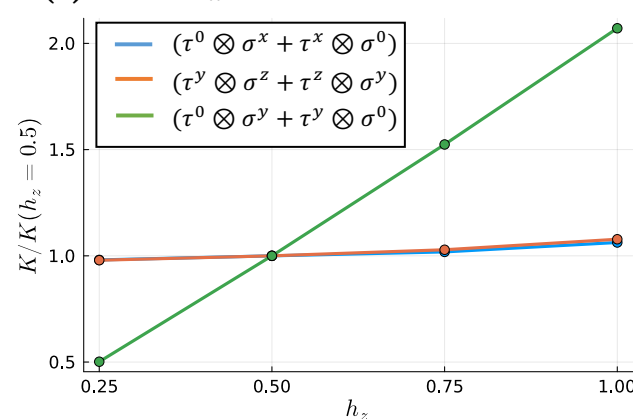
bl, or, gr $\propto J_x^0$

(d) $(\xi, J_x, h_z, \Omega) = (0.2, 0.7, 0.5, 10)$



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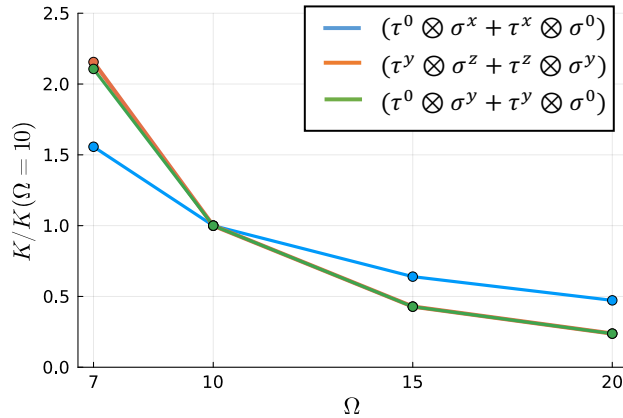
bl, or $\propto h_z^0$, gr $\propto h_z^1$

$$\hat{K}(t) = \xi \left[\frac{1}{\Omega} (1 - \cos(\Omega t)) (\tau^0 \otimes \sigma^x + \tau^x \otimes \sigma^0) + \frac{2J_z}{\Omega^2} \sin(\Omega t) (\tau^y \otimes \sigma^z + \tau^z \otimes \sigma^y) + \frac{2h_z}{\Omega^2} \sin(\Omega t) (\tau^0 \otimes \sigma^y + \tau^y \otimes \sigma^0) + \frac{2h_z J_z}{\Omega^3} (1 - \cos(\Omega t)) (\tau^x \otimes \sigma^z + \tau^z \otimes \sigma^x) \right]$$

Step 2: Convert the result to operator form

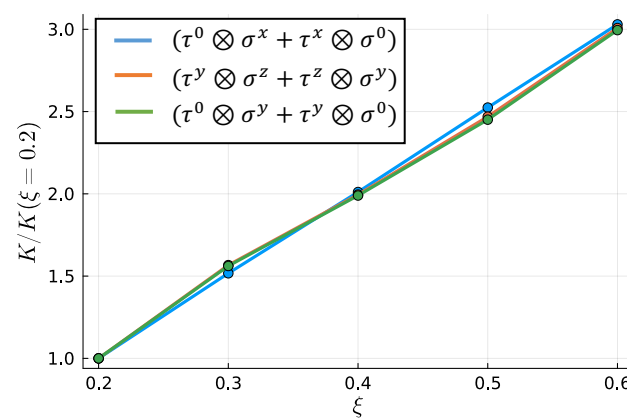
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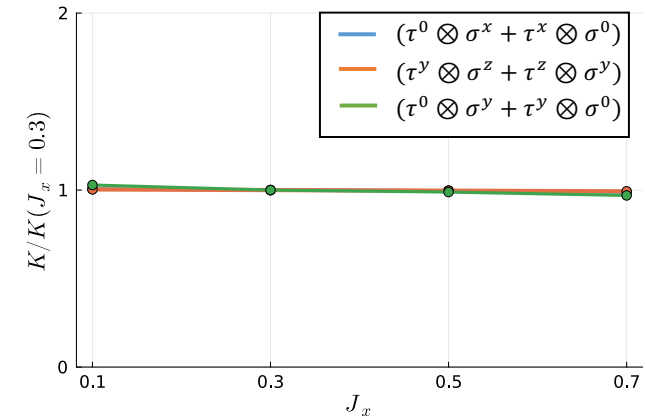
→ $bl \propto \Omega^{-1}$, $or \propto \Omega^{-2}$, $gr \propto \Omega^{-2}$

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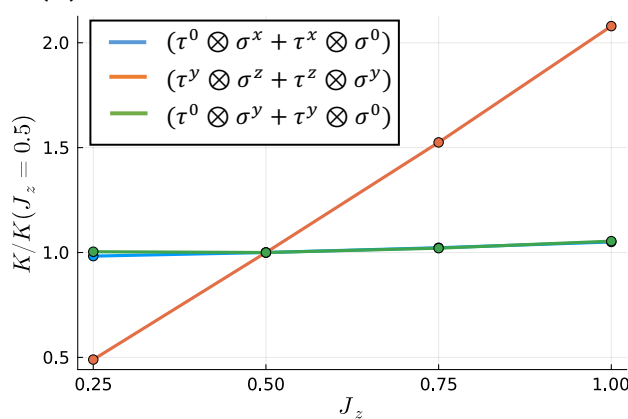
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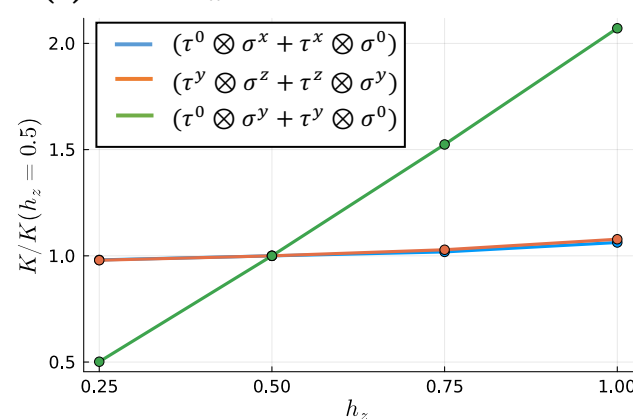
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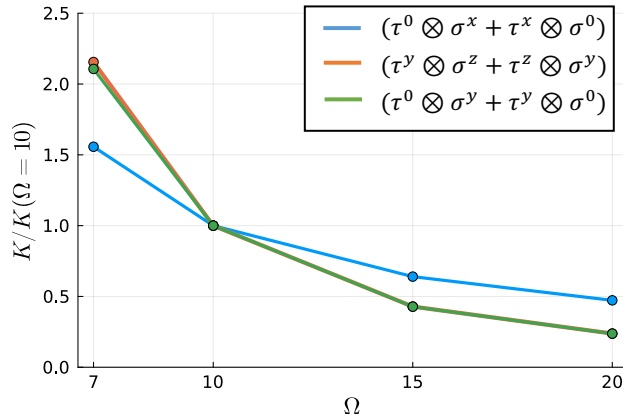
$$\hat{K}(t) = \xi \left[\frac{1}{\Omega} (1 - \cos(\Omega t)) (\tau^0 \otimes \sigma^x + \tau^x \otimes \sigma^0) + \frac{2J_z}{\Omega^2} \sin(\Omega t) (\tau^y \otimes \sigma^z + \tau^z \otimes \sigma^y) + \frac{2h_z}{\Omega^2} \sin(\Omega t) (\tau^0 \otimes \sigma^y + \tau^y \otimes \sigma^0) + \frac{2h_z J_z}{\Omega^3} (1 - \cos(\Omega t)) (\tau^x \otimes \sigma^z + \tau^z \otimes \sigma^x) \right]$$

$$\hat{K}(t) = \int dt' \{ \hat{V}(t') - i \int dt'' [\hat{V}(t''), \hat{H}_0] \}$$

Step 2: Convert the result to operator form

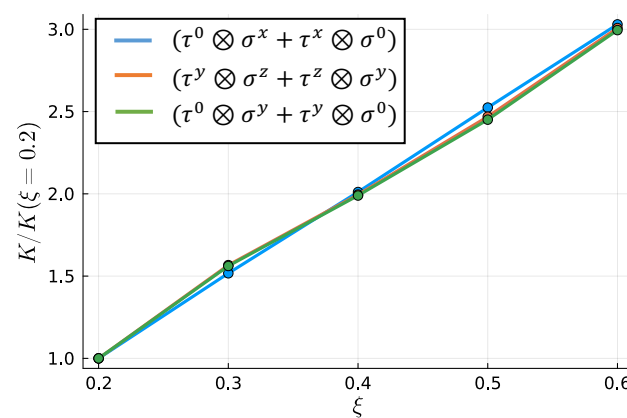
Parameter dependence & translate it to operator form

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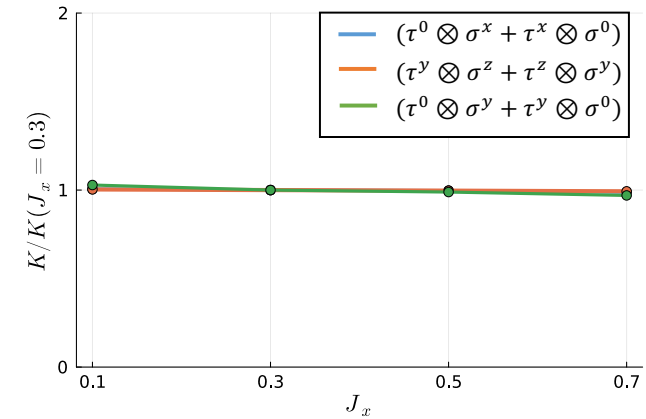
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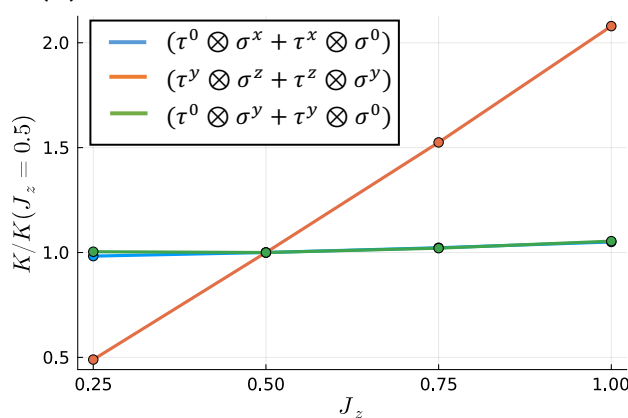
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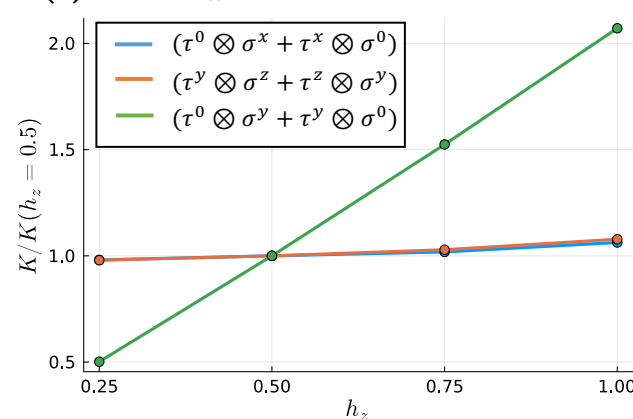
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$bl, or \propto h_z^0$, $gr \propto h_z^1$

$$\hat{K}(t) = \xi \left[\frac{1}{\Omega} (1 - \cos(\Omega t)) (\tau^0 \otimes \sigma^x + \tau^x \otimes \sigma^0) + \frac{2J_z}{\Omega^2} \sin(\Omega t) (\tau^y \otimes \sigma^z + \tau^z \otimes \sigma^y) + \frac{2h_z}{\Omega^2} \sin(\Omega t) (\tau^0 \otimes \sigma^y + \tau^y \otimes \sigma^0) + \frac{2h_z J_z}{\Omega^3} (1 - \cos(\Omega t)) (\tau^x \otimes \sigma^z + \tau^z \otimes \sigma^x) \right]$$



Floquet-Magnus expansion!

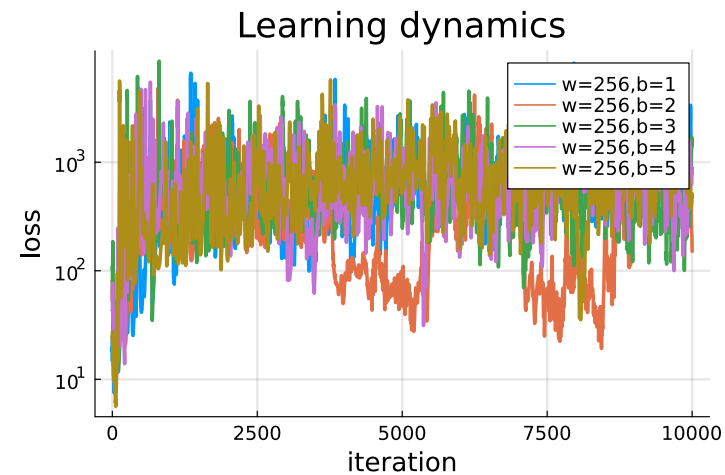
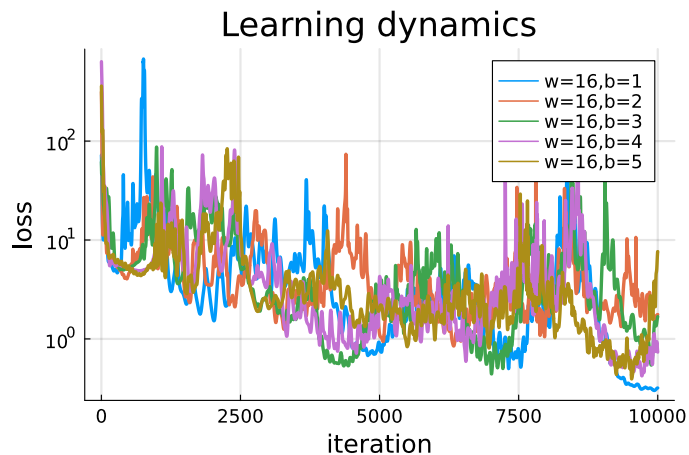
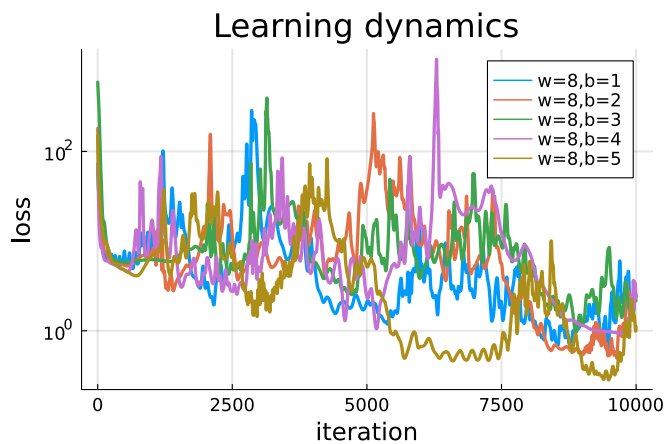
$$\hat{K}(t) = \int dt' \{ \hat{V}(t') - i \int dt'' [\hat{V}(t''), \hat{H}_0] \}$$

Results

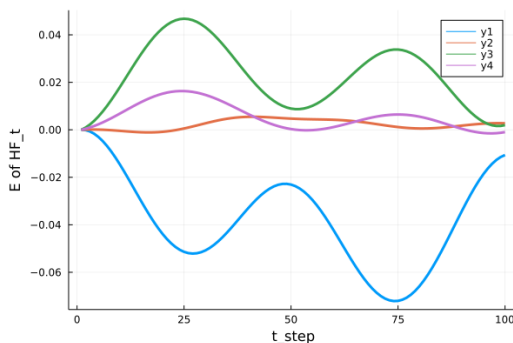
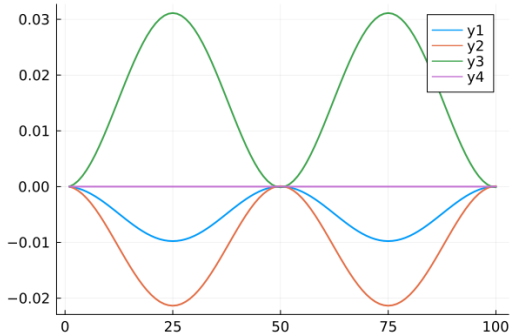
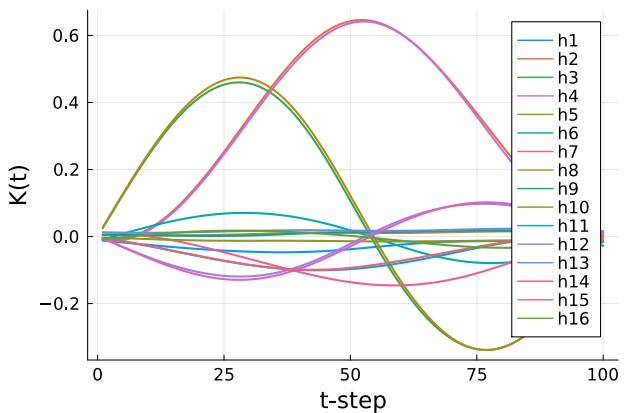
● Resonant Drive

$$\Omega = 2, \xi = 0.2, J_z = 1.0, h_z = 0.5$$

Learning dynamics is unstable



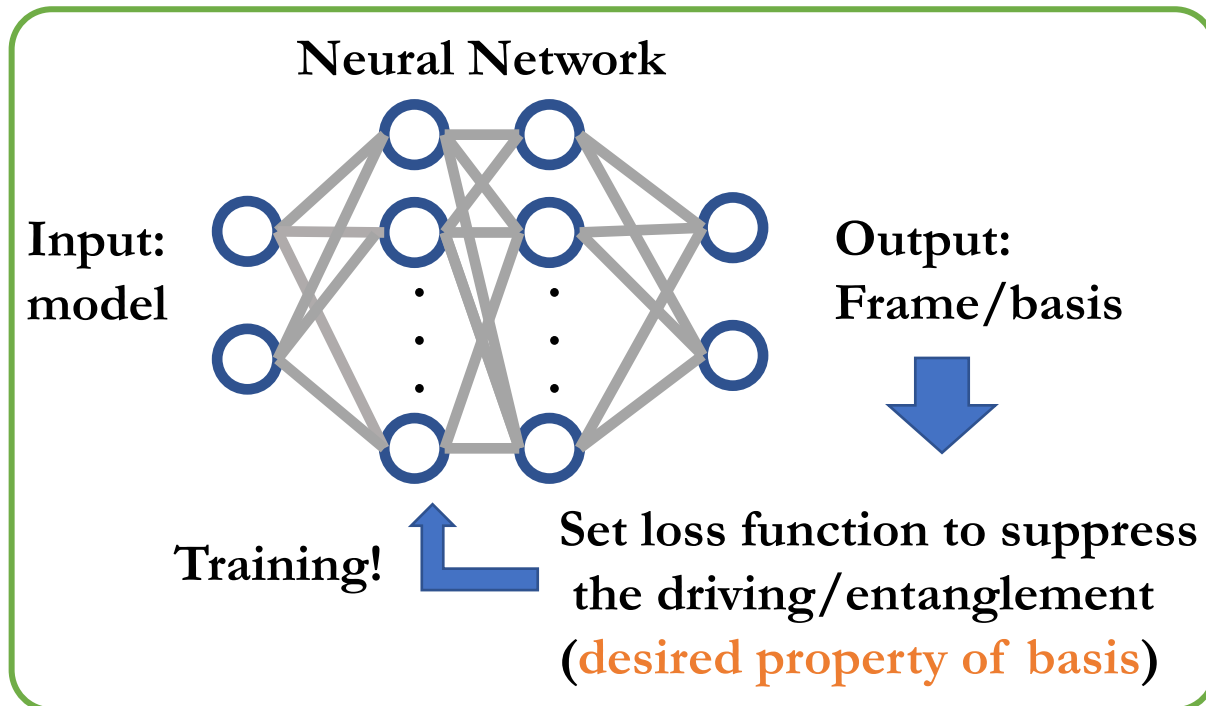
cannot suppress the time-dependence



Summary & Outlooks

- We propose the methods, and it can “derive” the high-frequency expansion with RNN.
- RNN derives the appropriate RF, not the exact one in the high-frequency regime.
- It cannot derive in the resonant regime.
- This should mean that there is a local minimum when there is scale separation. (Is it general?)

Step1: Numerically derive the unitary tr.



Step2: Convert the results into operators

We get (Rotating) frame numerically
 $\{U(t) = \exp[iK(t)]\}$

We can also calculate the parameter dependence

Physicist

$\hat{U} = \exp[-i\hat{K}(\psi^\dagger, \psi)]?$

Construct the framework of theoretical analysis