Emulating the Magnus Formulation of IMSRG

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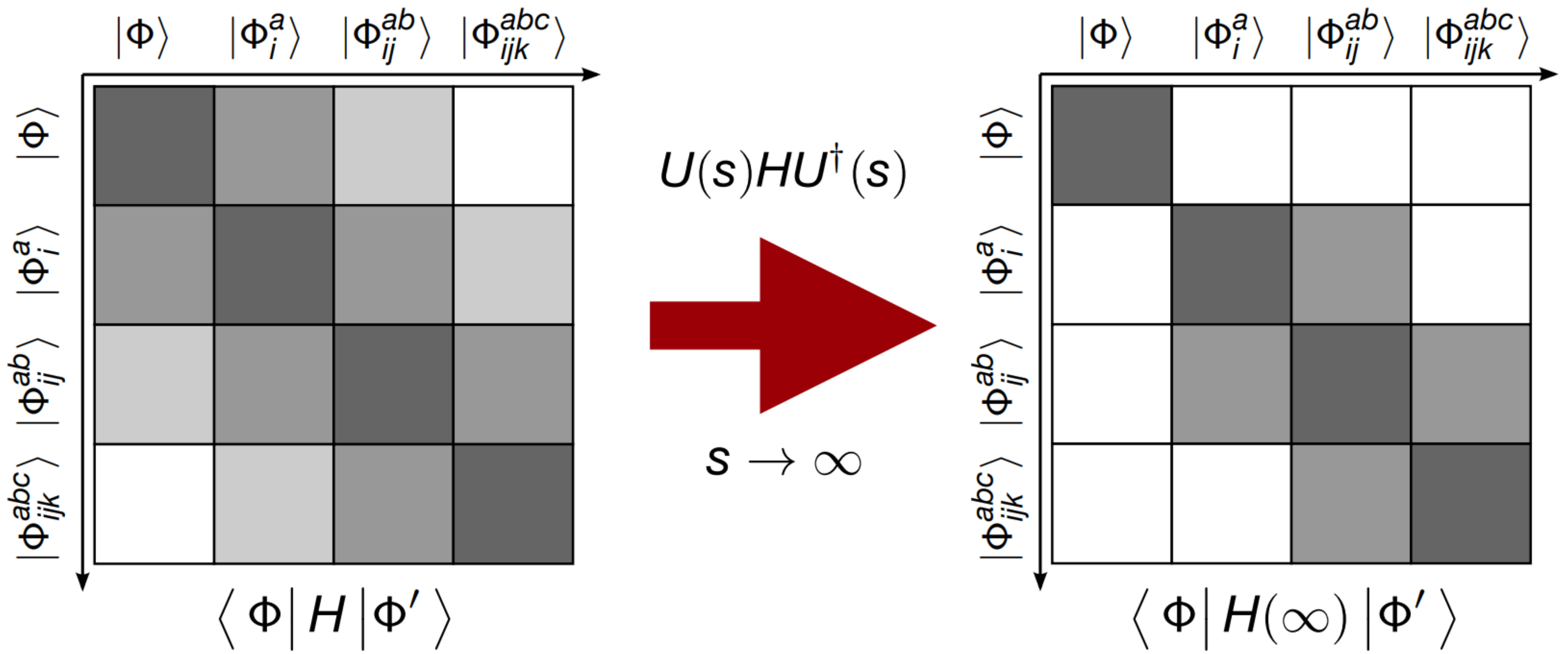
Outline

- Background / Motivation
- Emulation Techniques
- Preliminary Results

Background/ Motivation: What is IMSRG?



In Medium Similarity Renormalization Group (IMSRG) is a method used to decouple states or band diagonalize Hamiltonians via continuous unitary transformations.

Heiko Hergert, et. al. In-Medium Similarity Renormalization Group Approach to the Nuclear Many-Body Problem, pages477–570. Springer International Publishing, Cham, 2017.

What is IMSRG?

- IMSRG does this by working on **second quantized operators**.

$$\frac{d}{ds}\hat{H}(s) = [\hat{\eta}(s), \hat{H}(s)]\,.$$

$$\frac{dE}{ds} = \sum_{ab}(n_a - n_b)\eta_{ab}f_{ba} + \frac{1}{2}\sum_{abcd}\eta_{abcd}\Gamma_{cdab}n_a n_b \bar{n}_c \bar{n}_d\,,$$

$$\frac{df_{ij}}{ds} = \sum_{a}(1 + P_{ij})\eta_{ia}f_{aj} + \sum_{ab}(n_a - n_b)(\eta_{ab}\Gamma_{biaj} - f_{ab}\eta_{biaj}) + \frac{1}{2}\sum_{abc}(n_a n_b \bar{n}_c + \bar{n}_a \bar{n}_b n_c)(1 + P_{ij})\eta_{ciab}\Gamma_{abcj}\,,$$

$$\frac{d\Gamma_{ijkl}}{ds} = \sum_{a}\{(1 - P_{ij})(\eta_{ia}\Gamma_{ajkl} - f_{ia}\eta_{ajkl}) - (1 - P_{kl})(\eta_{ak}\Gamma_{ijal} - f_{ak}\eta_{ijal})\} + \frac{1}{2}\sum_{ab}(1 - n_a - n_b)(\eta_{ijab}\Gamma_{abkl} - \Gamma_{ijab}\eta_{abkl}) + \sum_{ab}(n_a - n_b)(1 - P_{ij})(1 - P_{kl})\eta_{aibk}\Gamma_{bjal}\,.$$

- **The time complexity here is roughly N^6 if we truncate at 2-body**, where N is the size of the single particle basis.

Purpose of IMSRG: Vanilla IMSRG

- IMSRG often works as a mediator to soften or decouple Hamiltonians so that we can extract observables.
- However, In vanilla IMSRG **to get these observables, we have to either do a separate evolution and save the generator values.**

$$\frac{d}{ds}\hat{O}(s) = [\hat{\eta}(s), \hat{O}(s)] \,,$$

- Or, coevolve the observable with the Hamiltonian, leading to a **doubling of computational cost.**
- The last thing we need is to have to STORE values for our generator and do a SECOND (or even third or fourth) evolution.

Purpose of IMSRG: Magnus IMSRG

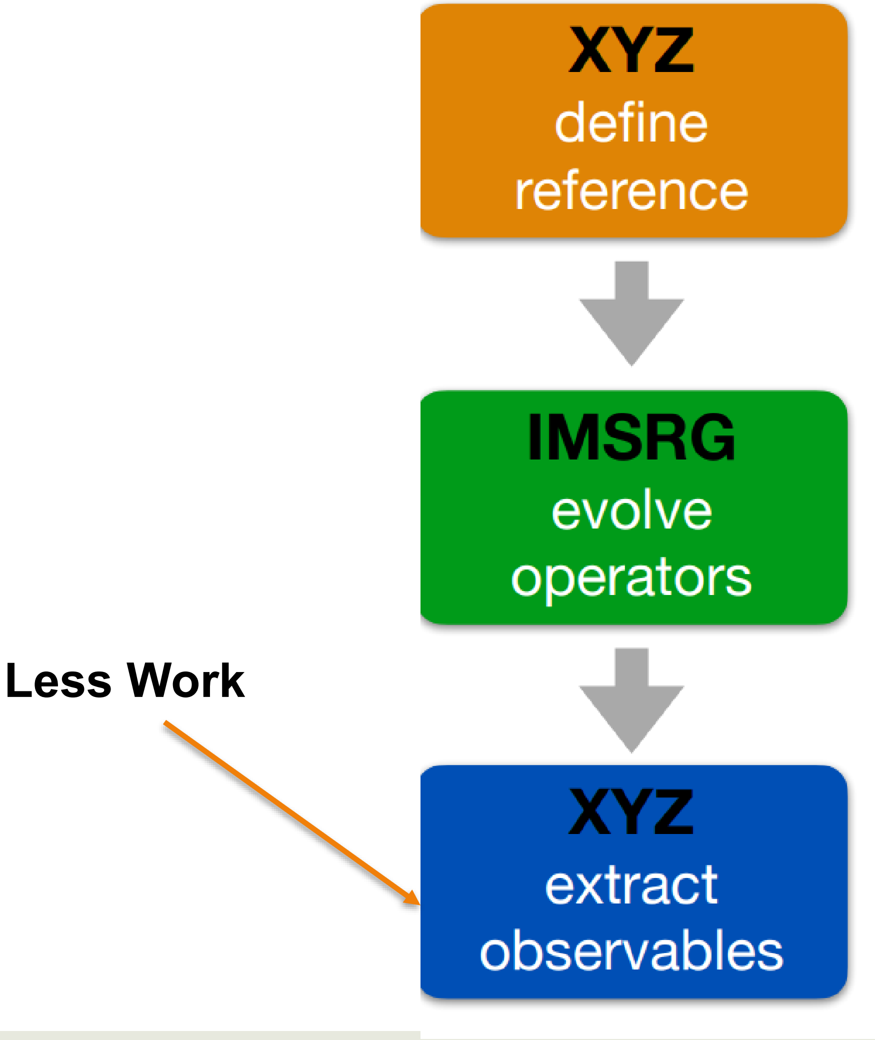
- In order to avoid these problem, we can use the **Magnus Formulation.**

$$\hat{U}(s) \equiv e^{\hat{\Omega}(s)}$$

$$\frac{d\hat{\Omega}}{ds} = \sum_{k=0}^{\infty} \frac{B_k}{k!} \mathrm{ad}^k_{\hat{\Omega}} (\hat{\eta})$$

- Allows us to **obtain any observable we want from just one evolution of one operator** by doing a simple similarity transformation.

$$\hat{O}(\infty) \equiv e^{\hat{\Omega}(\infty)} \hat{O}(0) e^{-\hat{\Omega}(\infty)}$$



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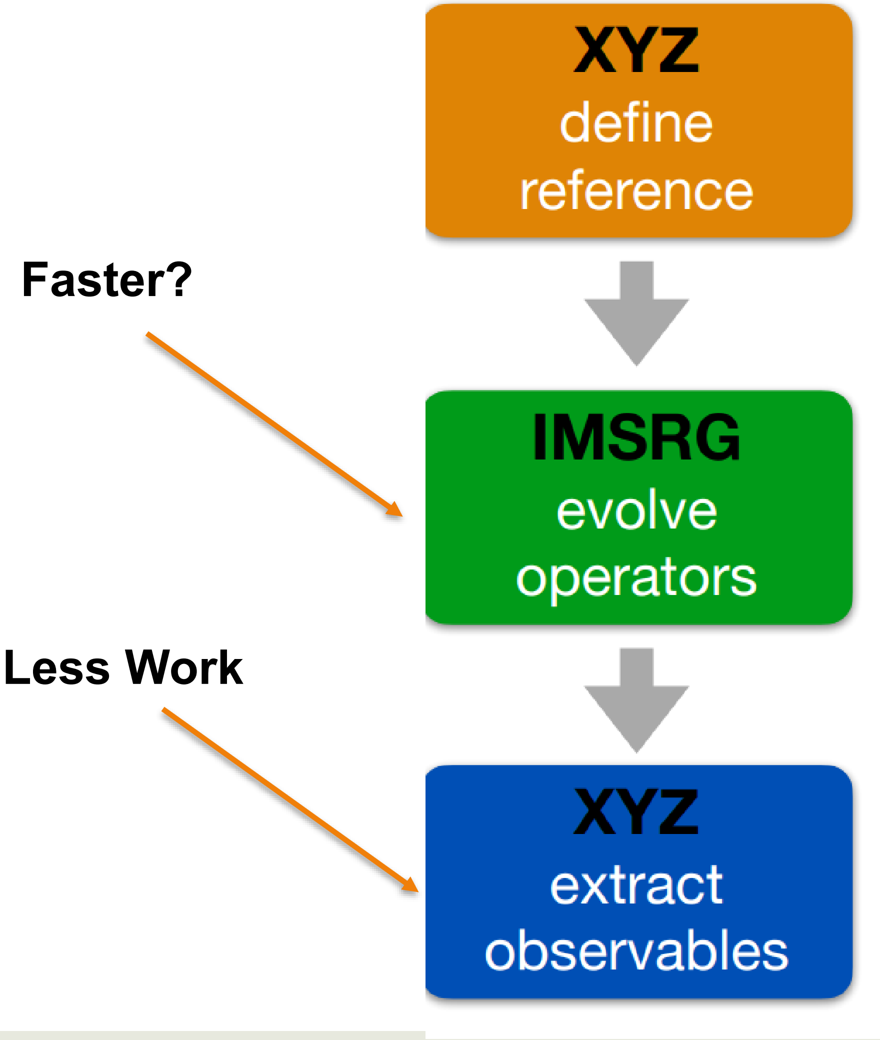
- **This is the method we will emulate in the talk.**



Outline

Background / Motivation

Emulation Techniques

Preliminary Results

Dynamic Mode Decomposition (DMD) for emulating Vanilla IMSRG

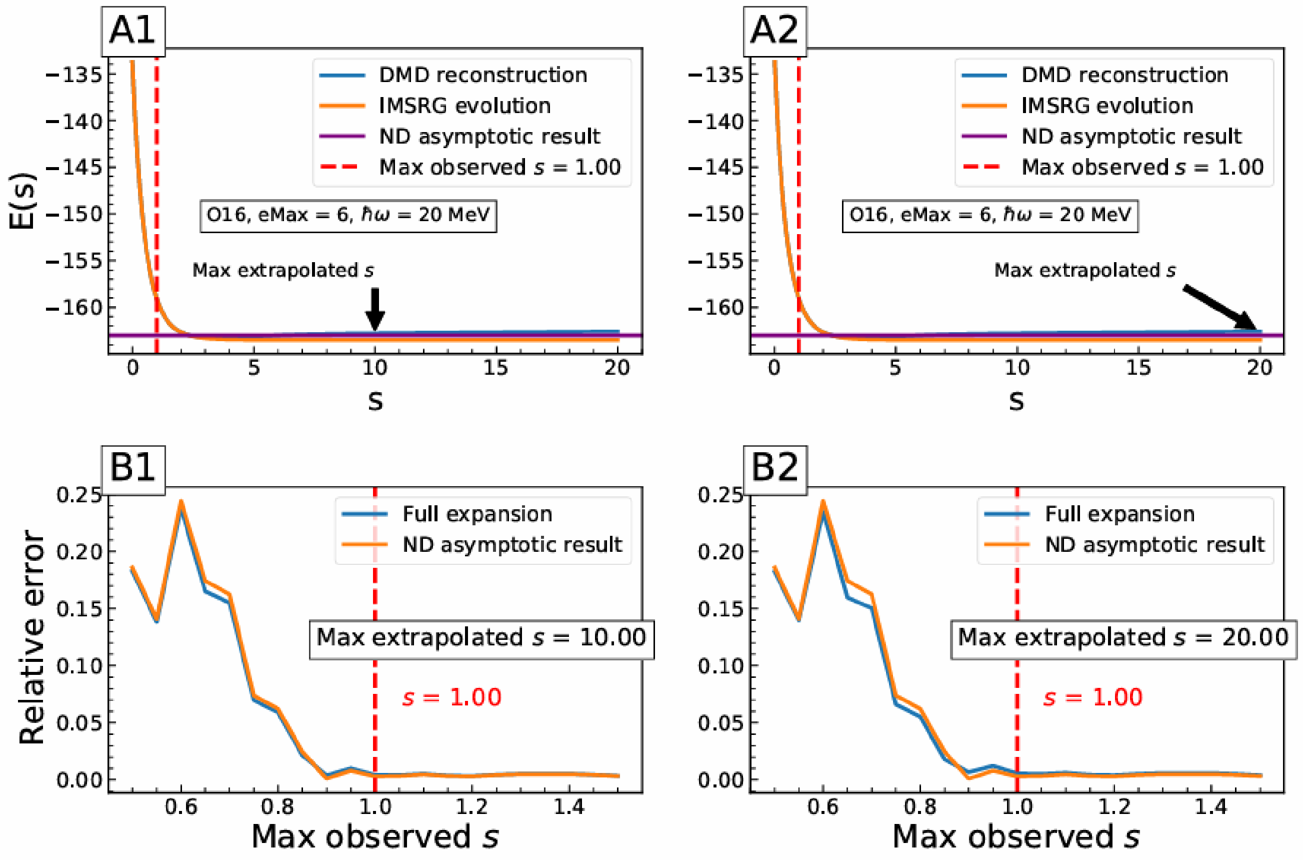
For Emulating the non-magnus formulation!

Pros

- Simple implementation
- Fast Training
- Fairly Accurate

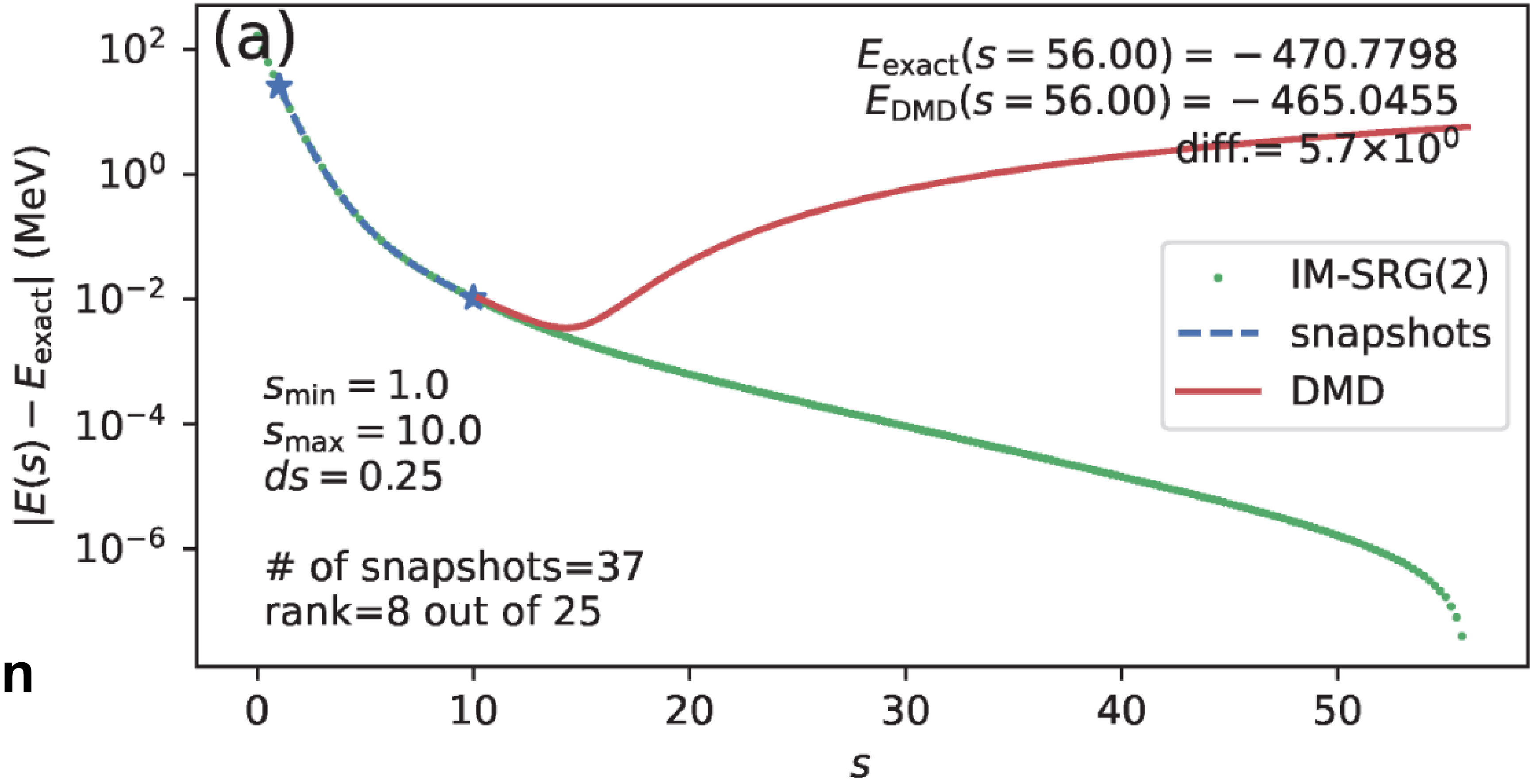
Cons

- **Struggles with Magnus IMSRG**
- Hard to modify



Jacob Davison. Theoretical and Computational Improvements to the In-Medium Similarity Renormalization Group. PhD. thesis, Michigan State University, East Lansing, MI, USA, 2023

DMD for Magnus IMSRG



Sota Yoshida. Surrogate Model for In-Medium Similarity Renormalization Group Method Using Dynamic Mode Decomposition. Particles, 8(1):13,2025.

Doesn't converge even with lots of training points

Solution: Modeling an Operator as an Eigenvector

Practically, when solving the IMSRG equations, the matrices are vectorized to be used in an ODE solver.

$$\Omega \approx \Omega^{(0)} + \Omega^{(1)} + \Omega^{(2)}$$

$$|\Omega\rangle = \begin{pmatrix} \Omega^{(0)} \\ \Omega^{(1)} \\ \cdots \\ \\ \Omega^{(2)} \\ \cdots \\ \cdots \end{pmatrix}$$

$$\frac{d\hat{\Omega}}{ds} = \sum_{k=0}^{\infty} \frac{B_k}{k!} \mathrm{ad}_{\hat{\Omega}}^{k}\,(\hat{\eta})$$

Original

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Original

We model $|\Omega\rangle$ as the flow-dependent ground-state eigenvector $|\phi(s)\rangle$ of a "Hamiltonian"

$$P(s) = A_{\text{Train}} + \frac{d}{ds} y(s) B_{\text{Train}}$$

$$P(s)|\phi(s)\rangle = \lambda(s)|\phi(s)\rangle$$

$$|\Omega(s)\rangle \approx |\phi'(s)\rangle$$

Where $y(s)$ is a function fit to $||\Omega(s)\rangle|^2$

And we can Use the **loss function**:

$$\mathcal{L}(\phi(s_i)) = \sum_i \| \, |\Omega_i\rangle \, \|^2 - \| \, \langle \phi'(s_i)| \, |\Omega_i\rangle \, \|$$

Emulator

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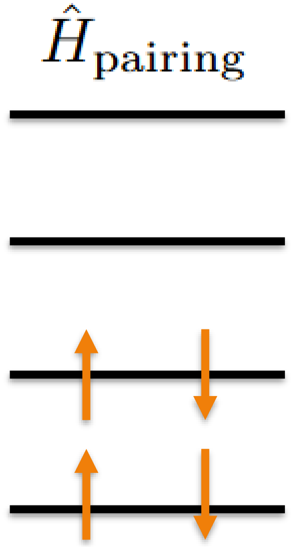
Pairing Model (with Pair Breaking)

$$\hat{H}_{\text{pairing}} = \delta \sum_{p\sigma} (p-1) a^\dagger_{p\sigma} a_{p\sigma} - \frac{1}{2} g \sum_{pq} a^\dagger_{p+} a^\dagger_{p-} a_{q-} a_{q+}$$



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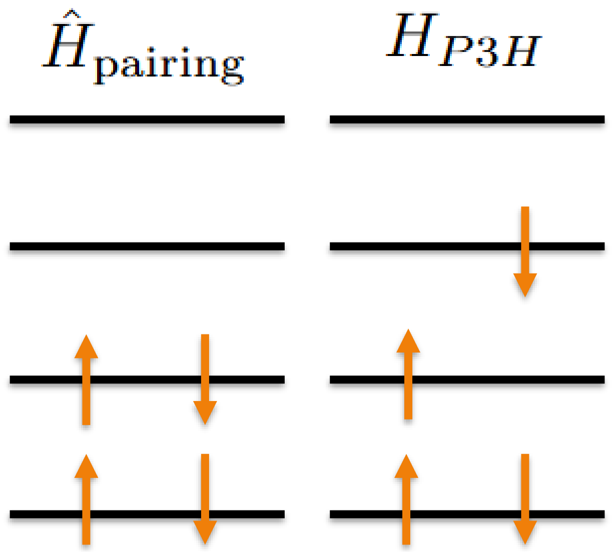
$$H_{P3H} = H_{\text{pairing}} - \frac{b}{2} \sum_{pp'q} \left(a^\dagger_{p+} a^\dagger_{p-} a_{p'-} a_{q+} + a^\dagger_{q+} a^\dagger_{p'-} a_{p-} a_{p+} \right)$$



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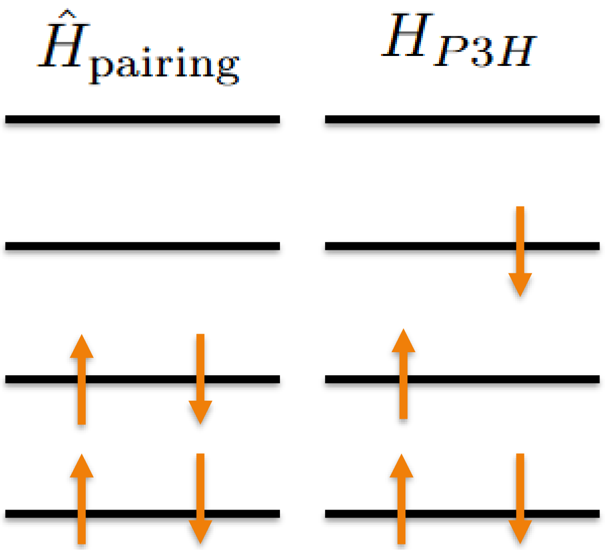
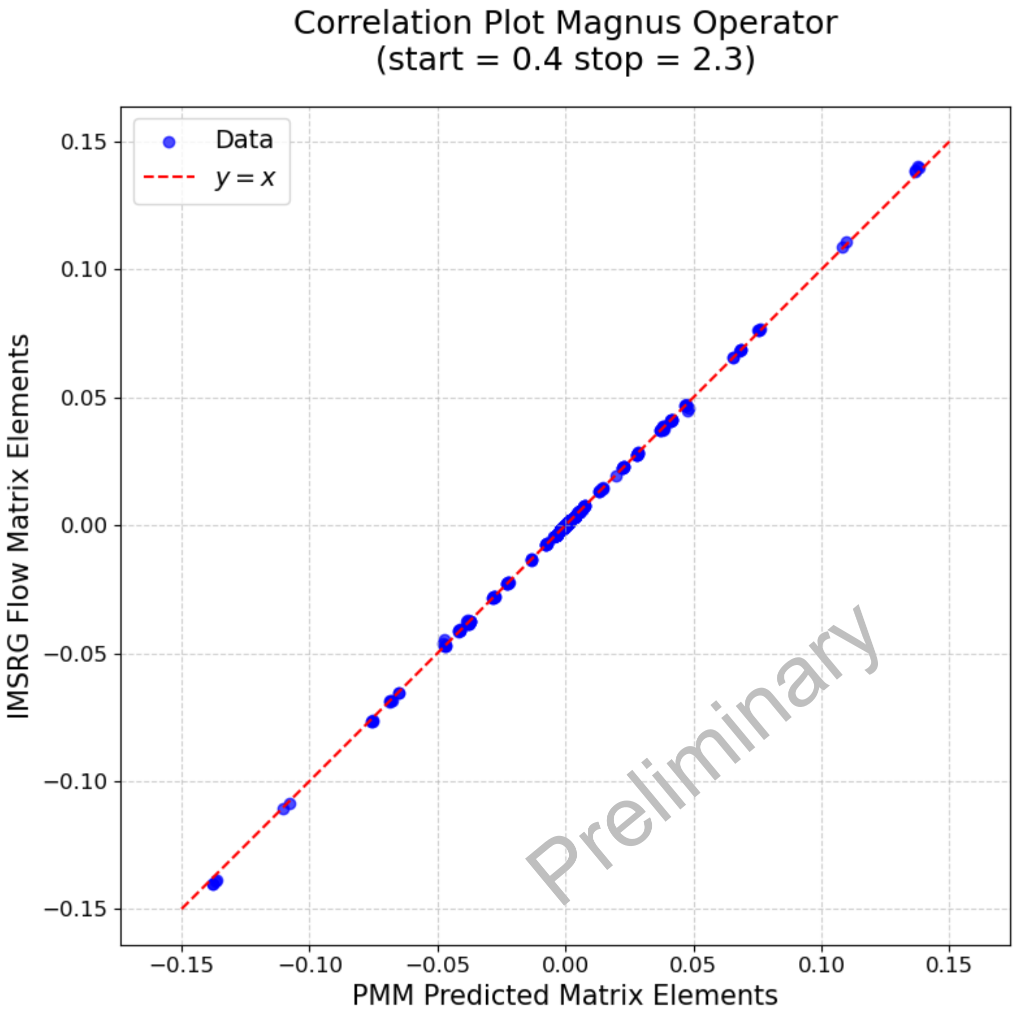


Normal Order

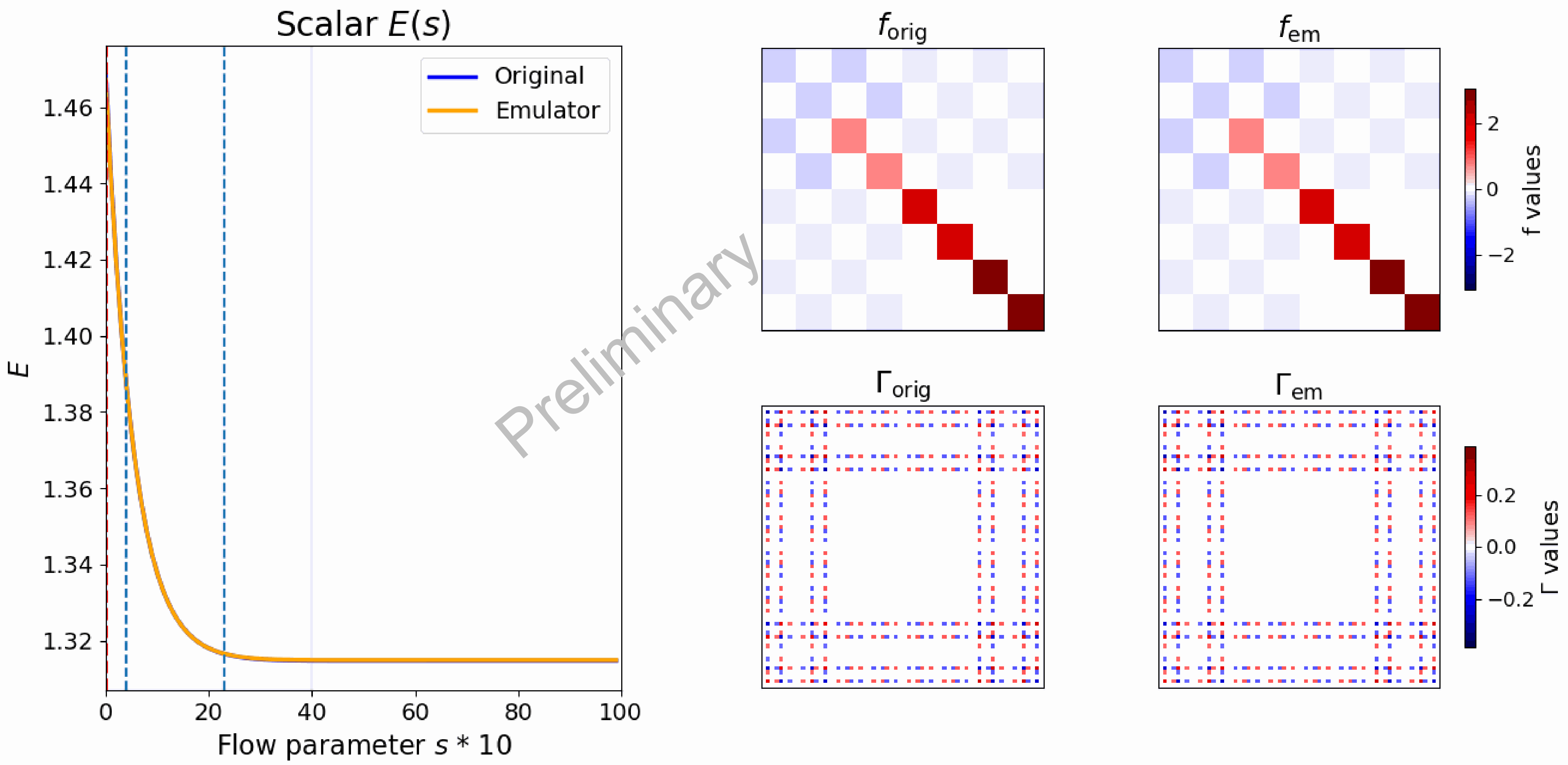
$$\hat{H} = E + \sum_{ij} f_{ij} \{a^\dagger_i a_j\} + \frac{1}{4} \sum_{ijkl} \Gamma_{ijkl} \{a^\dagger_i a^\dagger_j a_l a_k\}$$

Results using the Pairing Model (with pair breaking)

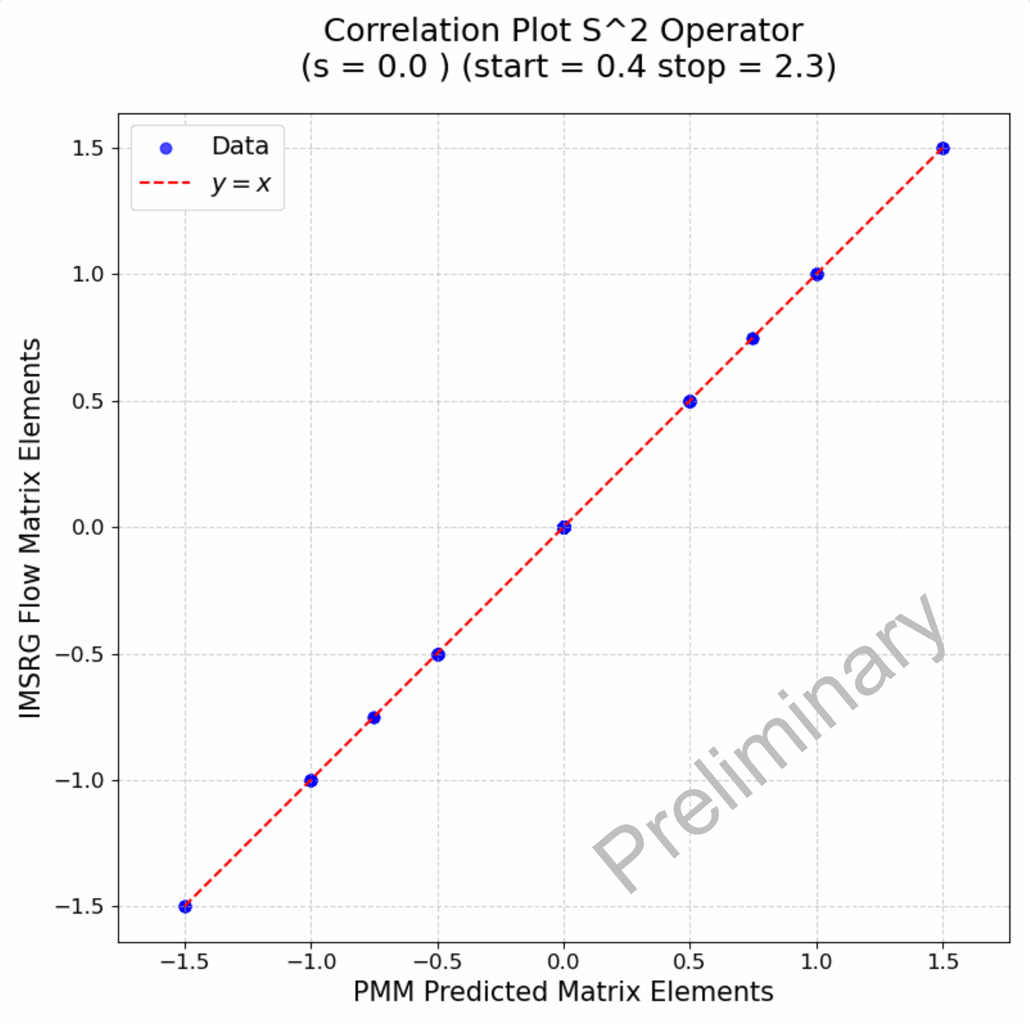


- 4 particles and 4 holes
- Extrapolated out to s =10.0

Reconstructing the Hamiltonian

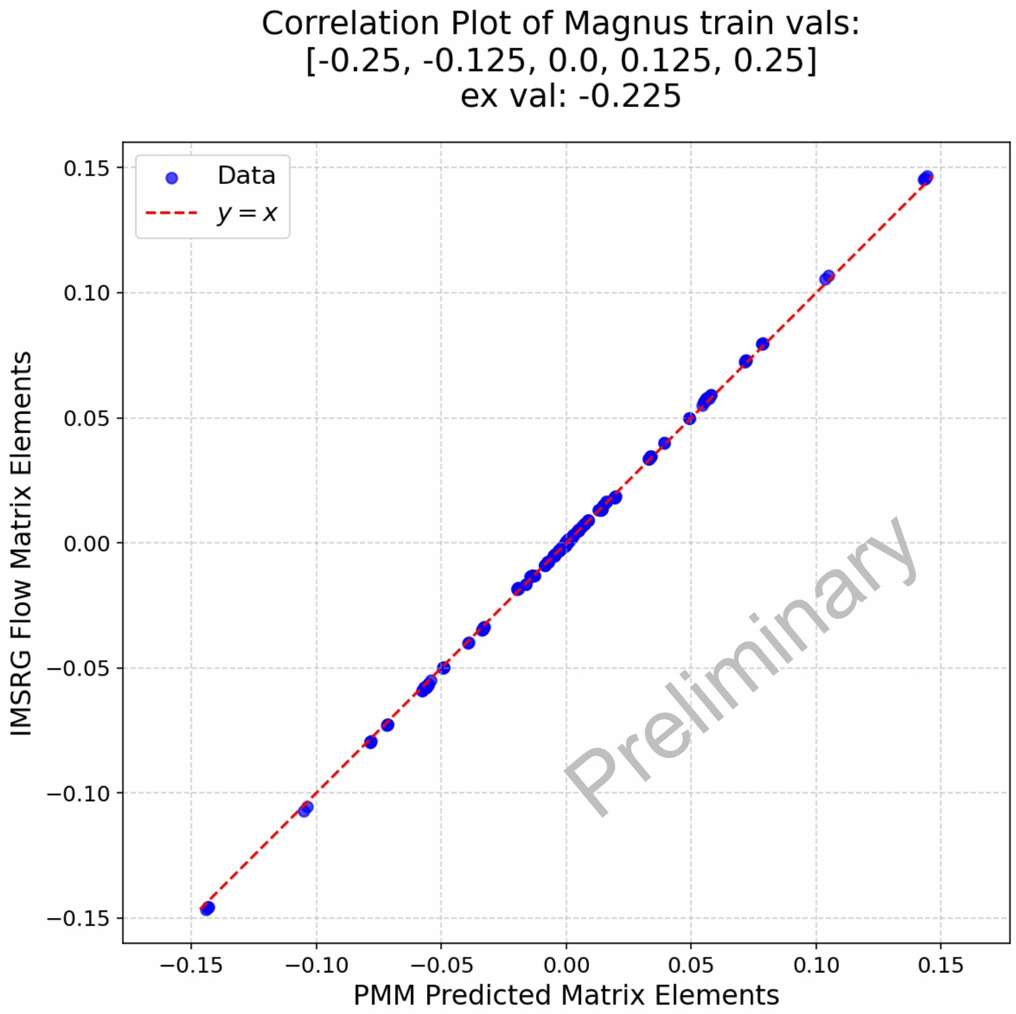


Using PMM to Evolve S^2 Operator



Can Predict the Flow of Other Observables

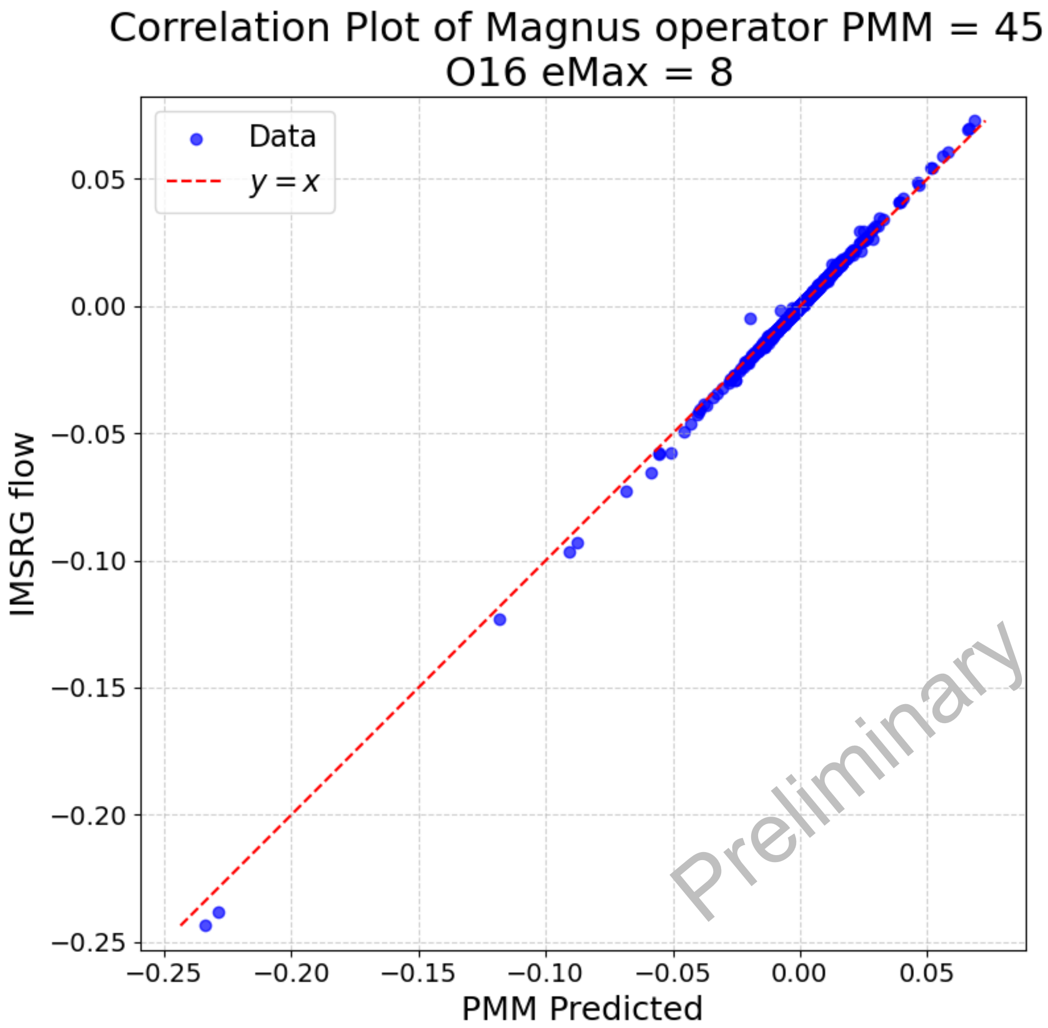
Interpolating the PMMs



Interpolating for different values of b

$$H_{P3H} = H_{\text{pairing}} - \frac{b}{2} \sum_{pp'q} \left(a^\dagger_{p+} a^\dagger_{p-} a_{p'-} a_{q+} + a^\dagger_{q+} a^\dagger_{p'-} a_{p-} a_{p+} \right)$$

Results with Realistic Interaction (EM 1.8 / 2.0)



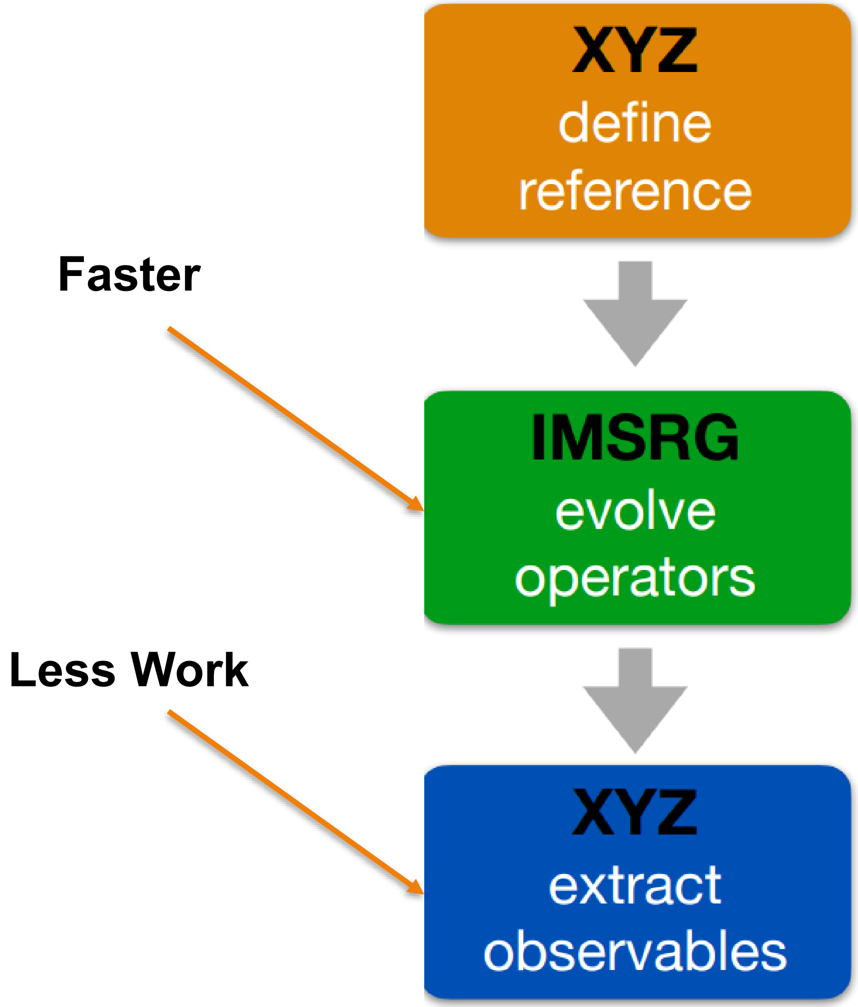
Trained from s = 0.18 to s = 2.92 and extrapolated to s = 10

~670,000 Parameters to ~4,000

Conclusions/ Future Work

Conclusions

- PMMs seem to strike a balance between the **speed and simplicity** of DMD with **flexibility and accuracy** of other methods.
- Can **Accurately Predict the Flow** of The Magnus Operator.
- Can **interpolate** the Magnus operator, allowing for **more information-per-flow**.



FRIB
Facility for Rare Isotope Beams
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References/ Acknowledgments

- [1] Heiko Hergert, Scott K. Bogner, Justin G. Lietz, Titus D. Morris, Samuel J.Novario, Nathan M. Parzuchowski, and Fei Yuan. In-Medium Similarity Renormalization Group Approach to the Nuclear Many-Body Problem, pages477–570. Springer International Publishing, Cham, 2017.
- [2] Jacob Davison. Theoretical and Computational Improvements to the In-Medium Similarity Renormalization Group. Ph.d. thesis, Michigan State University, East Lansing, MI, USA, 2023.
- [3] Sota Yoshida. Surrogate Model for In-Medium Similarity Renormalization Group Method Using Dynamic Mode Decomposition. Particles, 8(1):13,2025.
- [4] T. D. Morris, N. M. Parzuchowski, and S. K. Bogner. Magnus expansion and in-medium similarity renormalization group. Physical Review C, 92(3),September 2015.

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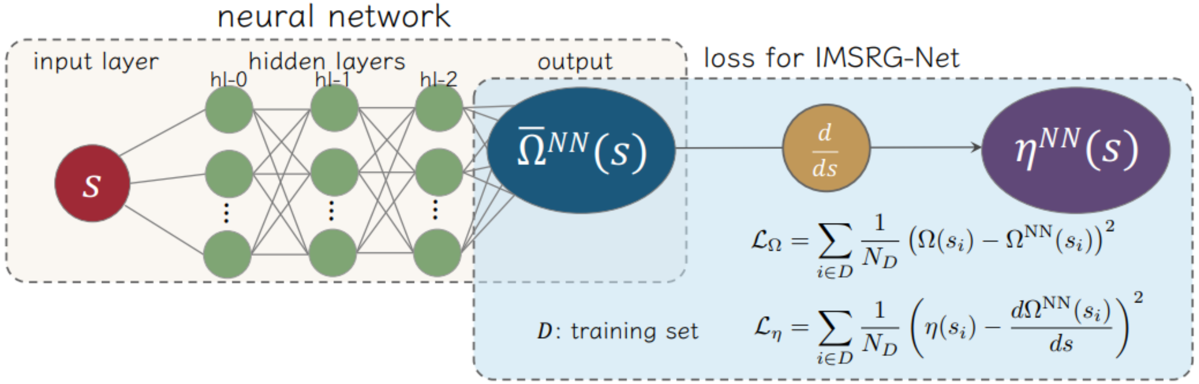
Neural Network Emulation of Magnus

- Pros
  - Accurate.
  - Still faster than IMSRG in some situations.

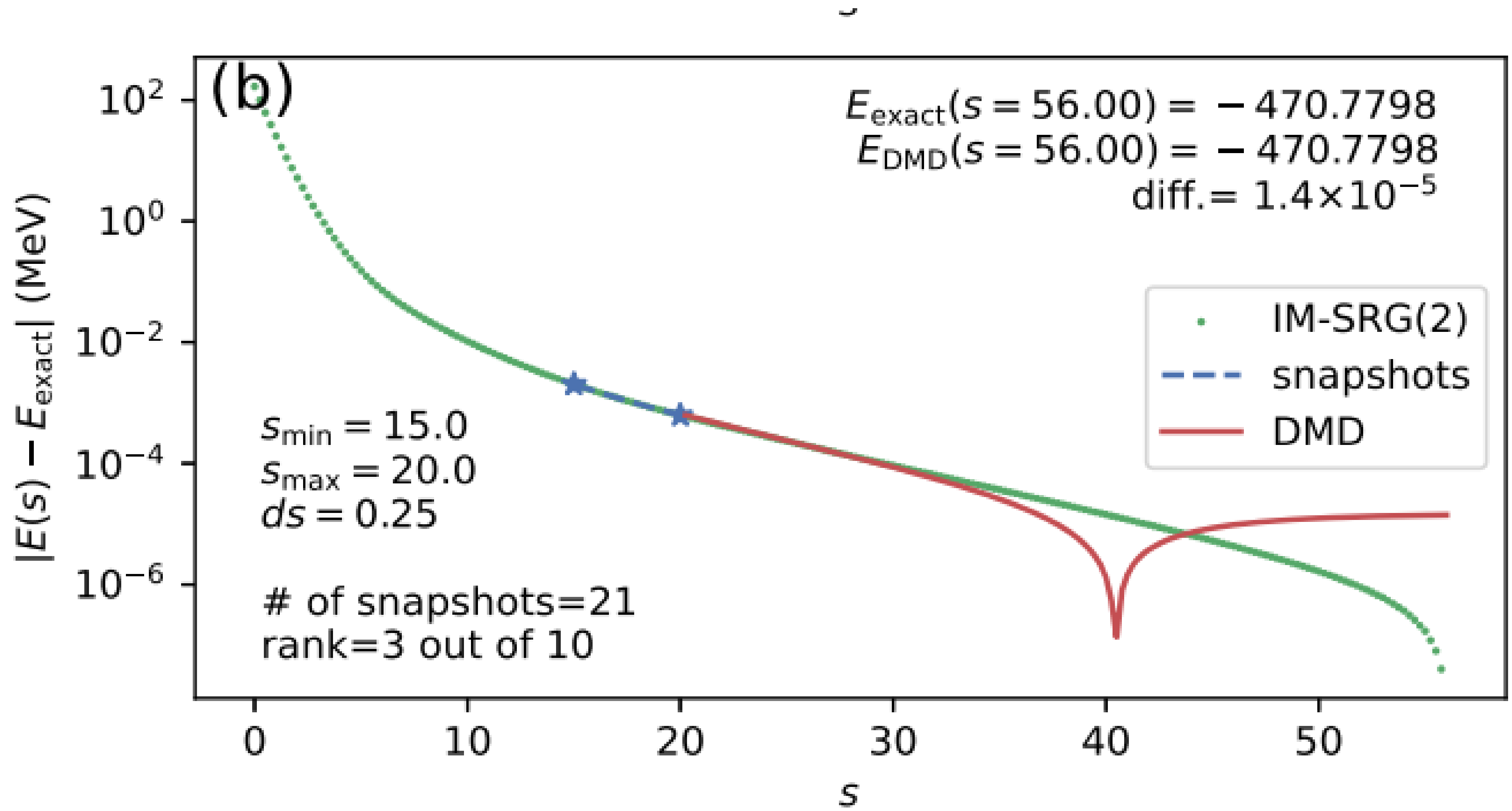


- Cons
  - Uses lots of VRAM (~20Gb).
  - Uses lots of training points.

			Energy (MeV)			
			$s = 20$		$s = \infty$	
target	interaction	$e_{\max}$	IMSRG(2)	IMSRG-Net	IMSRG(2)	IMSRG-Net
^{16}O	EM500	4	-156.9474	-156.9474	-156.9611	-156.9607
		6	-163.4079	-163.4079	-163.4153	-163.4150
		8	-165.1876	-165.1875	-165.1932	-165.1927
		10	-165.5309	-165.5309	-165.5359	-165.5357
	EMN500+2n3n	4	-111.8453	-111.8453	-111.8470	-111.8462
		6	-114.4895	-114.4895	-114.4925	-114.4918
		8	-115.5894	-115.5894	-115.5930	-115.5924
		10	-115.9040	-115.9040	-115.9079	-115.9082

Sota Yoshida. Imsrg-net: A machine-learning-based solver for the in-medium similarity renormalization group method. Phys. Rev. C, 108:044303, Oct2023.

DMD struggles with The Magnus Operator



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How PMMs can help

- The Solution to the Dyson series of a time-dependent Hamiltonian can be found by simply finding the ground-state eigenvector of the Hamiltonian at time $H(t)$. This is impractical for large Hamiltonians, but perfectly feasible if we find a small-space approximation of the Hamiltonian.

$$H(t)\left|\psi_0(t)\right\rangle = E_0(t)\left|\psi_0(t)\right\rangle$$

or

$$\left|\psi_0(t)\right\rangle = \sum_{n=0}^{\infty}\left(-\frac{i}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \cdots \int_{t_0}^{t_{n-1}} dt_n H\left(t_1\right) H\left(t_2\right) \cdots H\left(t_n\right)\left|\psi_0(0)\right\rangle$$

Observable Values	CI	IMSRG	IMSRG DMD	Magnus	Magnus PMM
First Excited State No PB	2	2	2	2.000002	2.00000203
First Excited State PB	2	1.999461	1.9997867	1.99928	1.99927903
Ground State No PB	0	0	0	0.000856	0.000854
Ground State PB	0	0	0	0.001356	0.001357

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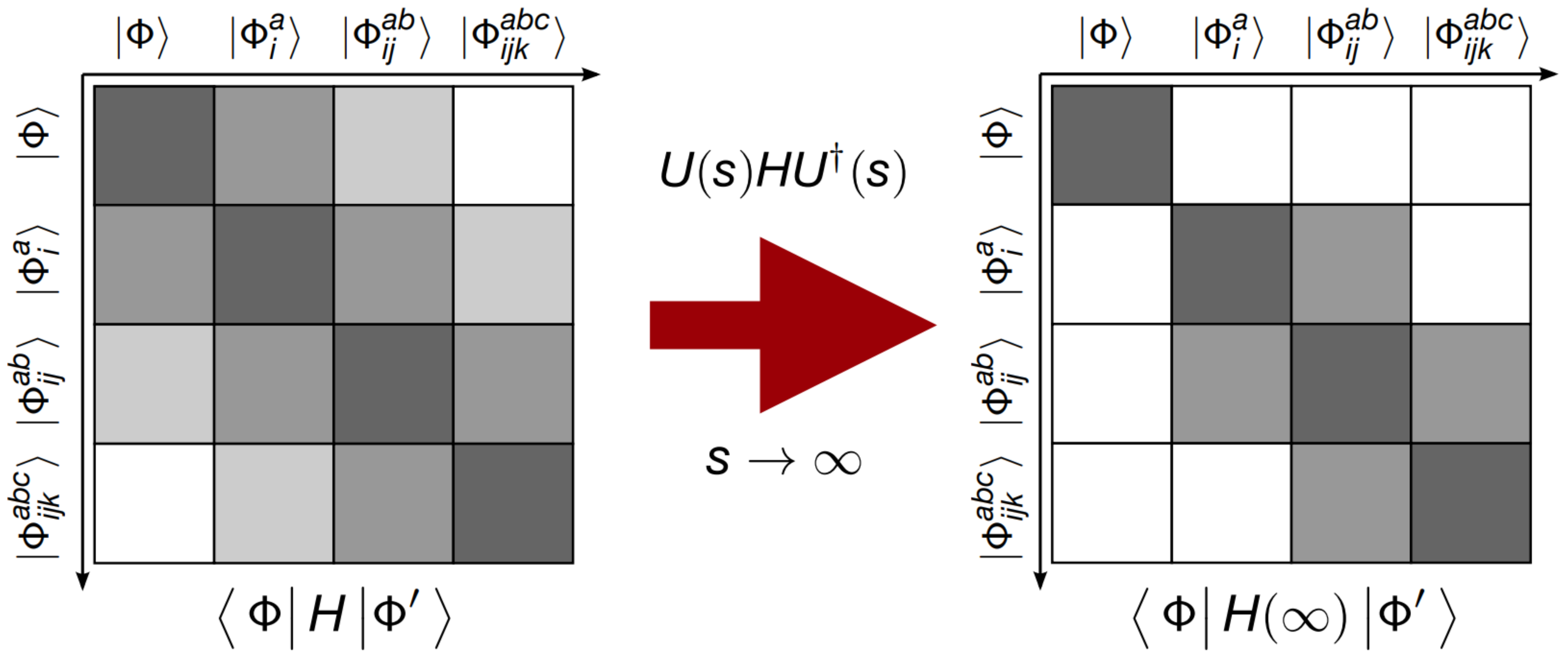

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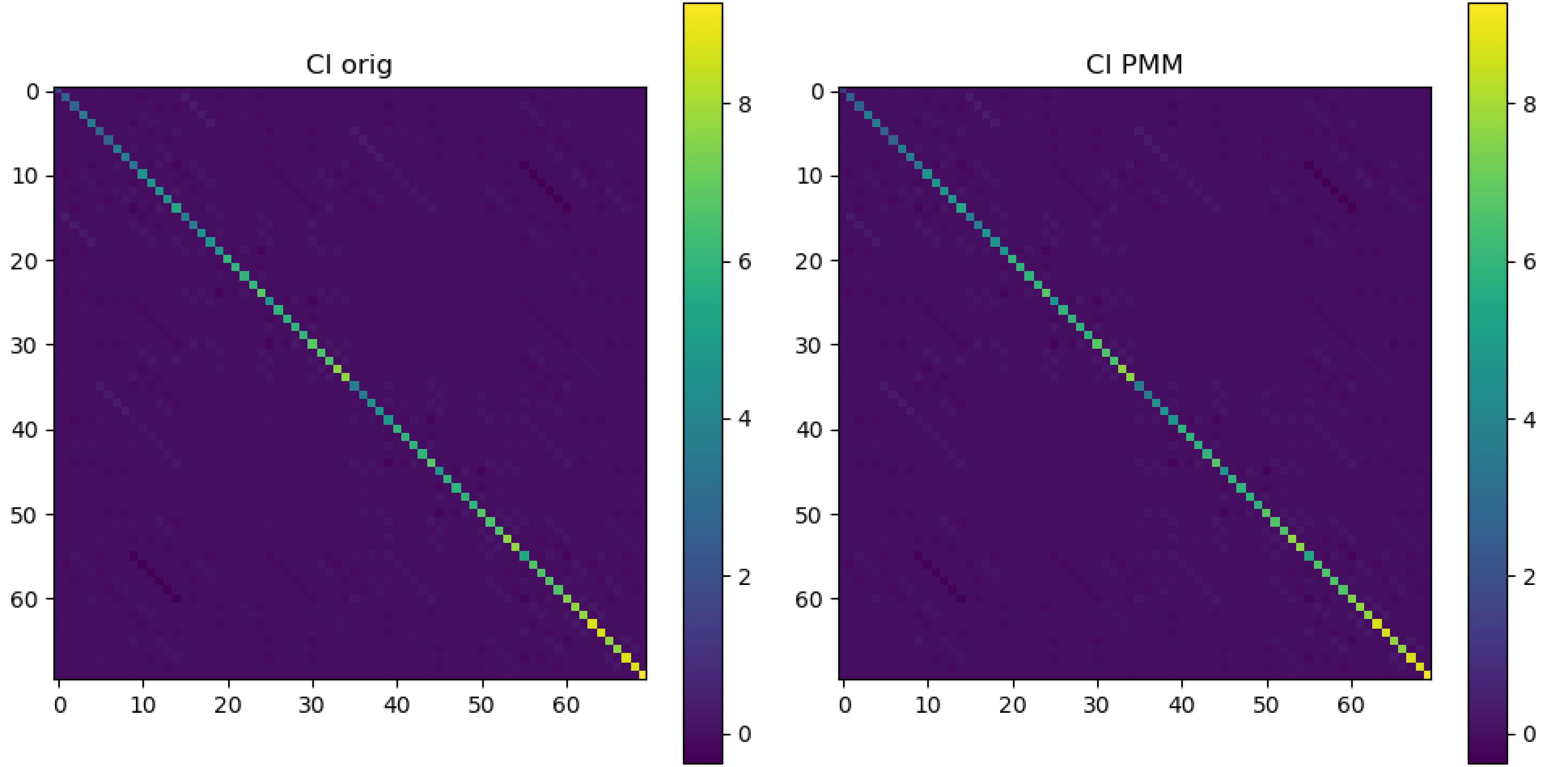

That was