VARIATIONAL NEURAL NETWORK ANSATZ FOR STEADY-STATES IN OPEN QUANTUM SYSTEMS

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ARXIV:1902.10104 [quant-ph]

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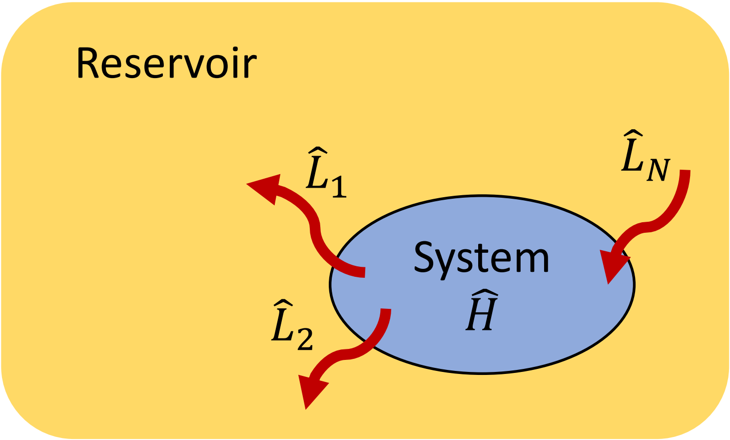
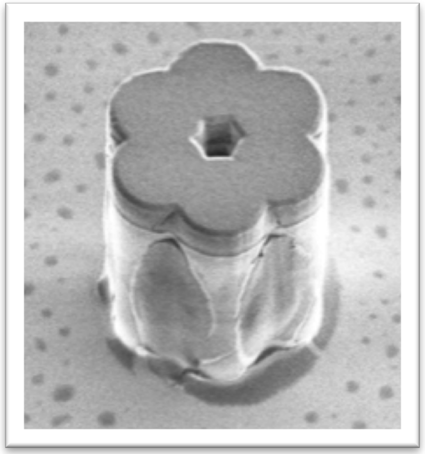
OPEN QUANTUM SYSTEMS

Describe the interaction of a quantum system H with its environment



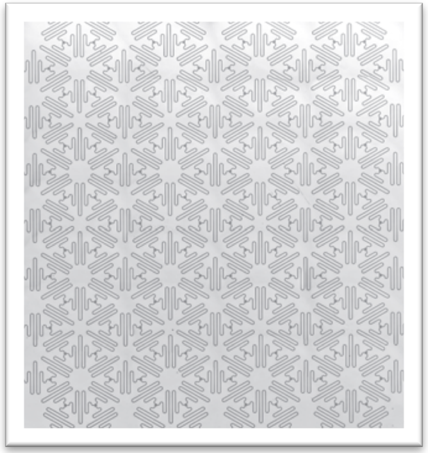
- Out of Equilibrium phenomena
- Reservoir Engineering
- *Dissipative* phase transitions

Semiconductor Micropillars



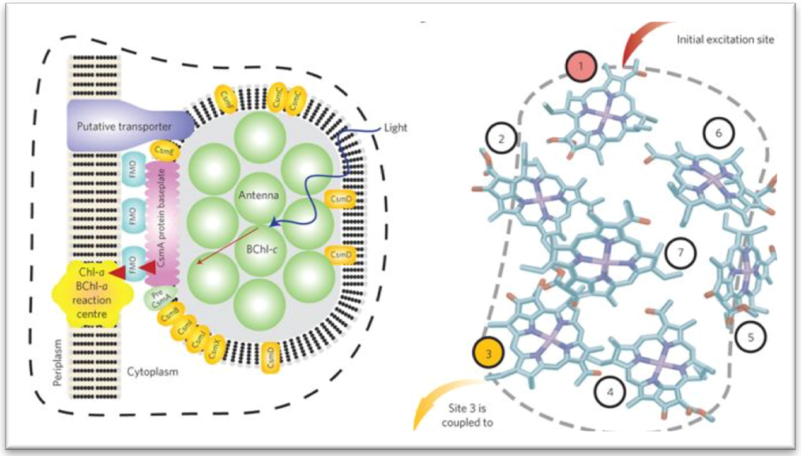
N. Carlon Zambon et Al.
arXiv:1812.06163

Superconducting circuits



A. A. Houck et Al.
Nat Phys 8, 292 (2012)

Quantum Biology



N. Lambert et Al.
Nat Phys 9, 10 (2013)

Schroedinger's Equation → Lindblad Master Eq.

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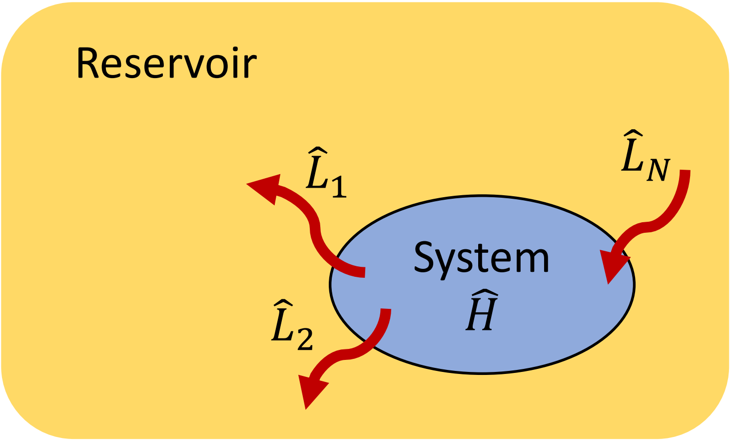


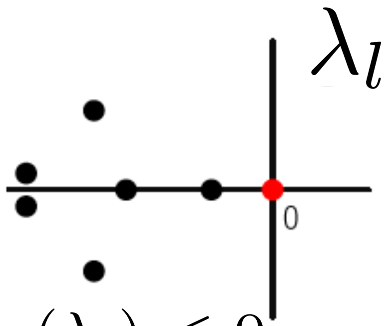
The state

$$|\psi\rangle \in \mathcal{H}_{\text{sys}} \otimes \mathcal{H}_{\text{E}} \quad \Longrightarrow \quad \hat{\rho} = \text{Tr}_{\text{E}}[|\psi\rangle\langle\psi|]$$

The master equation

$$\frac{\partial \hat{\rho}}{\partial t} = -i\left[\hat{H}, \hat{\rho}\right] + \sum_{j=1}^{N_{\text{channels}}} \left(\hat{L}_j \hat{\rho} \hat{L}_j^\dagger - \frac{1}{2}\left\{\hat{L}_j^\dagger \hat{L}_j, \hat{\rho}\right\}\right)$$

Coherent evolution — Incoherent Evolution



$$\text{Re}(\lambda_l) \leq 0$$

Rewritten as a linear super-operatorial equation

$$\partial_t \hat{\rho} = \mathcal{L}\hat{\rho}$$

We are usually interested in the steady-state

$$\hat{\rho}_{\text{ss}} = \lim_{t\to\infty} e^{\mathcal{L}t}\hat{\rho}$$

$$\mathcal{L}\hat{\rho}_{ss} = 0$$

$$\partial_t \rho_{ss} = 0$$

[HP Breuer, F Petruccione, The theory of quantum system (2012)]

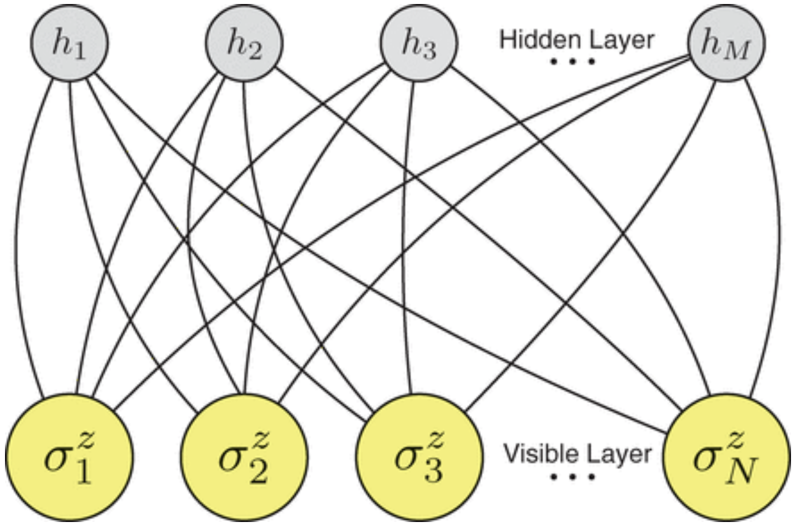
The dimensional curse

For N lattices of N sites, the Hilbert space has an exponentially big dimension $\dim \mathcal{H} \approx l^N$

Numerical Techniques try to reduce this size with physical insight (eg: MPS/MPOs, Cluster Mean Field..)

Neural Networks are Low-Dimensional approximations of high-dimensional functions…

$$|\psi\rangle = \begin{pmatrix} \psi(\uparrow\uparrow\ldots\uparrow) \\ \psi(\downarrow\uparrow\ldots\uparrow) \\ \psi(\uparrow\downarrow\ldots\uparrow) \\ \psi(\downarrow\downarrow\ldots\uparrow) \\ \vdots \\ \psi(\downarrow\downarrow\ldots\downarrow) \end{pmatrix}$$



[G. Carleo and M. Troyer, Science (2017)]

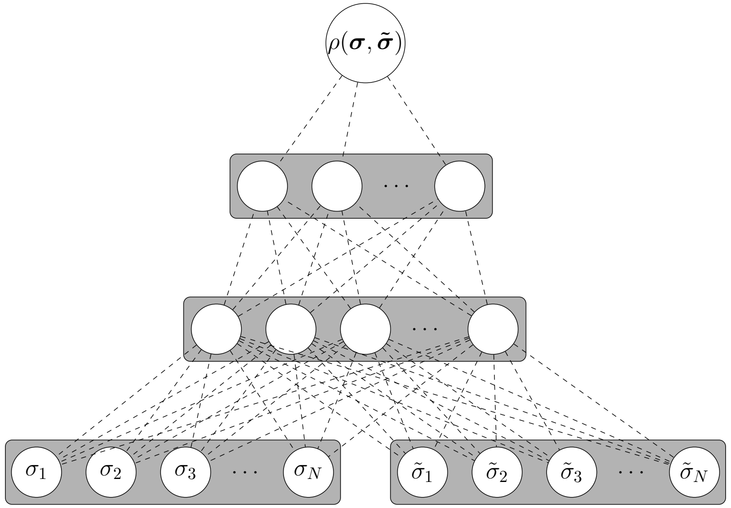
THE DIMENSIONAL CURSE

FOR N SPINS, THE HILBERT SPACE HAS AN EXPONENTIALLY BIG DIMENSION $\dim \hat{\rho} = \dim \mathcal{H} \otimes \mathcal{H} = 2^{2N}$

$$\hat{\rho} = \sum_{\substack{\sigma_1,\dots,\sigma_N,\\ \tilde{\sigma}_1,\dots,\tilde{\sigma}_N}} \underbrace{\rho(\sigma_1,\dots,\sigma_N,\tilde{\sigma}_1,\dots,\tilde{\sigma}_N)}_{\text{HIGH-DIMENSIONAL FUNCTION}} |\sigma_1,\dots,\sigma_N\rangle \langle \tilde{\sigma}_1,\dots,\tilde{\sigma}_N|$$

4 ARTICLES CAME OUT IN A WEEK WITH SIMILAR PROPOSALS

F.V, A. BIELLA, N. REGNAULT AND C.CIUTI	ARXIV:1902.10104
M.J. HARTMANN AND G.CARLEO	ARXIV:1902.05131
A. NAGY AND V. SAVONA	ARXIV:1902.09483
N. YOSHIOKA AND R: HAMAZAKI	ARXIV:1902.07006

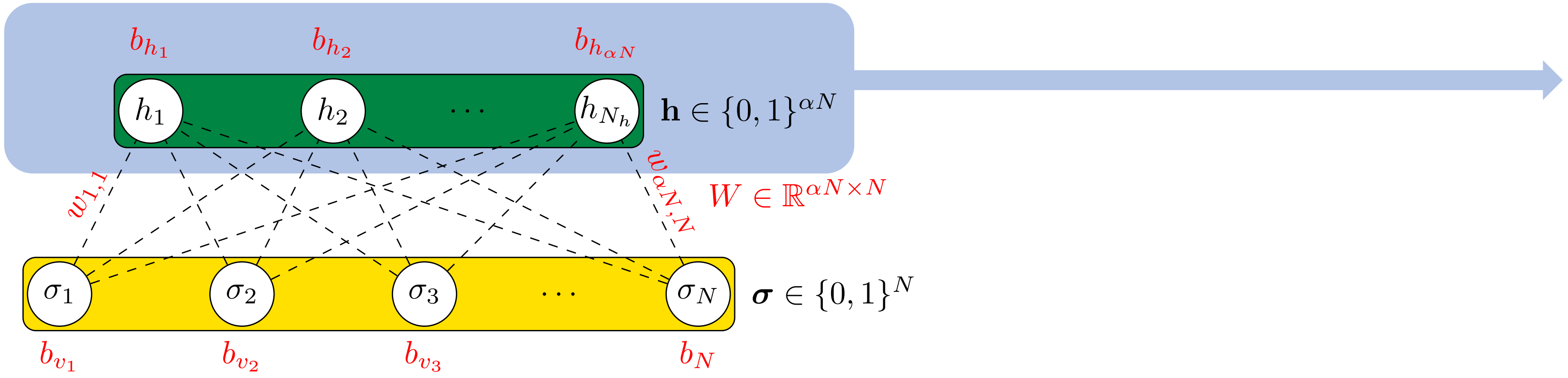


BUT $\hat{\rho}$ IS POSITIVE-SEMIDEFINITE AND HERMITIAN. WE WANT TO ENFORCE THOSE PROPERTIES.

[G. Carleo and M. Troyer, Science (2017)]

Neural Density Matrix

Drawing inspiration from RBMs (Restricted Boltzmann Machines)…



Tracing out the hidden layer gives a well-defined probability distribution

$$p(\boldsymbol{\sigma}) = \sum_{\mathbf{h}} e^{-E(\boldsymbol{\sigma},\mathbf{h})}$$

[G. Torlai and R. Melko, PRL (2018)]

NEURAL DENSITY MATRIX

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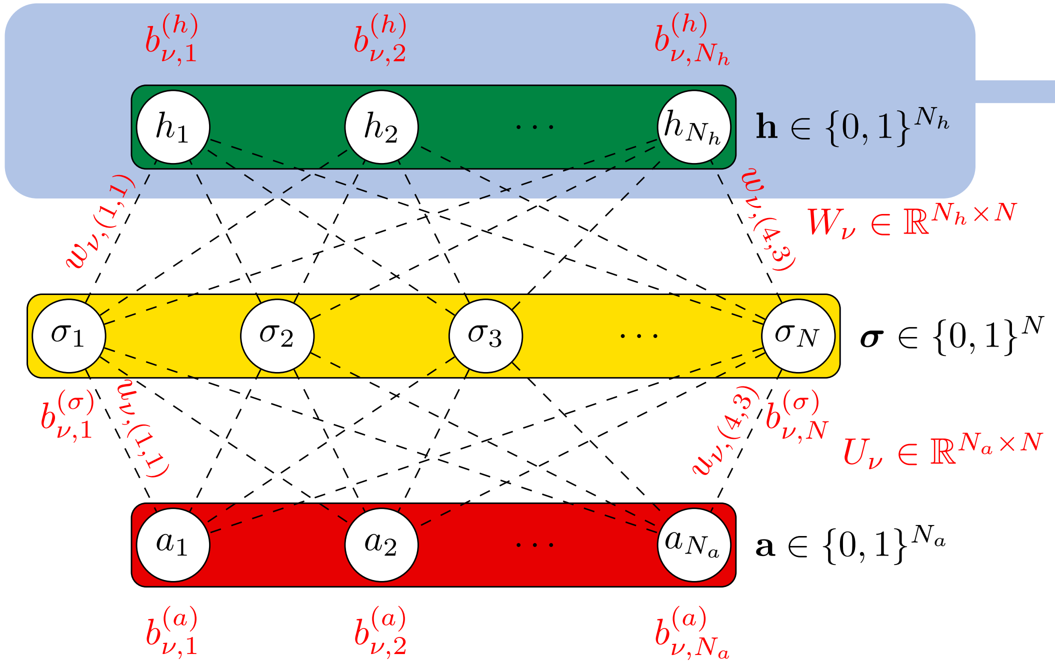

TRACING OUT THE HIDDEN LAYER GIVES A WELL-DEFINED PROBABILITY DISTRIBUTION

$$p(\boldsymbol{\sigma}) = \sum_{\mathbf{h}} e^{-E(\boldsymbol{\sigma},\mathbf{h})}$$

DOUBLE THE «HIDDEN» VARIABLES

$$p(\boldsymbol{\sigma},\mathbf{a}) = \sum_{\mathbf{h}} e^{-E(\boldsymbol{\sigma},\mathbf{a},\mathbf{h})}$$

[G. Torlai and R. Melko, PRL (2018)]

Neural Density Matrix

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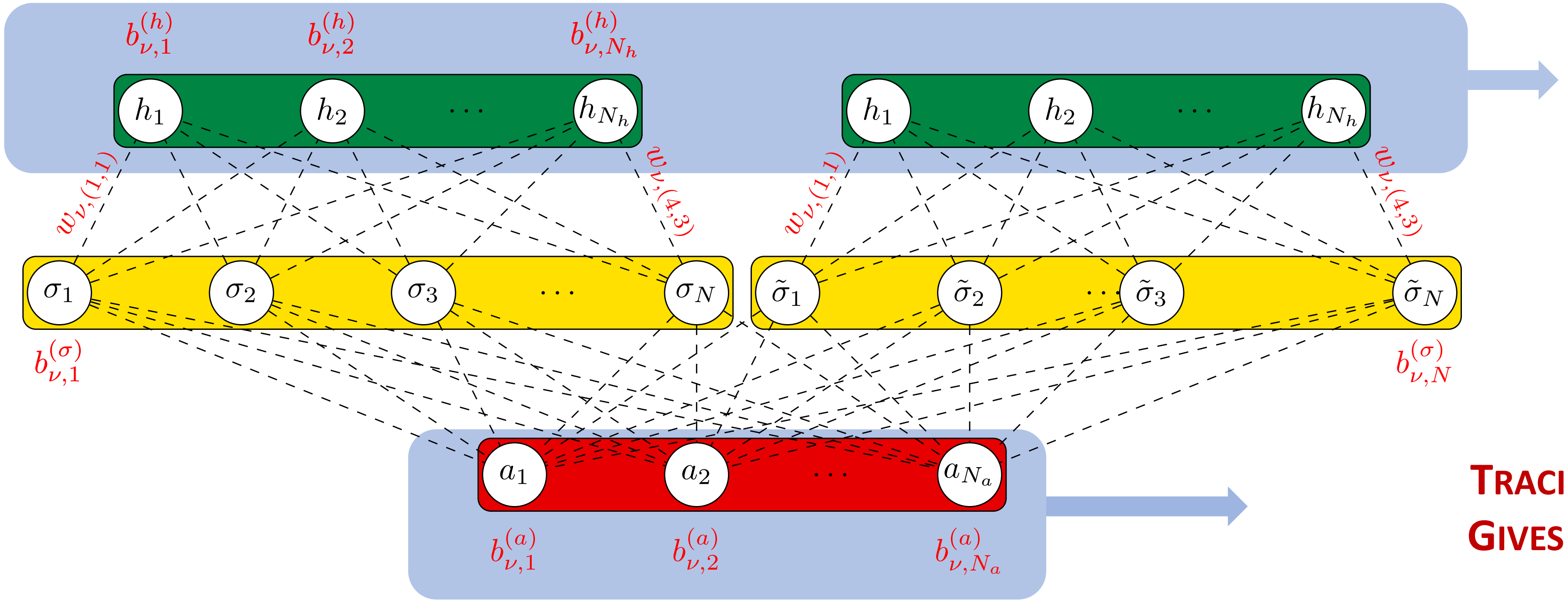


Tracing out the hidden layer gives a well-defined probability distribution

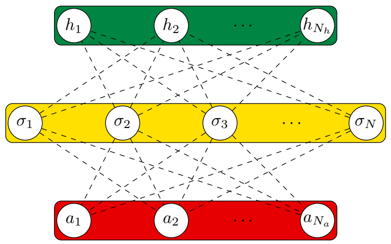
$$p(\boldsymbol{\sigma}) = \sum_{\mathbf{h}} e^{-E(\boldsymbol{\sigma},\mathbf{h})}$$

Double the «hidden» Variables

$$p(\boldsymbol{\sigma},\mathbf{a}) = \sum_{\mathbf{h}} e^{-E(\boldsymbol{\sigma},\mathbf{a},\mathbf{h})}$$

Tracing out another Hidden layer gives an ensemble of distributions

Formally equivalent to defining an RBM in the bigger space, summing over the hidden space and then



$$\psi(\vec{\sigma},\vec{a}) \in \mathcal{H}_s \otimes \mathcal{H}_a \qquad \Rightarrow \qquad \rho(\vec{\sigma},\vec{\sigma}') = \sum_{a\in\mathcal{H}_a} \left[\psi(\vec{\sigma},\vec{a})\psi^{\star}(\vec{\sigma}',\vec{a})\right]$$

Can be generalized to FFNN!

[G. Torlai and R. Melko, PRL (2018)]

OUT OF EQUILIBRIUM: FINDING THE STEADY STATE

We have a variational ansatz (where v are the variational parameters)

$$\rho_{\boldsymbol{v}}(\boldsymbol{\sigma}, \boldsymbol{\sigma}')$$

I want to find the steady state

$$\frac{d\rho_{\mathrm{ss}}}{dt} = \mathcal{L}\rho_{\mathrm{ss}} = 0$$

We need a variational principle: I define the `Cost Function`

$$\mathcal{C}(\boldsymbol{v}) = \frac{\|d\hat{\rho}_{\boldsymbol{v}}/dt\|_2^2}{\|\hat{\rho}_{\boldsymbol{v}}\|_2^2} = \frac{\mathrm{Tr}\left[\hat{\rho}_{\boldsymbol{v}}^{\dagger}\mathcal{L}^{\dagger}\mathcal{L}\hat{\rho}_{\boldsymbol{v}}\right]}{\mathrm{Tr}\left[\hat{\rho}_{\boldsymbol{v}}^{\dagger}\hat{\rho}_{\boldsymbol{v}}\right]}$$

Which has the nice properties:

$$\mathcal{C}(\boldsymbol{v}_{ss}) = 0 \iff \hat{\rho}_{\boldsymbol{v}_{ss}} = \hat{\rho}_{ss}$$

$$\mathcal{C}(\boldsymbol{v}) \geq 0$$

DIFFERENT COST FUNCTIONS ARE POSSIBLE!
SEE POSTER OF A. NAGY FOR A DIFFERENT ONE

[H. Weimer, PRL (2015)]

Out Of Equilibrium: Finding the steady state III

We recasted the problem of finding the steady state $\rho_{\rm SS}$ to a minimization problem for $\mathcal{C}(\boldsymbol{v})$

So we could perform a gradient-descent like minimization: $\boldsymbol{v} \rightarrow \boldsymbol{v} - \nabla_{\boldsymbol{v}}\mathcal{C}(\boldsymbol{v})$

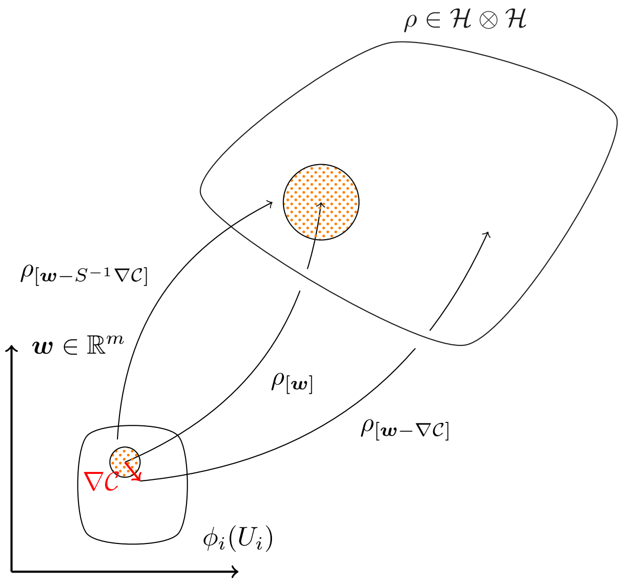
But there's a problem! Local Minimas! ➔ **NATURAL GRADIENT DESCENT**

But there's a problem! Computing the Cost Fun ➔ **SAMPLING**

$$\mathcal{C}(\boldsymbol{v}) = \frac{\mathrm{Tr}\left[\hat{\rho}_{\boldsymbol{v}}^{\dagger}\mathcal{L}^{\dagger}\mathcal{L}\hat{\rho}_{\boldsymbol{v}}\right]}{\mathrm{Tr}\left[\hat{\rho}_{\boldsymbol{v}}^{\dagger}\hat{\rho}_{\boldsymbol{v}}\right]} = \sum_{\boldsymbol{\sigma},\tilde{\boldsymbol{\sigma}}} p_{\boldsymbol{v}}(\boldsymbol{\sigma},\tilde{\boldsymbol{\sigma}})\mathcal{C}^{\rm Loc}(\boldsymbol{v},\boldsymbol{\sigma},\tilde{\boldsymbol{\sigma}}),$$

Exponentially
Many elements

$$p_{\boldsymbol{v}}(\boldsymbol{\sigma},\tilde{\boldsymbol{\sigma}}) = |\rho_{\boldsymbol{v}}(\boldsymbol{\sigma},\tilde{\boldsymbol{\sigma}})|^2 / \sum_{\boldsymbol{\sigma},\tilde{\boldsymbol{\sigma}}} \rho_{\boldsymbol{v}}(\boldsymbol{\sigma},\tilde{\boldsymbol{\sigma}})$$



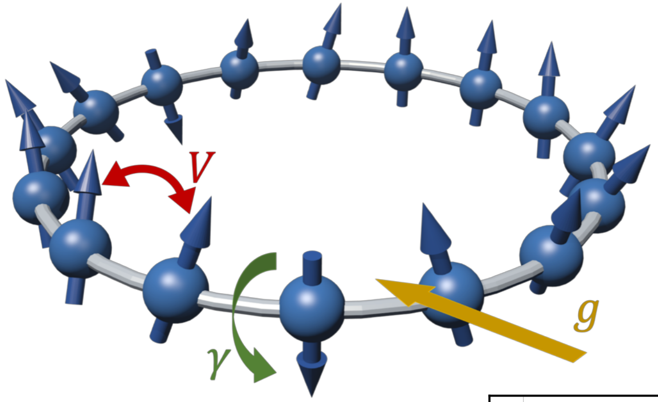
This is a probability distribution ➔ I can sample it! (and the gradient)

$$\mathcal{C}^{\rm Loc}(\boldsymbol{v},\boldsymbol{\sigma},\tilde{\boldsymbol{\sigma}}) = \sum_{\boldsymbol{\sigma}',\tilde{\boldsymbol{\sigma}}'} \frac{\rho_{\boldsymbol{v}}(\boldsymbol{\sigma}',\tilde{\boldsymbol{\sigma}}')}{\rho_{\boldsymbol{v}}(\boldsymbol{\sigma},\tilde{\boldsymbol{\sigma}})}(\mathcal{L}^{\dagger}\mathcal{L})(\boldsymbol{\sigma},\tilde{\boldsymbol{\sigma}};\boldsymbol{\sigma}',\tilde{\boldsymbol{\sigma}}').$$

Results for Driven-Dissipative Quantum Ising Model

The hamiltonian is

$$H = \frac{V}{4} \sum_{\langle j,l \rangle} \hat{\sigma}_j^z \hat{\sigma}_l^z + \frac{g}{2} \sum_j \hat{\sigma}_j^x$$



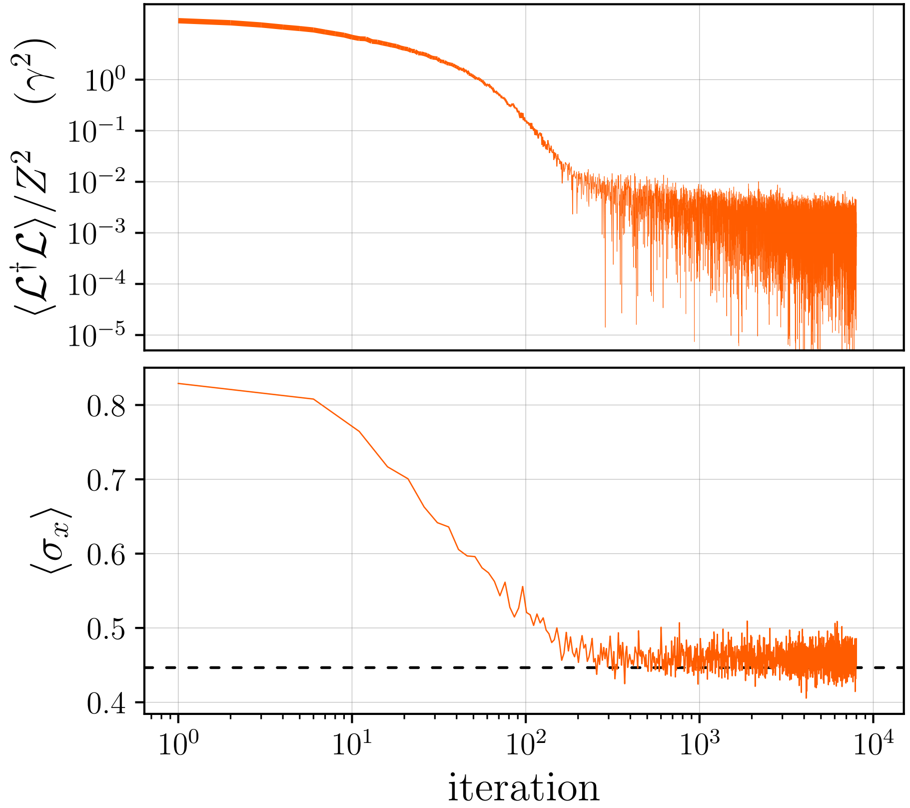
With de-exitation jump operators $L_j = \sigma_j^-$

We study the magnetizations $m^{(\alpha)} = \frac{1}{N} \sum_i \sigma_i^{(\alpha)}$

For a chain of N=16 sites (PBC)

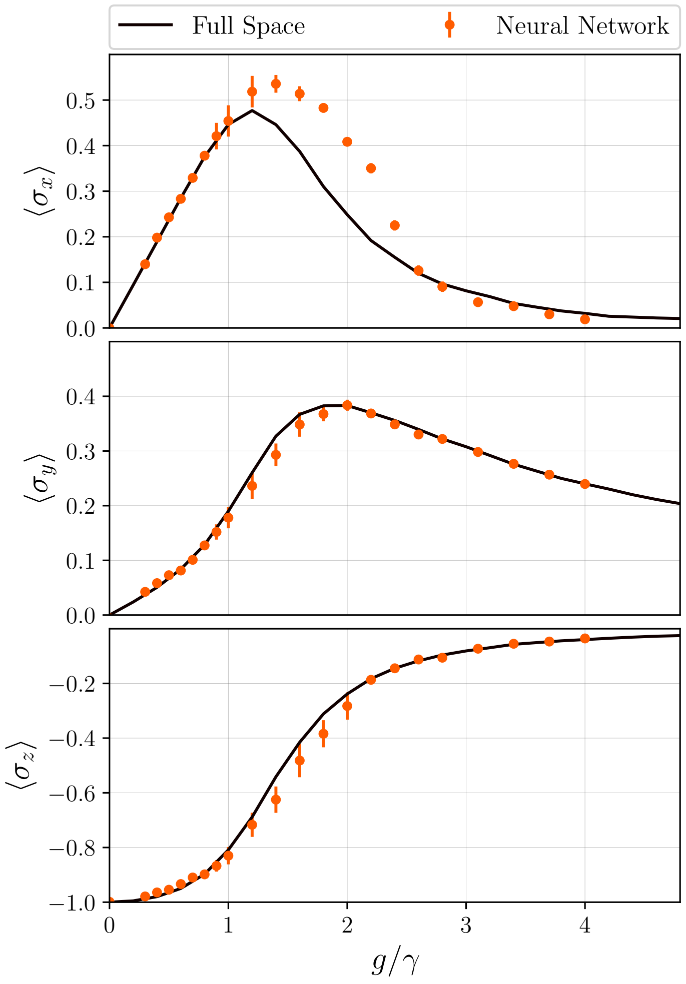
Observables are sampled like:

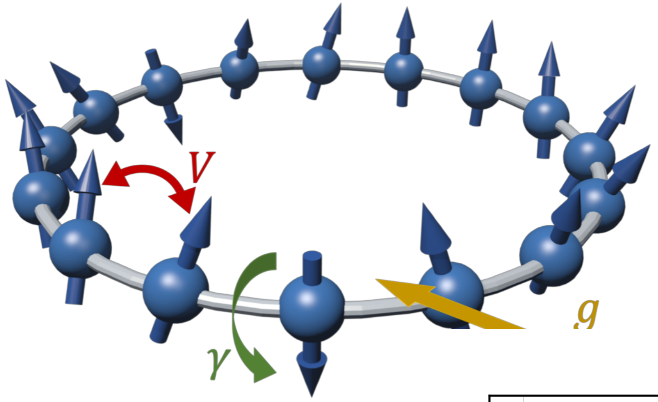
$$\langle \hat{m}^{(\alpha)} \rangle = \frac{\mathrm{Tr}\left[\hat{\rho}\ \hat{m}^{(\alpha)}\right]}{\mathrm{Tr}[\hat{\rho}]} = \sum_{\boldsymbol{\sigma}} p_{\boldsymbol{v}}^{\mathrm{obs}}(\boldsymbol{\sigma}) \sum_{\tilde{\boldsymbol{\sigma}}} \frac{\rho_{\boldsymbol{v}}(\boldsymbol{\sigma}, \tilde{\boldsymbol{\sigma}}) m^{(\alpha)}(\tilde{\boldsymbol{\sigma}}, \boldsymbol{\sigma})}{\rho_{\boldsymbol{v}}(\boldsymbol{\sigma}, \boldsymbol{\sigma})},$$

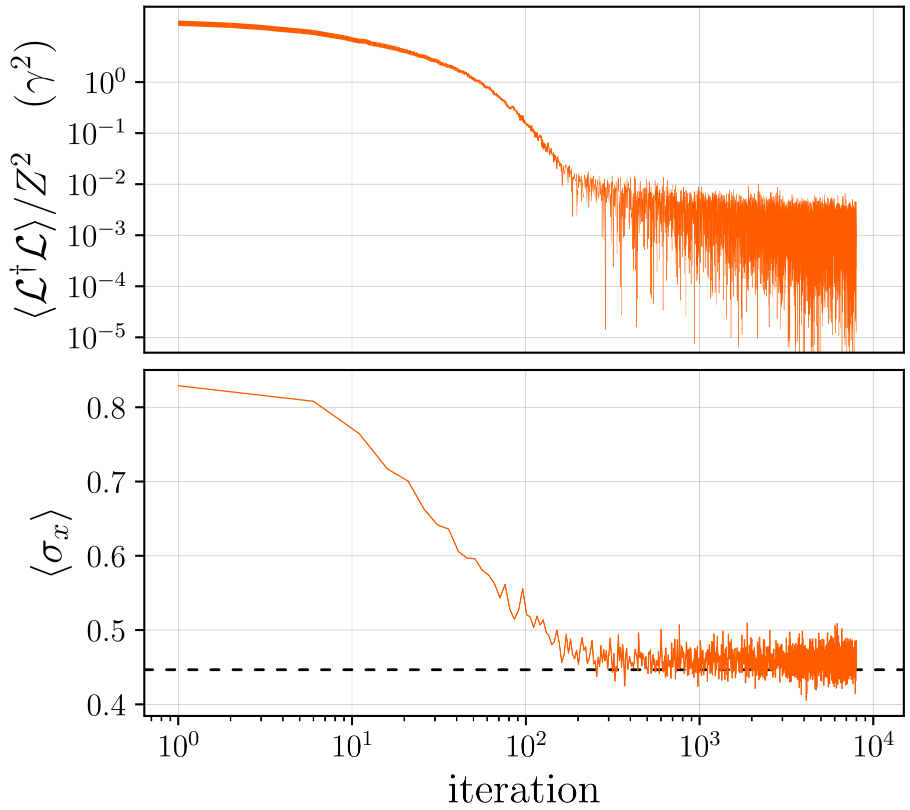


Results for Driven-Dissipative Quantum Ising Model II

A full scan in the transverse field gives:







CONCLUSIONS

- Density Matrices can be approximated with Neural Networks
- Variational Monte Carlo can be remapped to machine learning procedures
- We can solve the exponential growth problem

Perspectives:

- Try different topologies, layers to enforce simmetries…
- Test different cost functions
- [Also investigate Neural Network encodings for Digital Quantum Algorithm applications]

Aknowledgements

<u>F.V.</u>, A. Biella, N. Regnault and C. Ciuti

«Variational neural Network ansatz for steady states in Open Quantum Systems»

ArXiv:1902.10104

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Questions?

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CONTACT ME

QUESTIONS?

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CODE?

Will soon be available on GitHub. If you want to have a look now drop me an email.

COLLABORATE?

I am finalizing a framework written in Julia to perform MonteCarlo simulations using Neural Network ansatzes. If you would like to collaborate and/or help, I would love an hand.