Title: From Neural density Operators to Tensor Networks

Speakers: Filippo Vincentini

Series: Quantum Matter

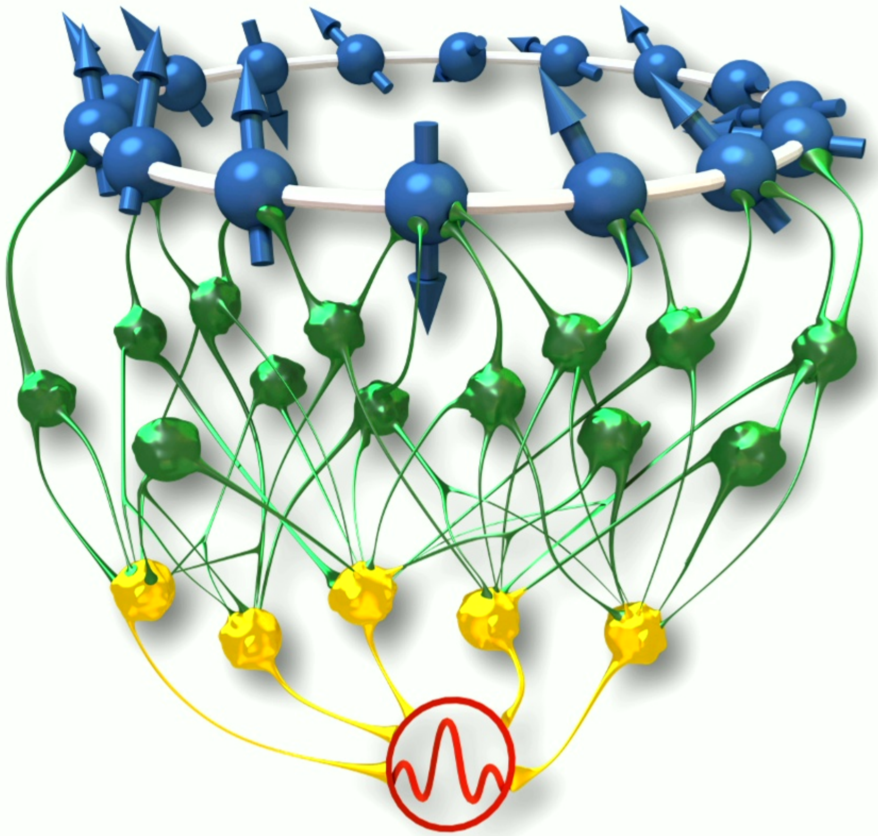
Date: July 22, 2022 - 10:30 AM

URL: https://pirsa.org/22070028

Abstract: In this talk I will discuss recent advances in Neural-Network parametrisations of pure and mixed quantum states that can be efficiently sampled. In the first part I will generalise the Neural Density Operator ansatz originally proposed by Torlai and Melko by combining two general ingredients that can be used to construct deep, autoregressive ansatze that automatically enforce positive definitness. In the second part, instead, I will show that any matrix product state can be exactly represented by a recurrent neural network with a linear memory update. I will then discuss how to generalise this linear RNN architecture to 2D lattices, comparing both approaches to standard DMRG calculations.

Zoom link: https://pitp.zoom.us/j/98833163484?pwd=bEZTeTB0c1l1QmkrQXdEc3dBQ0dJZz09

FROM NEURAL DENSITY OPERATORS TO TENSOR NETWORKS



FILIPPO VICENTINI

Computational Quantum Science Lab.

EPFL

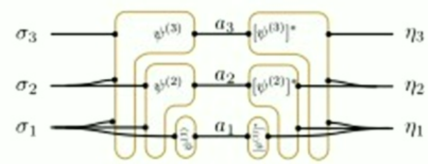
STUDYING FINITE TEMPERATURE SYSTEMS

VARIATIONAL PRINCIPLE FOR STEADY-STATE

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

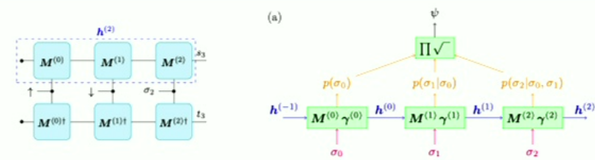
[**F.V.** et Al, PRL (2019)]

DEEP, POSITIVE DEFINITE NQS



[**F.V.** et Al, arXiv:2206.13488 (2022)]

MPS ⇔ RECURRENT NN MAPPING



[Wu, Rossi, **F.V.** et Al, arXiv:2206.12363 (2022)]

OPEN QUANTUM SYSTEMS

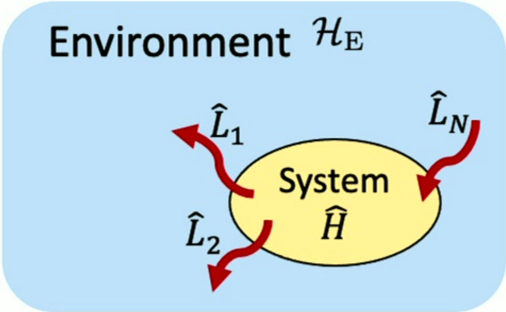
Introduction and Motivation

Machine Learning for Quantum Physics

My Research (Past and Future)

Open Quantum Systems

Study the properties of a system (strongly) coupled to the environment and driven far from equilibrium



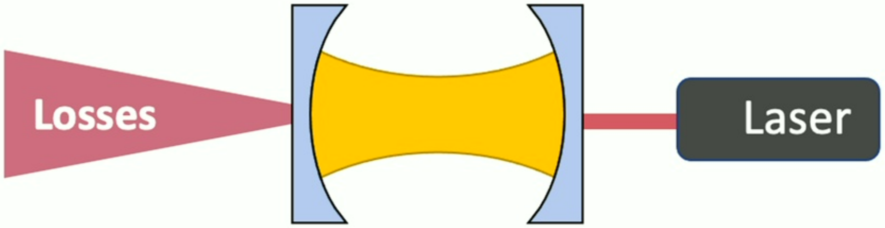
Environments

- Thermal Bath (trivial relaxation towards $e^{-\beta \hat{H}}$)
- Parametric Baths (reservoir engineering)

Pumping

- Drives the system away from the thermal state

Quantum Case



OPEN QUANTUM SYSTEMS

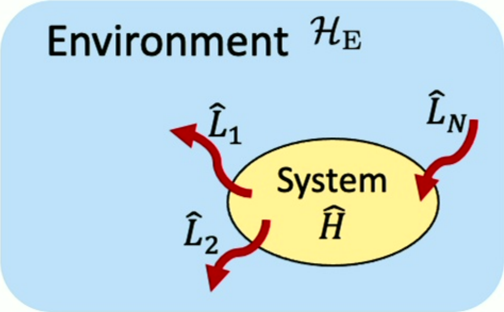
Study the properties of a system (strongly) coupled to the environment and driven far from equilibrium

ENVIRONMENTS

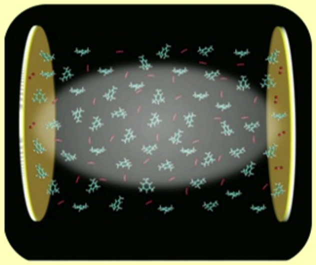
- Thermal Bath (trivial relaxation towards $e^{-\beta\hat{H}}$)
- Parametric Baths (reservoir engineering)

PUMPING

- Drives the system away from the thermal state

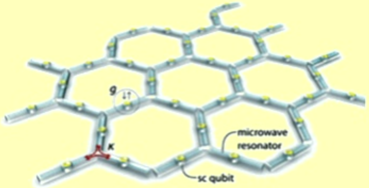


CAVITY QUANTUM CHEMISTRY



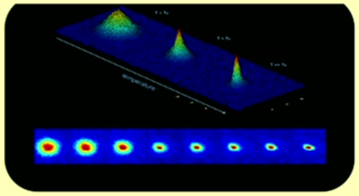
[Flick et Al, Nanophotonics (2018)]
[Rubio et Al, PNAS (2019)]
[Vidal et Al, Science (2021)]

ARRAY OF RESONATORS

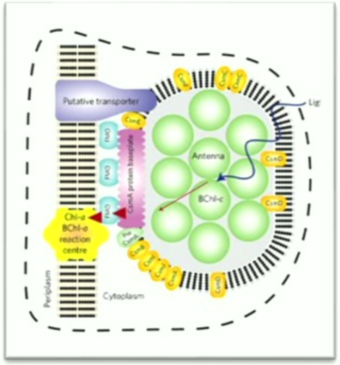


[Koch et Al, PRA 82 (2010)]

ULTRACOLD ATOMIC GASES



Quantum Biology



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

OPEN QUANTUM SYSTEMS

Study the properties of a system (strongly) coupled to the environment and driven far from equilibrium

ENVIRONMENTS

- Thermal Bath (trivial relaxation towards $e^{-\beta\hat{H}}$)
- Parametric Baths (reservoir engineering)

PUMPING

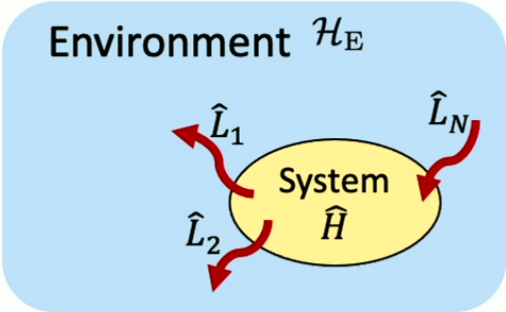
- Drives the system away from the thermal state

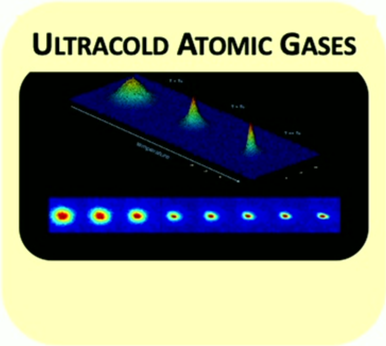
NOVEL PROPERTIES!

- *Dissipative* phase transitions
- Quantum-nonequilibrium critical exponents
- *Dissipative* symmetries

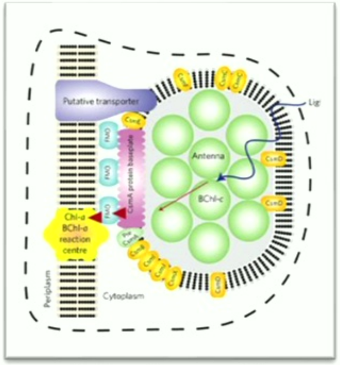
(SOME) FUNDAMENTAL OPEN QUESTIONS:

- Role of Long-range-correlations
- Role of Symmetries
- Transport properties (diffusive vs balistic)
- Differences different frameworks



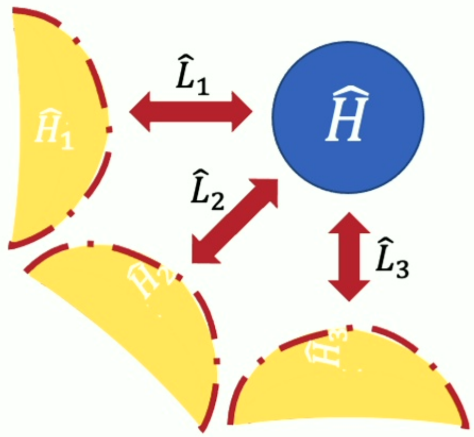


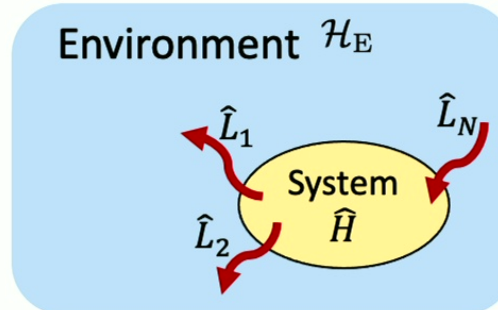
Quantum Biology



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

A RELATED PROBLEM: IMAGINARY TIME EVOLUTION





IMAGINARY-TIME EVOLUTION

$$\frac{d\hat{\rho}}{d\beta} = -\left\{\hat{H}, \hat{\rho}\right\}$$

Assumption:
- Secular Approx.
- Born-Markov Approx.

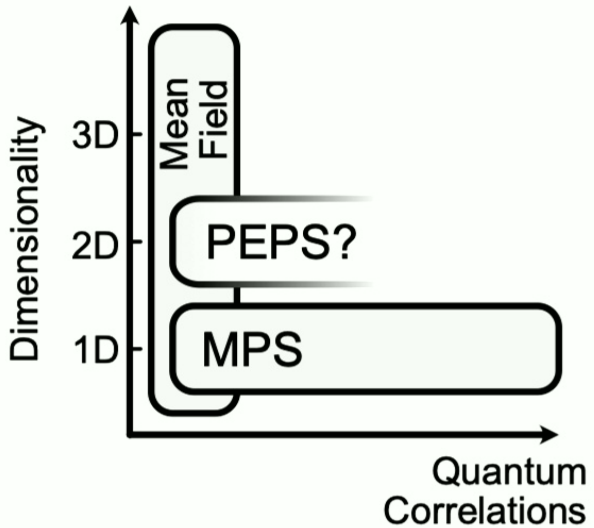
THE LINDBLAD MASTER EQUATION

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

COHERENT EVOLUTION **INCOHERENT EVOLUTION**

(Some) Computational Methods

$$|\psi\rangle = \sum_{\sigma_1,\sigma_2,\ldots,\sigma_N} \psi(\sigma_1,\sigma_2,\ldots,\sigma_N)\,|\sigma_1,\sigma_2,\ldots,\sigma_N\rangle$$



Mean-Field approaches

Mean Field
Cluster-Mean Field [Yamamoto..., PRB, **79** (2020)]
Gutzwiller wf [Krauth et al, PRB **45** (1992)]

Tensor Networks

long intro: [Montangero, Springer (2008)])
short intro: [Biamonte et al, arXiv:1708 (2017)]

DMRG [White et al, PRB, **48** (1993)]
MPS Ansatz [Verstraete et al, QIC **7** (2008)]
PEPS Ansatz [Cirac et al,RMP, **93** (2021)]

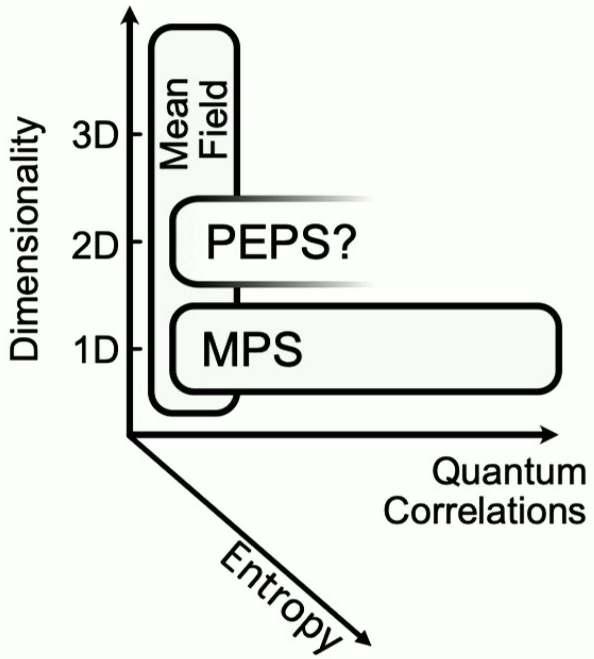
Quantum Monte Carlo

[Foulkes et al, RMP **73**, (2001)]
[Becca, Sorella CUP (2017)]

Green's function MC [Lee et al, CIP **6**, (1992)]
Diffusion MC [Reynolds et al, CIP **4**, (1990)]
Auxiliary-Field [Baeurle et al, JCP **184**, (2003)]
Path Integral [Herman et al, JCP **76**, (1982)]

(SOME) COMPUTATIONAL METHODS

$$\hat{\rho} = \sum_{\sigma_1,\ldots,\sigma_N,\eta_1,\ldots,\eta_N} \rho(\sigma_1,\eta_1,\ldots,\sigma_N,\eta_N)\,|\sigma_1,\ldots,\sigma_N\rangle\langle\eta_1,\ldots,\eta_N|$$



MEAN-FIELD APPROACHES

Mean Field
Cluster-Mean Field [Yamamoto..., PRB, **79** (2020)]
Gutzwiller wf [Krauth et al, PRB **45** (1992)]
Truncated Wigner [Vogel et al, PRA **39** (1989)]

TENSOR NETWORKS

long intro: [Montangero, Springer (2008)])
short intro: [Biamonte et al, arXiv:1708 (2017)]

DMRG [White et al, PRB, **48** (1993)]
MPS Ansatz [Verstraete et al, QIC **7** (2008)]
PEPS Ansatz [Cirac et al,RMP, **93** (2021)]

Positive TN [Werner et al, PRL, **116** (2016)]
Dissipative MPO [Orus et al, NRP, 1 (2019)]

QUANTUM MONTE CARLO

[Foulkes et al, RMP **73**, (2001)]
[Becca, Sorella CUP (2017)]

Green's function MC [Lee et al, CIP **6**, (1992)]
Diffusion MC [Reynolds et al, CIP **4**, (1990)]
Auxiliary-Field [Baeurle et al, JCP **184**, (2003)]
Path Integral [Herman et al, JCP **76**, (1982)]
Liouville-FCI [Nagy et al, PRA **97**, (2018)]

LIOUVILLE SPACE METHODS

Gauge-P repr. [Deuar et al, PRA, **66** (2002)]
Gaussian Trajectories [Verstraelen (2018)]
Correlation Hierarchy [Casteels..., NJP, **18** (2016)]
Corner Renormaliz. [Finazzi et al, PRL **115** (2015)]
Arnoldi-Lindblad [Minganti..., Quantum **6** (2022)]

NQS: 2 INGREDIENTS

VARIATIONAL ANSATZ

$$\hat{\rho} \approx \hat{\rho}_w$$

Lowers Memory complexity

COST FUNCTION

$$\mathcal{C}(w)$$

To update the variational parameters

OPTIMISING THE PARAMETERS

GROUND-STATE OPTIMISATION (VMC)

GROUND STATE

$$\hat{H}\,|\psi_{gs}\rangle = E_{gs}\,|\psi_{gs}\rangle$$

VARIATIONAL PRINCIPLE

$$E(\mathcal{W}) = \left\langle \hat{H} \right\rangle = \frac{\langle \psi(\mathcal{W})|\hat{H}|\psi(\mathcal{W})\rangle}{\langle \psi(\mathcal{W})|\psi(\mathcal{W})\rangle} \geq E_{gs}$$

$$E(\mathcal{W}) = E_{gs} \quad \Rightarrow \quad |\psi(\mathcal{W})\rangle = |\psi_{gs}\rangle$$

Optimising the Parameters

Steady-state optimisation (VMC)

Steady State

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

Variational Principle

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

Ground-state optimisation (VMC)

Ground State

$$\hat{H}\,|\psi_{gs}\rangle = E_{gs}\,|\psi_{gs}\rangle$$

Variational Principle

$$E(\mathcal{W}) = \left\langle \hat{H} \right\rangle = \frac{\langle\psi(\mathcal{W})|\hat{H}|\psi(\mathcal{W})\rangle}{\langle\psi(\mathcal{W})|\psi(\mathcal{W})\rangle} \geq E_{gs}$$

$$E(\mathcal{W}) = E_{gs} \quad \Rightarrow \quad |\psi(\mathcal{W})\rangle = |\psi_{gs}\rangle$$

So we want to determine the

$$\min_{\mathcal{W}}[E(\mathcal{W})]$$

Optimising the Parameters

Steady-State optimisation (VMC)

Steady State

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

Variational Principle

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

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

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

Ground-State optimisation (VMC)

Ground State

$$\hat{H}\,|\psi_{gs}\rangle = E_{gs}\,|\psi_{gs}\rangle$$

Variational Principle

$$E(\mathcal{W}) = \left\langle \hat{H} \right\rangle = \frac{\langle\psi(\mathcal{W})|\hat{H}|\psi(\mathcal{W})\rangle}{\langle\psi(\mathcal{W})|\psi(\mathcal{W})\rangle} \geq E_{gs}$$

$$E(\mathcal{W}) = E_{gs} \quad \Rightarrow \quad |\psi(\mathcal{W})\rangle = |\psi_{gs}\rangle$$

So we want to determine the

$$\min_{\mathcal{W}}[E(\mathcal{W})]$$

Optimising the Parameters

Steady-State optimisation (VMC)

Steady State

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

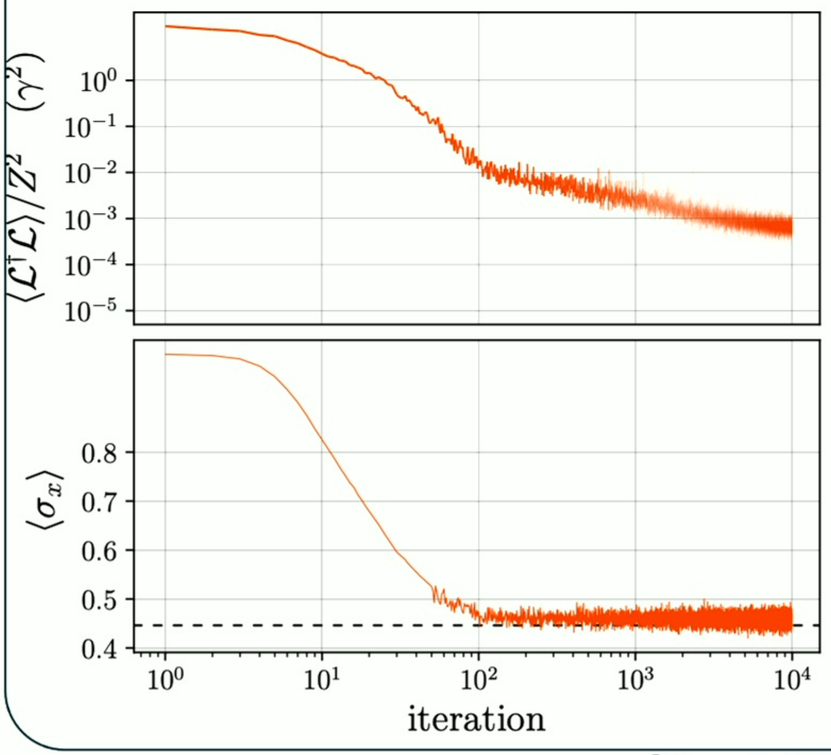
Variational Principle

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

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

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

16 sites dissipative TFIM (V=2, g=1)



[Vicentini PRL 2019]

Optimising the Parameters

Steady-State optimisation (VMC)

Steady State

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

Variational Principle

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

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

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

Dynamics

Dynamical Equation (Akin to Schroeding.)

$$\frac{d\rho(t)}{dt} = \mathcal{L}\rho(t)$$

dTDVP

$$\frac{d\mathbf{v}}{dt} = S^{-1}F$$

$$S_{i,j} = \mathrm{Tr}\left[(\partial_{v_i}\rho_{\mathbf{v}}^{\dagger})\partial_{v_j}\rho_{\mathbf{v}}\right]$$

$$F_i = \mathrm{Tr}[(\partial_{v_i}\log\hat{\rho}_{\mathbf{v}})\mathcal{L}\hat{\rho}_{\mathbf{v}}]$$

NEURAL QUANTUM STATES

Pure states

$$|\psi\rangle = \sum_{\sigma} \exp[\log \psi(\sigma)]\, |\sigma\rangle$$

Encoded in a neural network

Nice property: whatever the output of logpsi, this is always a valid (unnormalized) state.

But Mixed states?

$$\hat{\rho} = \sum_{\sigma,\eta} \exp[\log \rho(\sigma,\eta)]\, |\sigma\rangle \langle\eta|$$

Matricial description

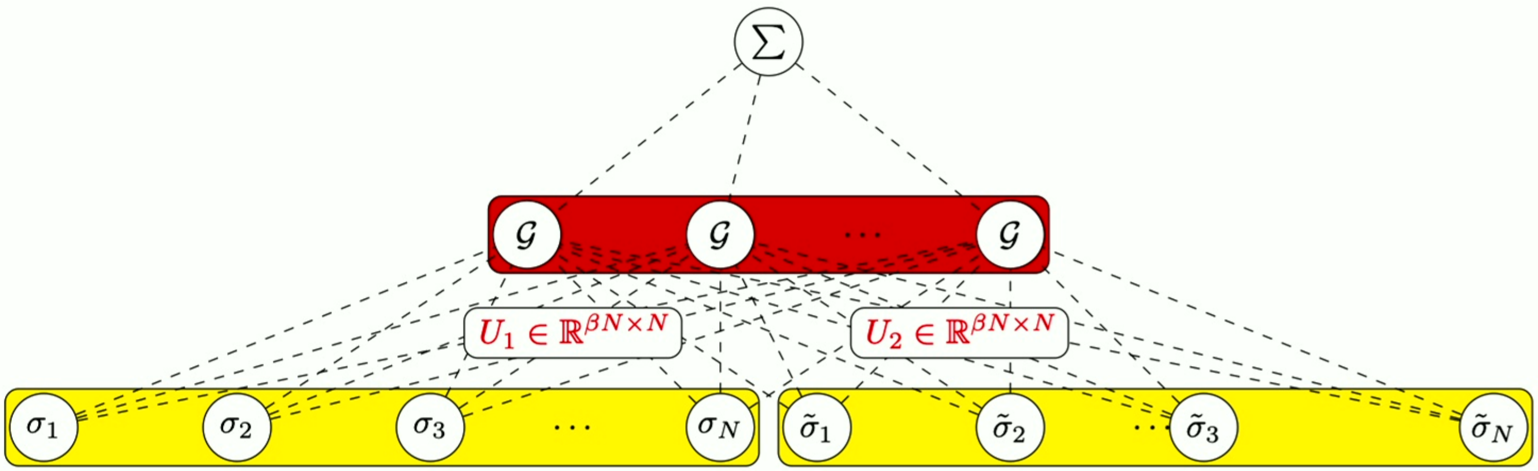
$$\hat{\rho} = \sum_{a} p(a)\hat{M}_a$$

POVM Description

NEURAL NETWORK DENSITY MATRIX

$$\hat{\rho} = \sum_{\sigma,\eta} \exp[\log \rho(\sigma, \eta)] \, |\sigma\rangle \langle \eta|$$

$$\log \rho(\sigma, \eta) = \sum_{j} \mathcal{G}(U_{1,i}^{[j]}\sigma_i + U_{2,i}^{[j]}\eta_i + d^{[j]})$$

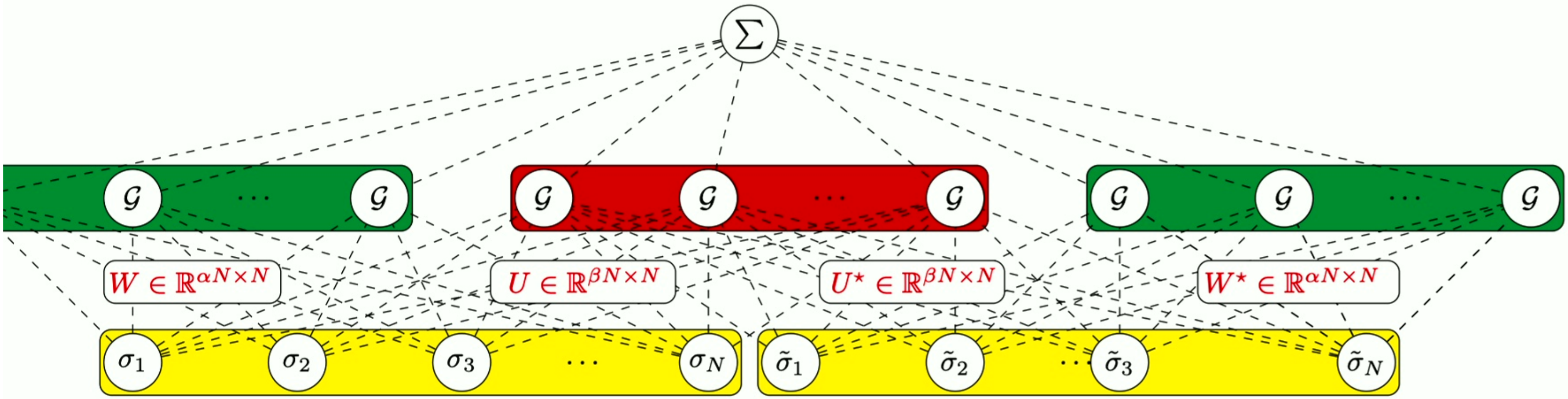


POSITIVE DEFINITE: PURIFICATION

Can we make the ansatz Positive-Semidefinite?

$$\rho(\boldsymbol{\sigma}, \boldsymbol{\eta}) = \sum_{\boldsymbol{a}} \psi(\boldsymbol{\sigma}, \mathbf{a}) \psi^{\star}(\boldsymbol{\eta}, \mathbf{a})$$

$$\psi(\boldsymbol{\sigma}, \boldsymbol{a}) = \Gamma_{\psi}(\boldsymbol{\sigma}) \exp\left[-\mathbf{a}^T (U\boldsymbol{\sigma} + \mathbf{d})\right]$$



[Torlai, PRL 120, 240503 (2018)]

Positive Definite: DeepNDM

Can we make the ansatz Positive-Semidefinite?

$$\rho(\boldsymbol{\sigma}, \boldsymbol{\eta}) = \sum_{\boldsymbol{a}} \psi(\boldsymbol{\sigma}, \mathbf{a}) \psi^\star(\boldsymbol{\eta}, \mathbf{a})$$

$$\psi(\boldsymbol{\sigma}, \boldsymbol{a}) = \Gamma_\psi(\boldsymbol{\sigma}) \exp\left[-\mathbf{a}^T \left(U\boldsymbol{\sigma} + \mathbf{d}\right)\right]$$

$$\psi(\boldsymbol{\sigma}, \boldsymbol{a}) = \Gamma_\psi(\boldsymbol{\sigma}) \exp\left[-\mathbf{a}^T \left(U\boldsymbol{\phi}(\boldsymbol{\sigma}) + \mathbf{d}\right)\right]$$

$$\rho(\boldsymbol{\sigma}, \boldsymbol{\eta}) = \prod_i^M \mathcal{G}\left[\mathbf{U}^{[i],T}\boldsymbol{\phi}(\boldsymbol{\sigma}) + \mathbf{U}^{[i],\dagger}\boldsymbol{\phi}(\boldsymbol{\eta}) + d^{[i]}\right]$$

[**F.V.**, Rossi, Carleo, arXiv:2206.13488]

POSITIVE DEFINITE: GRAM-HADAMARD DENSITY MATRIX

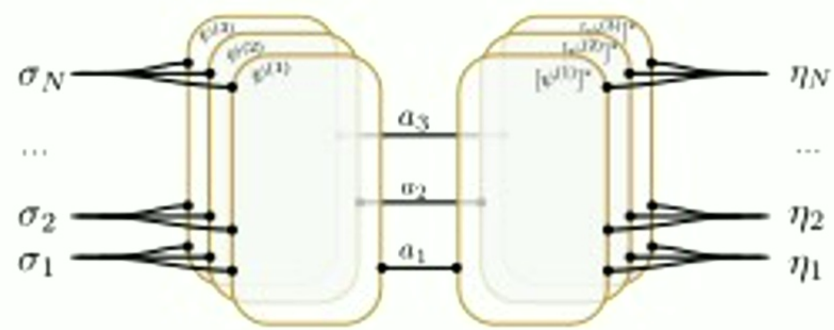
This corresponds to a more general statement:

$$\rho(\boldsymbol{\sigma}, \boldsymbol{\eta}) = \prod_{i}^{M} \pi_i(\boldsymbol{\sigma}, \boldsymbol{\eta}) \qquad \text{Rank}\,[\hat{\rho}] = \prod_{i}^{M} \text{Rank}\,[\pi_i]$$

If $\hat{\pi}_i$ is positive-definite, then the hadamard product of several PD matrices is positive definite

$$\pi_i(\boldsymbol{\sigma}, \boldsymbol{\eta}) = \sum_{a_i=1}^{K} \psi_{a_i}^{(i)}(\boldsymbol{\sigma})[\psi_{a_i}^{(i)}(\boldsymbol{\eta})]^\star$$

The $\hat{\pi}_i$ defined here is PD because it's a Gram Matrix



[**F.V.**, Rossi, Carleo, arXiv:2206.13488]

POSITIVE DEFINITE: GRAM-HADAMARD DENSITY MATRIX

I want to perform Autoregressive Sampling of the diagonal

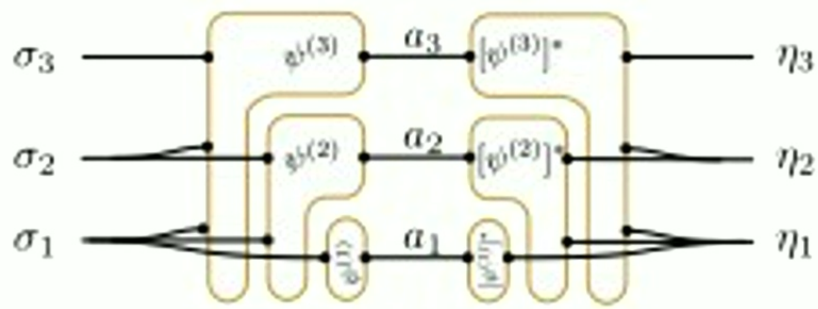
$$\rho(\boldsymbol{\sigma},\boldsymbol{\sigma}) = p_1(\sigma_1)p_2(\sigma_2|\sigma_1)p_3(\sigma_3|\sigma_2,\sigma_1)\dots p_N(\sigma_N|\sigma_{<N})$$

I then consider ϕ_i in autoregressive order:

$$\psi_{a_i}^{(i)}(\sigma_i|\boldsymbol{\sigma}_{<i}) = \frac{\tilde{\psi}_{a_i}^{(i)}(\sigma_i|\boldsymbol{\sigma}_{<i})}{\sum_{\sigma_i=\{\pm1\}}\tilde{\psi}_{a_i}^{(i)}(\sigma_i|\boldsymbol{\sigma}_{<i})}$$

Therefore:

$$p_i(\sigma_i|\boldsymbol{\sigma}_{<i}) = \pi_i(\boldsymbol{\sigma}_{\leq i},\boldsymbol{\sigma}_{\leq i}) = \frac{\sum_{a_i}^{K}\left|\tilde{\psi}_{a_i}^{(i)}(\boldsymbol{\sigma}_{\leq i})\right|^2}{\sum_{a_i,\sigma_i=\{\pm1\}}\left|\tilde{\psi}_{a_i}^{(i)}(\boldsymbol{\sigma}_{\leq i})\right|^2}$$



[**F.V.**, Rossi, Carleo, arXiv:2206.13488]

IMPORTANCE SAMPLING

I can only sample efficiently the diagonal

$$\rho(\boldsymbol{\sigma},\boldsymbol{\sigma}) = p_1(\sigma_1)p_2(\sigma_2|\sigma_1)p_3(\sigma_3|\sigma_2,\sigma_1)\dots p_N(\sigma_N|\sigma_{<N})$$

Use Importance Sampling

$$\mathop{\mathbb{E}}_{\rho^2}[f(\sigma,\eta)] := \frac{\sum_{\sigma,\eta} |\langle\sigma|\hat{\rho}|\eta\rangle|^2 f(\sigma,\eta)}{\sum_{\sigma,\eta} |\langle\sigma|\hat{\rho}|\eta\rangle|^2}$$

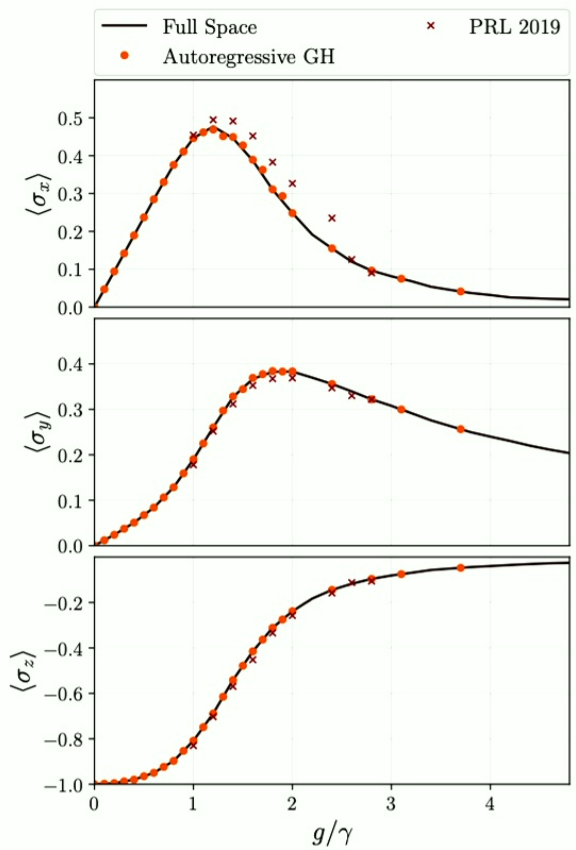
$$\mathop{\mathbb{E}}_{\rho^2}[f(\sigma,\eta)] \propto \mathop{\mathbb{E}}_{\sigma,\eta\sim p_\alpha(\sigma,\eta)}\left[\frac{|\langle\sigma|\hat{\rho}|\eta\rangle|^2}{p_\alpha(\sigma,\eta)} f(\sigma,\eta)\right].$$

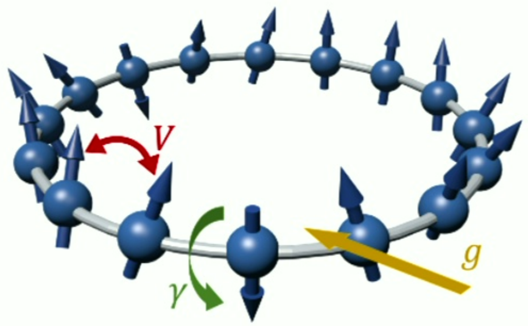
With a convex combination of autoregressive distributions

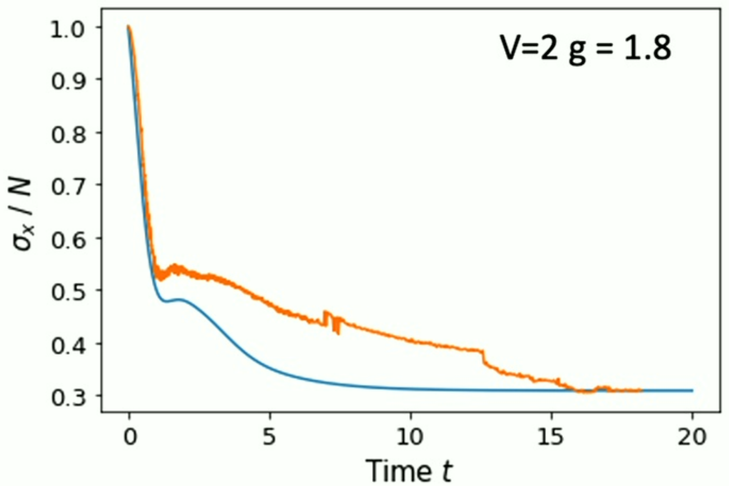
[F Vicentini et Al, in prep]

Benchmark: D-D Transverse Field Ising

A full scan in the transverse field gives:







Neural Density Matrices

- Gram-Hadamard constructions are a generalisation of the Purification of a pure state.
- Can efficiently encode completely pure and mixed states
- Autoregressive order of the diagonal probability can be defined
- Improves on past results

- (Mixed) Quantum State reconstruction?
- Imaginary-Time evolution

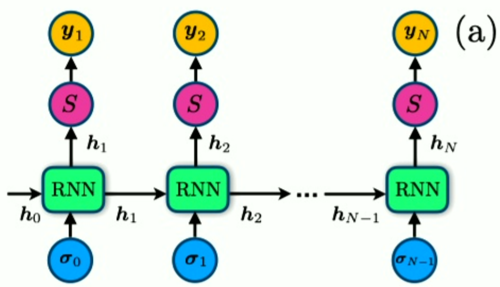
QUESTIONS?

MPS-RNN & Tensor-RNN

Positive Definite: Gram-Hadamard Density Matrix

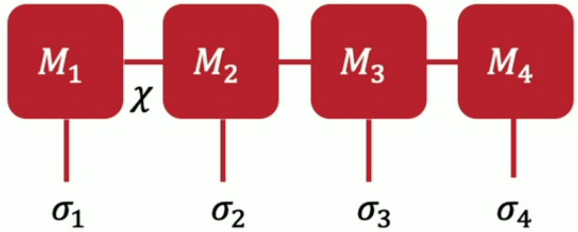
RNN– Quantum State

$$\psi(\boldsymbol{\sigma}) = \left(\prod_i \sqrt{p(\sigma_i|\boldsymbol{\sigma}_{<i})}\right) \mathrm{e}^{\mathrm{i}\phi(\boldsymbol{\sigma})},$$



MPS– Quantum State

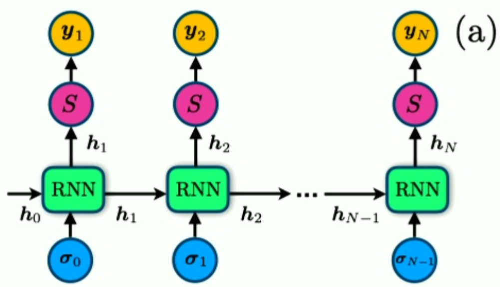
$$\psi(\boldsymbol{\sigma}) = \sum_{s_0,\dots,s_V=0}^{\chi-1} \prod_{i=0}^{V-1} M^{(i)}_{\sigma_i;s_{i+1},s_i},$$



POSITIVE DEFINITE: GRAM-HADAMARD DENSITY MATRIX

RNN– Quantum State

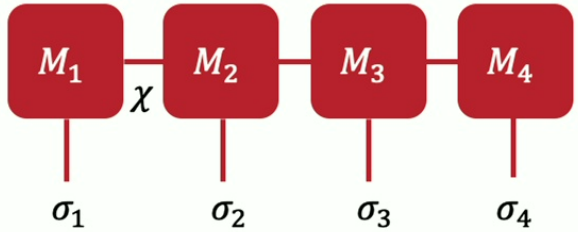
$$\psi(\boldsymbol{\sigma}) = \left(\prod_i \sqrt{p(\sigma_i|\boldsymbol{\sigma}_{<i})}\right) e^{i\phi(\boldsymbol{\sigma})},$$

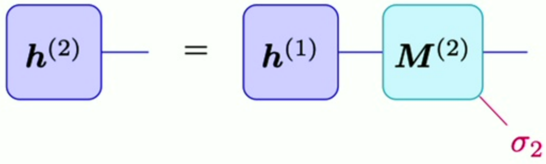


$$\mathbf{h}^{(i)} = f^{(i)}_{RNN}(\sigma_i, \mathbf{h}^{(i-1)}) = \mathbf{M}^{(i)}_{\sigma_i}\mathbf{h}^{(i-1)}$$

MPS– Quantum State

$$\psi(\boldsymbol{\sigma}) = \sum_{s_0,\ldots,s_V=0}^{\chi-1} \prod_{i=0}^{V-1} M^{(i)}_{\sigma_i; s_{i+1}, s_i},$$

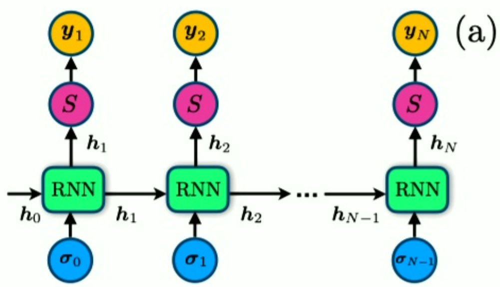




Positive Definite: Gram-Hadamard Density Matrix

RNN– Quantum State

$$\psi(\boldsymbol{\sigma}) = \left(\prod_i \sqrt{p(\sigma_i|\boldsymbol{\sigma}_{<i})}\right) \mathrm{e}^{\mathrm{i}\phi(\boldsymbol{\sigma})},$$

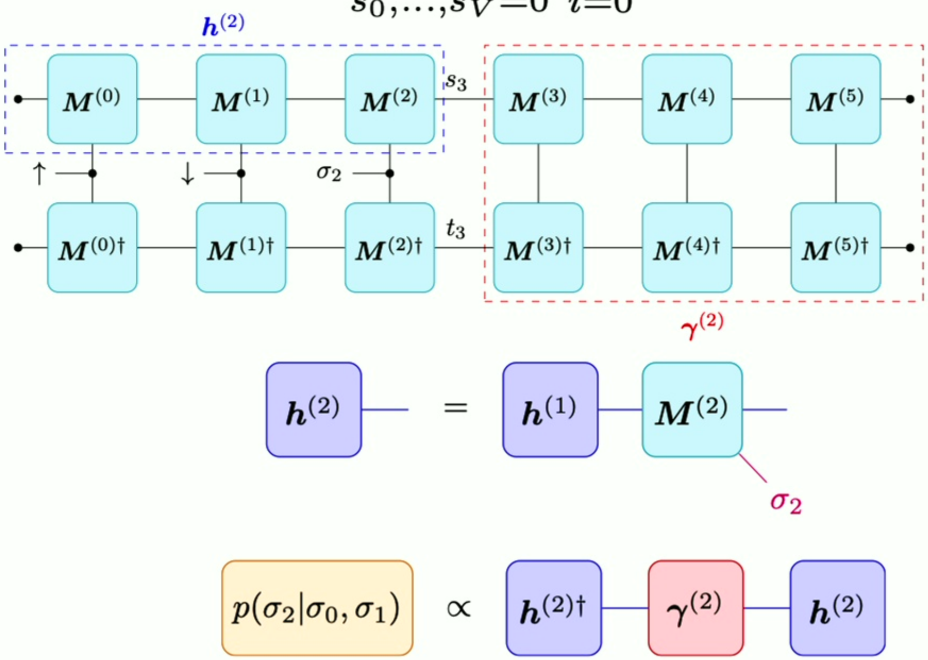


$$\mathbf{h}^{(i)} = f^{(i)}_{RNN}(\sigma_i, \mathbf{h}^{(i-1)}) = \mathbf{M}^{(i)}_{\sigma_i}\mathbf{h}^{(i-1)}$$

$$p(\sigma_i|\boldsymbol{\sigma}_{<i}) \propto [\boldsymbol{h}^{(i)}]^\dagger \boldsymbol{\gamma}^{(i)} \boldsymbol{h}^{(i)},$$

MPS– Quantum State

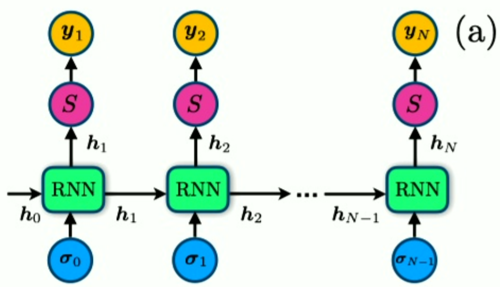
$$\psi(\boldsymbol{\sigma}) = \sum_{s_0,\ldots,s_V=0}^{\chi-1} \prod_{i=0}^{V-1} M^{(i)}_{\sigma_i;s_{i+1},s_i},$$



Positive Definite: Gram-Hadamard Density Matrix

RNN– Quantum State

$$\psi(\boldsymbol{\sigma}) = \left(\prod_i \sqrt{p(\sigma_i|\boldsymbol{\sigma}_{<i})}\right) \mathrm{e}^{\mathrm{i}\phi(\boldsymbol{\sigma})},$$



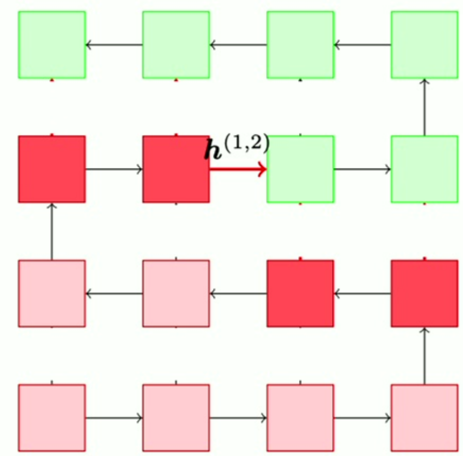
$$\mathbf{h}^{(i)} = f^{(i)}_{RNN}(\sigma_i, \mathbf{h}^{(i-1)}) = \mathbf{M}^{(i)}_{\sigma_i}\mathbf{h}^{(i-1)}$$

$$p(\sigma_i|\boldsymbol{\sigma}_{<i}) \propto [\boldsymbol{h}^{(i)}]^\dagger \boldsymbol{\gamma}^{(i)} \boldsymbol{h}^{(i)},$$

MPS Variational Parameters

$$M^{(i)}_{\sigma_i} \qquad \gamma^{(i)}$$

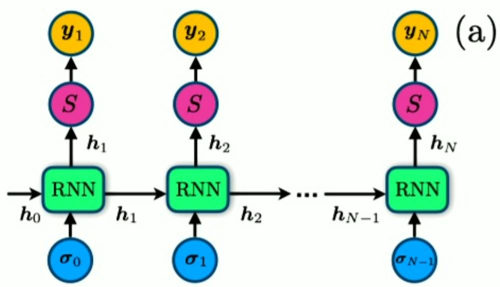
1D MPS-RNN Contraction order



POSITIVE DEFINITE: GRAM-HADAMARD DENSITY MATRIX

RNN– Quantum State

$$\psi(\boldsymbol{\sigma}) = \left(\prod_i \sqrt{p(\sigma_i|\boldsymbol{\sigma}_{<i})}\right) \mathrm{e}^{\mathrm{i}\phi(\boldsymbol{\sigma})},$$



$$\mathbf{h}^{(x,y)} = \mathbf{M}^{(x,y)}_{\mathrm{x};\sigma_{x,y}} \mathbf{h}^{(x\pm1,y)} + \mathbf{M}^{(x,y)}_{\mathrm{y};\sigma_{x,y}} \mathbf{h}^{(x,y-1)} + \mathbf{v}^{(x,y)}_{\sigma_{x,y}}$$

$$p(\sigma_i|\boldsymbol{\sigma}_{<i}) \propto [\boldsymbol{h}^{(i)}]^\dagger \boldsymbol{\gamma}^{(i)} \boldsymbol{h}^{(i)},$$

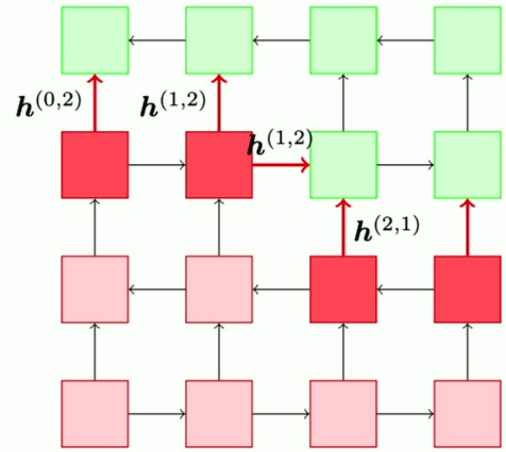
MPS Variational Parameters

$$M^{(i)}_{\sigma_i} \qquad \gamma^{(i)}$$

1D MPS-RNN Variational Parameters

$$\mathbf{v}^{(i)}$$

2D MPS-RNN Contraction order



Ansatz Hierarchy

Matrix Product States (RNN-Style) $M_{\sigma_i}^{(i)}$ $\gamma^{(i)}$

$$\mathbf{h}^{(i)} = \mathbf{M}_{\sigma_i}^{(i)} \mathbf{h}^{(i-1)}$$

1D MPS-RNN $M_{\sigma_i}^{(i)}$ $\gamma^{(i)}$ $v^{(i)}$

$$\mathbf{h}^{(i)} = \mathbf{M}_{\sigma_i}^{(i)} \mathbf{h}^{(i-1)} + \mathbf{v}^{(i)}$$

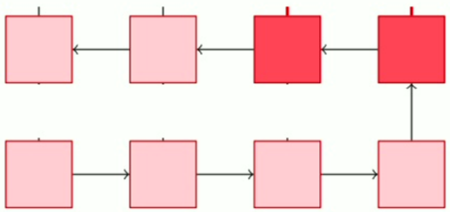
2D MPS-RNN

$$\mathbf{h}^{(x,y)} = \mathbf{M}_{\mathrm{x};\sigma_{x,y}}^{(x,y)} \mathbf{h}^{(x\pm1,y)} + \mathbf{M}_{\mathrm{y};\sigma_{x,y}}^{(x,y)} \mathbf{h}^{(x,y-1)} + \mathbf{v}_{\sigma_{x,y}}^{(x,y)}$$

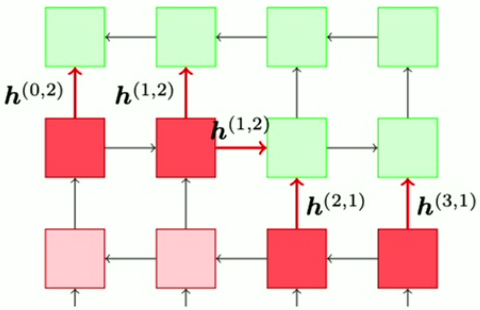
Tensor-RNN

$$\mathbf{h}^{(x,y)} = \mathbf{M}_{\mathrm{x};\sigma_{x,y}}^{(x,y)} \mathbf{h}^{(x\pm1,y)} + \mathbf{M}_{\mathrm{y};\sigma_{x,y}}^{(x,y)} \mathbf{h}^{(x,y-1)} + \mathbf{v}_{\sigma_{x,y}}^{(x,y)} + \mathbf{T}_{\sigma_{x,y};t,u}^{(x,y)} h_t^{(x\pm1,y)} h_u^{(x,y-1)}$$

MPS / 1D MPS-RNN

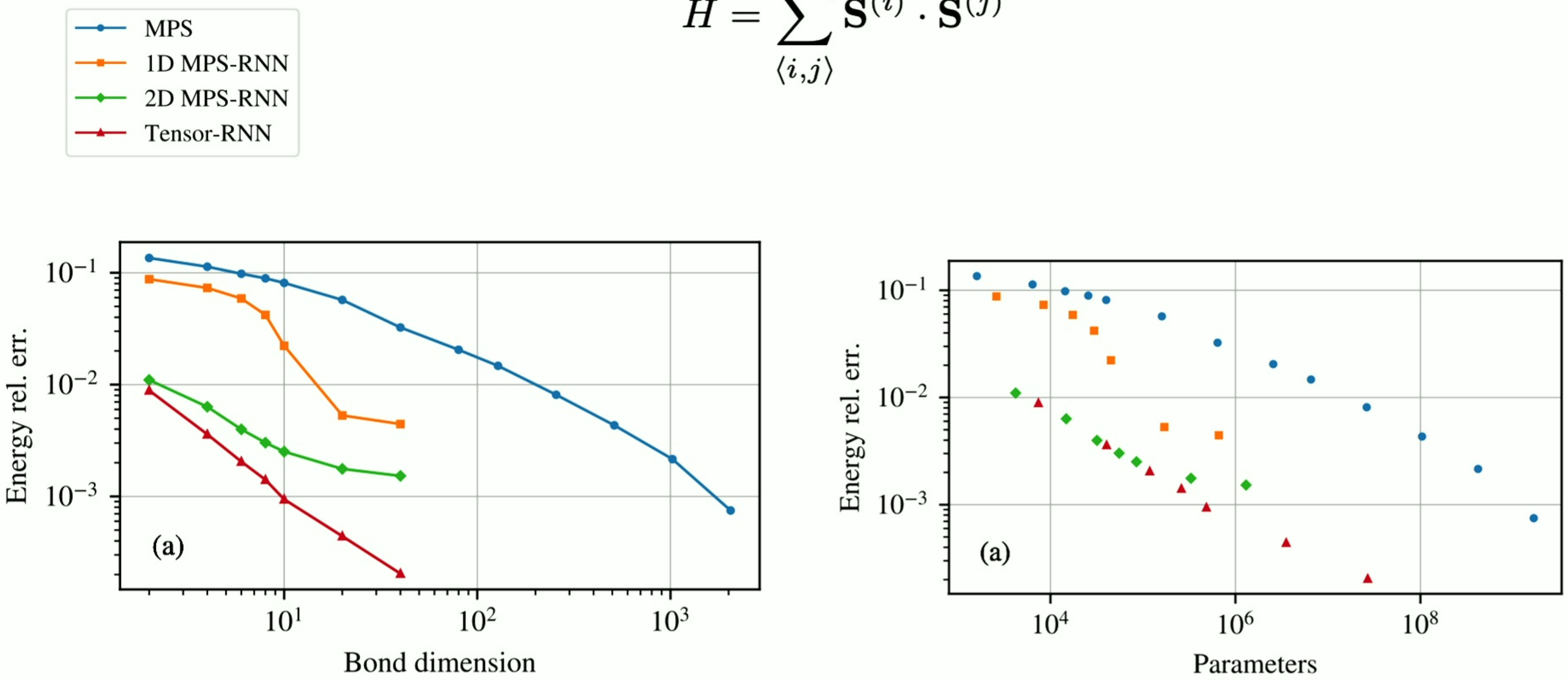


Tensor- / 2D MPS-RNN



Results: AF Heisenberg Model

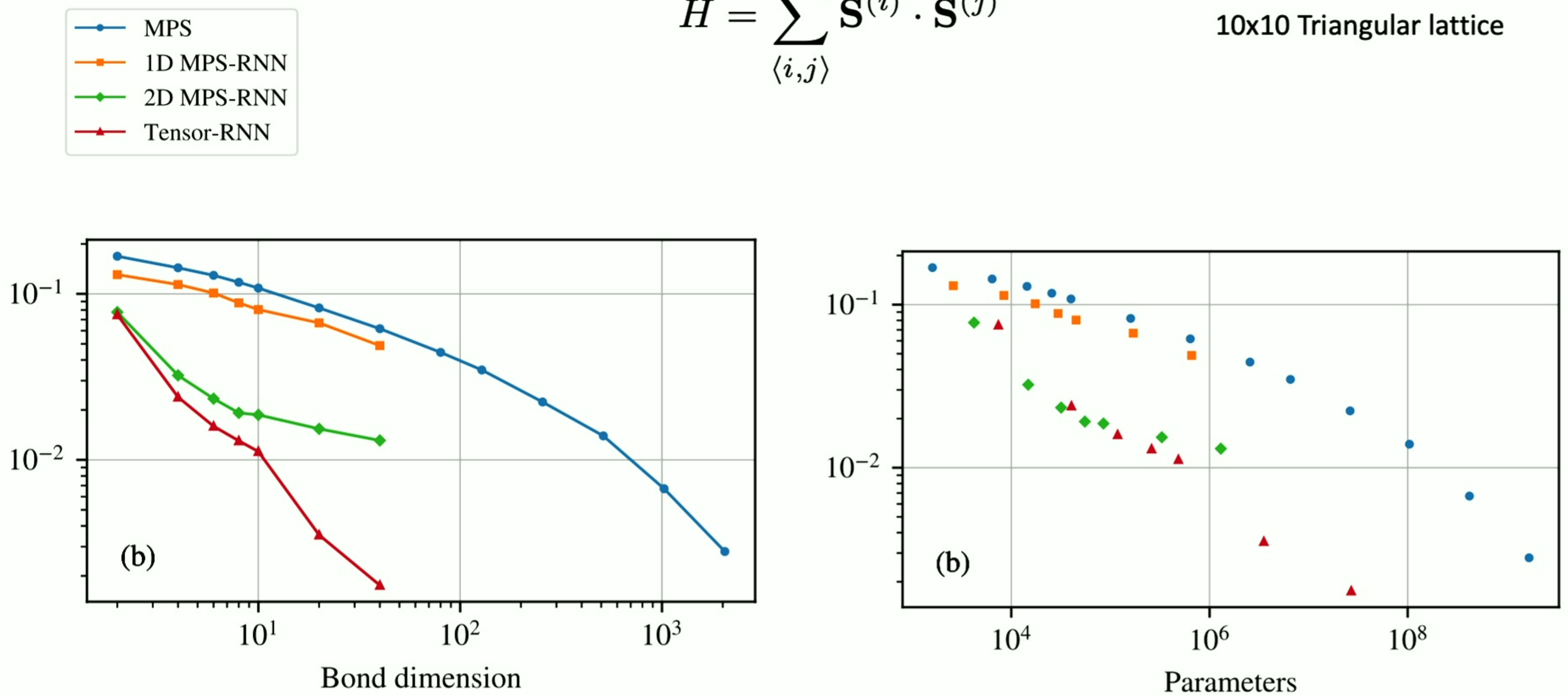
$$\hat{H} = \sum_{\langle i,j \rangle} \mathbf{S}^{(i)} \cdot \mathbf{S}^{(j)}$$



RESULTS: AF HEISENBERG MODEL, TRIANGULAR LATTICE

$$\hat{H} = \sum_{\langle i,j \rangle} \mathbf{S}^{(i)} \cdot \mathbf{S}^{(j)}$$

10x10 Triangular lattice



ANSATZ HIERARCHY

Matrix Product States (RNN-Style) $M_{\sigma_i}^{(i)}$ $\gamma^{(i)}$

$$\mathbf{h}^{(i)} = \mathbf{M}_{\sigma_i}^{(i)} \mathbf{h}^{(i-1)}$$

1D MPS-RNN $M_{\sigma_i}^{(i)}$ $\gamma^{(i)}$ $v^{(i)}$

$$\mathbf{h}^{(i)} = \mathbf{M}_{\sigma_i}^{(i)} \mathbf{h}^{(i-1)} + \mathbf{v}^{(i)}$$

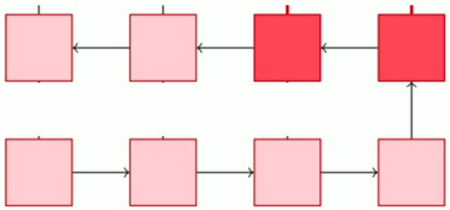
2D MPS-RNN

$$\mathbf{h}^{(x,y)} = \mathbf{M}_{\mathrm{x};\sigma_{x,y}}^{(x,y)} \mathbf{h}^{(x\pm1,y)} + \mathbf{M}_{\mathrm{y};\sigma_{x,y}}^{(x,y)} \mathbf{h}^{(x,y-1)} + \mathbf{v}_{\sigma_{x,y}}^{(x,y)}$$

Tensor-RNN

$$\mathbf{h}^{(x,y)} = \mathbf{M}_{\mathrm{x};\sigma_{x,y}}^{(x,y)} \mathbf{h}^{(x\pm1,y)} + \mathbf{M}_{\mathrm{y};\sigma_{x,y}}^{(x,y)} \mathbf{h}^{(x,y-1)} + \mathbf{v}_{\sigma_{x,y}}^{(x,y)} + \mathbf{T}_{\sigma_{x,y};t,u}^{(x,y)} h_t^{(x\pm1,y)} h_u^{(x,y-1)}$$

MPS / 1D MPS-RNN



Tensor- / 2D MPS-RNN