Violating Bell's inequality with Langevin dynamics in a deep belief network

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Cold Quantum Coffee

20.11.2018

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Center for Quantum Dynamics

CLUSTER OF EXCELLENCE STRUCTURES

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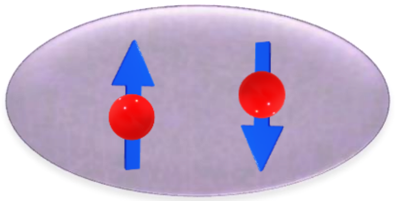
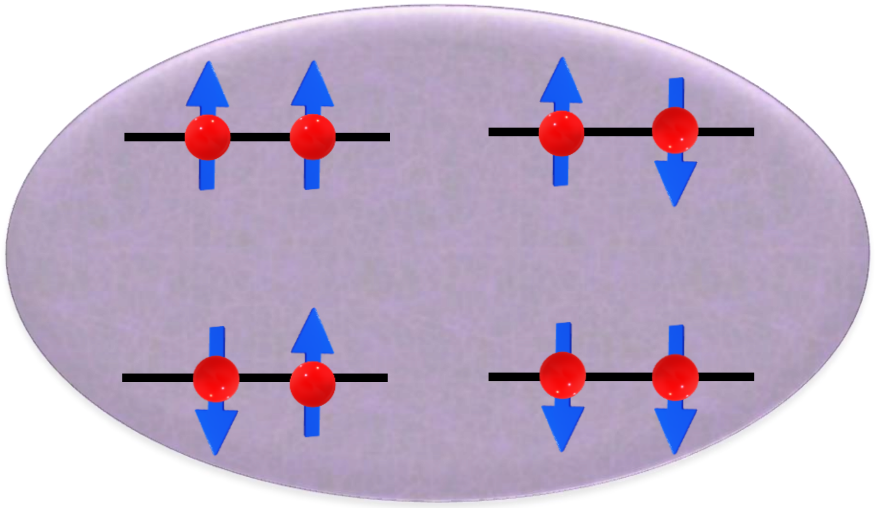
Spin-½ Systems

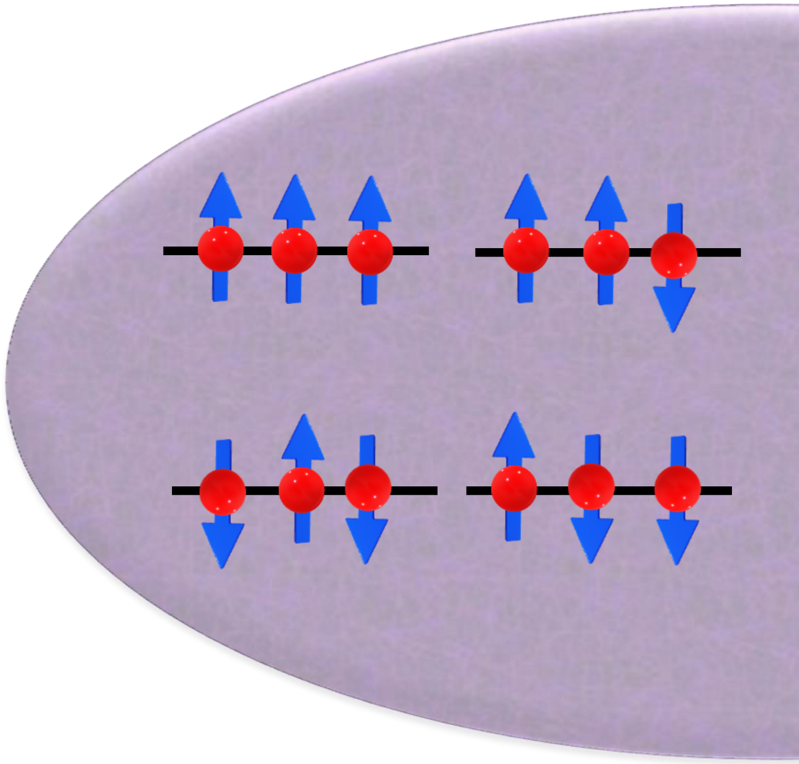
One spin:
two configurations



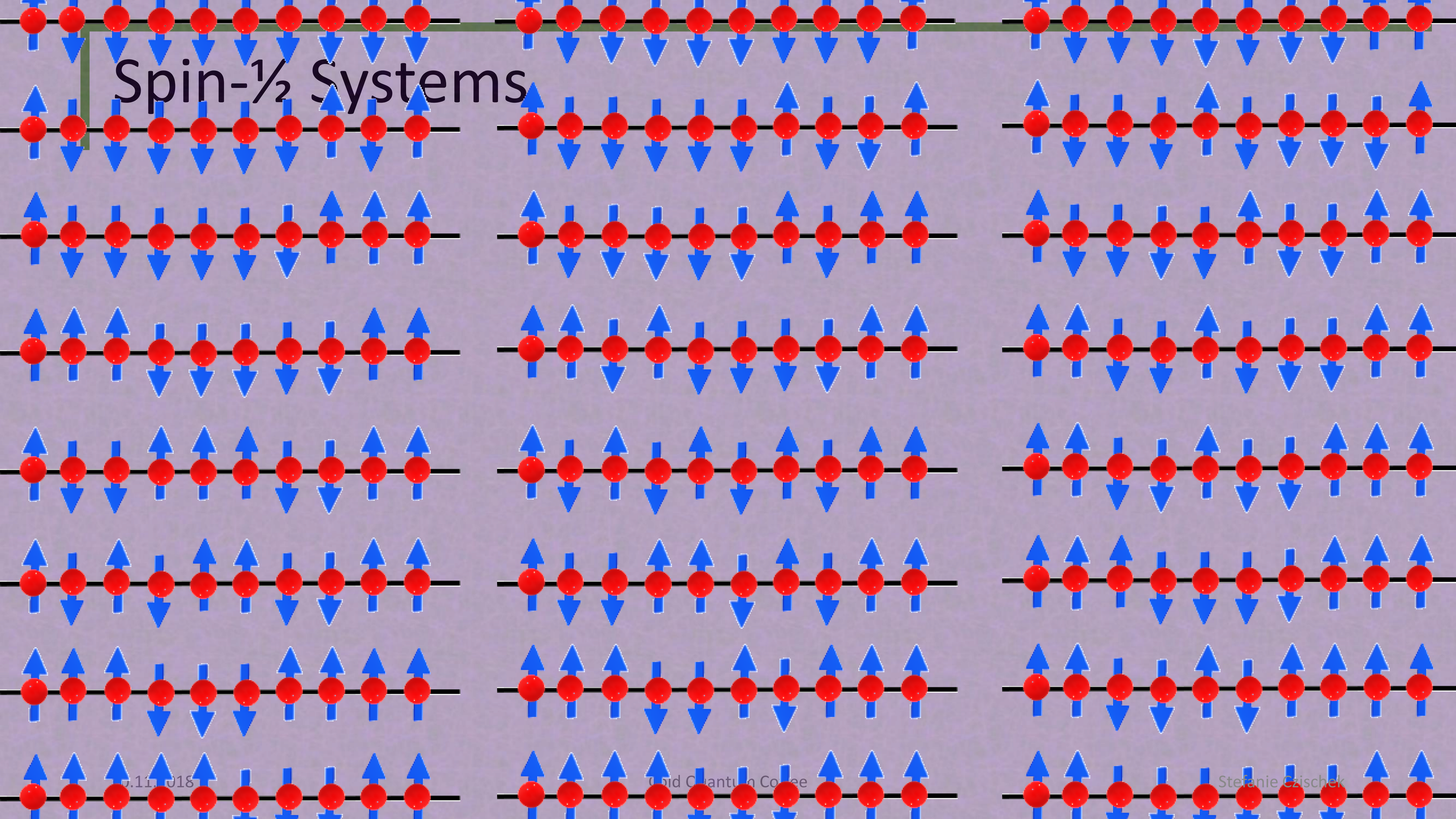
Two spins:
four configurations



Three spins:
eight configurations



Spin-½ Systems



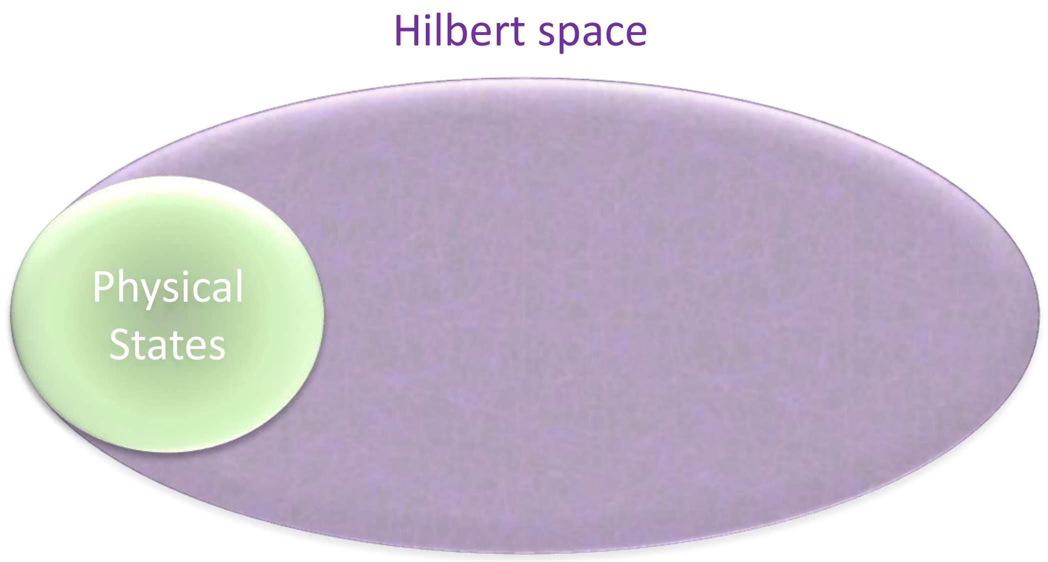
Spin-½ Systems

- Wave function as weighted sum over all product states

$$|\Psi\rangle = \sum_{i_1 \dots i_N} c_{i_1 \dots i_N} |i_1 \dots i_N\rangle$$

- Look for functional
  $\{0,1\}^N \rightarrow \mathbb{C} \qquad (i_1 \dots i_N) \rightarrow c_{i_1 \dots i_N} = f(i_1 \dots i_N; W)$

Analogy to Machine Learning!



Machine Learning

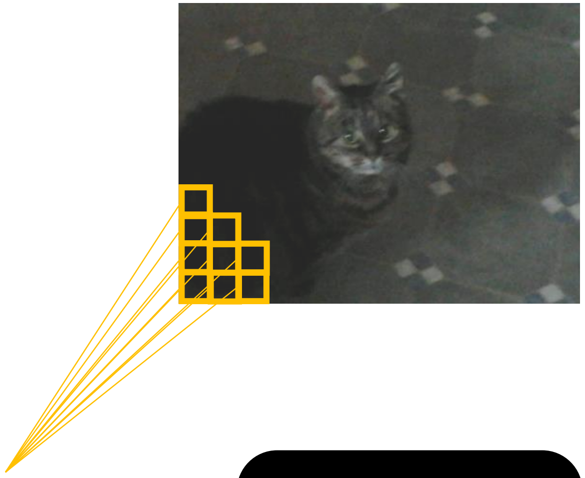
Netflix Prize

- Predict user ratings for films based on previous ratings

Films rated by user → Machine Learning System → Rating for a given film

Pattern Recognition

- Is there a cat in the picture?

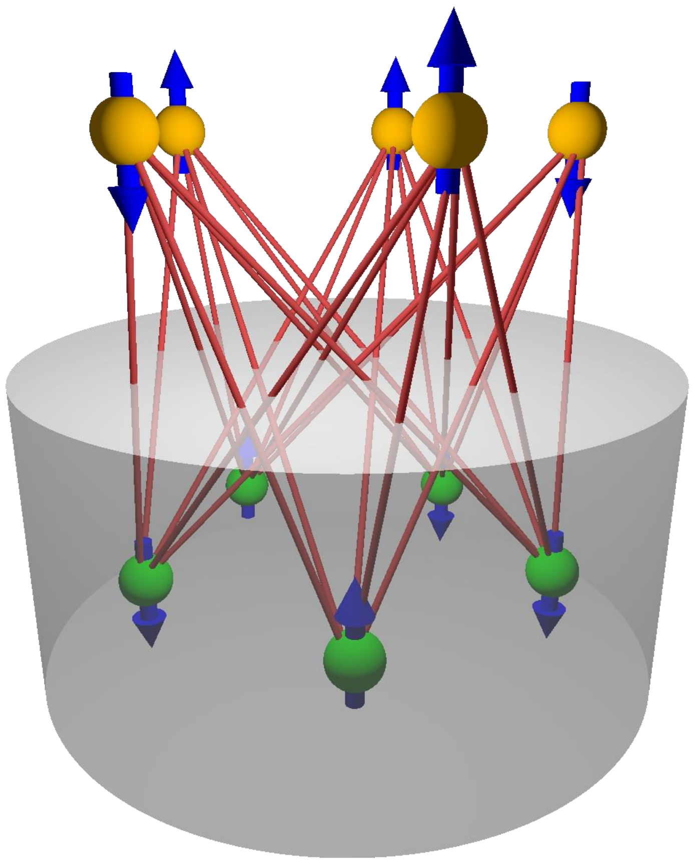


Color value for each pixel → Machine Learning System → Cat or not

Quantum Dynamics and Machine Learning

[Carleo and Troyer, Science 2017]

- Represent Spin-½ system using artificial neural networks
- Use unsupervised learning to find ground states and calculate dynamics
- Where is the simulation method efficient?
- Where does it struggle?

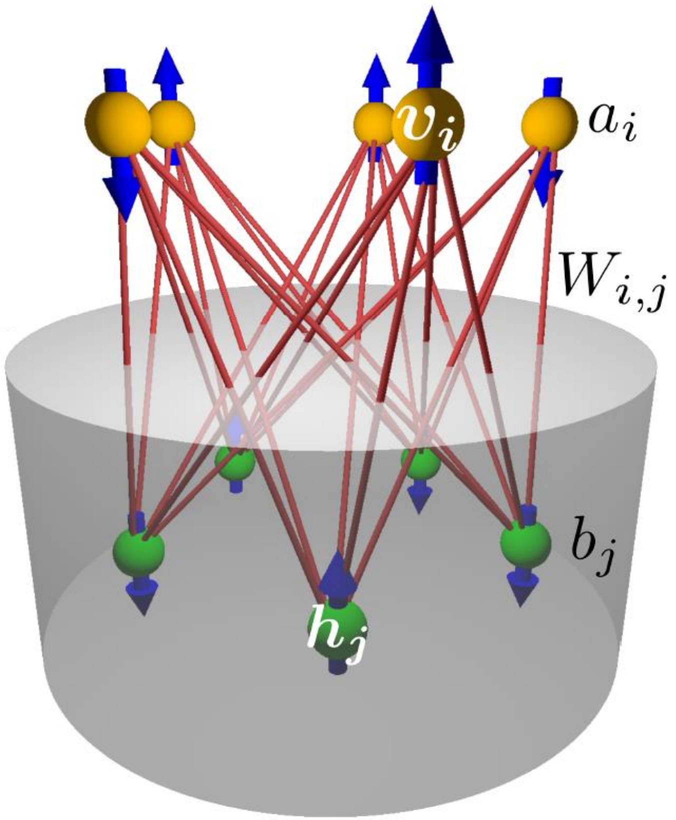


Neural-network quantum states

[Carleo and Troyer, Science 2017]

Restricted Boltzmann machine:

- N visible variables v_z^i
- $M = \alpha N$ hidden variables h_j
- Biases a_i, b_j and weights $W_{i,j}$ as variational parameters



$v_i^z, h_j \epsilon \{-1,1\}$

$$|\Psi\rangle = \sum_{i_1 \dots i_N} c_{i_1 \dots i_N} |i_1 \dots i_N\rangle = \sum_{\boldsymbol{v}^z} c_{\boldsymbol{v}^z} |\boldsymbol{v}^z\rangle$$

$$c_{\boldsymbol{v}^z} = \sum_{\{\boldsymbol{h}\}} e^{-E[\boldsymbol{v}^z, \boldsymbol{h}]}$$

$$E[\boldsymbol{v}^z, \boldsymbol{h}] = -\sum_{i,j} v_i^z W_{i,j} h_j - \sum_i a_i v_i^z - \sum_j b_j h_j$$

$$c_{\boldsymbol{v}^z} = e^{\sum_i a_i v_i^z} \prod_j 2\cosh\left(b_j + \sum_i v_i^z W_{i,j}\right)$$

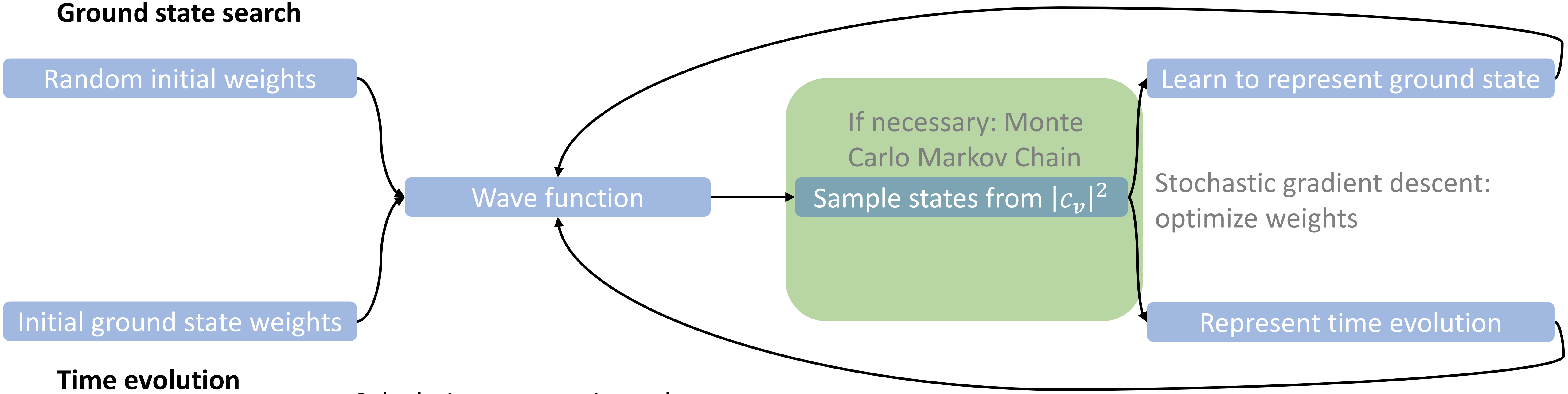
Neural-network quantum states

[Carleo and Troyer, Science 2017]

$$W_k(p+1) = W_k(p) - \gamma \frac{\partial E}{\partial W_k}$$

Imaginary time evolution

Ground state search



Time evolution

Calculating expectation values:

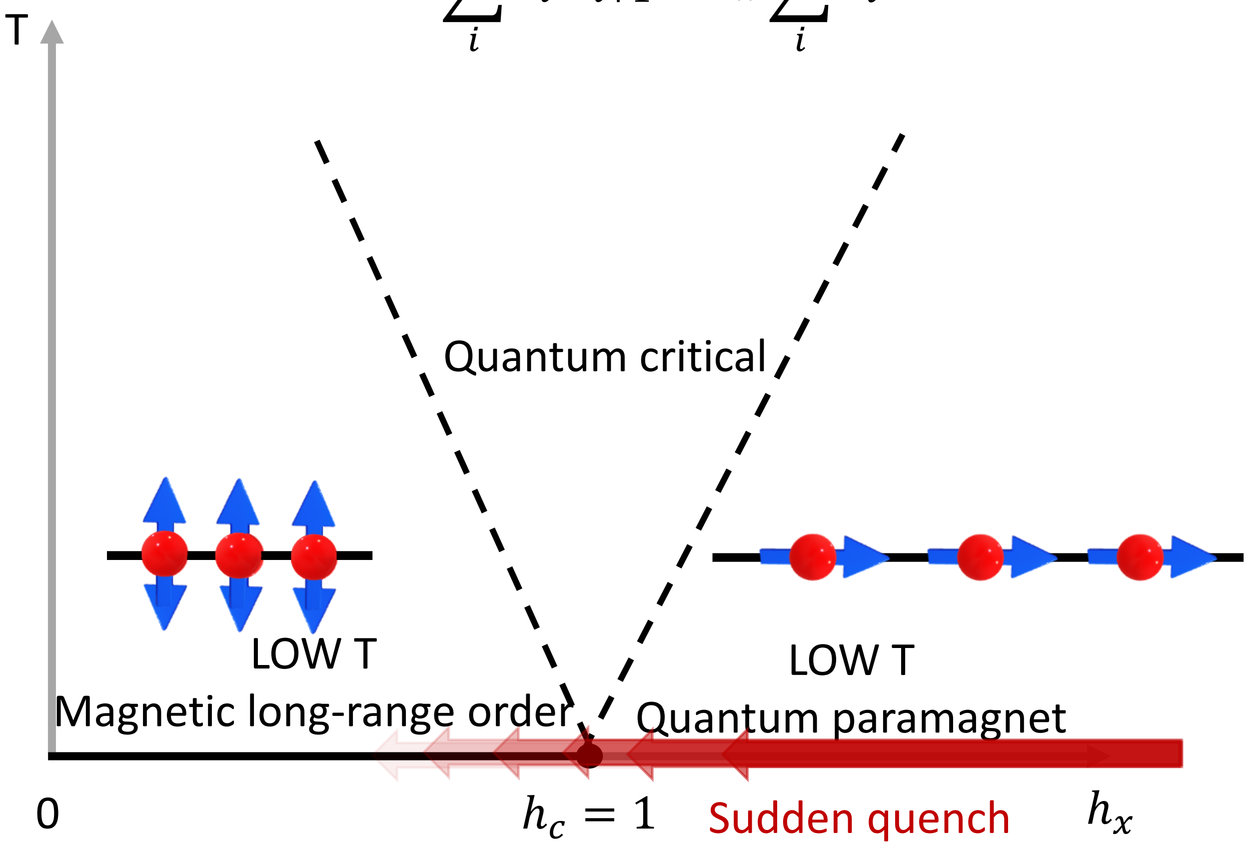
$$\langle \hat{\mathcal{O}} \rangle = \frac{1}{Z} \sum_{\{\boldsymbol{v}^z\}} \mathcal{O}(\boldsymbol{v}^z) |c_{\boldsymbol{v}^z}|^2 \approx \frac{1}{P} \sum_{p=1}^{P} \mathcal{O}\left(\boldsymbol{v}_p^z\right)$$

$$W_k(t+\Delta t) = W_k(t) - i\Delta t \frac{\partial E}{\partial W_k}$$

Real time evolution

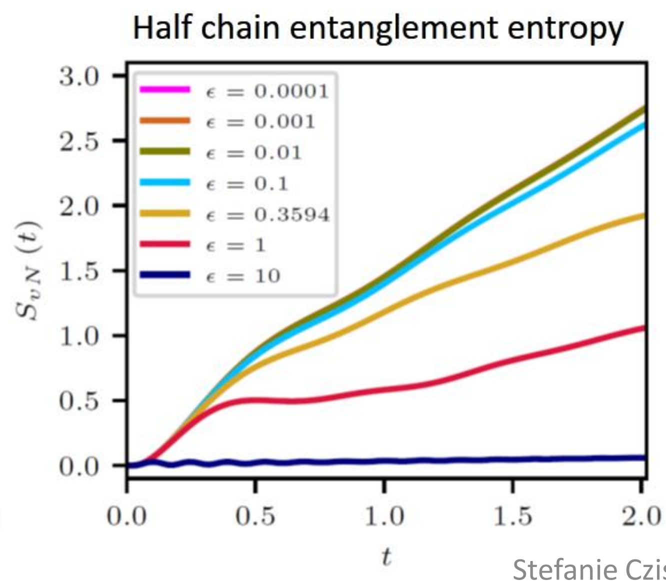
Transverse Field Ising Model (TFIM)

$$\hat{H} = -\sum_i \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z - h_x \sum_i \hat{\sigma}_i^x$$



Picture from: S. Sachdev, Quantum Phase Transitions

- Quantum critical point at $h_c = 1$
- Analytical solutions available [Lieb, Calabrese,…]
- Quenches studied in detail [Karl, Cakir et al. PRE 2017]
- Hard for MPS based methods



$$\epsilon = \frac{h_x - h_c}{h_c}$$

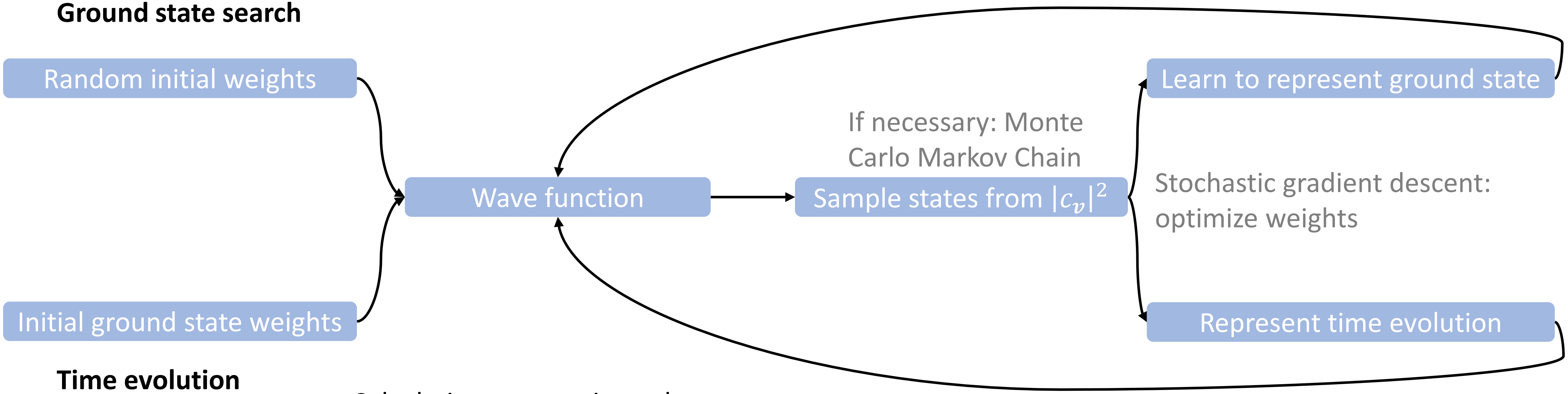
Neural-network quantum states

[Carleo and Troyer, Science 2017]

$$W_k(p+1) = W_k(p) - \gamma \frac{\partial E}{\partial W_k}$$

Imaginary time evolution

Ground state search



Time evolution

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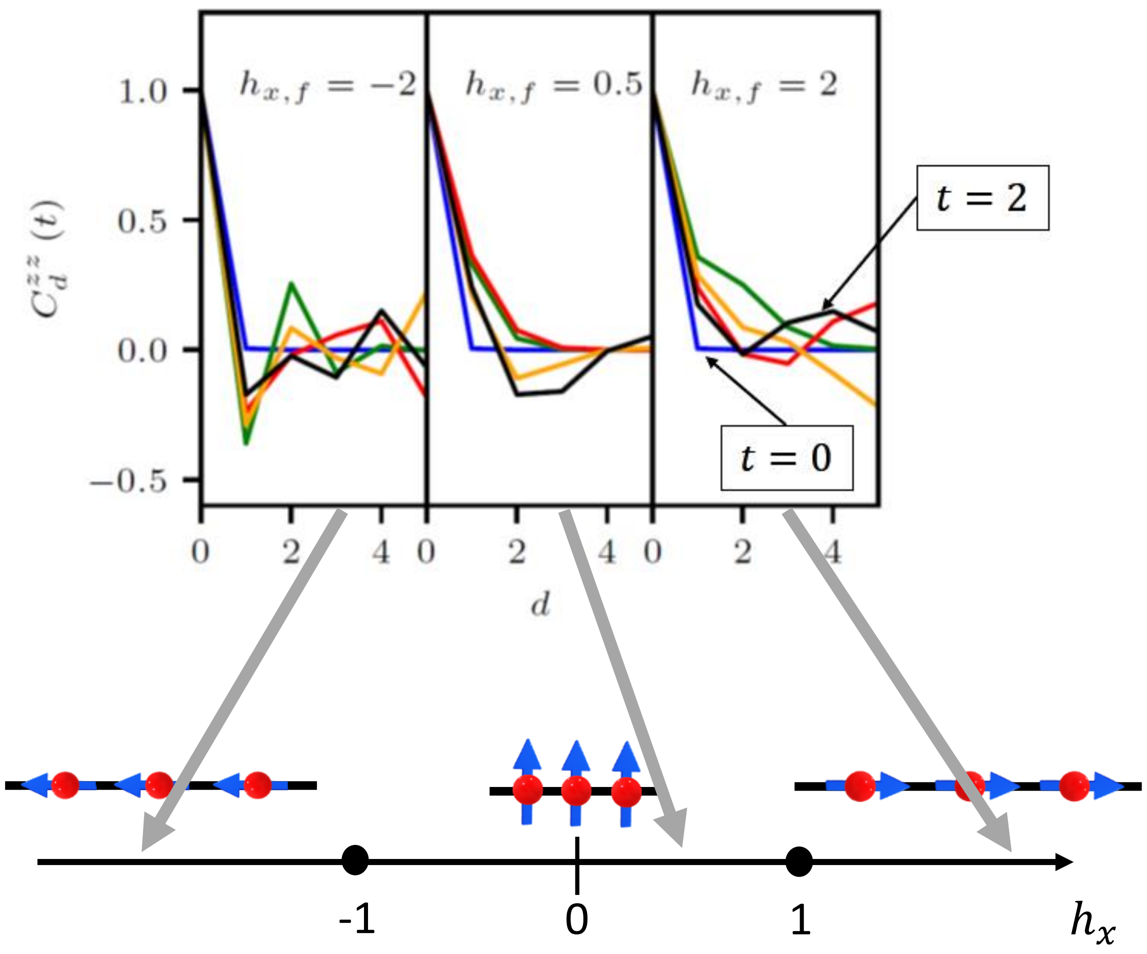
$$W_k(t+\Delta t) = W_k(t) - i\Delta t \frac{\partial E}{\partial W_k}$$

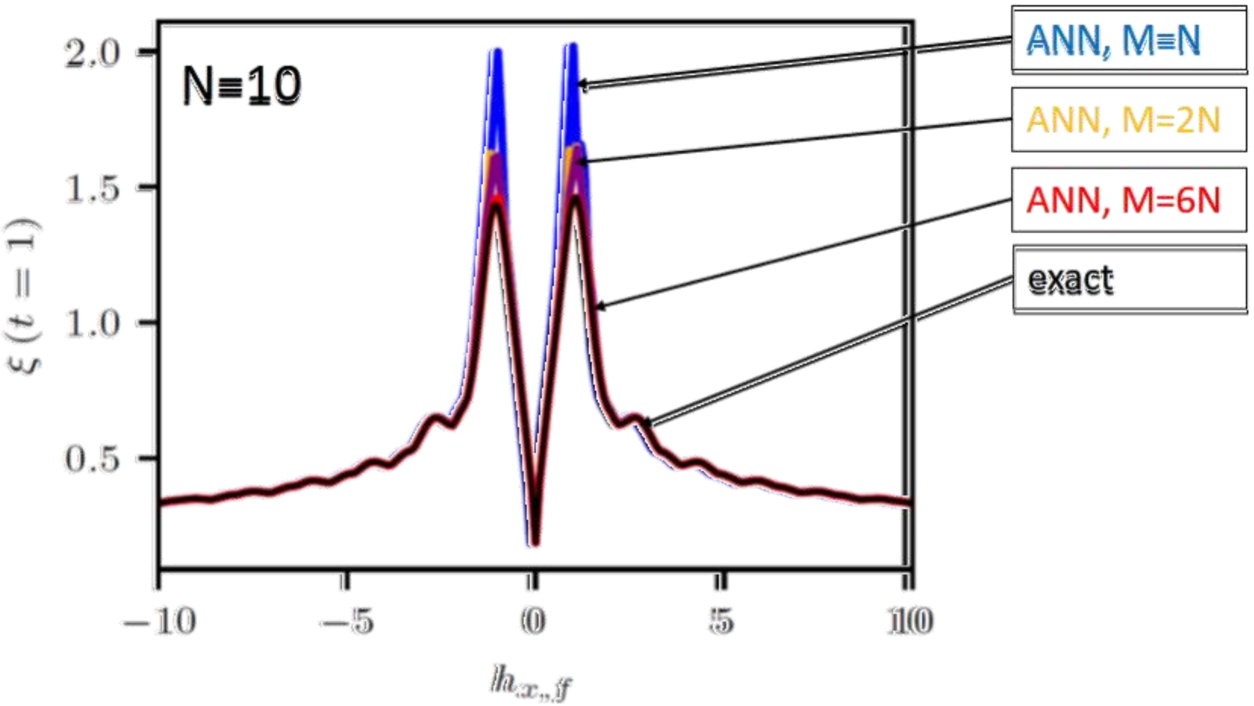
Real time evolution

Quenches in the TFIM

Analytical solutions, N=10



Correlation length



$$C_d^{zz}(t) = \langle \hat{\sigma}_i^z \hat{\sigma}_{i+d}^z \rangle$$

$$|C_d^{zz}(t)| = e^{-d/\xi(t)}$$

N visible, M hidden neurons

TFIM in a longitudinal field

$$\hat{H} = -\sum_i \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z - h_x \sum_i \hat{\sigma}_i^x - h_z \sum_i \hat{\sigma}_i^z$$

$$|C_d^{zz}(t)| = e^{-d/\xi(t)}$$

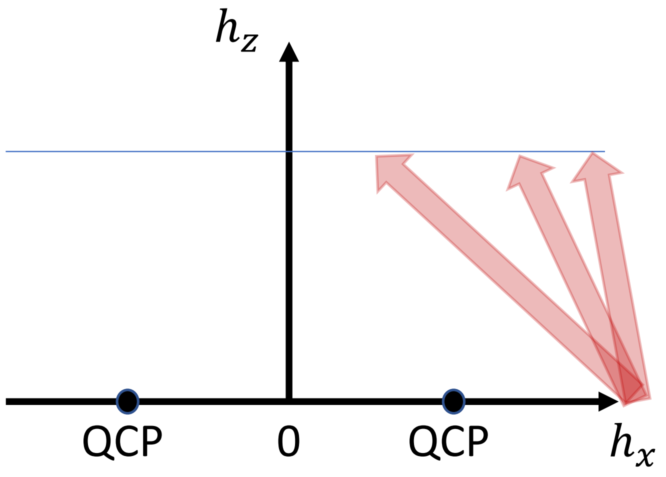
$$\Delta\xi(t) = |\xi - \xi_{\mathrm{exact}}|$$

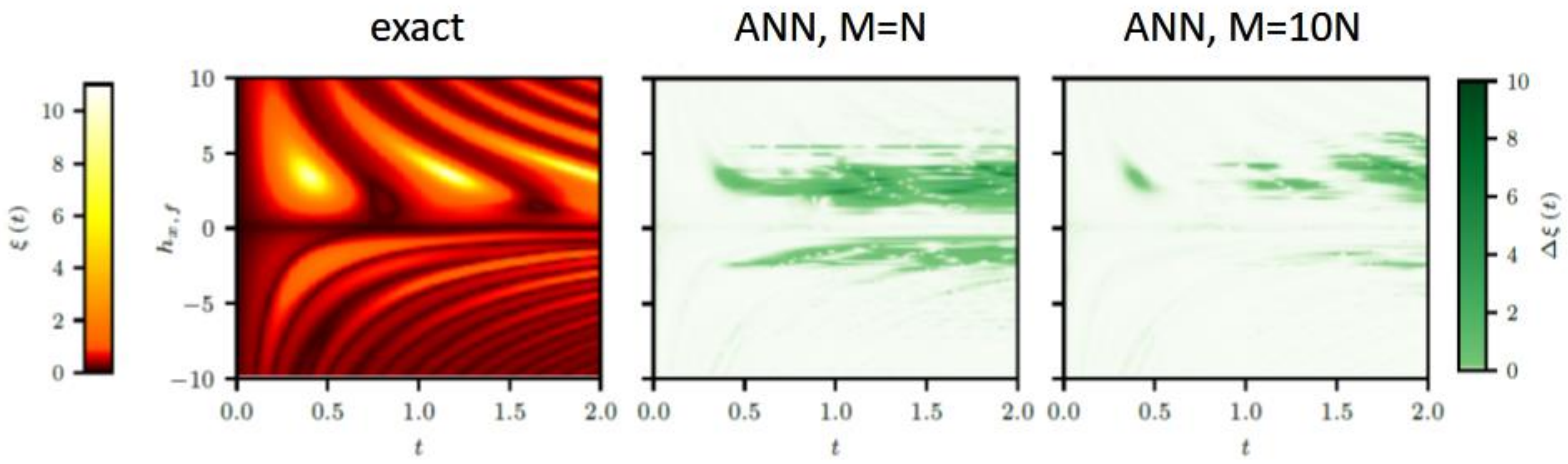
$h_{x,i} = 100$

$h_{z,i} = 0$

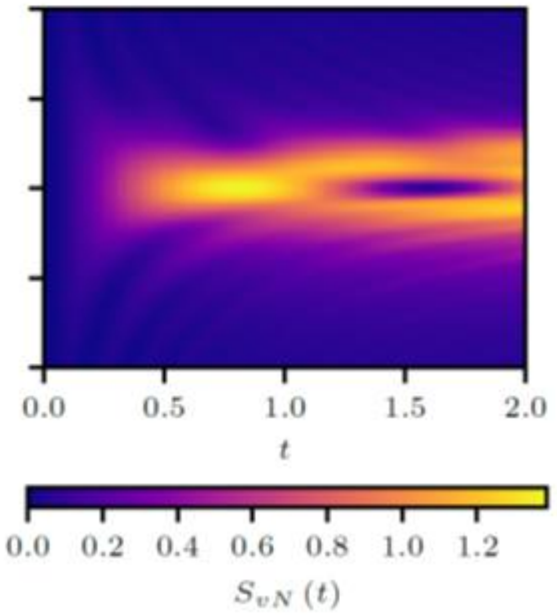
$N = 10$

$h_{z,f} = 2$





Entanglement entropy



Simulating large spin systems

$$\hat{H} = -\sum_i \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z - h_x \sum_i \hat{\sigma}_i^x - h_z \sum_i \hat{\sigma}_i^z$$

$N = 42$

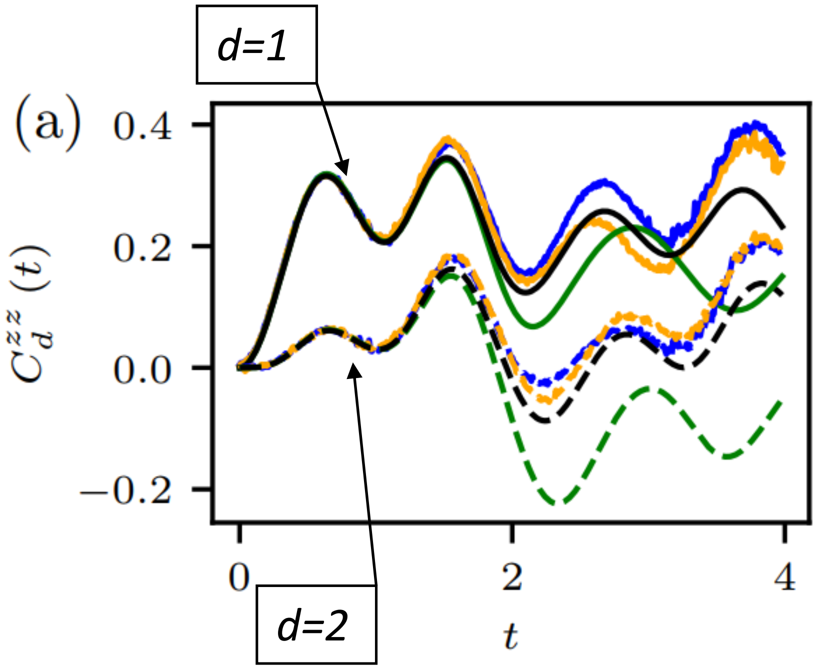
$h_{x,f} = 0.5, \quad h_{z,f} = 1$

ANN, *M=N*

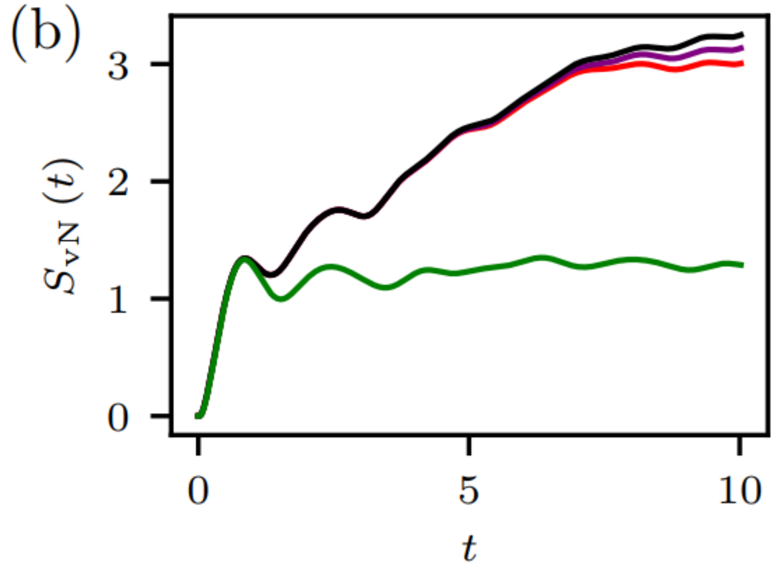
ANN, *M=2N*

tDMRG, *D=5*

tDMRG, *D=128*



Half chain entanglement entropy



tDMRG, *D=5*

tDMRG, *D=64*

tDMRG, *D=96*

tDMRG, *D=128*

Bond dimension *D*

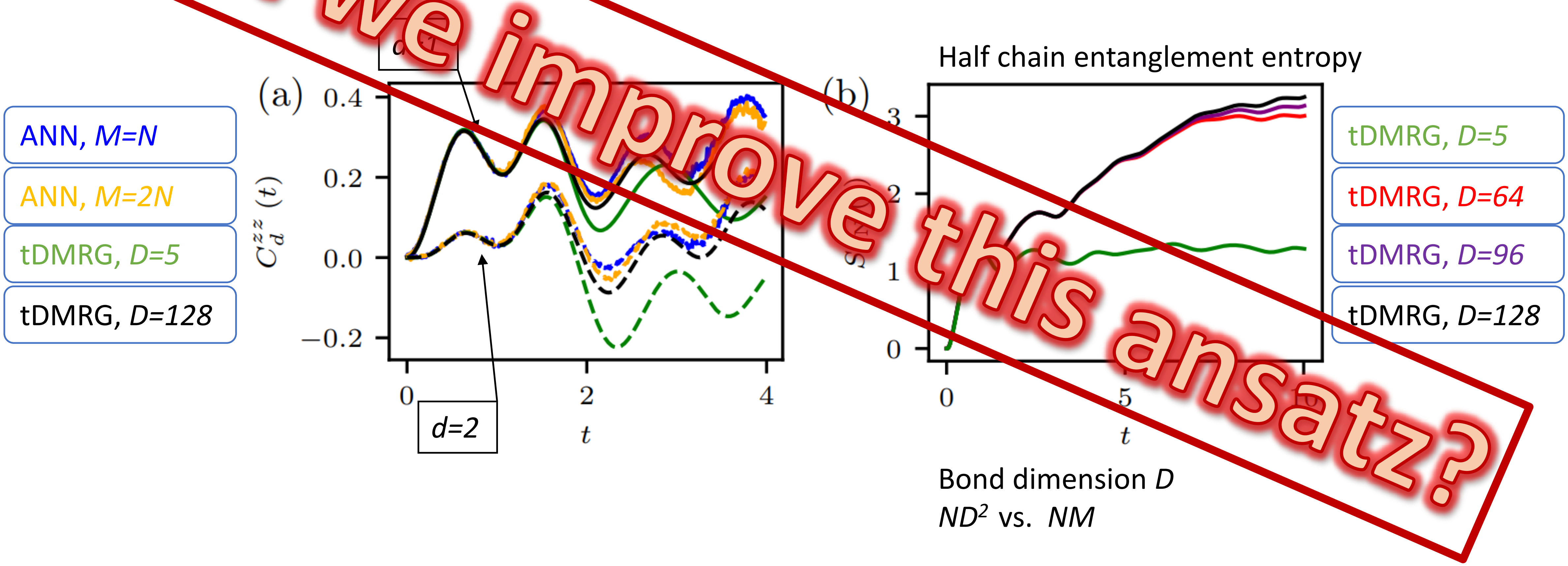
ND^2 vs. NM

Simulating large spin systems

$$\hat{H} = -\sum_i \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z - h_x \sum_i \hat{\sigma}_i^x - h_z \sum_i \hat{\sigma}_i^z$$

$N = 42$ $h_{x,f} = 0.5, \quad h_{z,f} = 1$

Half chain entanglement entropy



Bond dimension D

ND^2 vs. NM

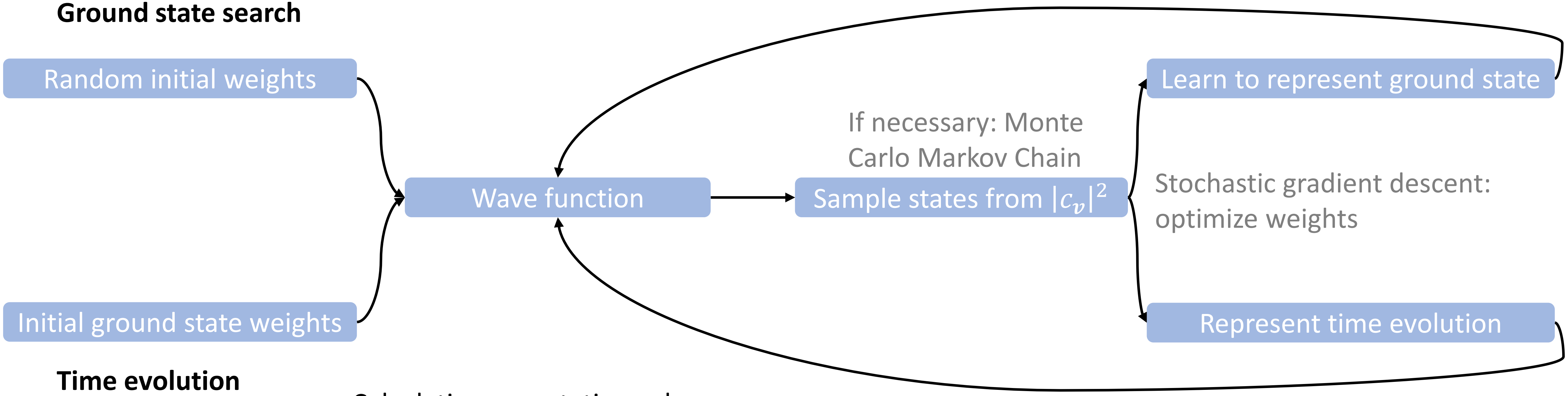
Neural-network quantum states

[Carleo and Troyer, Science 2017]

$$W_k(p+1) = W_k(p) - \gamma \frac{\partial E}{\partial W_k}$$

Imaginary time evolution

Ground state search



Time evolution

$$W_k(t+\Delta t) = W_k(t) - i\Delta t \frac{\partial E}{\partial W_k}$$

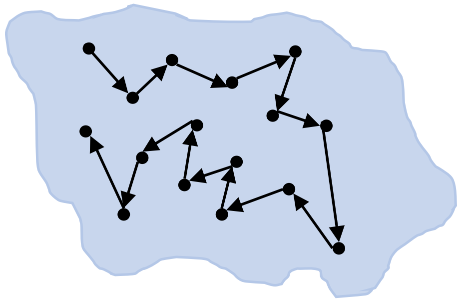
Real time evolution

Calculating expectation values:

$$\langle \hat{\mathcal{O}} \rangle = \frac{1}{Z} \sum_{\{\boldsymbol{v}^z\}} \mathcal{O}(\boldsymbol{v}^z) |c_{\boldsymbol{v}^z}|^2 \approx \frac{1}{P} \sum_{p=1}^{P} \mathcal{O}\left(\boldsymbol{v}_p^z\right)$$

Going to Langevin Dynamics

Brownian motion: Particle in a fluid



Equation of motion: Langevin equation

$$m\ddot{x}(t) = -\lambda\dot{x}(t) + \boldsymbol{\eta}(t)$$

Friction coefficient

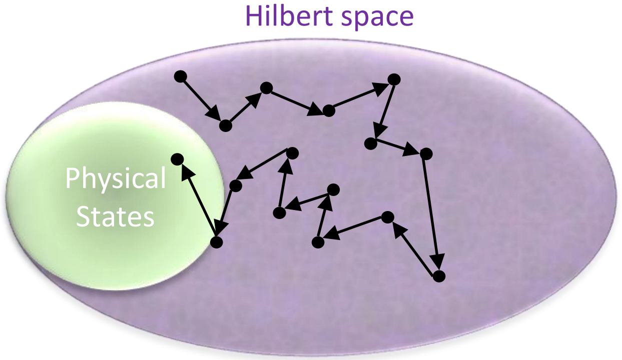
Noise term (representing collisions)

Gaussian white noise:

$$\langle\eta_i(t)\rangle = 0$$
$$\left\langle\eta_i(t)\eta_j(t')\right\rangle = 2\lambda k_B T\delta_{i,j}\delta(t-t')$$

Analogy to sampling spin states

Sampling spin states: Walk around in Hilbert space



Equation of motion: Langevin equation

$$m\dot{\boldsymbol{v}}^z(t) = -\lambda\boldsymbol{v}^z(t) + \boldsymbol{\eta}^z(t)$$

What is the force?

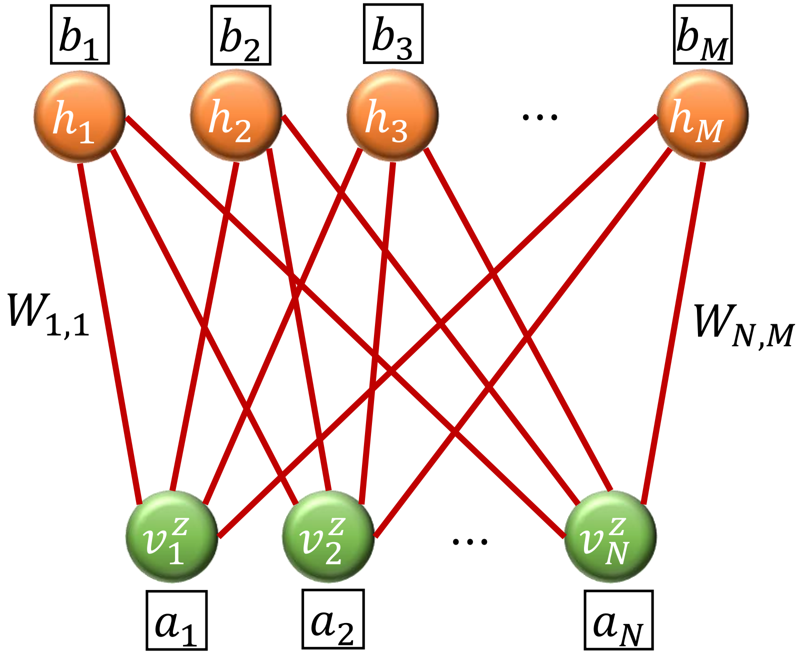
Gaussian white noise:

$$\langle\eta_i^z(t)\rangle = 0$$
$$\left\langle\eta_i^z(t)\eta_j^z(t')\right\rangle = 2\delta_{i,j}\delta(t-t')$$

Sampling with the Langevin Equation

$$c_{\boldsymbol{v}^z,\boldsymbol{h}} = e^{\sum_i a_i v_i^z + \sum_{i,j} v_i^z W_{i,j} h_j + \sum_j b_j h_j} =: e^{-S}$$

Action: $$S = -\sum_i a_i v_i^z - \sum_{i,j} v_i^z W_{i,j} h_j - \sum_j b_j h_j$$



Langevin Equations:

$$\dot{v}_i^z = -\frac{\partial S}{\partial v_i^z} + \eta_i^z = a_i + \sum_j W_{i,j} h_j + \eta_i^z$$

$$\dot{h}_j = -\frac{\partial S}{\partial h_j} + \eta_j^h = \sum_i v_i^z W_{i,j} + b_j + \eta_j^h$$

Real

Complex

Sampling with the Langevin Equation

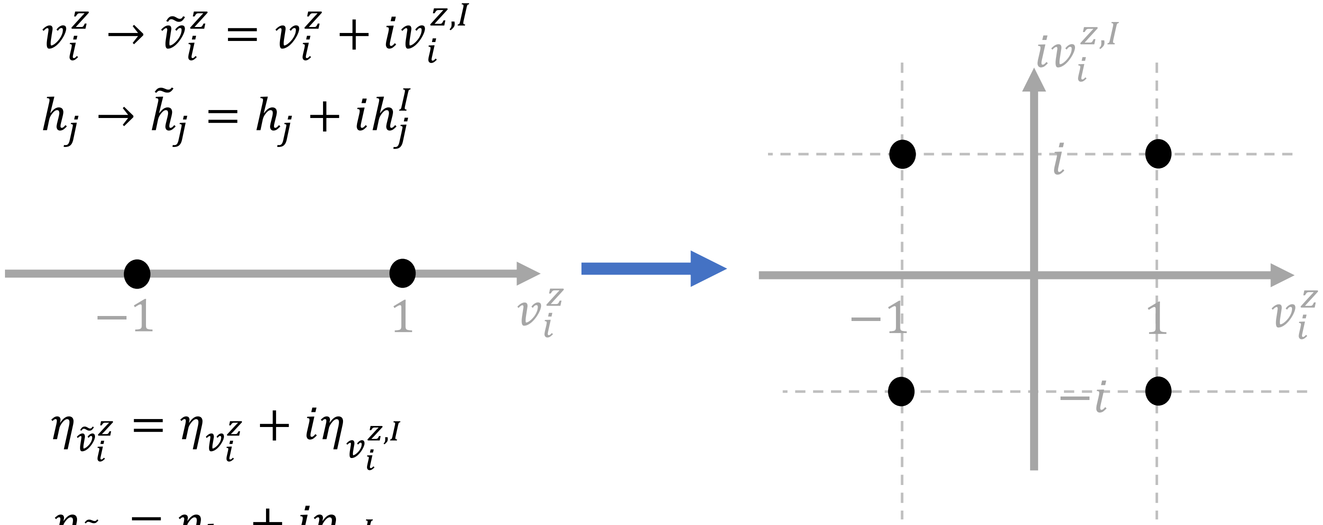
Idea: Complex Langevin equations can be applied to complex actions

Action: $$S = -\sum_i a_i v_i^z - \sum_{i,j} v_i^z W_{i,j} h_j - \sum_j b_j h_j$$

Complexification:

$$v_i^z \rightarrow \tilde{v}_i^z = v_i^z + i v_i^{z,I}$$

$$h_j \rightarrow \tilde{h}_j = h_j + i h_j^I$$



$$\eta_{\tilde{v}_i^z} = \eta_{v_i^z} + i\eta_{v_i^{z,I}}$$

$$\eta_{\tilde{h}_i} = \eta_{h_i} + i\eta_{h_i^I}$$

Complexified equations of motion:

$$\dot{\tilde{v}}_i^z = -\frac{\partial S(v_i^z \rightarrow \tilde{v}_i^z)}{\partial \tilde{v}_i^z} + \eta_{\tilde{v}_i^z} = a_i + \sum_j W_{i,j}\, h_j + \eta_{\tilde{v}_i^z}$$

$$\dot{\tilde{h}}_j = -\frac{\partial S(h_j \rightarrow \tilde{h}_j)}{\partial \tilde{h}_j} + \eta_{\tilde{h}_j} = b_j + \sum_i v_i^z W_{i,j} + \eta_{\tilde{h}_j}$$

Sampling with the Langevin Equation

CAUTION
$f(x) = mx + b$
FORMULAE AHEAD

We can not sample the phase!

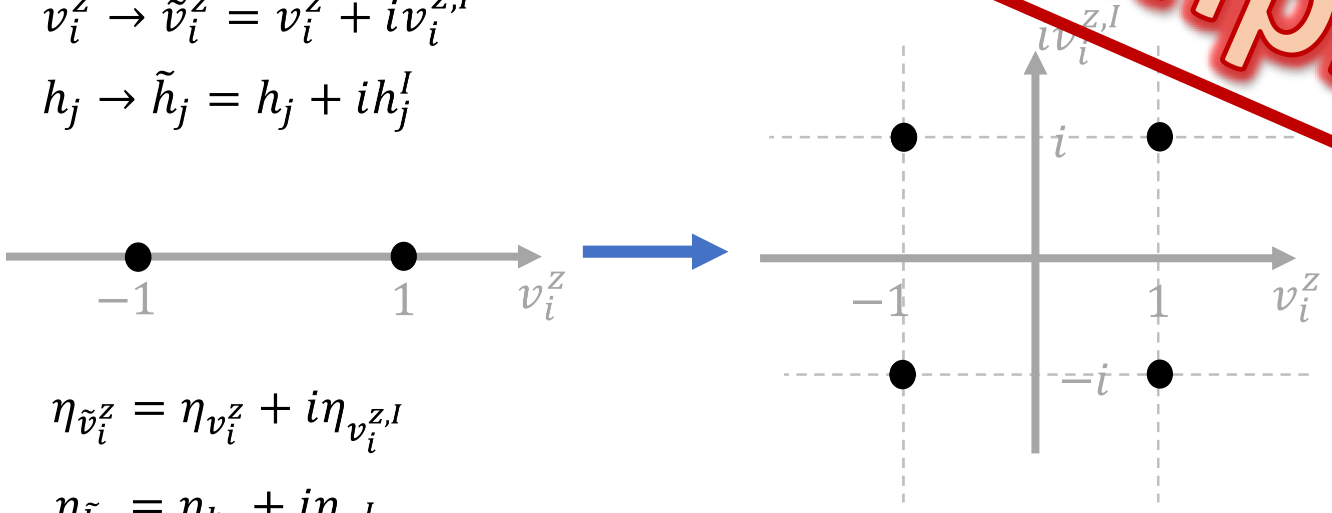
Idea: Complex Langevin equations can be applied to complex actions

Action: $S = -\sum_i a_i v_i^z - \sum_{i,j} v_i^z W_{i,j} h_j - \sum_j b_j h_j$

Complexification:

$v_i^z \to \tilde{v}_i^z = v_i^z + i v_i^{z,I}$

$h_j \to \tilde{h}_j = h_j + i h_j^I$



$\eta_{\tilde{v}_i^z} = \eta_{v_i^z} + i\eta_{v_i^{z,I}}$

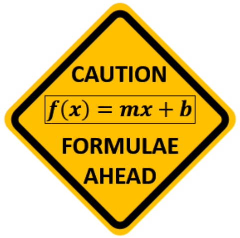
$\eta_{\tilde{h}_i} = \eta_{h_i} + i\eta_{h_i^I}$

Complexified equations of motion:

$$\dot{\tilde{v}}_i^z = -\frac{\partial S(v_i^z \to \tilde{v}_i^z)}{\partial \tilde{v}_i^z} + \eta_{\tilde{v}_i^z} = a_i + \sum_j W_{i,j} h_j + \eta_{\tilde{v}_i^z}$$

$$\dot{\tilde{h}}_j = -\frac{\partial S(h_j \to \tilde{h}_j)}{\partial \tilde{h}_j} + \eta_{\tilde{h}_j} = b_j + \sum_i v_i^z W_{i,j} + \eta_{\tilde{h}_j}$$

Use Langevin Dynamics for the real part



Action: $S = -\sum_i a_i v_i^z - \sum_{i,j} v_i^z W_{i,j} h_j - \sum_j b_j h_j =: \underbrace{S^R\big(\mathrm{Re}(\boldsymbol{a}), \mathrm{Re}(\boldsymbol{b}), \mathrm{Re}(W)\big)} + i\underbrace{S^I\big(\mathrm{Im}(\boldsymbol{a}), \mathrm{Im}(\boldsymbol{b}), \mathrm{Im}(W)\big)}$

Real Langevin:

$$\dot{v}_i^z = \mathrm{Re}(a_i) + \sum_j \mathrm{Re}(W_{i,j}) h_j + \eta_{v_i^z}$$

$$\dot{h}_j = \mathrm{Re}(b_j) + \sum_i v_i^z \mathrm{Re}(W_{i,j}) + \eta_{h_j}$$

Include phase in expectation values!

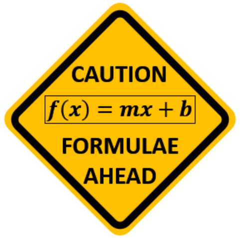
Sign problem!

Calculate observables:
(for diagonal operators)

$$\langle \hat{\mathcal{O}} \rangle = \frac{1}{Z} \sum_{\{\boldsymbol{v}^z\}} \sum_{\{\boldsymbol{v}^{z\prime}\}} \mathcal{O}(\boldsymbol{v}^z) c_{\boldsymbol{v}^z} c^*_{\boldsymbol{v}^{z\prime}} \, \delta_{\boldsymbol{v}^z, \boldsymbol{v}^{z\prime}}$$

$$\approx \frac{1}{\tilde{P}} \sum_{p=1}^{P} \sum_{q=1}^{P} \mathcal{O}(\boldsymbol{v}_p^z) e^{iS^I(\boldsymbol{v}_p^z, \boldsymbol{h}_p) - iS^I(\boldsymbol{v}_q^z, \boldsymbol{h}_q)} \delta_{\boldsymbol{v}_p^z, \boldsymbol{v}_q^z}, \qquad \tilde{P} = \sum_{p=1}^{P} \sum_{q=1}^{P} e^{iS^I(\boldsymbol{v}_p^z, \boldsymbol{h}_p) - iS^I(\boldsymbol{v}_q^z, \boldsymbol{h}_q)} \delta_{\boldsymbol{v}_p^z, \boldsymbol{v}_q^z}$$

Measuring in different bases



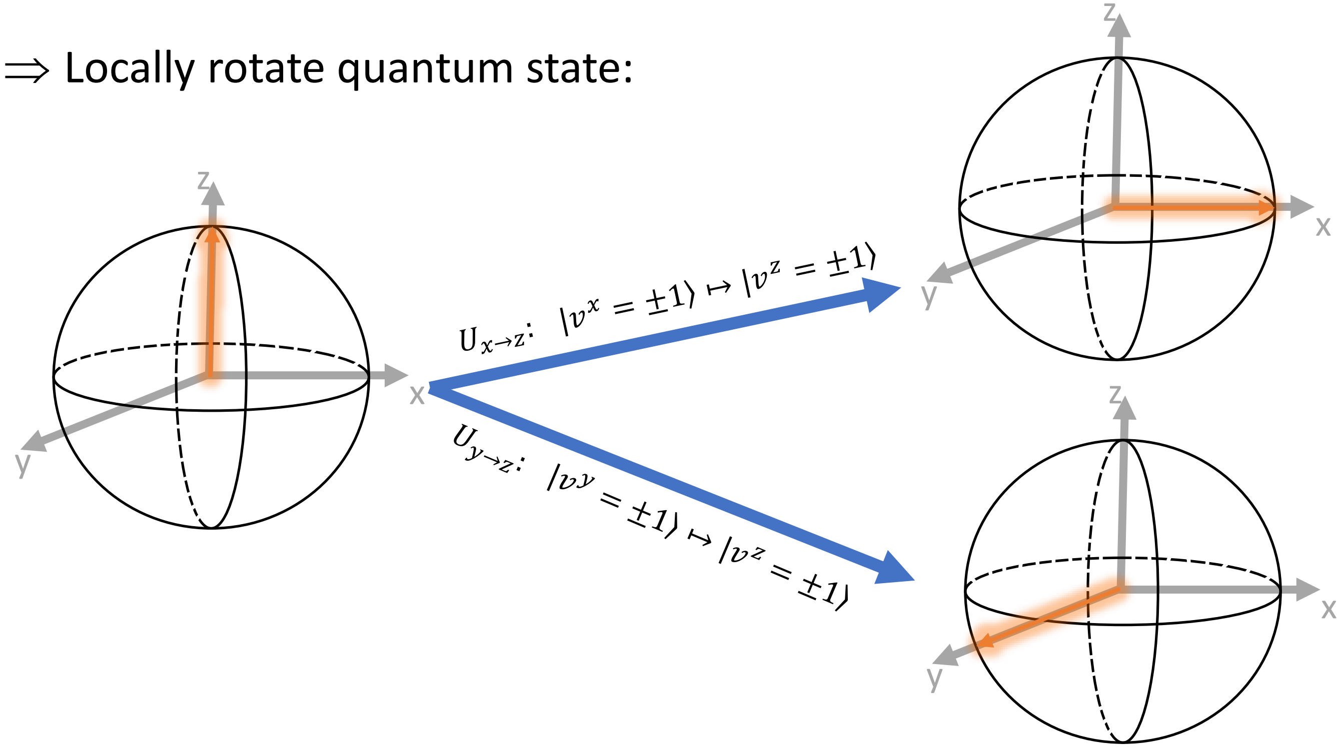
Expectation values of diagonal operators:

$$\langle \hat{\sigma}_i^z \rangle = \sum_{\{\boldsymbol{v}\}} v_i^z |c_{\boldsymbol{v}^z}|^2 \approx \frac{1}{\tilde{P}} \sum_{p=1}^{P} \sum_{q=1}^{P} v_{i,p}^z e^{iS^I(\boldsymbol{v}_p^z, \boldsymbol{h}_p) - iS^I(\boldsymbol{v}_q^z, \boldsymbol{h}_q)} \delta_{\boldsymbol{v}_p^z, \boldsymbol{v}_q^z}$$

$$\tilde{P} = \sum_{p=1}^{P} \sum_{q=1}^{P} e^{iS^I(\boldsymbol{v}_p^z, \boldsymbol{h}_p) - iS^I(\boldsymbol{v}_q^z, \boldsymbol{h}_q)} \delta_{\boldsymbol{v}_p^z, \boldsymbol{v}_q^z}$$

But what about operators in other bases, such as $\langle \hat{\sigma}_i^x \rangle$ or $\langle \hat{\sigma}_i^y \rangle$?

$\Rightarrow$ Locally rotate quantum state:



$$c_{\boldsymbol{v}^x} = \sum_{\boldsymbol{v}^z, \boldsymbol{h}} e^{\boldsymbol{v}^z W \boldsymbol{h} + \boldsymbol{a}\boldsymbol{v}^z + \boldsymbol{b}\boldsymbol{h} + i\frac{\pi}{4}(\boldsymbol{v}^x \boldsymbol{v}^z - \boldsymbol{v}^x - \boldsymbol{v}^z + 1)}$$

$$c_{\boldsymbol{v}^y} = \sum_{\boldsymbol{v}^z, \boldsymbol{h}} e^{\boldsymbol{v}^z W \boldsymbol{h} + \boldsymbol{a}\boldsymbol{v}^z + \boldsymbol{b}\boldsymbol{h} + i\frac{\pi}{4}(\boldsymbol{v}^y \boldsymbol{v}^z - 1)}$$

Setting up a deep belief network (DBN)

$$c_{v^x} = \sum_{\boldsymbol{v}^z,\boldsymbol{h}} e^{\boldsymbol{v}^z W \boldsymbol{h} + \boldsymbol{a}\boldsymbol{v}^z + \boldsymbol{b}\boldsymbol{h} + i\frac{\pi}{4}(\boldsymbol{v}^x \boldsymbol{v}^z - \boldsymbol{v}^x - \boldsymbol{v}^z + 1)}$$

$$c_{v^y} = \sum_{\boldsymbol{v}^z,\boldsymbol{h}} e^{\boldsymbol{v}^z W \boldsymbol{h} + \boldsymbol{a}\boldsymbol{v}^z + \boldsymbol{b}\boldsymbol{h} + i\frac{\pi}{4}(\boldsymbol{v}^y \boldsymbol{v}^z - 1)}$$

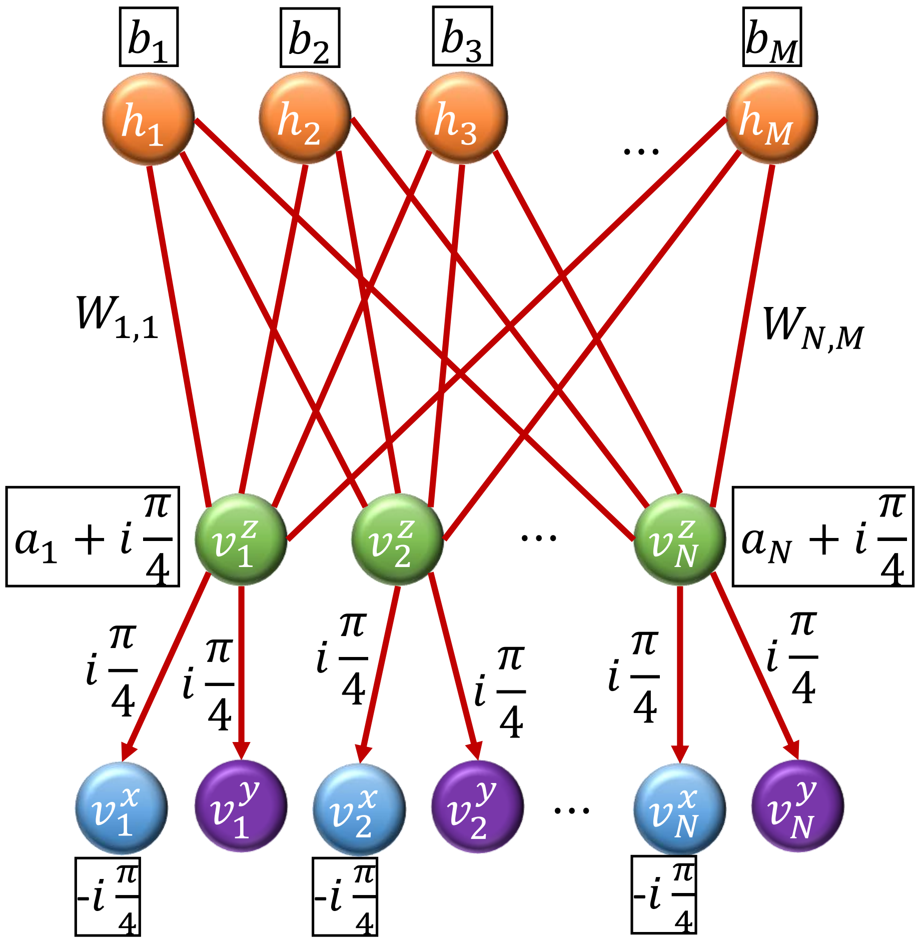
$$c_{v^z} = \sum_{\boldsymbol{h}} e^{\boldsymbol{v}^z W \boldsymbol{h} + \boldsymbol{a}\boldsymbol{v}^z + \boldsymbol{b}\boldsymbol{h}}$$

Equations of motion:

$\dot{\boldsymbol{v}}^x = \dot{\boldsymbol{v}}^y = 0 + \boldsymbol{\eta}^{x/y}$ (only complex phase)

$$\dot{\boldsymbol{v}}^z = \mathrm{Re}(W)\boldsymbol{h} + \mathrm{Re}(\boldsymbol{a}) + \boldsymbol{\eta}^z$$

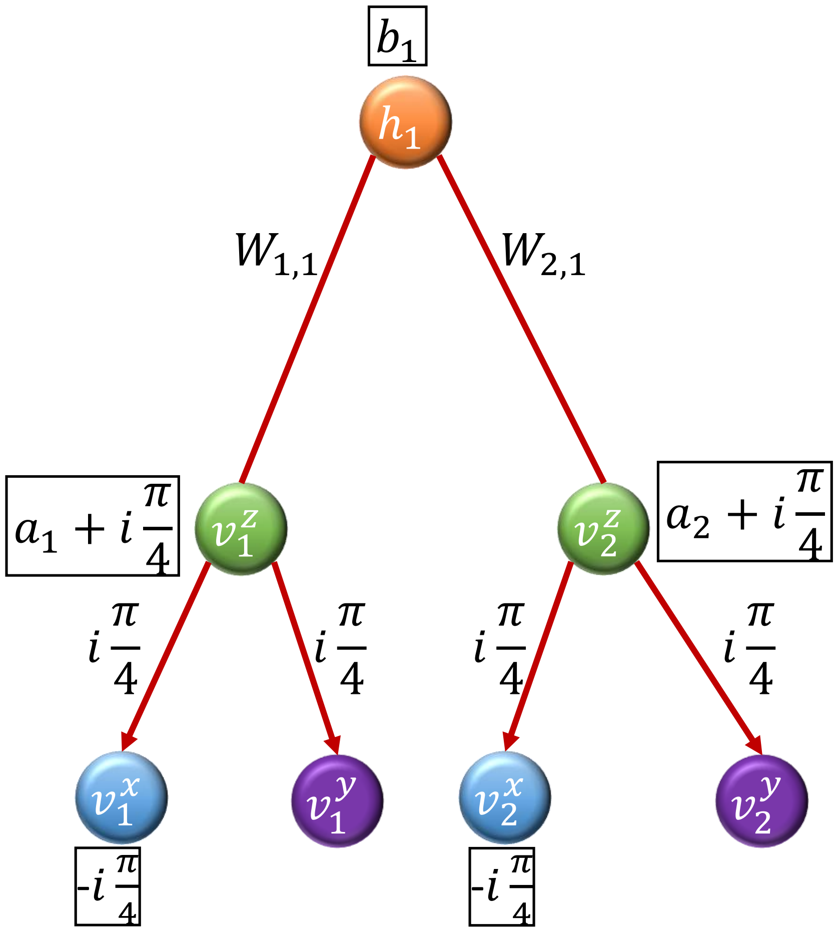
$$\dot{\boldsymbol{h}} = \boldsymbol{v}^z \mathrm{Re}(W) + \mathrm{Re}(\boldsymbol{b}) + \boldsymbol{\eta}^h$$



The Bell-pair state

$$\left|\Psi\right\rangle = \frac{1}{\sqrt{2}}[|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle] = \sum_{\{v^z\}} c_{v^z}\left|v_1^z, v_2^z\right\rangle \quad \Rightarrow \quad c_{v^z} = \begin{cases} \frac{1}{\sqrt{2}} & \text{if } v_1^z = -v_2^z \\ 0 & \text{else} \end{cases}$$

There are many possible choices for the weights!



Choice for complex weights:

$$W_{1,1} = -\omega_e + i\frac{\pi}{2},$$
$$W_{2,1} = \omega_e + i\frac{\pi}{2},$$
$$a_1 = i\frac{\pi}{2}, \qquad a_2 = 0,$$
$$b_1 = i\frac{\pi}{2},$$
$$\omega_e = \frac{1}{2}\sinh^{-1}\left[\frac{1}{\sqrt{8}}\right]$$

Choice for imaginary weights:

$$W_{1,1} = i\left(-\omega_o + \frac{\pi}{4}\right),$$
$$W_{2,1} = i\left(\omega_o + \frac{\pi}{4}\right),$$
$$a_1 = 0, \qquad a_2 = 0,$$
$$b_1 = 0,$$
$$\omega_o = \frac{1}{2}\cos^{-1}\left[\frac{1}{\sqrt{8}}\right]$$

Quantum entanglement: Bell’s inequality

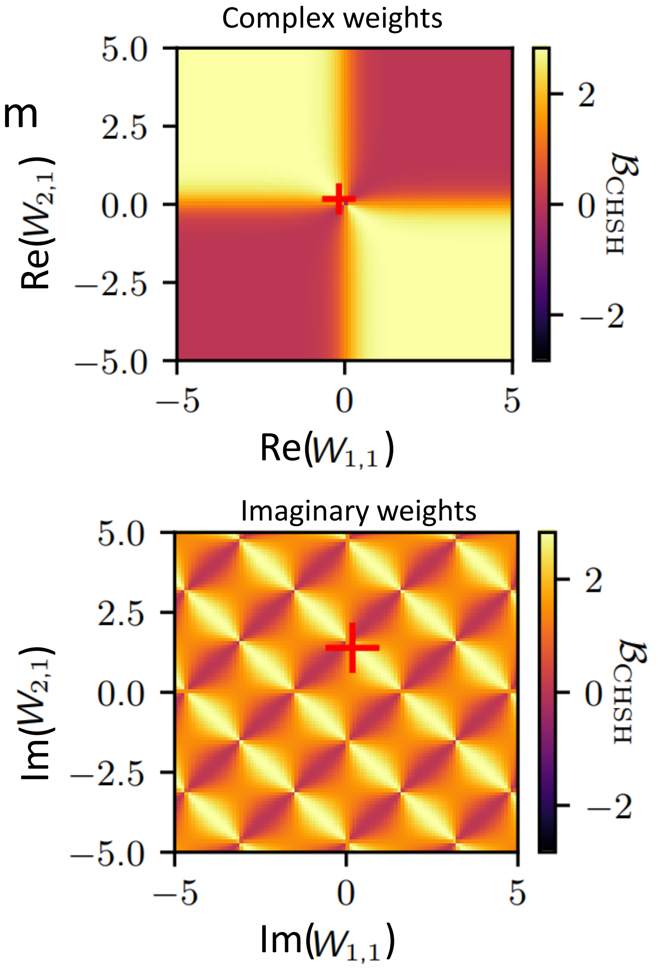
CHSH-inequality (J. Clauser, M. Horne, A. Shimony, R. Holt):

$$\mathcal{B}_{\mathrm{CHSH}} = \langle \hat{A}_1 \otimes \hat{B}_1 \rangle + \langle \hat{A}_1 \otimes \hat{B}_2 \rangle + \langle \hat{A}_2 \otimes \hat{B}_1 \rangle - \langle \hat{A}_2 \otimes \hat{B}_2 \rangle \leq 2 \quad \text{in a classical system}$$

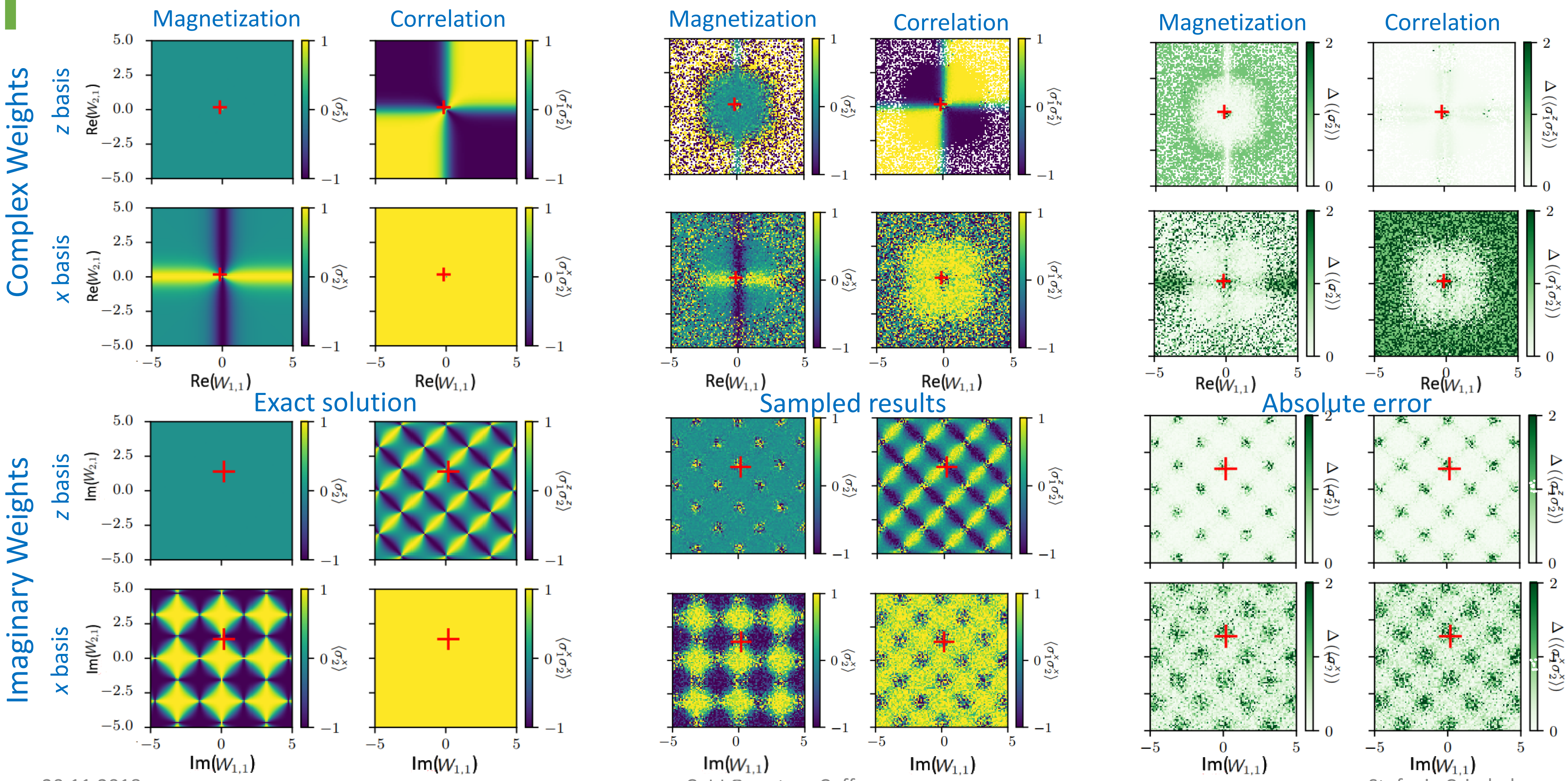
Choose:

$$\hat{A}_1 = \hat{\sigma}_1^x$$
$$\hat{A}_2 = \hat{\sigma}_1^z$$
$$\hat{B}_1 = \frac{1}{\sqrt{2}}(\hat{\sigma}_2^x - \hat{\sigma}_2^z)$$
$$\hat{B}_2 = \frac{1}{\sqrt{2}}(\hat{\sigma}_2^x + \hat{\sigma}_2^z)$$

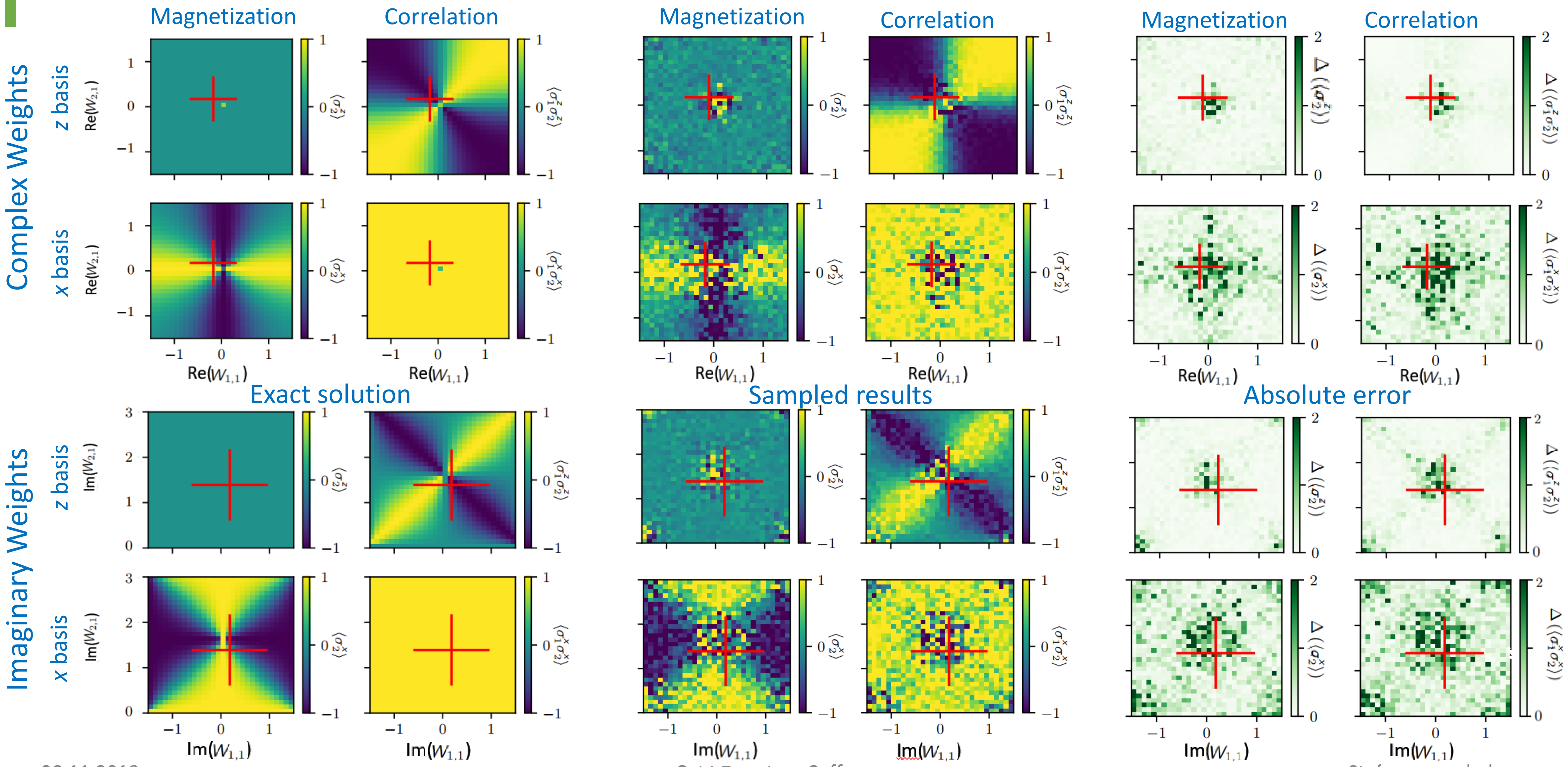
$$\Rightarrow \mathcal{B}_{\mathrm{CHSH}} = \sqrt{2}[\langle \hat{\sigma}_1^x \hat{\sigma}_2^x \rangle - \langle \hat{\sigma}_1^z \hat{\sigma}_2^z \rangle] = 2\sqrt{2} > 2 \quad \text{for the Bell-pair state}$$



Violating Bell's inequality with a DBN

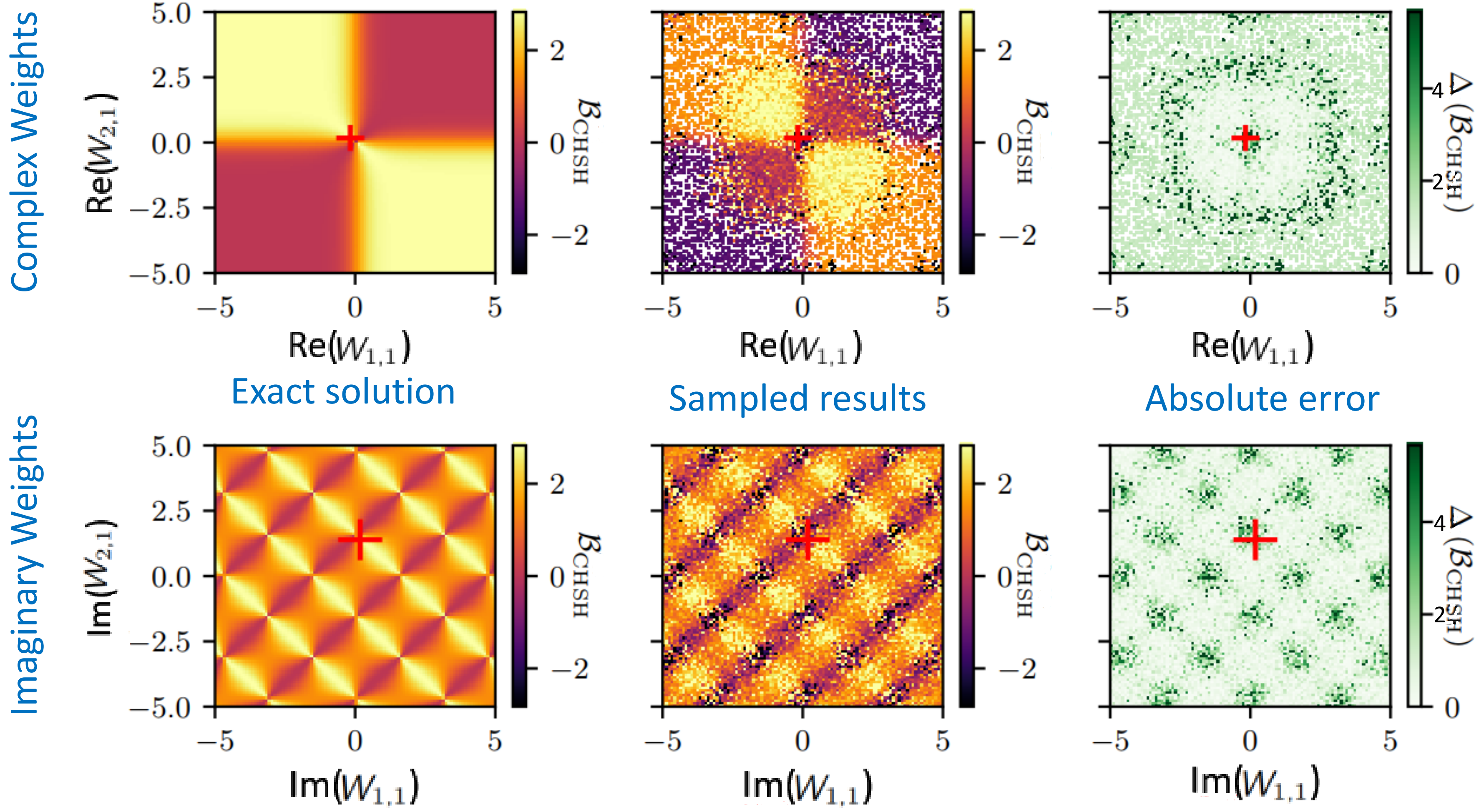


Violating Bell's inequality with a DBN



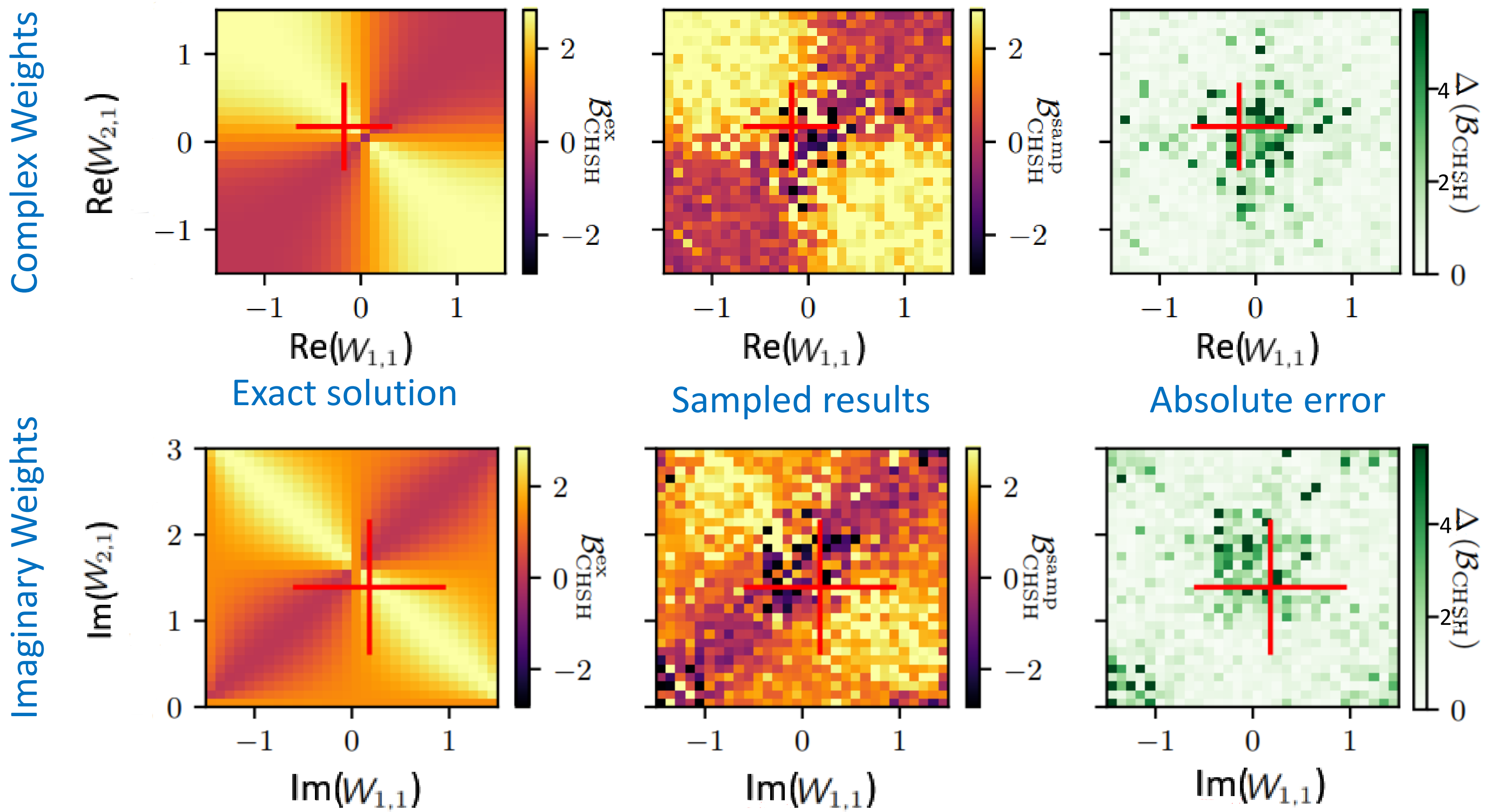
Violating Bell's inequality with a DBN

$\mathcal{B}_{\text{CHSH}} = \sqrt{2}[\langle \hat{\sigma}_1^x \hat{\sigma}_2^x \rangle - \langle \hat{\sigma}_1^z \hat{\sigma}_2^z \rangle]$

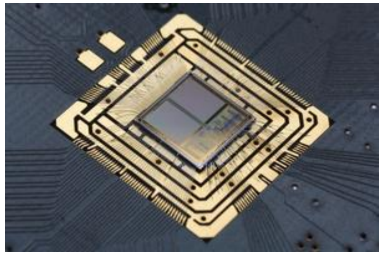


Violating Bell's inequality with a DBN

$$\mathcal{B}_{\mathrm{CHSH}} = \sqrt{2}[\langle\hat{\sigma}_1^x\hat{\sigma}_2^x\rangle - \langle\hat{\sigma}_1^z\hat{\sigma}_2^z\rangle]$$



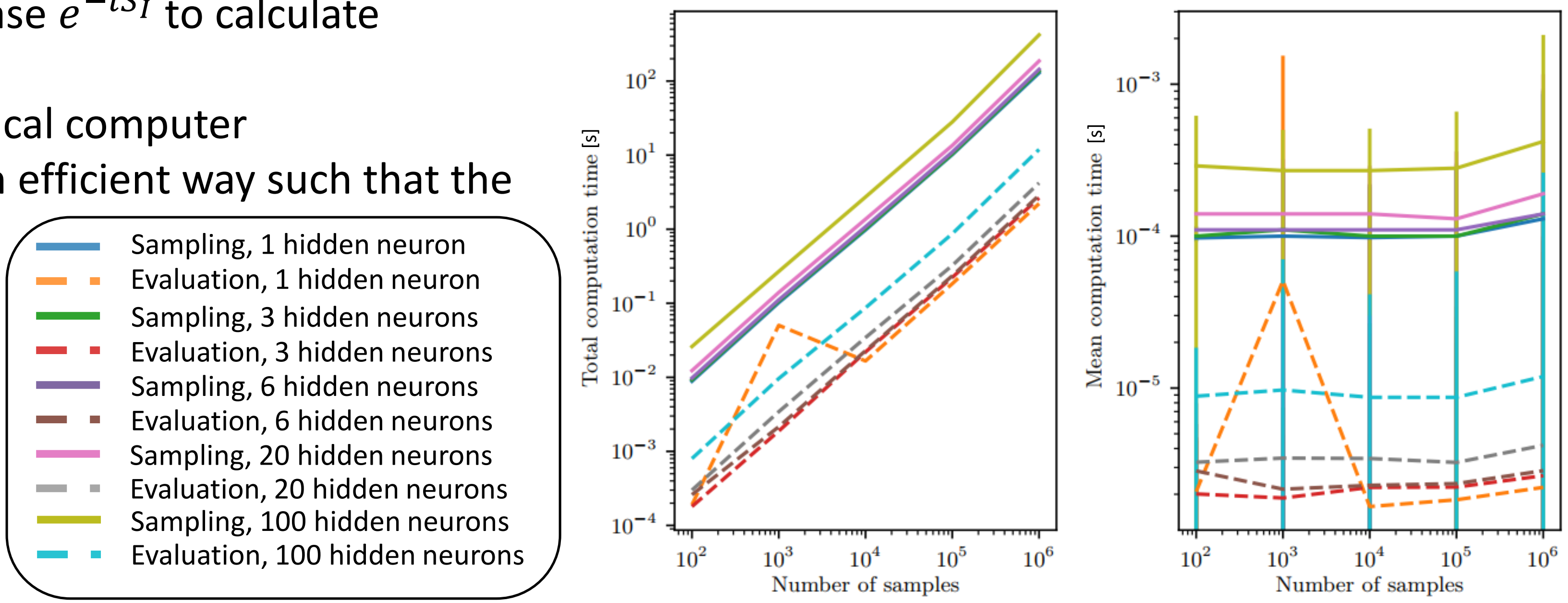
Outlook: Connection to the BrainScaleS group



- Sampling with Leaky-Integrate-and-Fire (LIF) neurons can be described via Langevin dynamics
- Sampling can be done in a very efficient and fast way on the neuromorphic hardware
- Huge sample sets can be created in short times (help with sign problem?)

BUT:

- We still need to evaluate the phase e^{-iS_I} to calculate expectation values
- This needs to be done on a classical computer
- Can the evaluation be done in an efficient way such that the sampling is the bottleneck?



Conclusion

- We can use Langevin dynamics in a deep belief network to sample spin states which show qantum entanglement

- With this ansatz we can go to deeper and more complex networks

- We can perform measurements in different bases

- We still need to evaluate the phase separately, this can end up in the sign problem

- We can create many samples efficiently with the neuromorphic hardware, but for large networks the evaluation becomes expensive