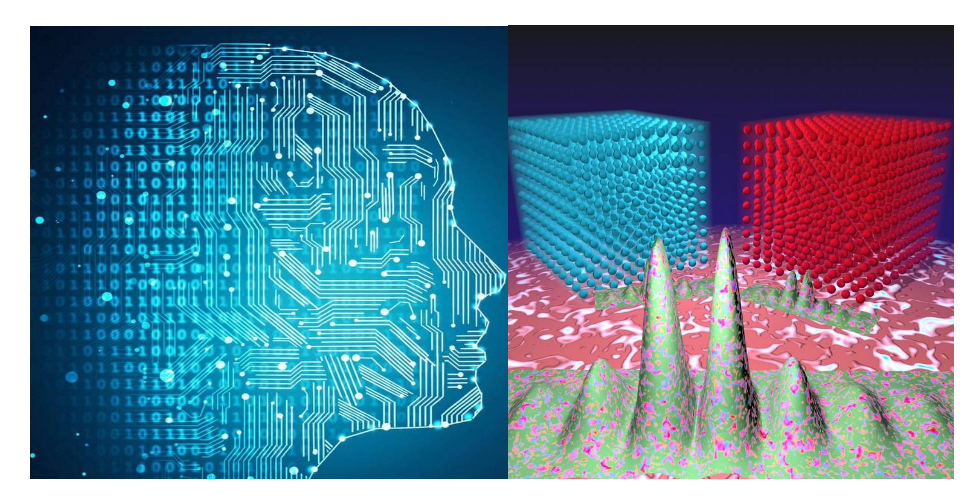
Designing quantum many-body matter with conditional generative adversarial networks (cGANs)



arXiv:2201.12127

Rouven Koch

Aalto University, Finland

AMLD 22 – 29.03.2022

Aalto University
School of Science

QUIZ: Which image is real?

Cat 1

Cat 2

https://thesecatsdonotexist.com/

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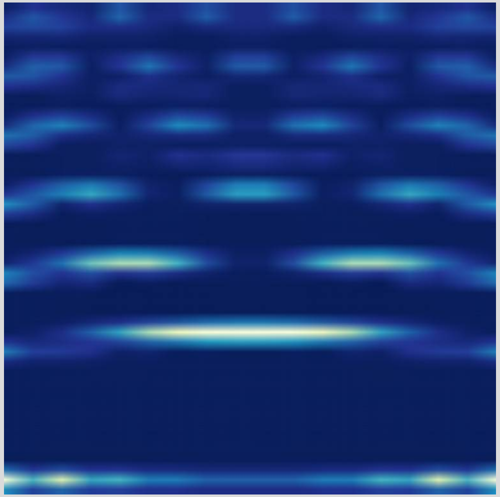
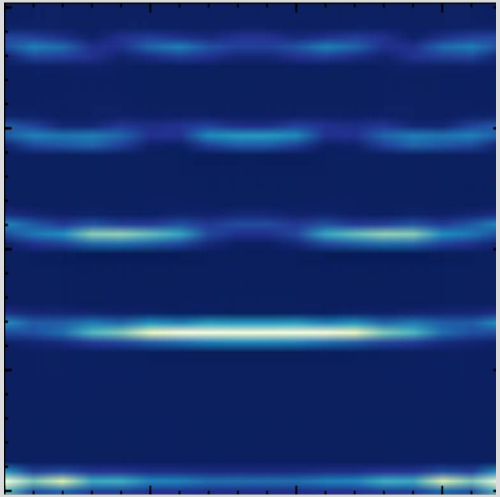
Spectrum 1



Spectrum 2



QUIZ: Which image is real?

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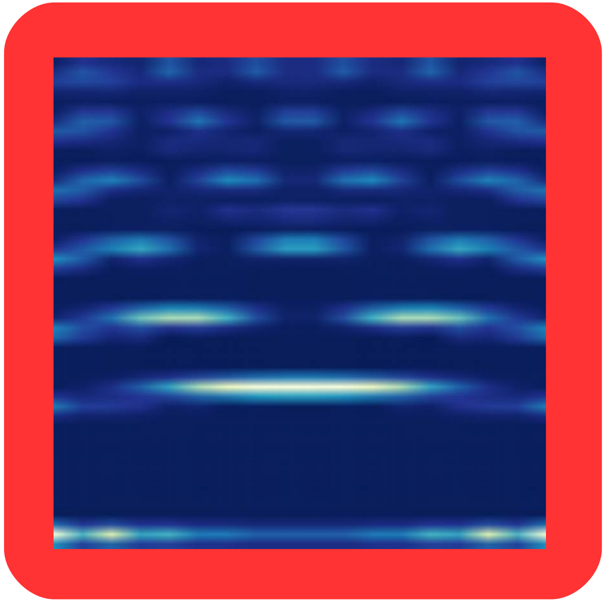
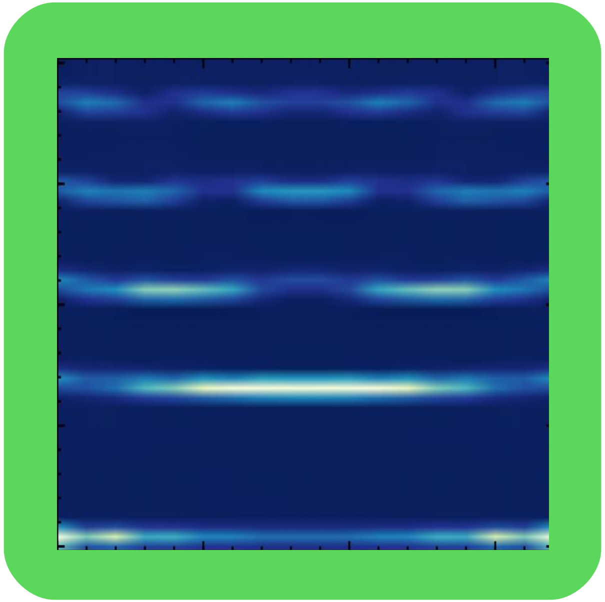


Spectrum 2



Motivation

<u>Example</u>: many-body Hamiltonian (*1d gapless spin-1/2 Heisenberg-model*)

$$H(\mathcal{N}_y, B_x) = \sum_n \mathbf{S}_n \cdot \mathbf{S}_{n+1} + \mathcal{N}_y (-1)^n S_n^y + B_x S_n^y + \xi_n^x S_n^x + \xi_n^y S_n^y$$

conditional parameter　　hidden parameter

N_y: local alternating Neel magnetic field

B_x: uniform Zeeman field

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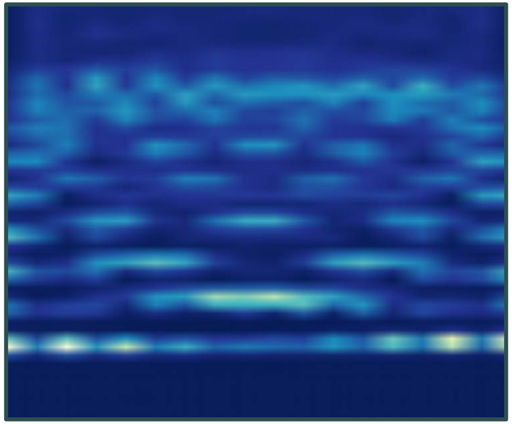
conditional parameter hidden parameter

N_y: local alternating Neel magnetic field

B_x: uniform Zeeman field

$$\chi(\omega) = \langle GS|\hat{A}\delta(\omega - \hat{H}(\alpha, \beta) + E_0)\hat{B}|GS\rangle$$

dynamical correlator



→ exact solvable with tensor-network calculations

Motivation

Question: What if we are interested in the full parameter space of this Hamiltonian?

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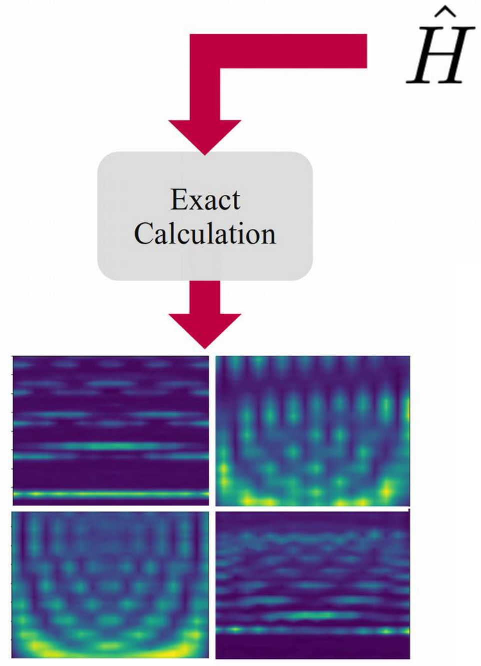
Answer 1:

- compute each parameter combination

→ inefficient and numerically demanding for most many-body systems

→ neglects hidden parameters in Hamiltonian



Motivation

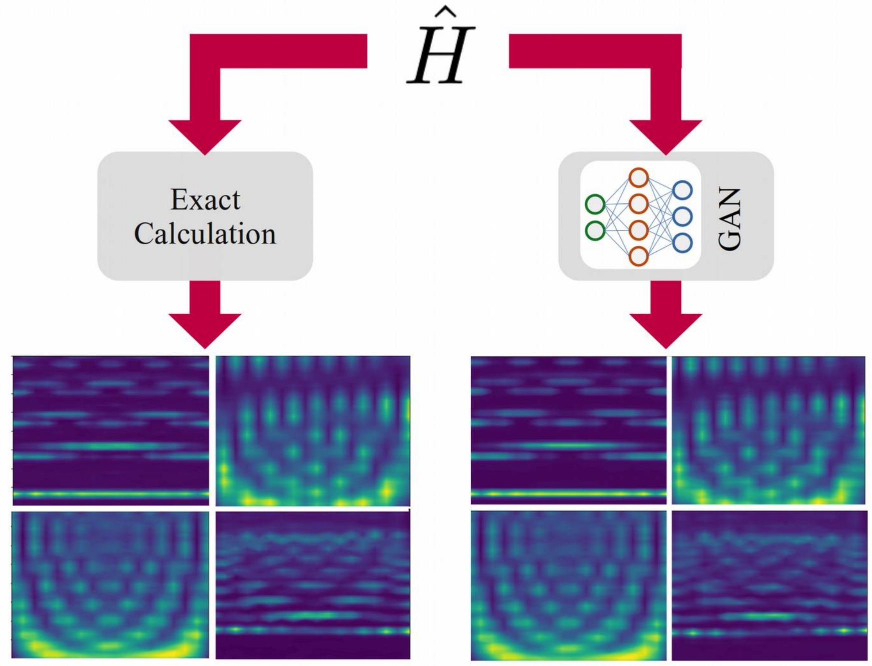
Question: What if we are interested in the full parameter space of this Hamiltonian?

Answer 2:

- using deep *generative learning* methods

→ train the algorithm on a subset of parameter combinations

→ **cGANs** incorporate the hidden parameters with intrinsic randomness



dynamical correlator

Background: Kernel Polynomial Method & Tensor Networks

→ expansion in terms of Chebyshev Polynomials $T_n(x)$

$$f(x) = \alpha_0 + 2\sum_{n=1}^{\infty} \alpha_n T_n(x)$$

Chebyshev moments

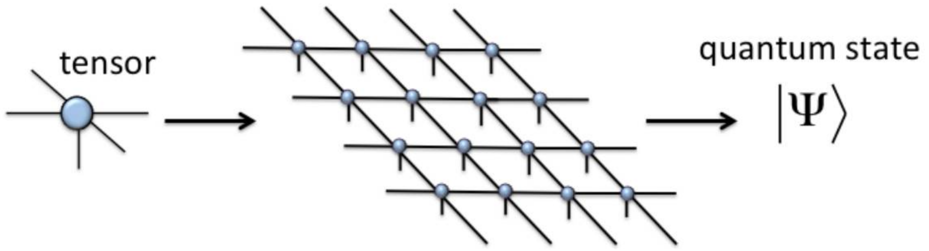
$$\mu_n = \langle \beta | T_n(H) | \alpha \rangle$$

$|\alpha\rangle, |\beta\rangle$: state of the system

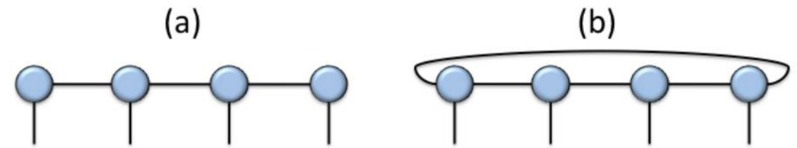
H : Hamiltonian

A. Weiße, et al., Rev. Mod. Physik 78.1 (2006): 275

- *Quantum states* as a collection of tensors interconnected by contraction

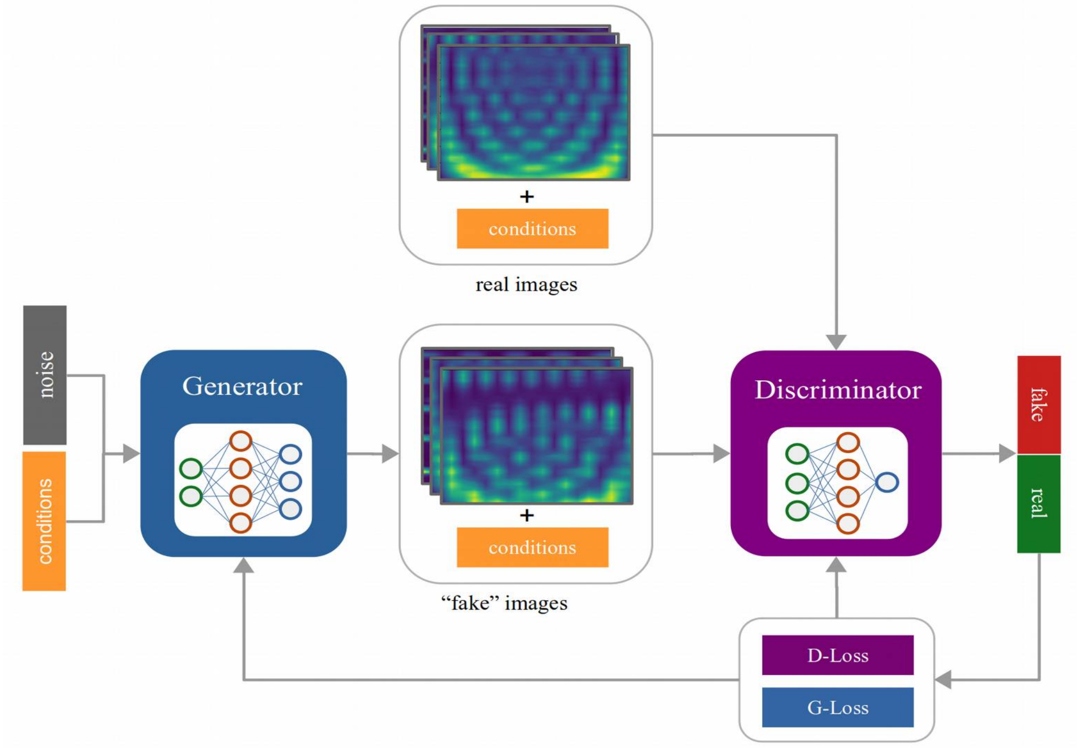


- TNs for 1D systems in condensed matter are the so-called *matrix product states*



Roman Orus, *A practical introduction to tensor networks: Matrix product states and projected entangled pair states*. Annals of Physics, 349:117–158, October 2014.

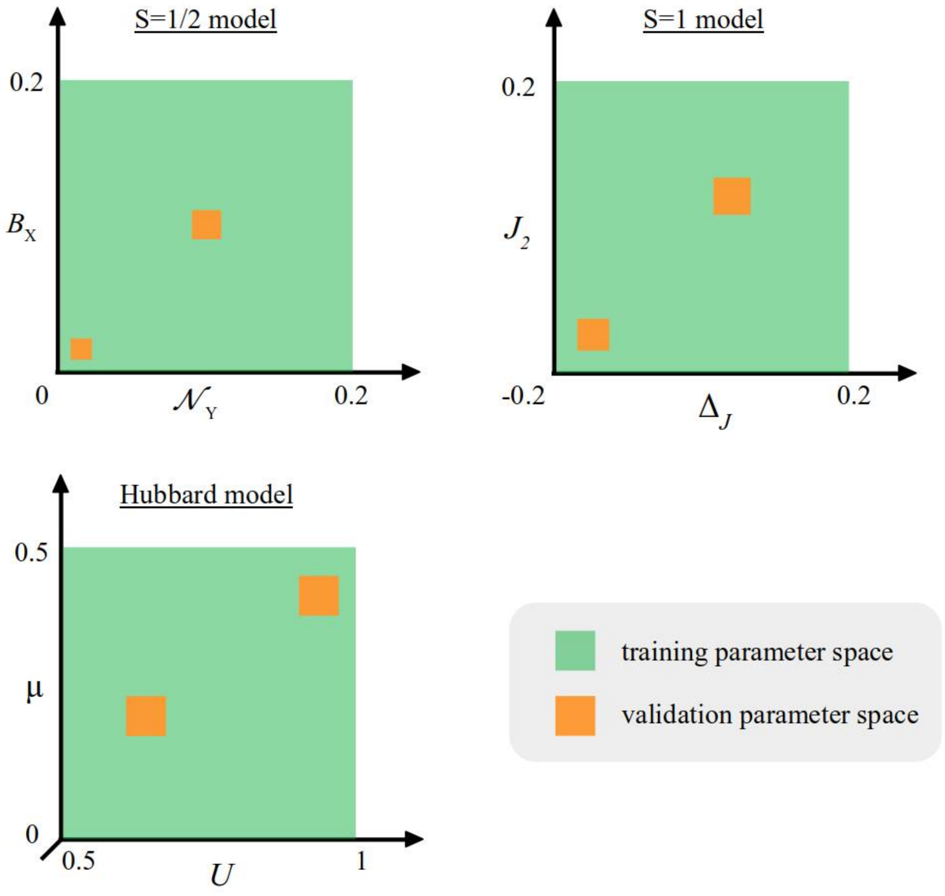
conditional Generative Adversarial Networks: architecture



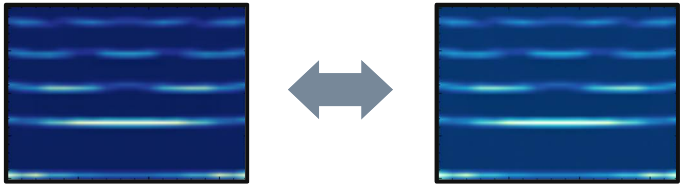
value function: $$\min_G \max_D V(D,G) = \mathbb{E}_{\boldsymbol{x}\sim p_{\text{data}}(\boldsymbol{x})}[\log D(\boldsymbol{x}|\boldsymbol{y})] + \mathbb{E}_{\boldsymbol{z}\sim p_z(\boldsymbol{z})}[\log(1 - D(G(\boldsymbol{z}|\boldsymbol{y})))]$$

→ two-player min-max game

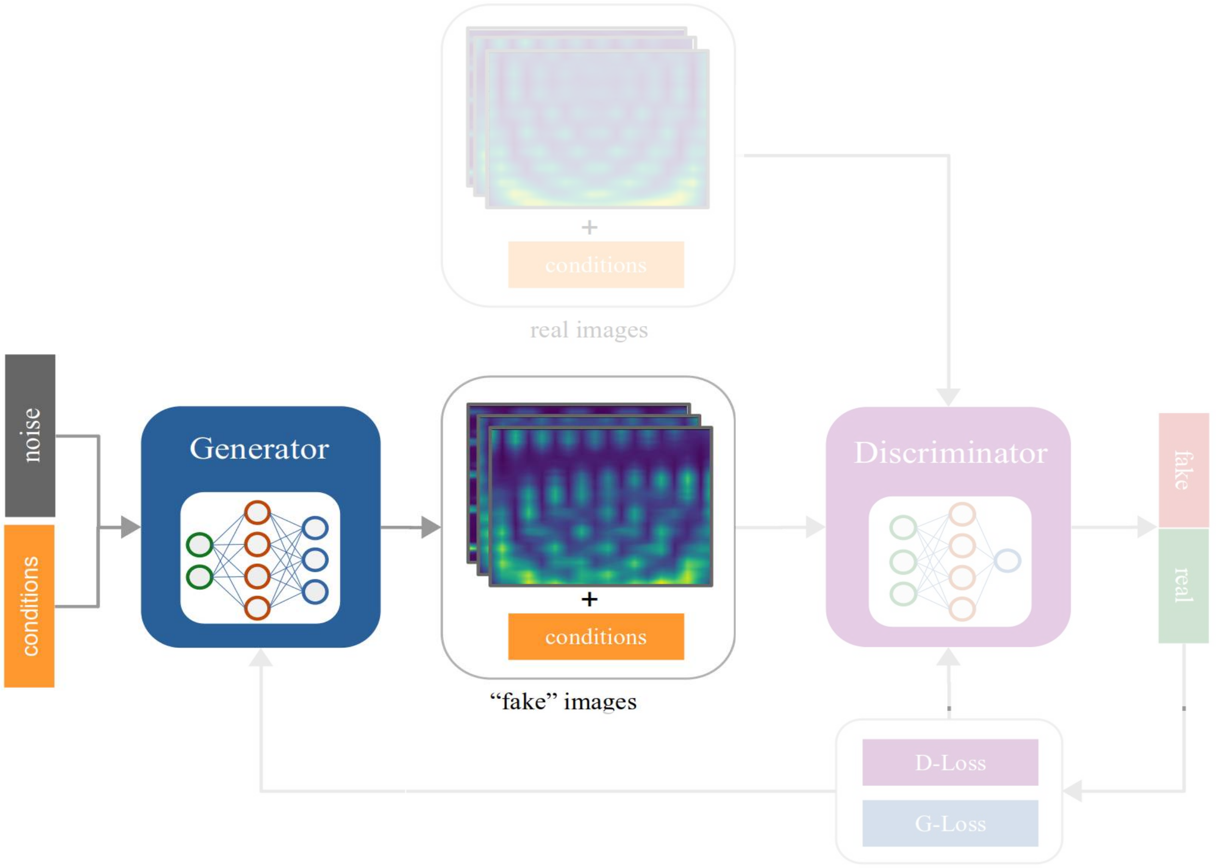
GAN: training and evaluation



Similarity measure of two images:
structural similarity index measure
(SSIM)



GAN as many-body simulator: the generator



Many-body systems (1d)

S=1/2-model

$$H = \sum_n \mathbf{S}_n \cdot \mathbf{S}_{n+1} + \xi_n^x S_n^x + \xi_n^y S_n^y + \mathcal{N}_y (-1)^n S_n^x + B_x S_n^y$$

conditional parameter:

N_y: local alternating Neel magnetic field

B_x: uniform Zeeman field

- gapless many-body Hamiltonian

S=1-model

$$H = \sum_n \left[1 + (-1)^n \Delta_J + \xi_1\right] \mathbf{S}_n \cdot \mathbf{S}_{n+1} + \left[J_2 + \xi_2\right] \mathbf{S}_n \cdot \mathbf{S}_{n+2}$$

conditional parameter:

Δ_J: variation in first neighbor interaction

J_2: second neighbor interaction

- interacting spin-1 system with topological order

Hubbard model

$$H = t \sum_{n,s} c_{n,s}^\dagger c_{n+1,s} + \sum_n U\left(\rho_{n,\uparrow} - 1/2\right)\left(\rho_{n,\downarrow} - 1/2\right) + \mu \sum_\sigma c_{n,\sigma}^\dagger c_{n,\sigma} + \sum_n + \xi (-1)^n S_n^y$$

conditional parameter:

U: Hubbard interaction

μ: chemical potential

- interacting fermionic system

Predictions: Many-body systems (validation set)

Hubbard model

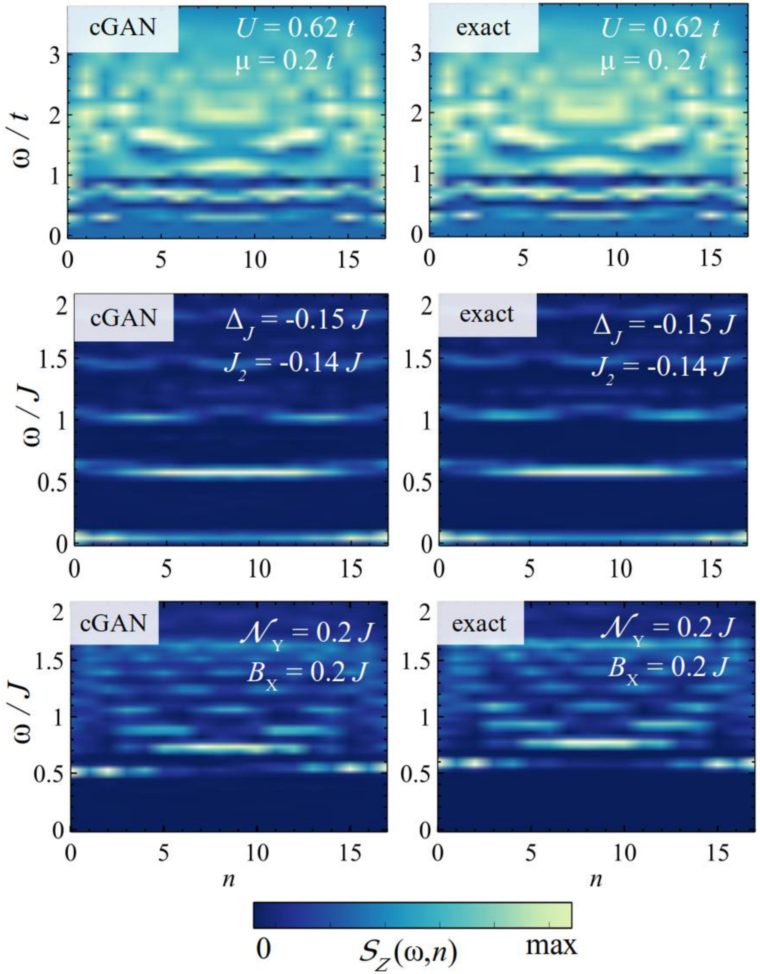
SSIM = 0.993

S=1

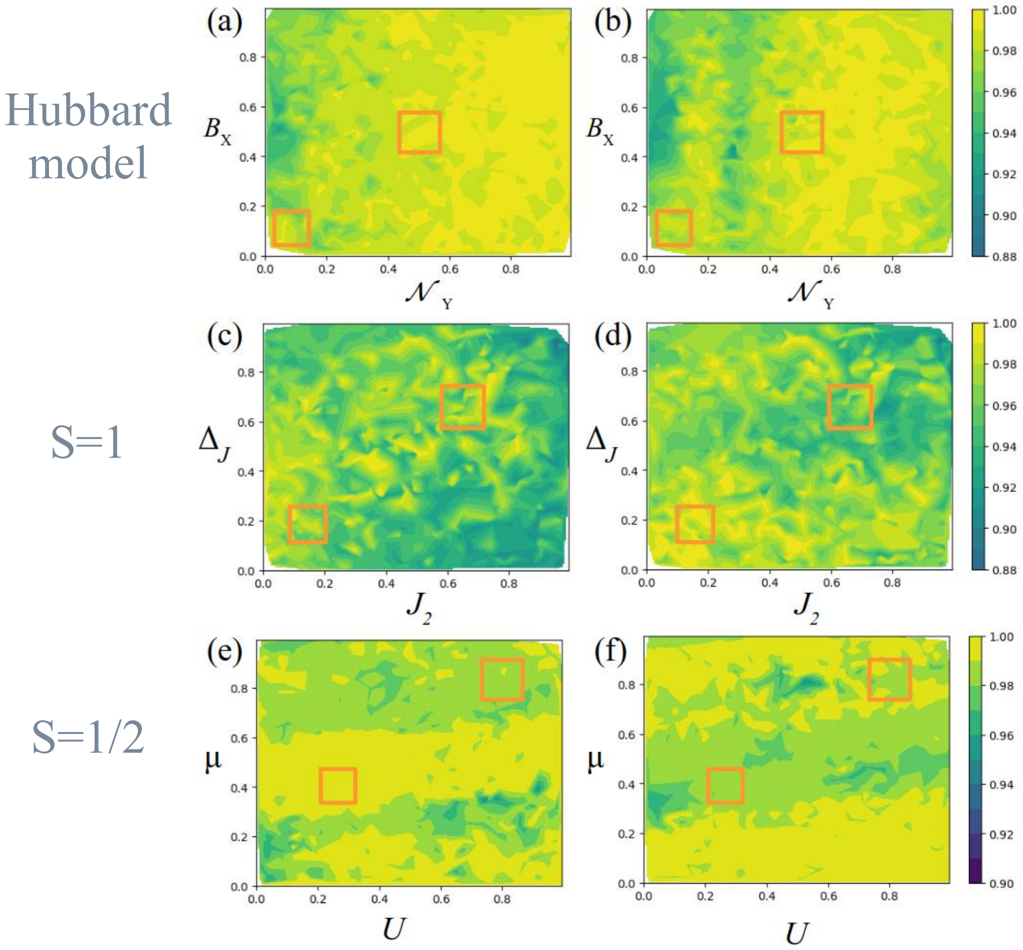
SSIM = 0.990

S=1/2

SSIM = 0.991

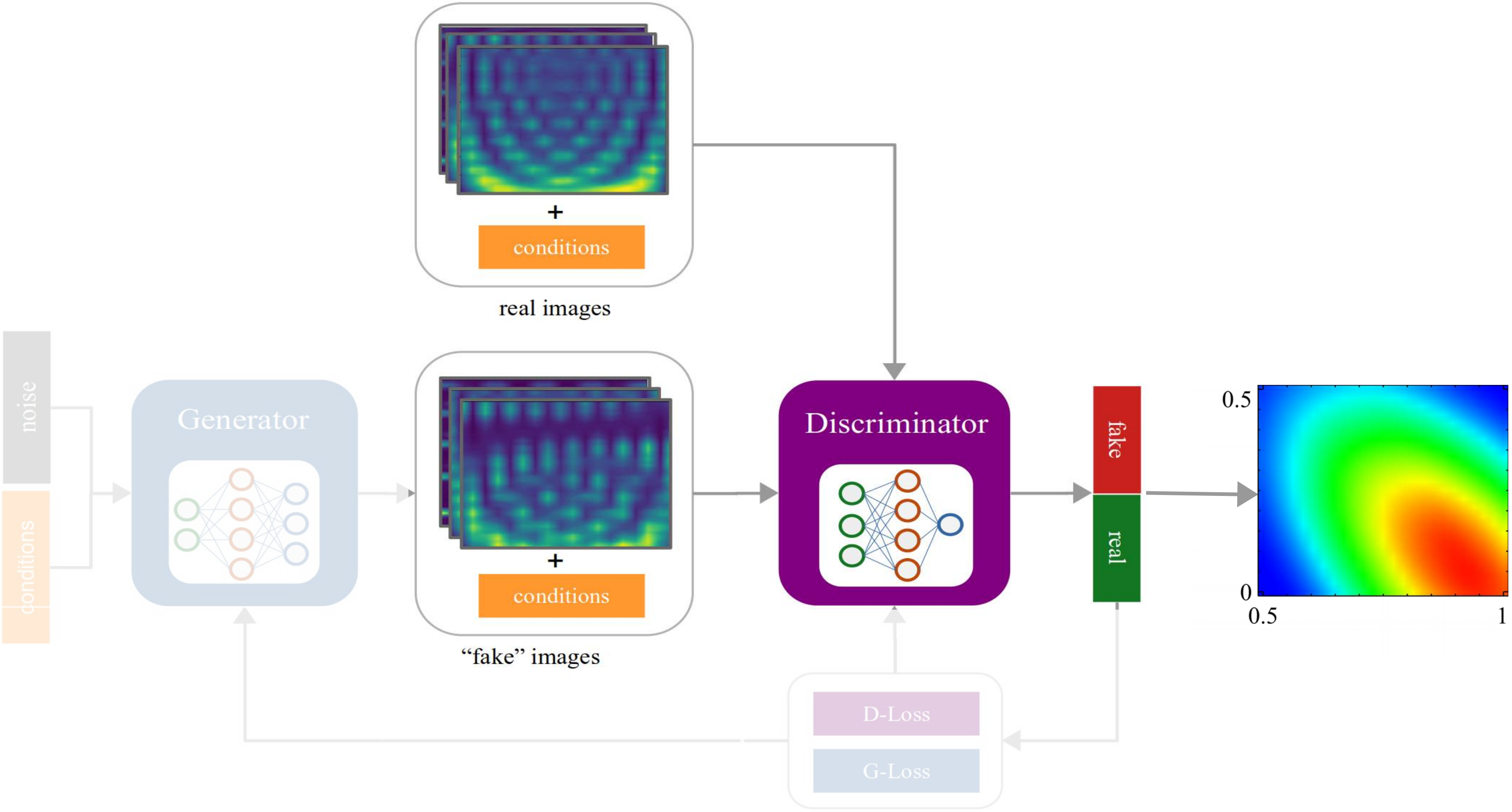


GAN: SSIM parameterspace



- SSIM in interval [0,1]
- *left*: trained on full parameterspace
- *right*: train-validation split
- homogeneous fluctuations due to intrinsic randomnes of cGAN

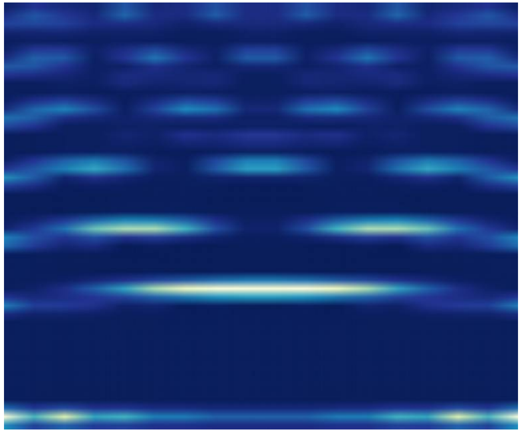
GAN as many-body assessor: the discriminator



Question: Can you guess the Hamiltonian?

spin-1 Heisenberg-model

$$H(\Delta_J, J_2) = \sum_n \left[1 + (-1)^n \Delta_J + \xi_1\right] \mathbf{S}_n \cdot \mathbf{S}_{n+1} + \left[J_2 + \xi_2\right] \mathbf{S}_n \cdot \mathbf{S}_{n+2}$$



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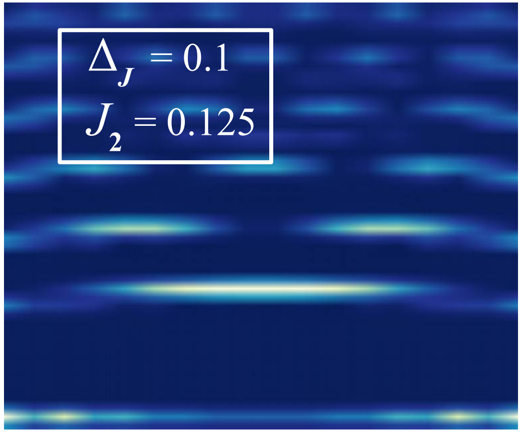
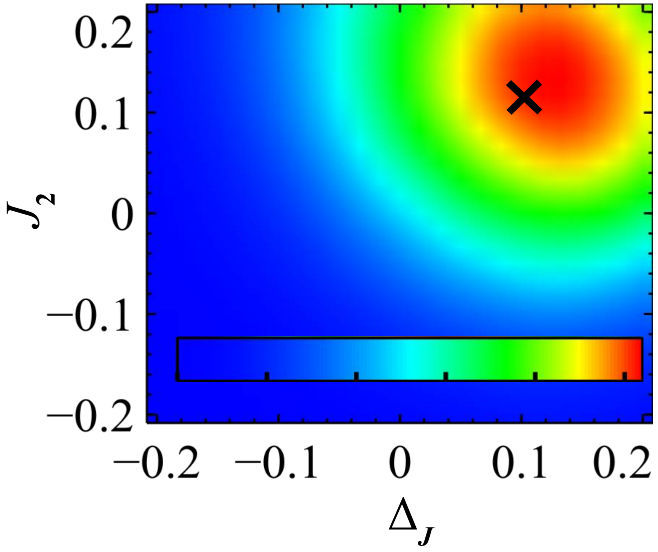
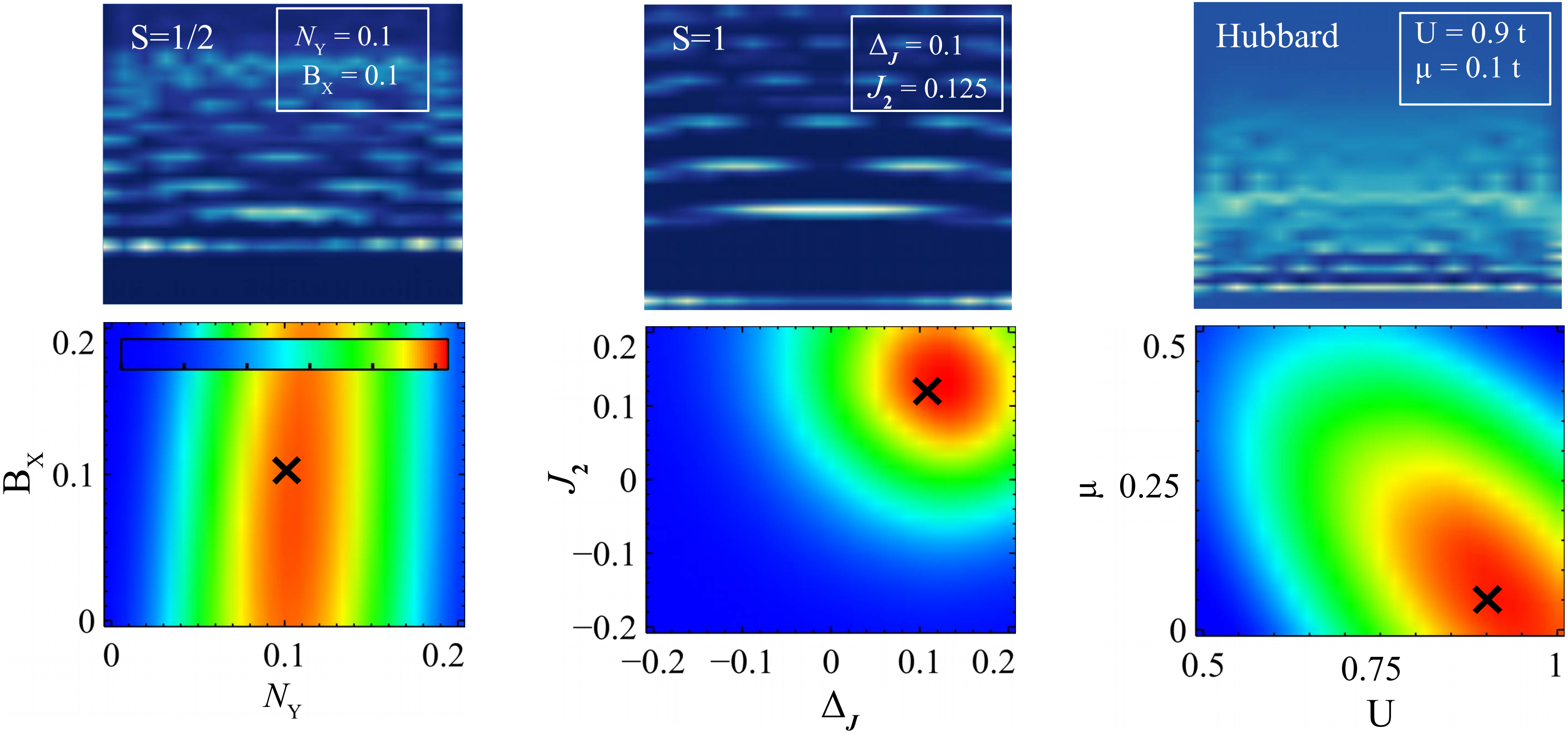
$$H(\Delta_J, J_2) = \sum_n [1 + (-1)^n \Delta_J + \xi_1]\, \mathbf{S}_n \cdot \mathbf{S}_{n+1} + [J_2 + \xi_2]\, \mathbf{S}_n \cdot \mathbf{S}_{n+2}$$



cGAN

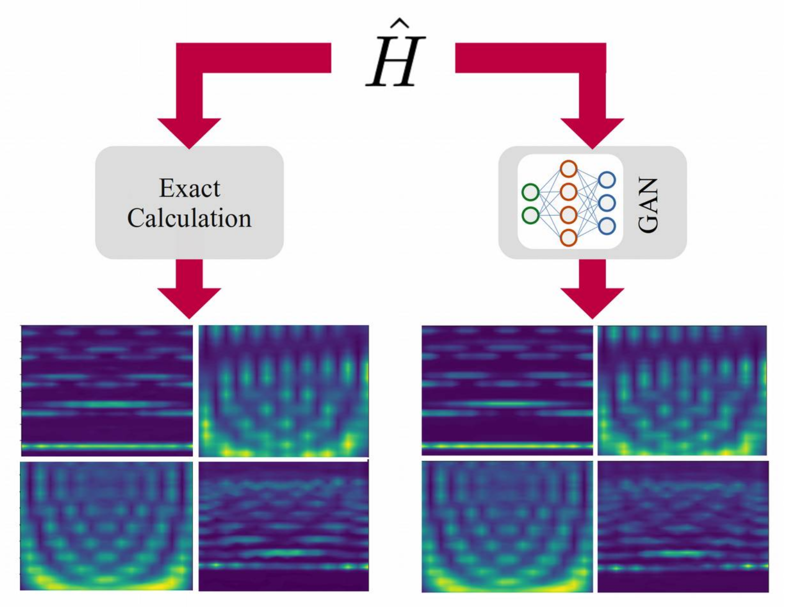


GAN as many-body assessor: Hamiltonian estimation



Take home message

Generative deep learning models can be a powerful tool for the **simulation** and **analysis** of many-body systems



arXiv:2201.12127

EXTRA SLIDES

Single-particle case: tight-binding systems

tight-binding Hamiltonian

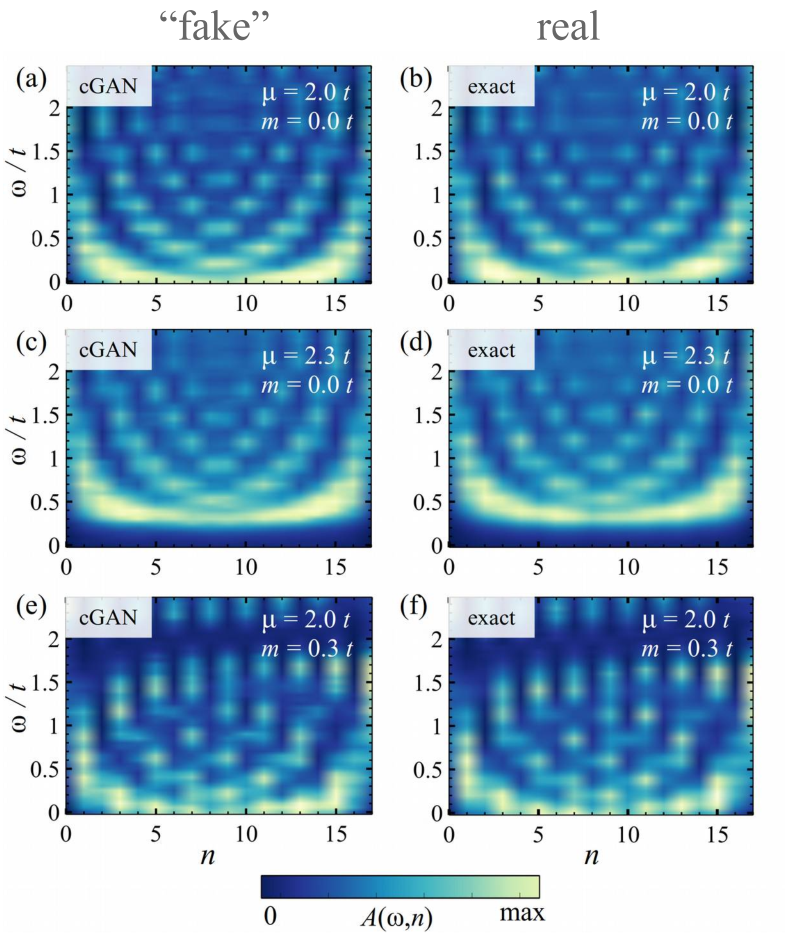
$$H(\mu, m) = \sum_{\langle n,m \rangle} t_{nm} c_n^\dagger c_m + \sum_n v_n c_n^\dagger c_n + \sum_n \mu\, c_n^\dagger c_n + m_n (-1)^n c_n^\dagger c_n$$

conditional parameter: μ, m

randomness: v_n

local density of states

$$A(\omega, n) = \langle n | \delta(\mathcal{H} - \omega) | n \rangle$$



(1) gapless many-body spin-1/2-model (1d)

$$H(\mathcal{N}_y, B_x) = \sum_n \mathbf{S}_n \cdot \mathbf{S}_{n+1} + \xi_n^x S_n^x + \xi_n^y S_n^y + \mathcal{N}_y(-1)^n S_n^x + B_x S_n^y$$

conditional parameter:

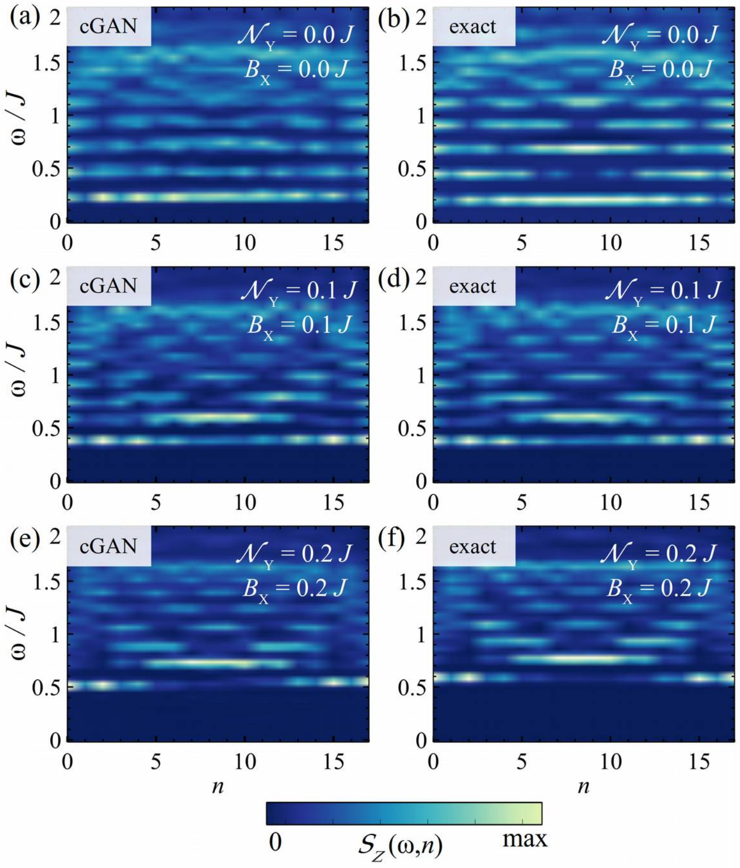
N_y: local alternating Neel magnetic field

B_x: uniform Zeeman field

dynamical spin correlator

$$\mathcal{S}(\omega, n) = \langle GS|S_n^z \delta(H - \omega + E_{GS}) S_n^z|GS\rangle$$

“fake” real



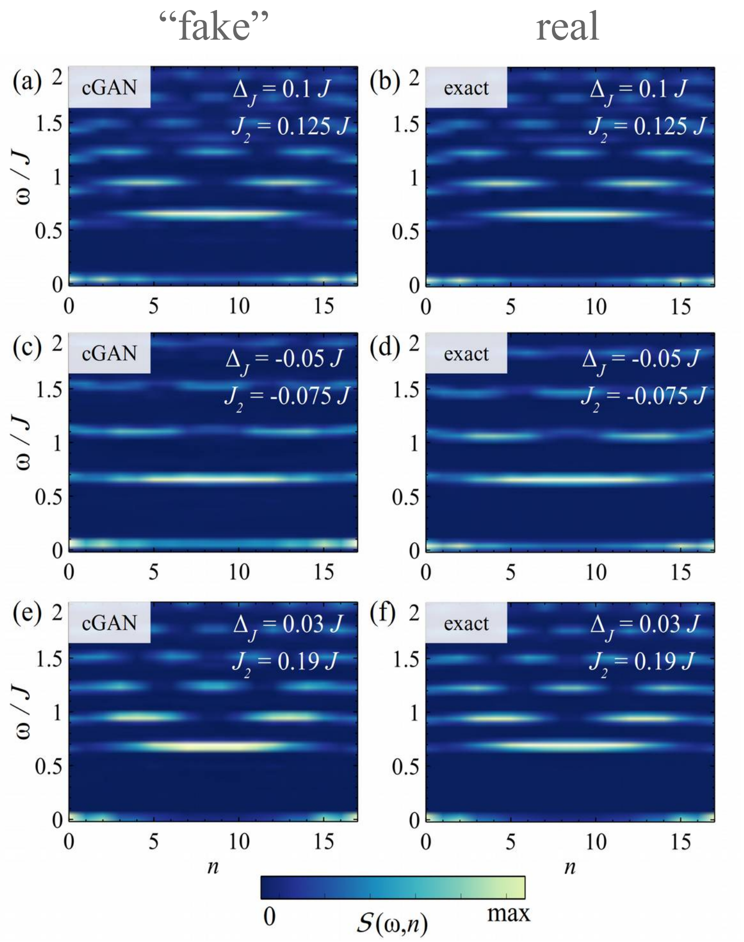
(2) Interacting spin-1 system with topological order

$$H(\Delta_J, J_2) = \sum_n [1 + (-1)^n \Delta_J + \xi_1] \mathbf{S}_n \cdot \mathbf{S}_{n+1} + [J_2 + \xi_2] \mathbf{S}_n \cdot \mathbf{S}_{n+2}$$

conditional parameter: Δ_J, J_2

full dynamical spin correlator

$$\mathcal{S}(\omega, n) = \sum_\alpha \langle GS | S_n^\alpha \delta(H - \omega + E_{GS}) S_n^\alpha | GS \rangle$$



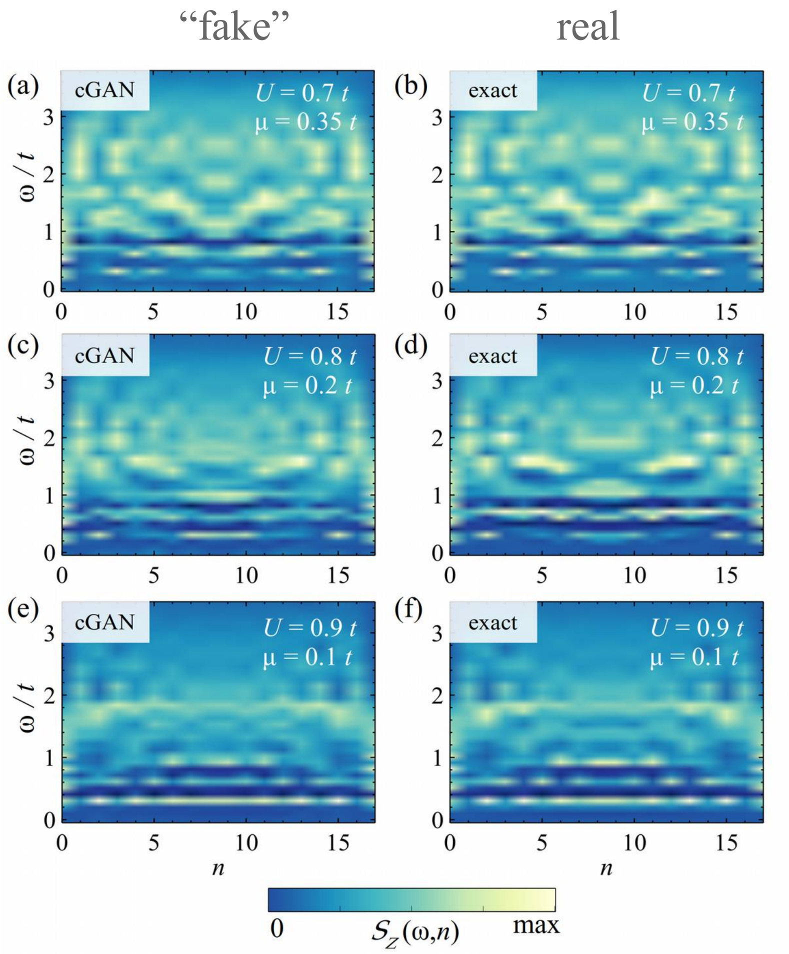
(3) 1d Hubbard model (interacting fermionic system)

$$H(U,\mu) = t\sum_{n,s} c^\dagger_{n,s}c_{n+1,s} + \sum_{n} +\xi(-1)^n S^y_n + \sum_n U\,(\rho_{n,\uparrow}-1/2)(\rho_{n,\downarrow}-1/2) + \mu\sum_\sigma c^\dagger_{n,\sigma}c_{n,\sigma}$$

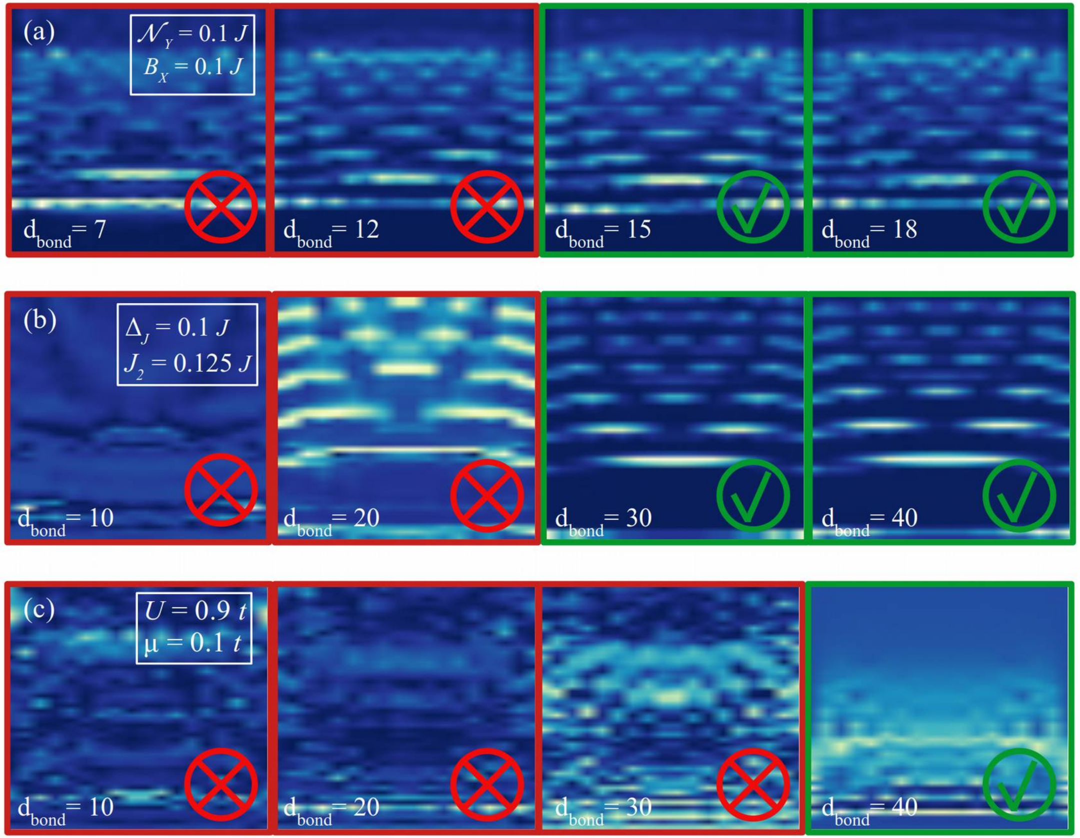
conditional parameter: U, μ

dynamical spin correlator

$$\mathcal{S}(\omega,n) = \langle GS|S^z_n\delta(H-\omega+E_{GS})S^z_n|GS\rangle$$



GAN as many-body assessor: outlier detection



- faulty nonphysical dynamical spectra for each many-body system

  → emulated by insufficient bond dimension of tensor-network calculations

- cGAN: distinguishes between physical and numerical noise / artifacts