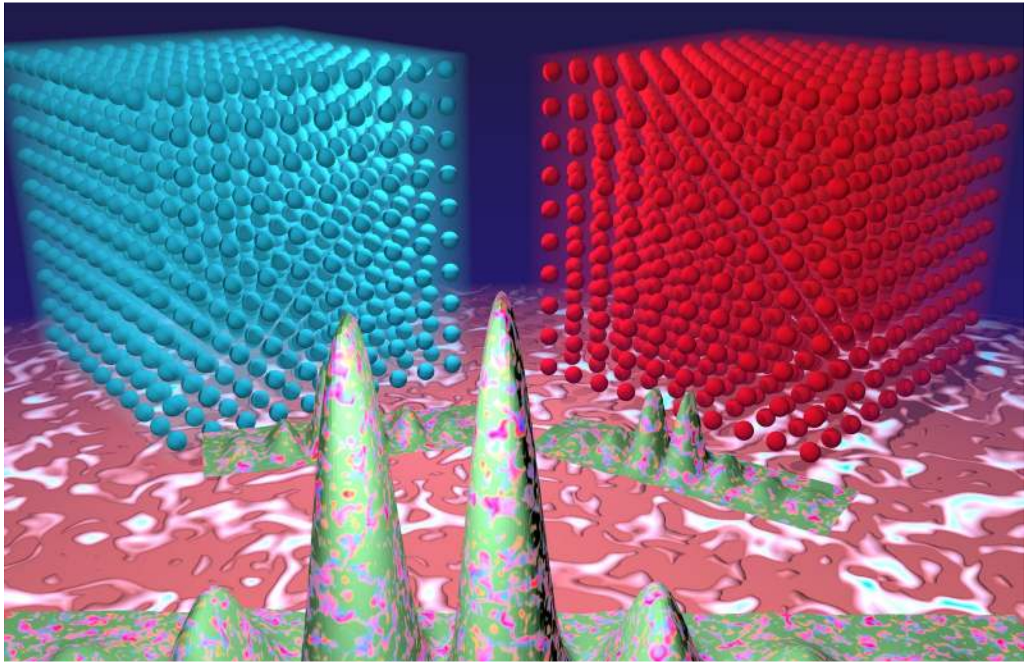
Designing and learning quantum many-body matter with generative adversarial networks

Jose Lado

Department of Applied Physics, Aalto University, Finland



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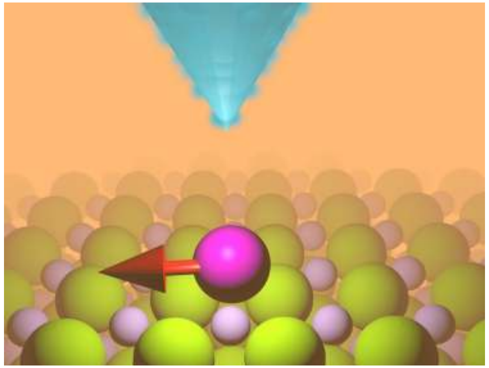
arXiv:2304.10852 (2023)

April 12th 2023, Machine Learning and (Quantum) Physics Workshop, Obergurgl

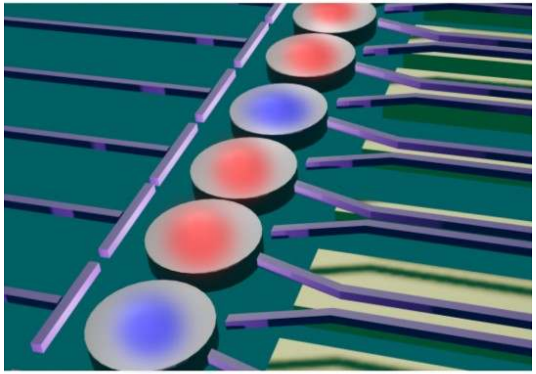
Knowledge and uncertainty

How can we navigate phenomena in quantum systems in the presence of hidden and unknown contributions?

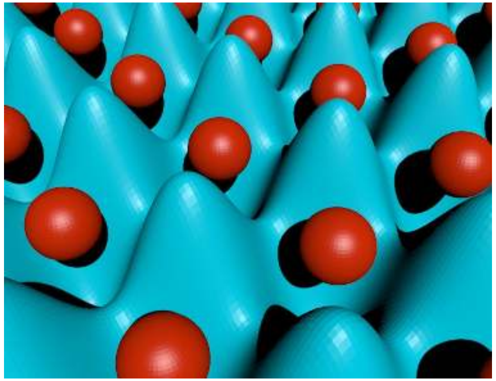
Quantum materials



Quantum devices



Quantum simulators



Often, there are things that we know about our system, and things that we do not

We want to navigate the possible phenomenologies incorporating both knowledge and randomness

Navigating the manifold of Hamiltonians

How can we navigate a complex manifold of Hamiltonians

$$H(\lambda_i, w_i)$$

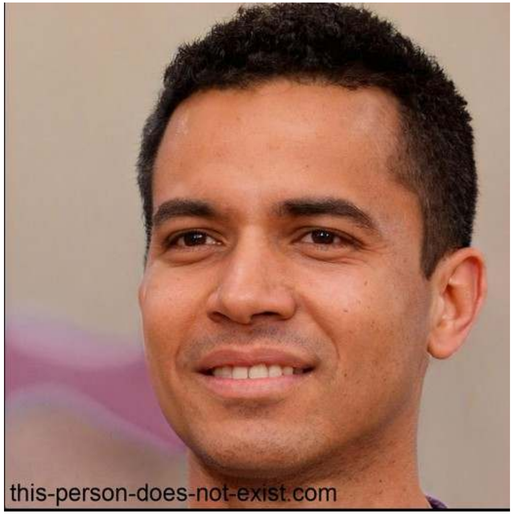
Parameters of our system
- Magnetic and electric fields
- Hopping
- Many-body interactions

Hidden variables
- Smaller marginal parameters
- Disorder
- Computational limitations
- Pure randomness

How can we do it with high quality and limited amount of data?

Navigating the manifold of humans

Generative adversarial learning allows to create ultra-high quality realistic fake data



https://this-person-does-not-exist.com

Navigating the manifold of cats

Generative adversarial learning allows to create ultra-high quality realistic fake data

https://thesecatsdonotexist.com/

Generative conditional adversarial learning

The generator

Generate real-looking data

(given conditions)

VS

The discriminator

Guess if some data is real or fake

(given conditions)

Behind the scenes

cGAN for quantum many-body generation, assessment and learning

Rouven Koch

Aalto (Finland)

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cGAN for experimental Hamiltonian learning

Alberto Bordin

TU Delft & QuTech (Netherlands)

David van Driel

TU Delft & QuTech (Netherlands)

Eliska Greplova

TU Delft (Netherlands)

arXiv:2304.10852 (2023)

Designing quantum many-body matter with conditional generative adversarial networks

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The generative many-body problem

We will take interacting many-body one dimensional systems

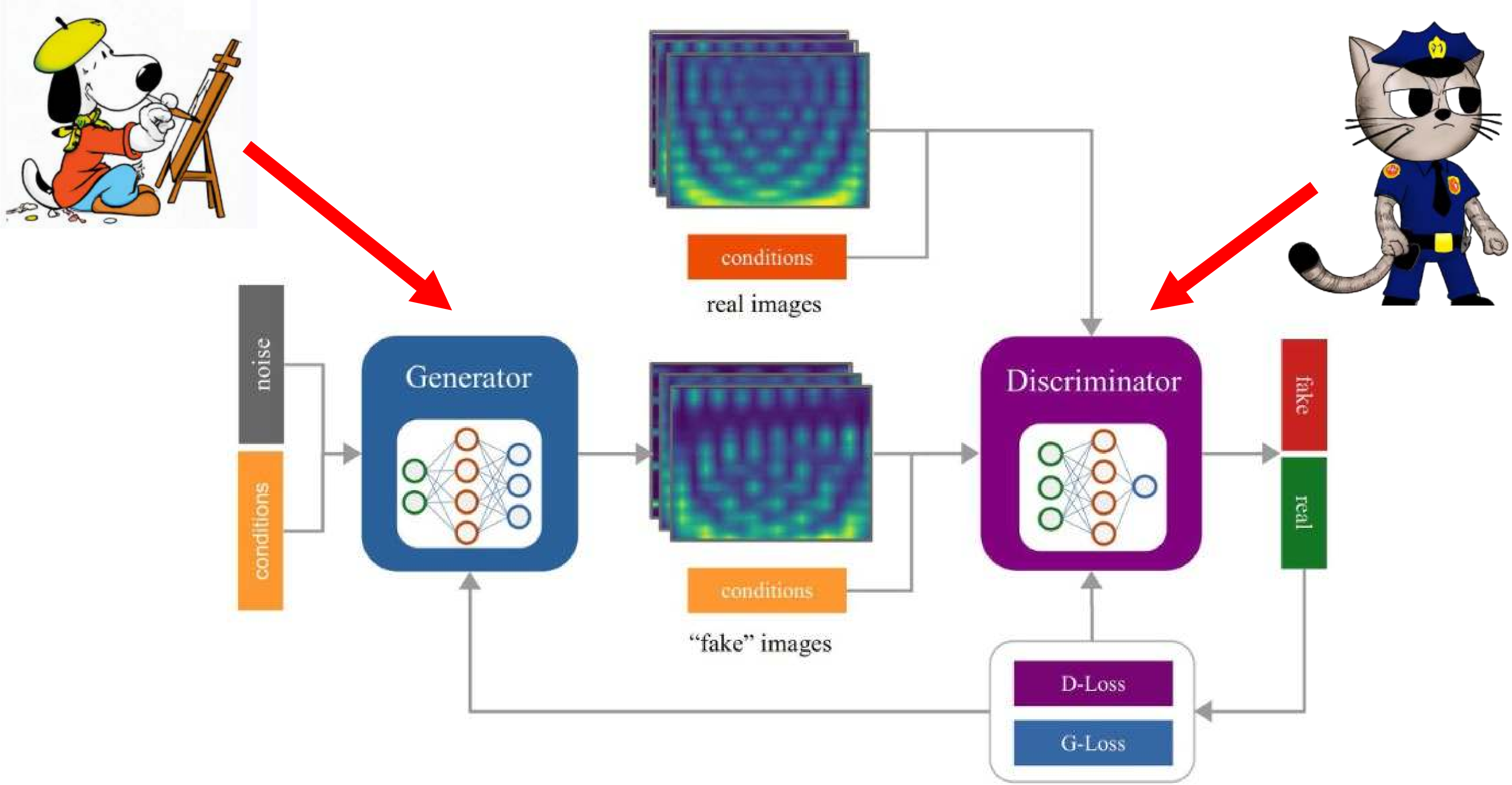
$$H \sim \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

We will take Hamiltonian with controlled terms and hidden variables $H(\lambda_i, w_i)$

With the objective of the discriminator to compute the dynamical spin excitation spectra

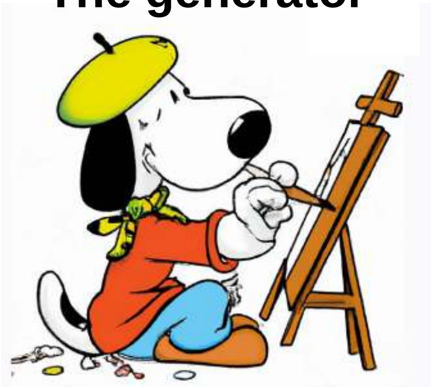
$$\mathcal{S}_z(\omega, n) = \langle \mathrm{GS} | \hat{S}_n^z \delta(\omega \mathcal{I} - \hat{H} + E_{\mathrm{GS}}) \hat{S}_n^z | \mathrm{GS} \rangle$$

The architecture of a conditional generative neural network



The value of a generator and a discriminator

The generator



- Explore the phase space of highly complex models
- Account for unknown variables and noise

The discriminator

- Know if some data is physical
- Measure the likelihood of certain model parameters

The training of a cGAN

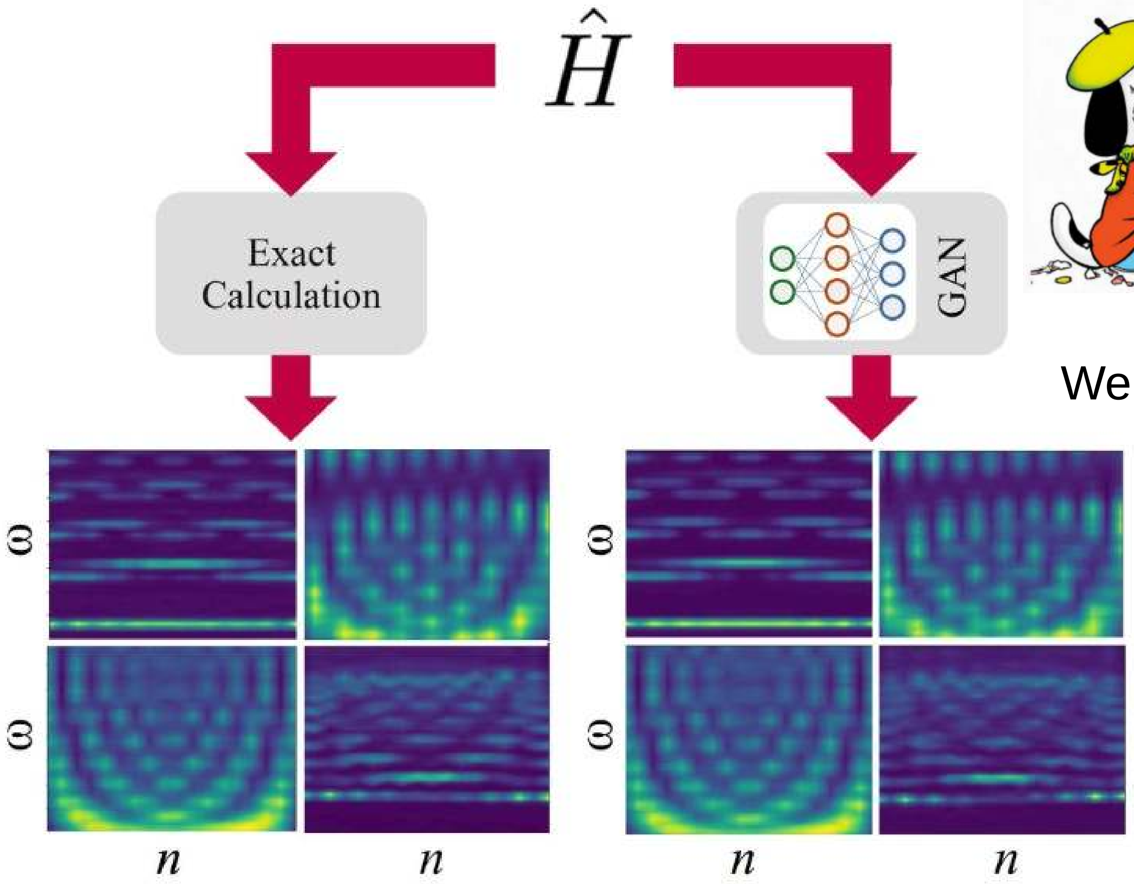
The loss function of the adversarial game

$$\min_G \max_D V(D,G) = \mathbb{E}_{x\sim p_{\text{data}}(\mathbf{x})}[\log D(\mathbf{x})] + \mathbb{E}_{z\sim p_z(\mathbf{z})}(\log\{1 - D[G(\mathbf{z})]\}).$$

After training, the generator is capable of creating data indistinguishable from the real one

The generator: solving quantum many-body Hamiltonians with the cGAN

Direct calculation VS cGAN

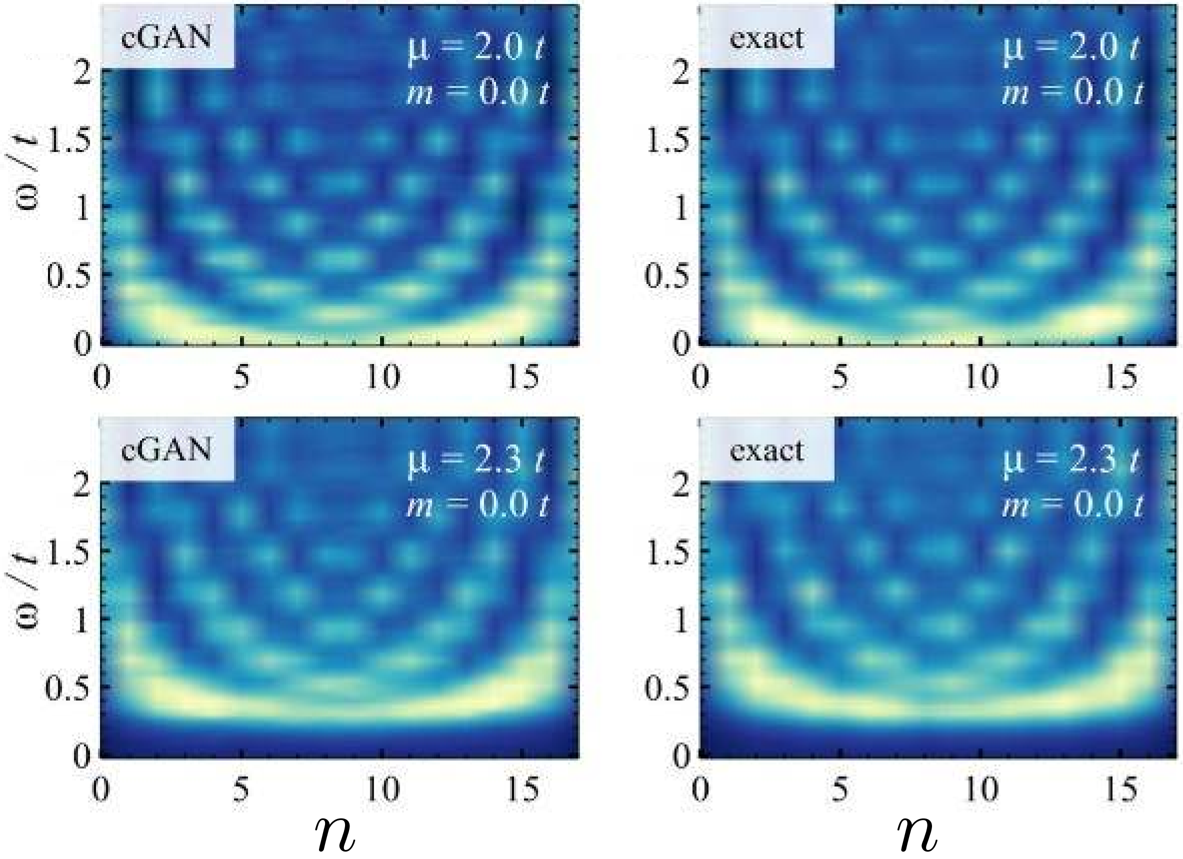


We will demonstrate this with different models

- A non-interacting model
- A spin model with spinon excitations
- A spin model with topological order
- An interacting fermionic model

(solved exactly with tensor-networks)

A non-interacting model: tight binding model



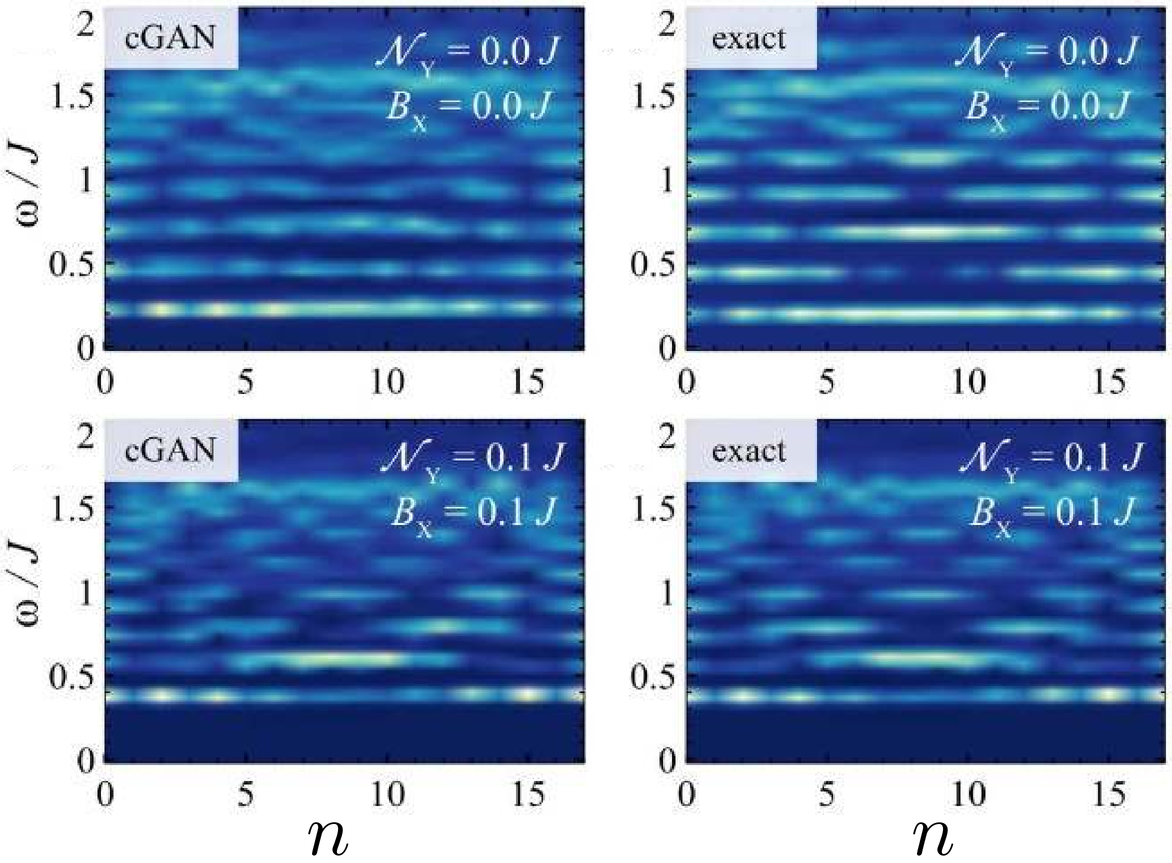
The Hamiltonian manifold

$$H(\mu, m) = t \sum_n c_n^\dagger c_{n+1} + \text{H.c.} + \mu \sum_n c_n^\dagger c_n + m \sum_n (-1)^n c_n^\dagger c_n + \sum_n v_n c_n^\dagger c_n,$$

Local spectral function
(density of states)

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

A spin model with spinon excitations: the S=1/2 Heisenberg chain



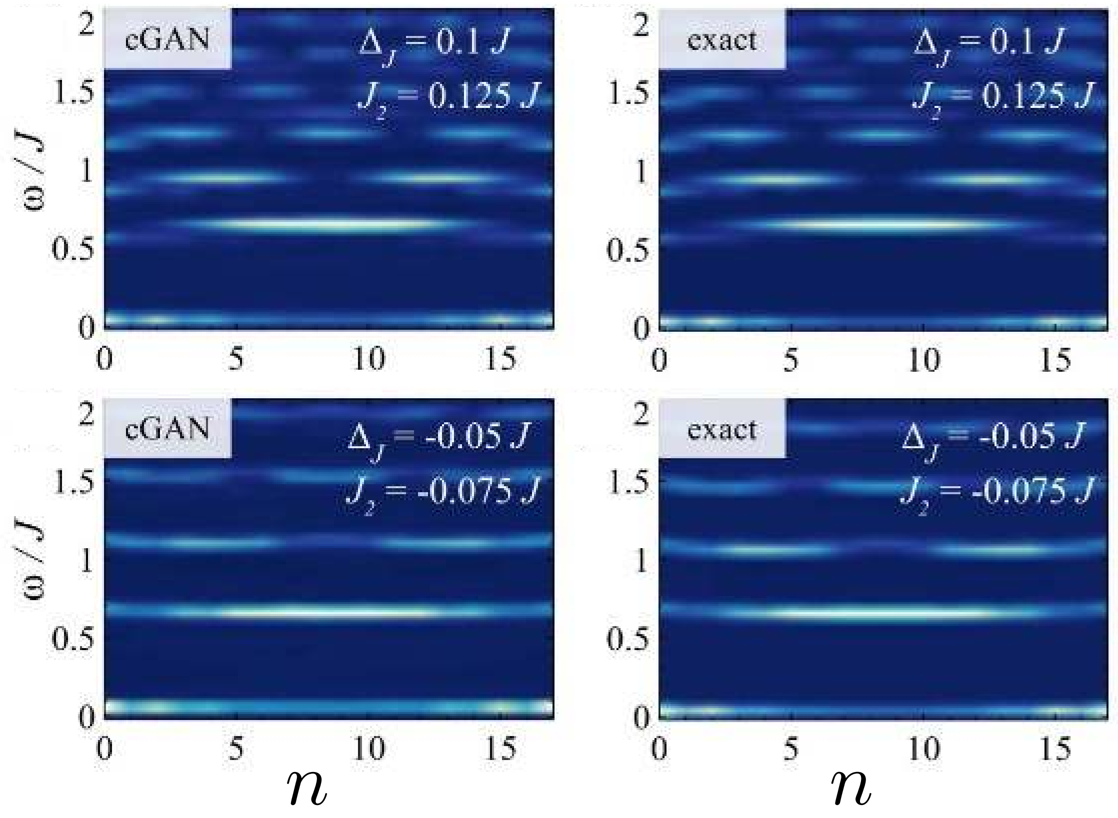
The Hamiltonian manifold

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

Local spin structure factor

$$\mathcal{S}_z(\omega, n) = \langle \mathrm{GS} | \hat{S}_n^z \delta(\omega \mathcal{I} - \hat{H} + E_{\mathrm{GS}}) \hat{S}_n^z | \mathrm{GS} \rangle$$

A spin model with topological order: the S=1 Heisenberg chain



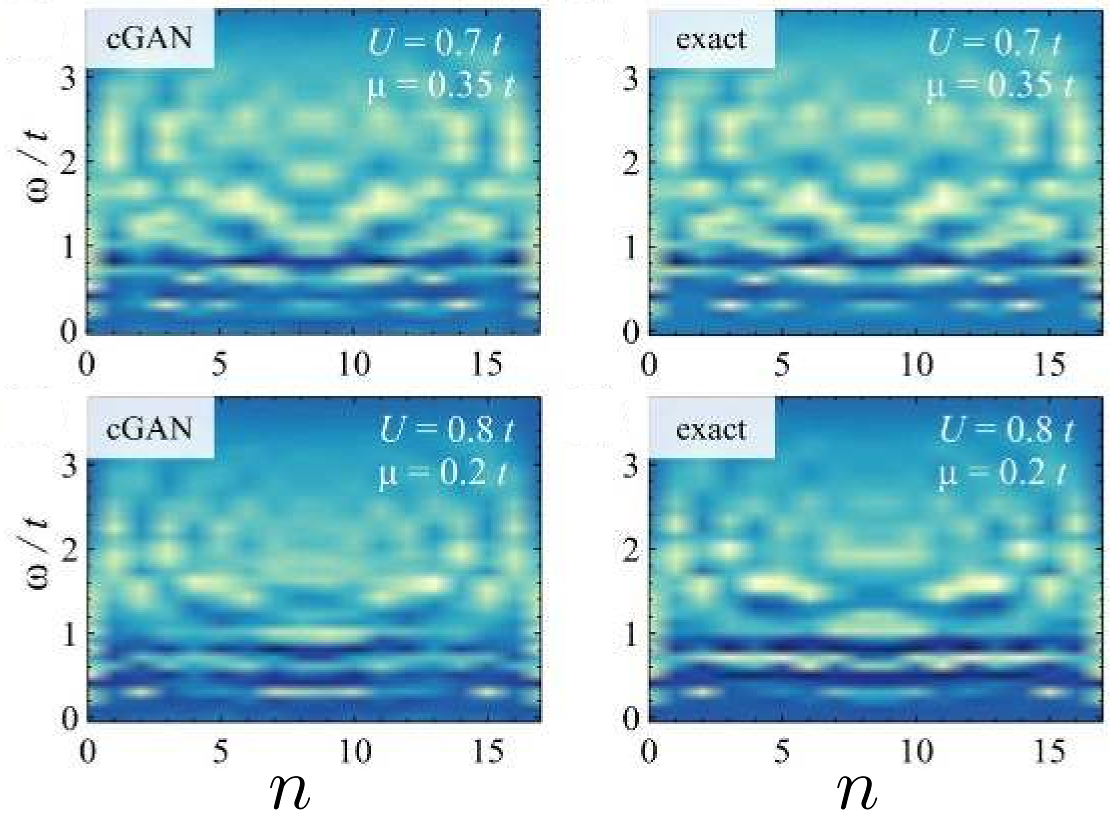
The Hamiltonian manifold

$$H(\Delta_J, J_2) = J\sum_n \mathbf{S}_n\cdot\mathbf{S}_{n+1} + J_2\sum_n \mathbf{S}_n\cdot\mathbf{S}_{n+2}$$
$$+\,\Delta_J\sum_n(-1)^n\,\mathbf{S}_n\cdot\mathbf{S}_{n+1}$$
$$+\sum_n \xi_n^J\,\mathbf{S}_n\cdot\mathbf{S}_{n+1} + \sum_n \xi_n^{J_2}\,\mathbf{S}_n\cdot\mathbf{S}_{n+2}$$

Local spin structure factor

$$\mathcal{S}_z(\omega, n) = \langle\mathrm{GS}|\hat{S}_n^z\,\delta(\omega\mathcal{I} - \hat{H} + E_{\mathrm{GS}})\,\hat{S}_n^z|\mathrm{GS}\rangle$$

An interacting fermionic model: the doped Hubbard model



The Hamiltonian manifold

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

The local spin structure factor

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

The discriminator: assessing and learning data with the cGAN

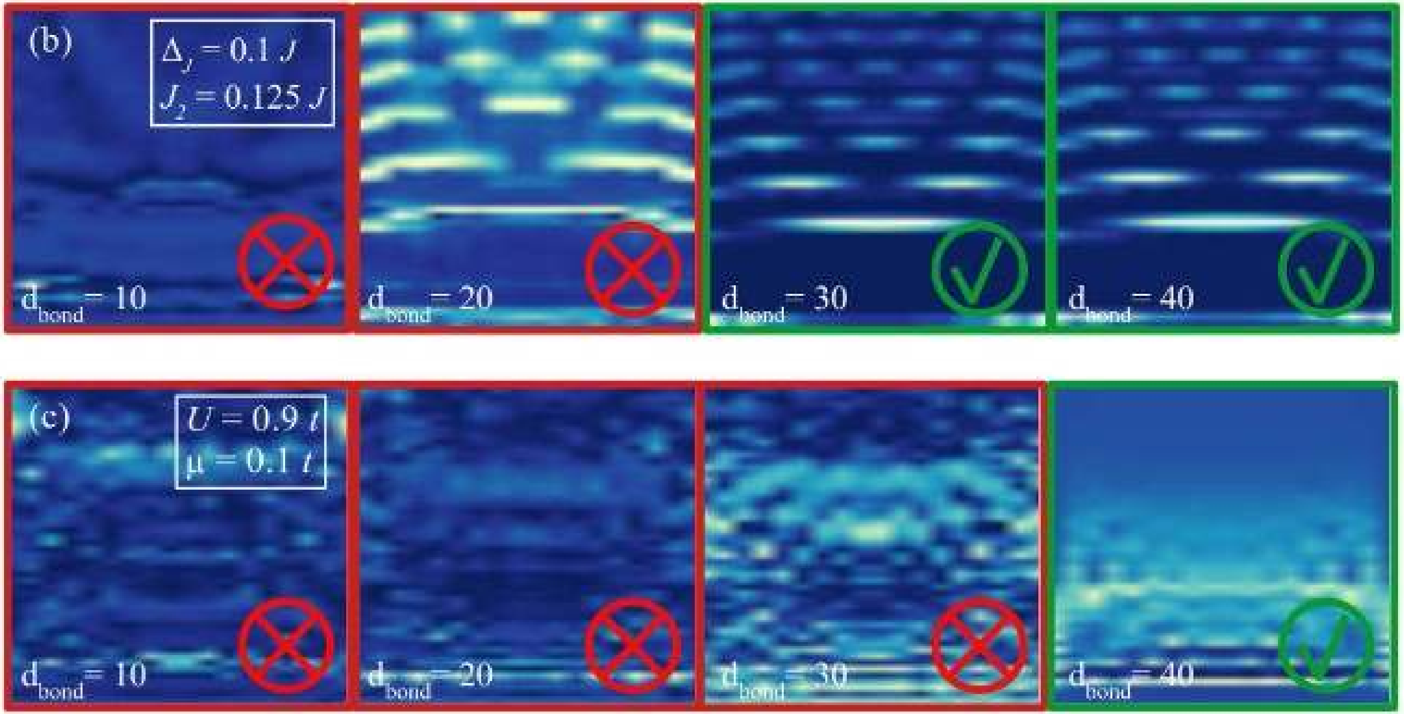
Anomaly detection with the discriminator

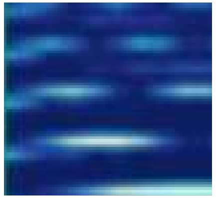
Given a certain data, does it correspond to a physical system?

- Is this a real dynamical correlator?
- Or is it just unphysical?

(in our simulations we can continuously go from physical to unphysical results by changing the bond dimension of the tensor-network)

Anomaly detection with the discriminator





The discriminator intrinsically allows assessing certain data is physically meaningful

Hamiltonian learning with the discriminator

Given a certain data, to which parameters does it correspond?

- Due to the hidden variables, there can be several different data consistent for the same Hamiltonian parameters
- There can be several Hamiltonians consistent with this data

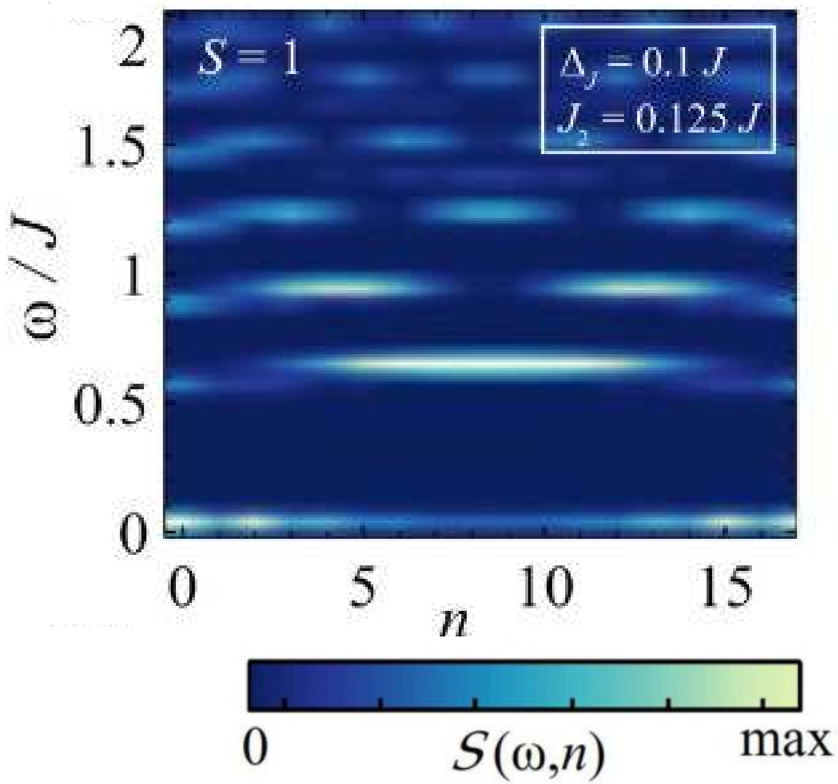
$$H(\lambda_i, w_i)$$

Physical parameters

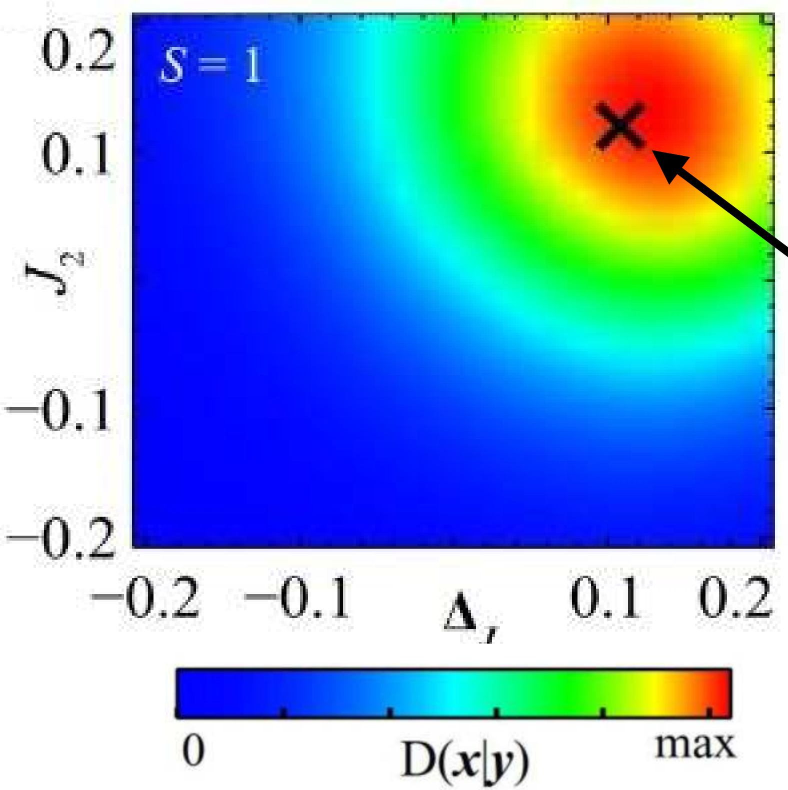
Hidden parameters

Hamiltonian learning with the discriminator

The data



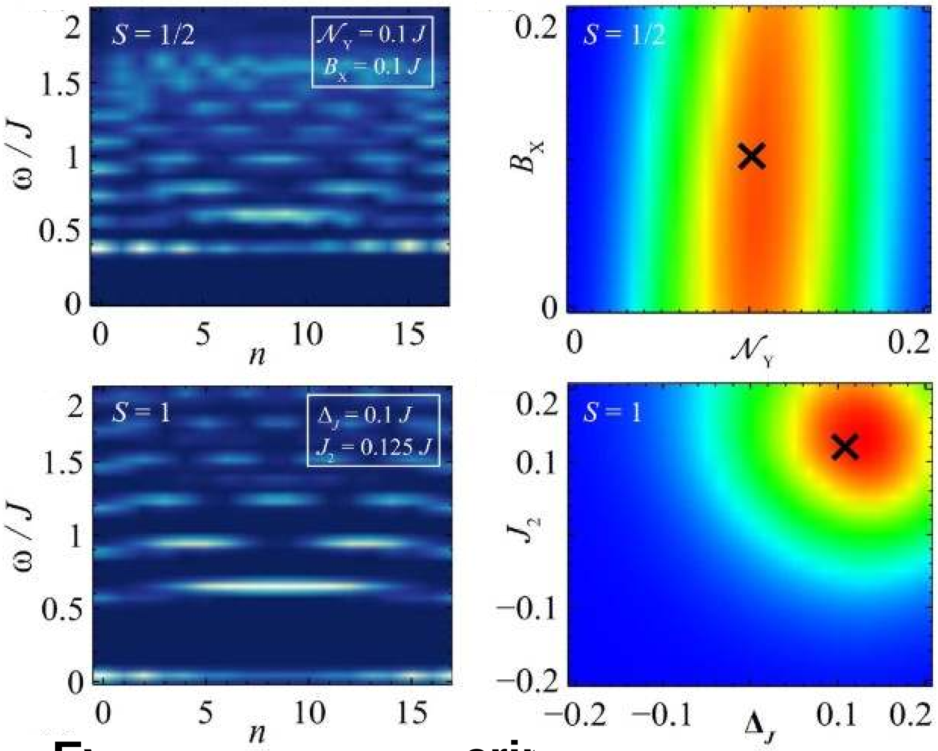
The rating of the discriminator



Real value
of the parameters

Hamiltonian learning with the discriminator

Dynamical correlator **Parameter rating**



Parameter set		Rating
$\{\lambda_i\}_0$	$\longrightarrow$	“unlikely”
$\{\lambda_i\}_1$	$\longrightarrow$	“perhaps”
$\{\lambda_i\}_2$	$\longrightarrow$	“very likely”

Evaluating the discriminator in the phase space yields the compatible Hamiltonians

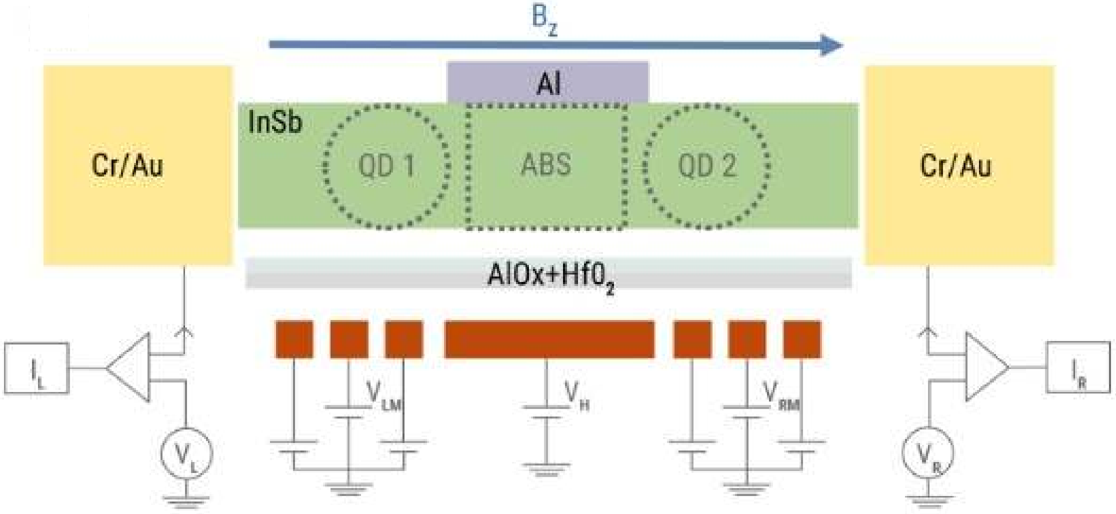
Experimental adversarial Hamiltonian learning of quantum dots in a minimal Kitaev chain

arXiv:2304.10852 (2023)

A minimal experimental device for Hamiltonian learning

The device

Gated nanowire proximitized
to superconductors, with
magnetic field and spin-orbit coupling



Nature 614, 445–450 (2023)

The low energy model

A two site model

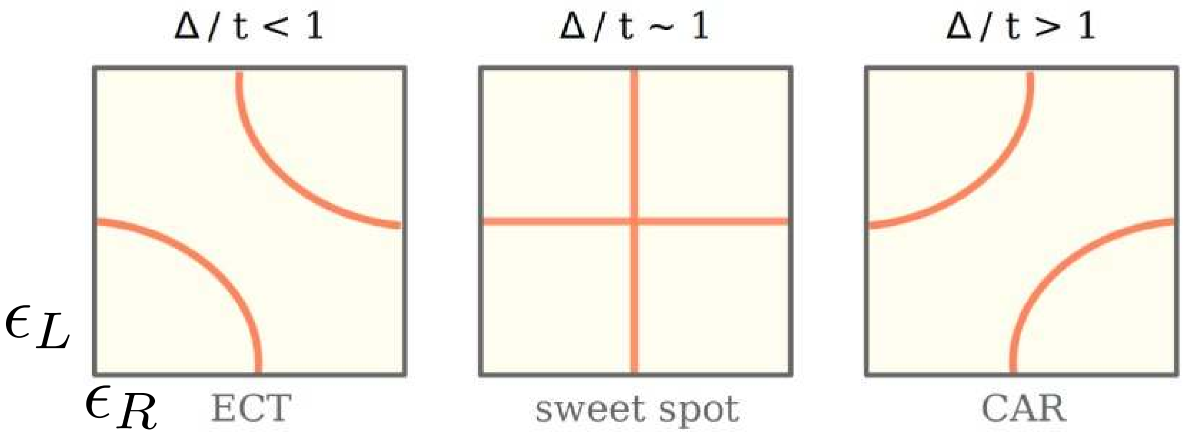
The theoretical model to train the cGAN

The model: Kitaev model $H = td_L^\dagger d_R + \Delta d_L^\dagger d_R^\dagger + \epsilon_L d_L^\dagger d_L + \epsilon_R d_R^\dagger d_R + h.c.$

The observable: the differential conductance $G^0_{\alpha\beta} = dI_\alpha / dV_\beta$

(we include temperature and finite lead coupling non-pertubatively)

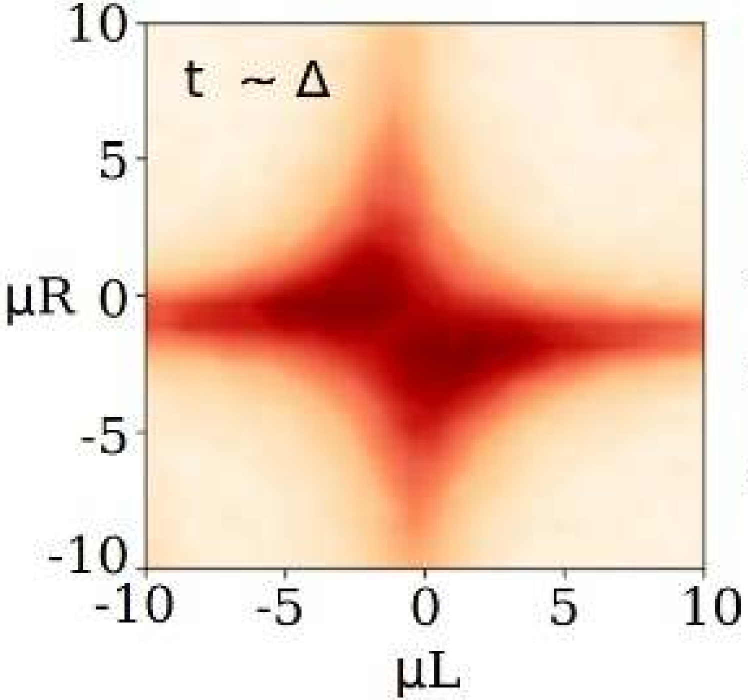
The main regimes of the model



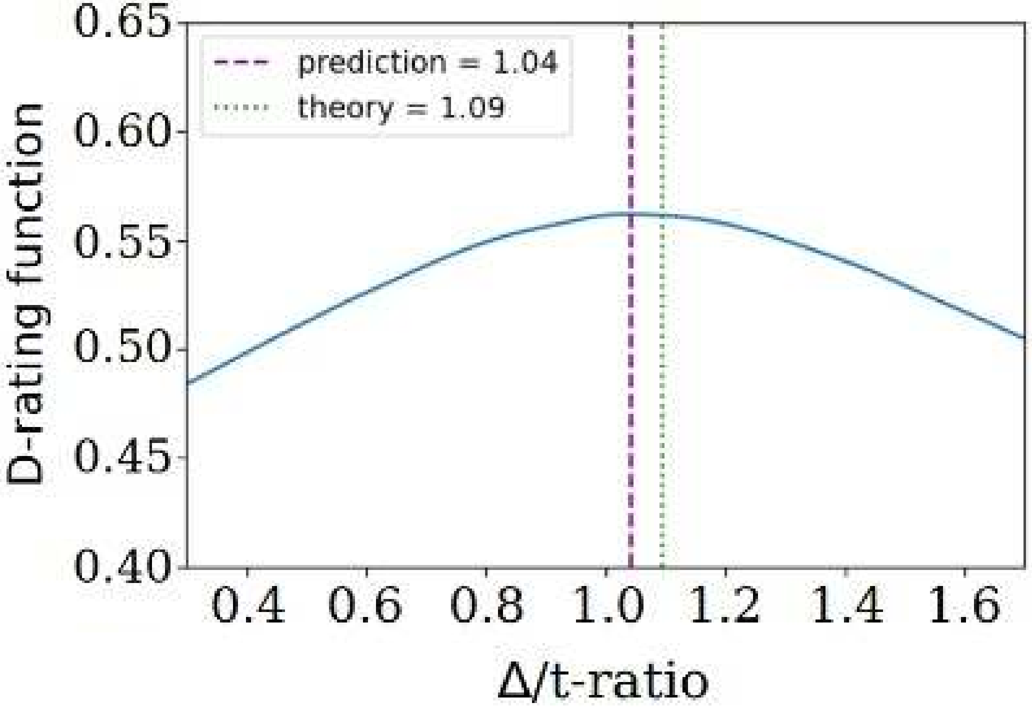
Learning Hamiltonian parameters from conductance

The likelihood of each parameters is evaluated with the trained discriminator

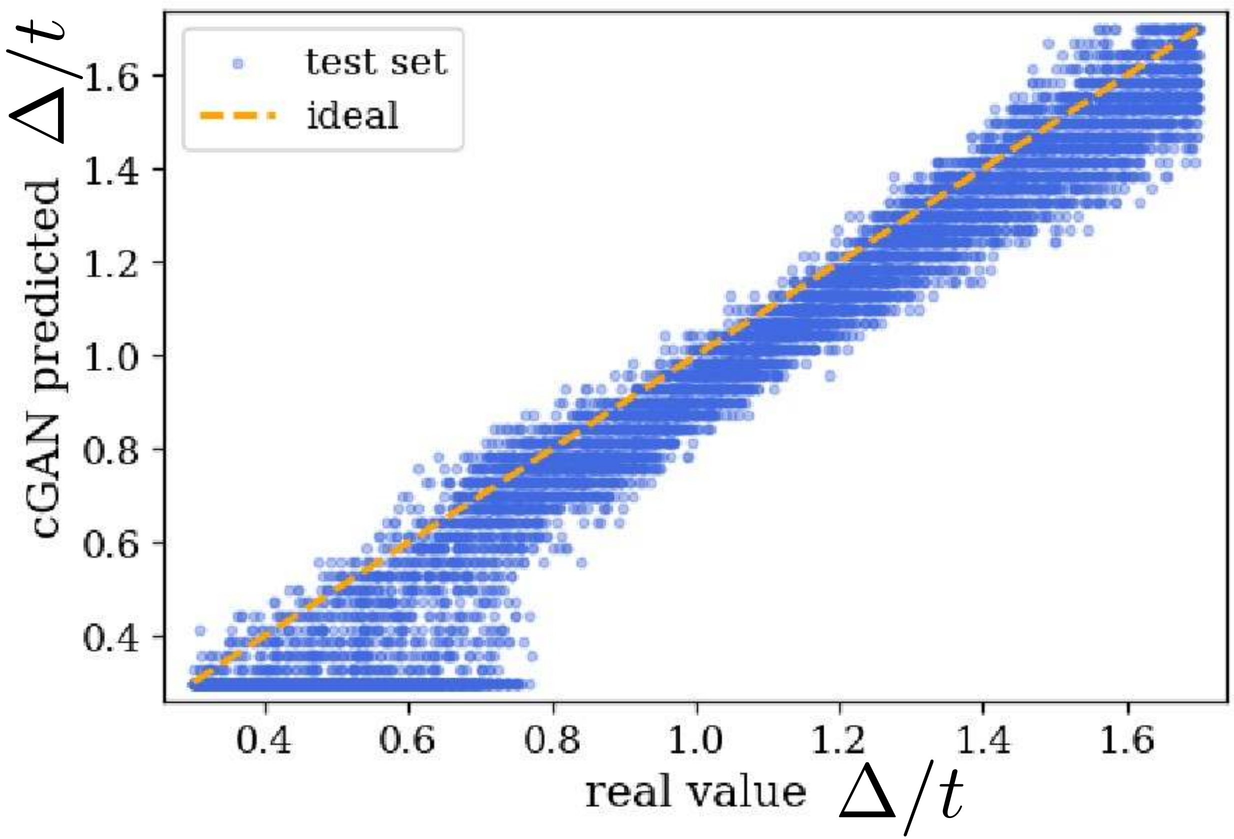
Conductance



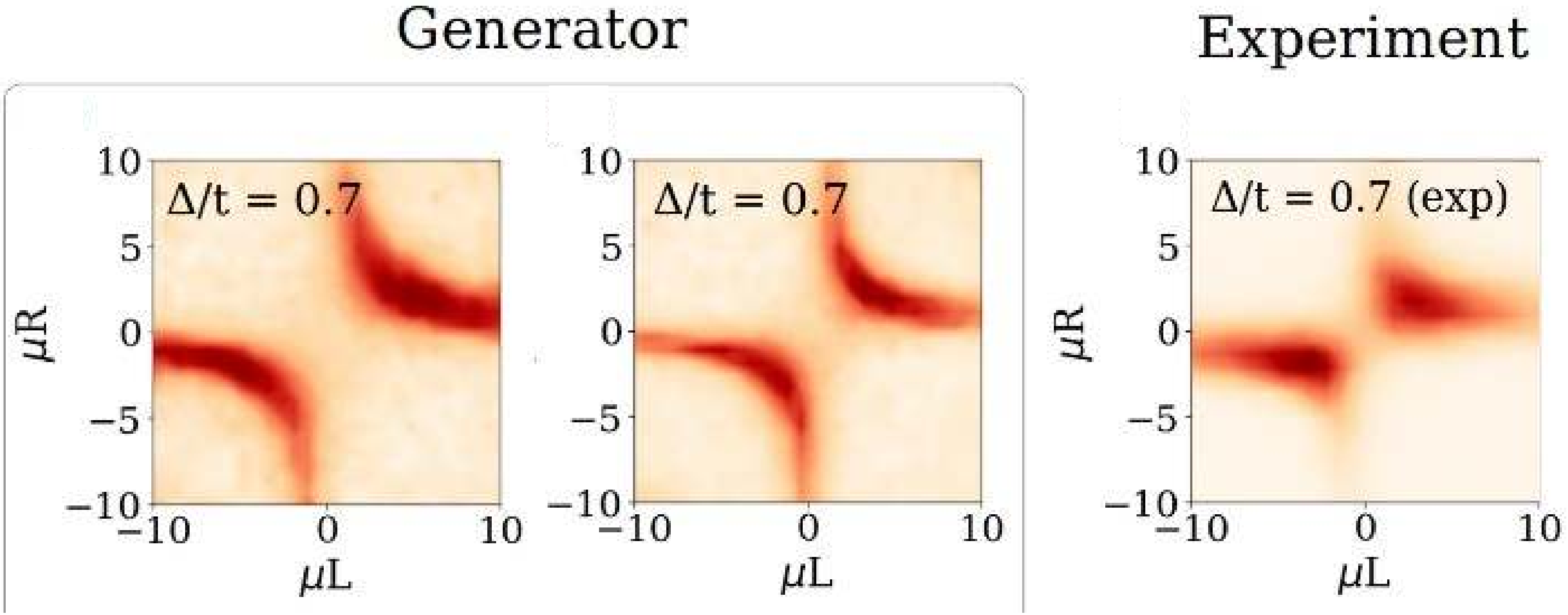
Discriminator rating



Learning Hamiltonian parameters from conductance



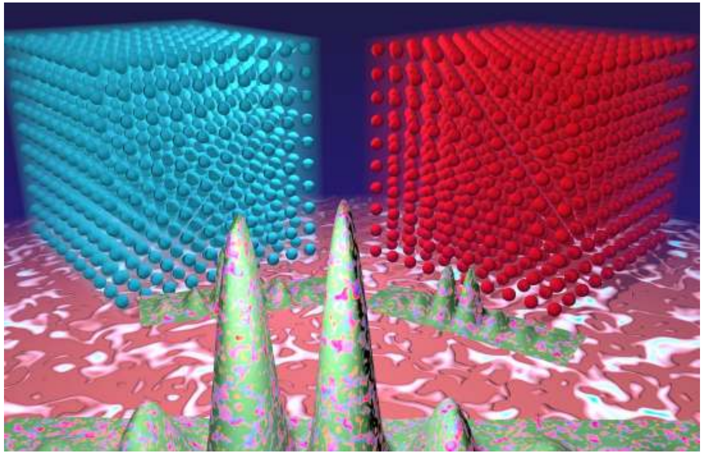
Hamiltonian inference with theoretical and experimental data



Evaluating the cGAN on experimental data allows extracting Hamiltonian parameters

Take home

Conditional generative adversarial learning allows exploring quantum many-body Hamiltonian manifolds and perform Hamiltonian inference of experimental data



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