Time-dependent Neural Quantum States

a new approach for quantum dynamics

Exploring the quantum chromodynamics phase diagram:
from hadrons and nuclei to matter under extreme conditions

Alejandro Romero-Ros
28th January 2025

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Plan de Recuperación, Transformación y Resiliencia
AGENCIA ESTATAL DE INVESTIGACIÓN
ICCUB
Institut de Ciències del Cosmos
UNIVERSITAT DE BARCELONA
EXCELENCIA MARÍA DE MAEZTU 04/2025-03/2031
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Learning the Ground State with Neural Quantum States

J. Rozalén Sarmiento, A. Rios

HadNucMat Workshop, 2025, Barcelona

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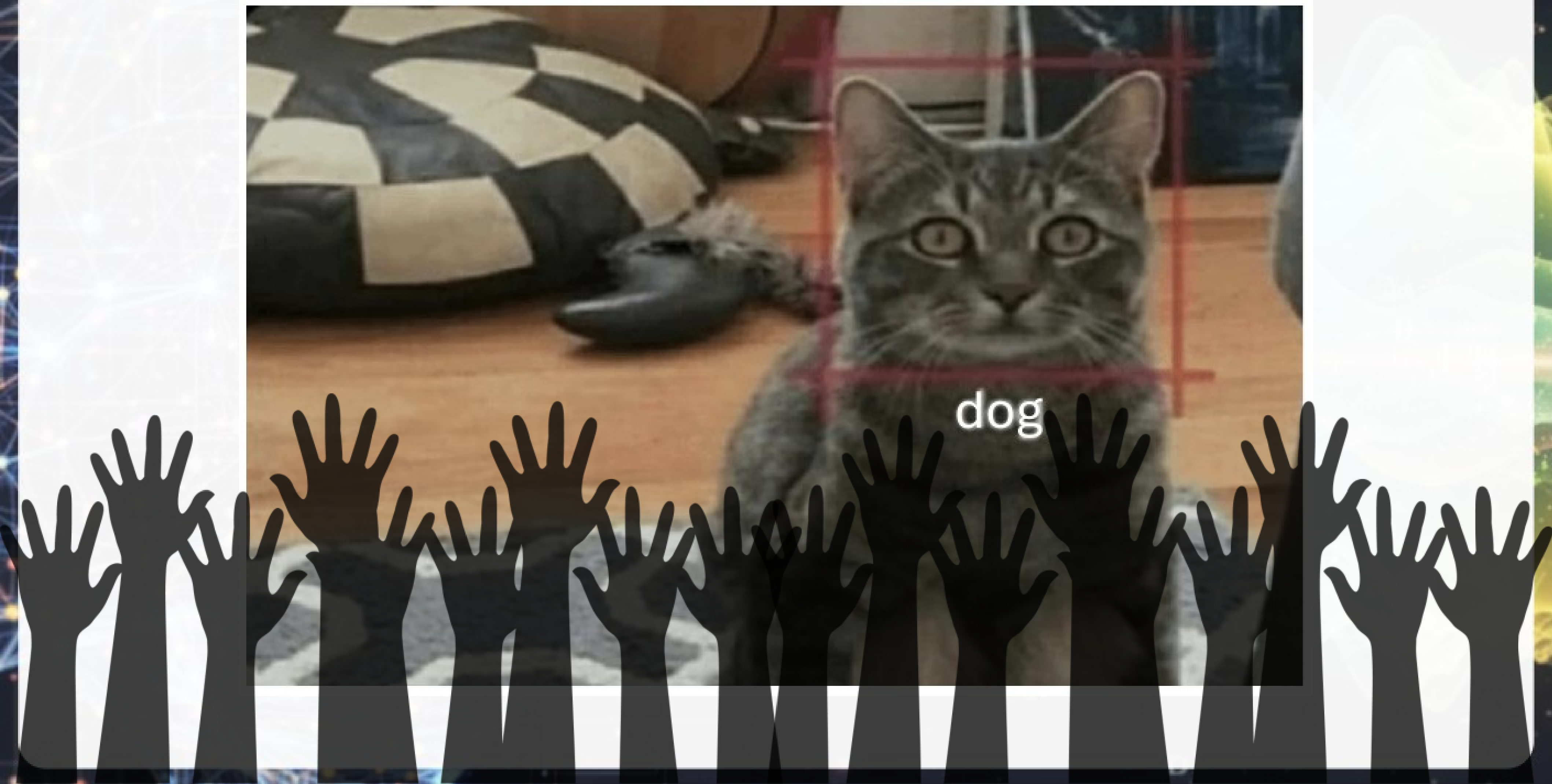
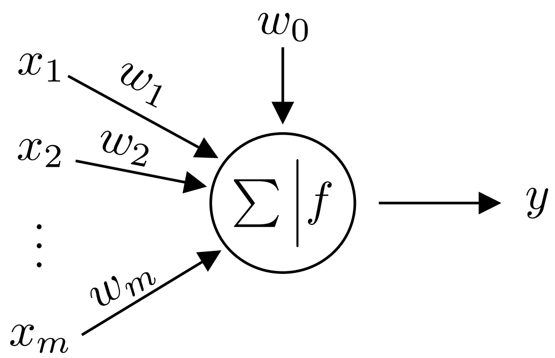
dog


dog

Artificial Neural Networks

Neuron or Perceptron



Artificial Neural Networks

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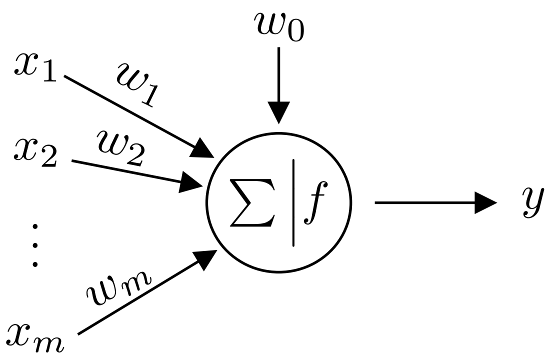
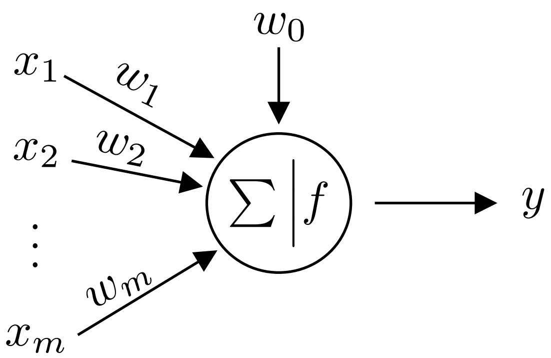


$$y = f\left(w_0 + \sum_{k}^{m} x_k w_k\right)$$

Neuron or Perceptron



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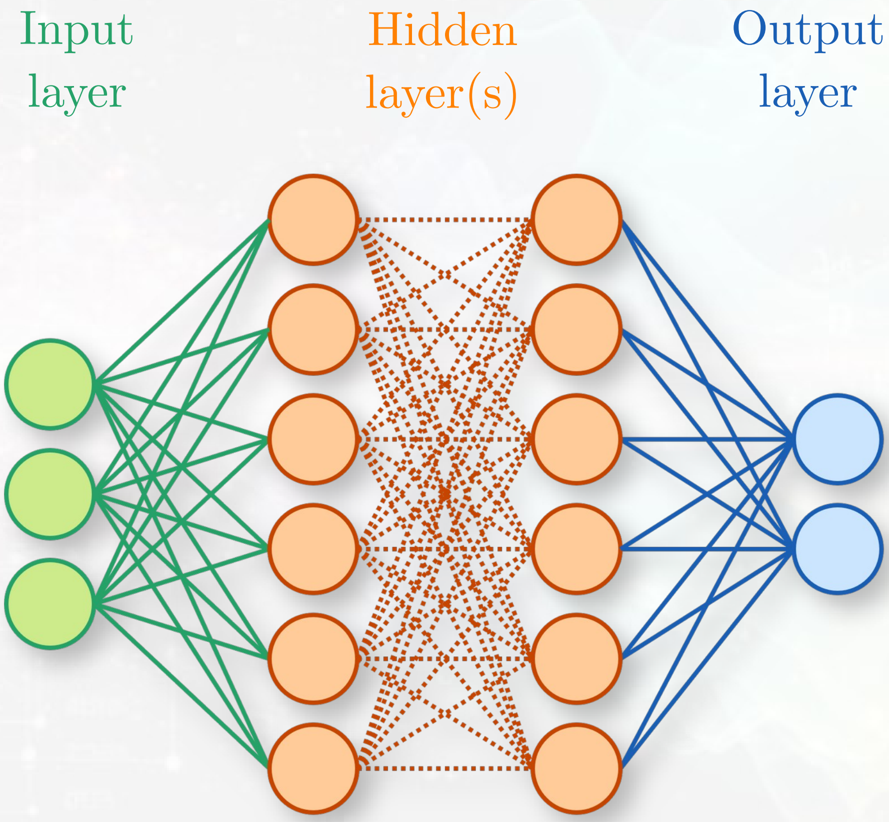

Neural Quantum States

Neural Quantum States

1) Universal Function Approximators

[1] K. Hornik, M. Stinchcombe, and H. White, Neural Networks **2**, 359 (1989).

Neural Quantum States

1) Universal Function Approximators

2) Polynomial Scaling

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Neural Quantum States

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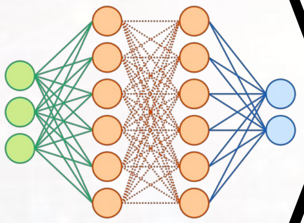

$$\left| \quad \right\rangle \equiv \left| \Psi_{\vec{\theta}} \right\rangle$$

Parametrized wavefunction ansatz[3]

[1] K. Hornik, M. Stinchcombe, and H. White, Neural Networks **2**, 359 (1989).

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[3] G. Carleo and M. Troyer, Science **355**, 602 (2017).

Classic ANN & NQS (minimize)

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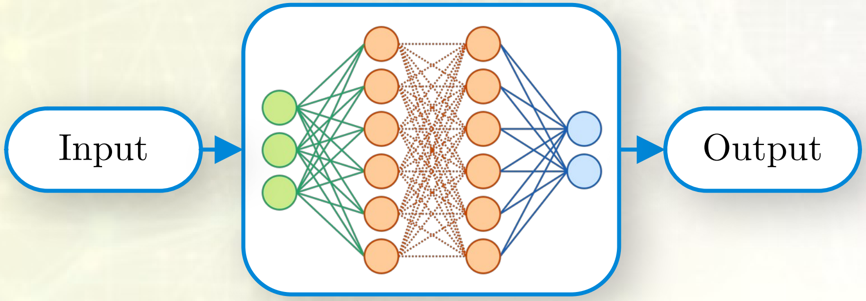

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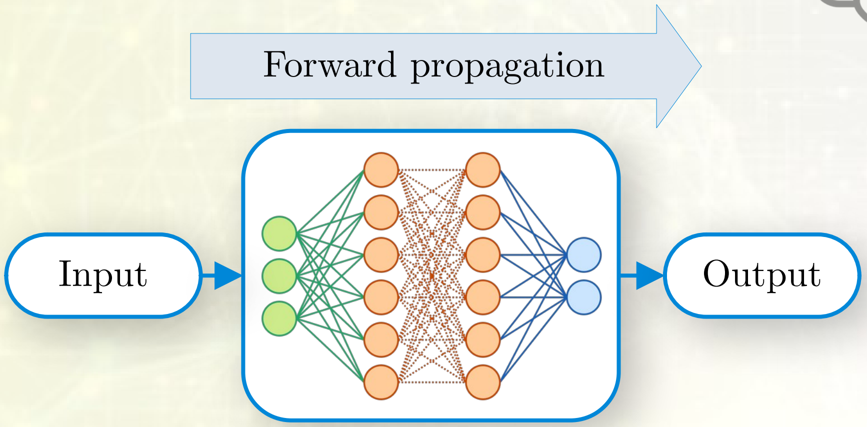

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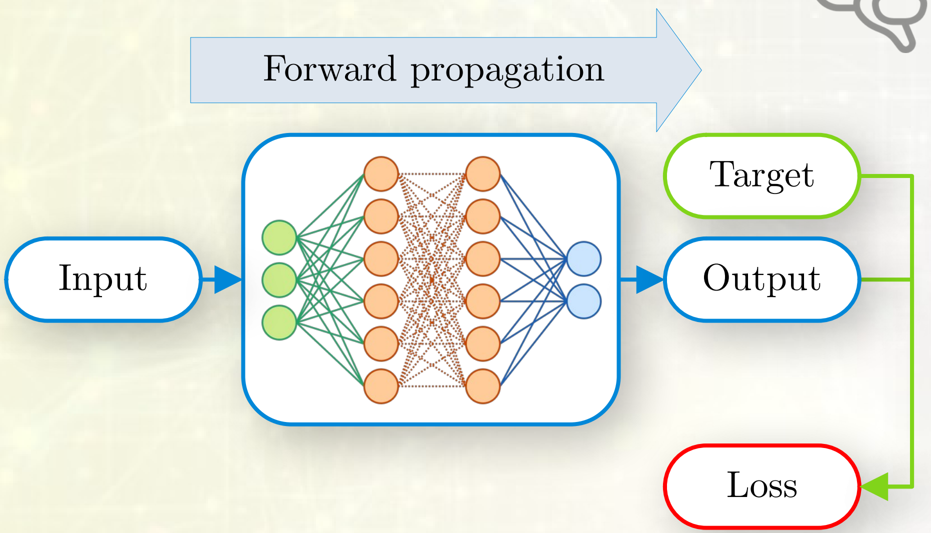

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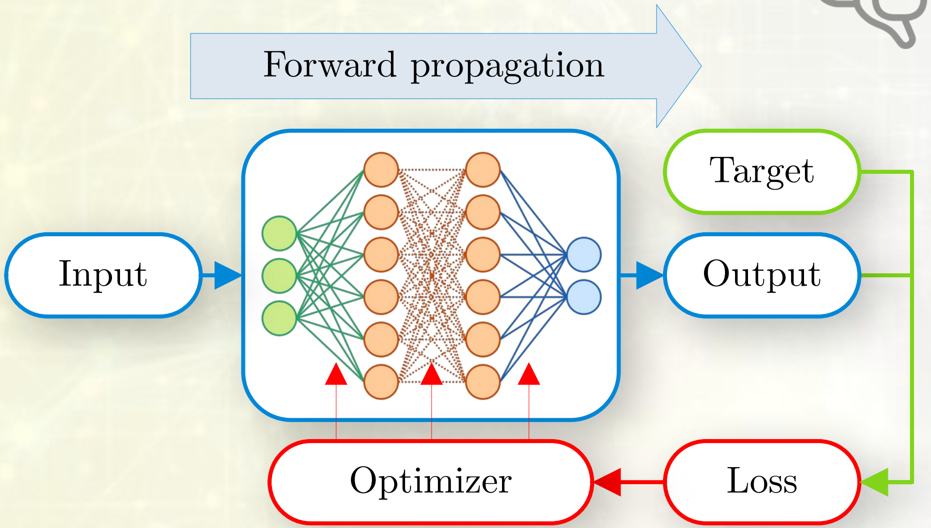

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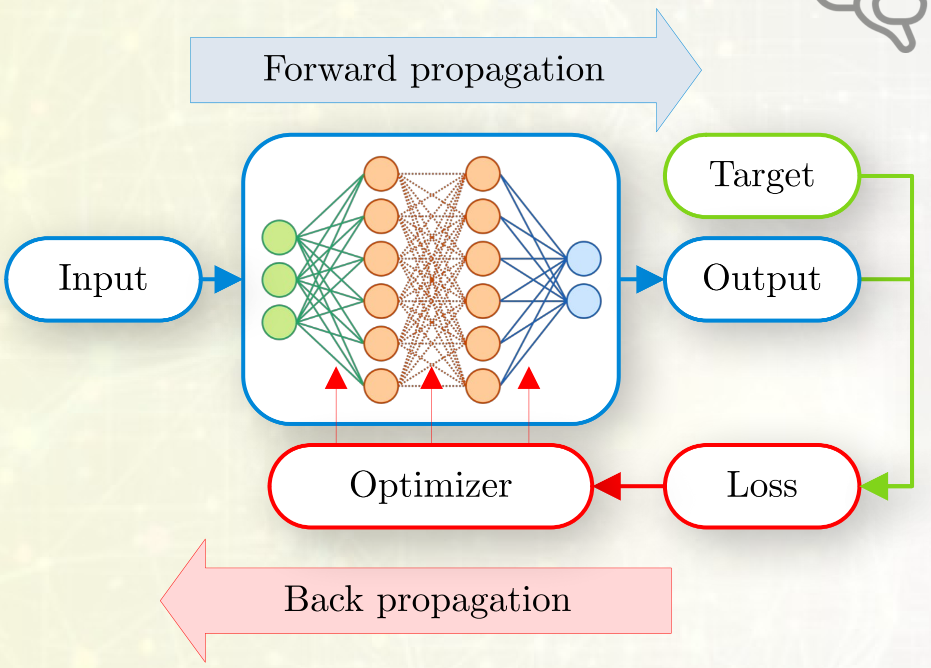

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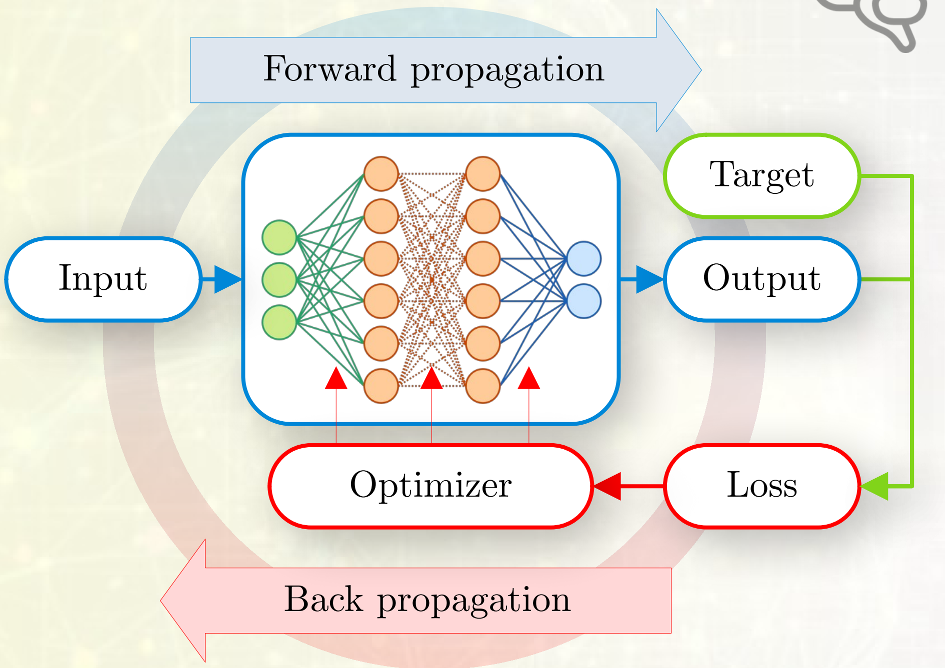

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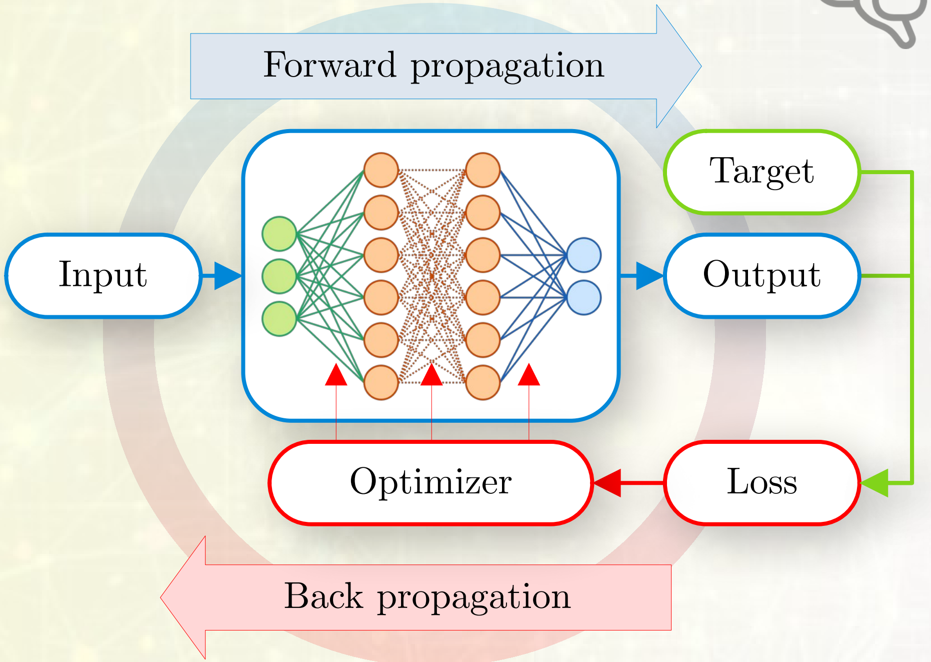
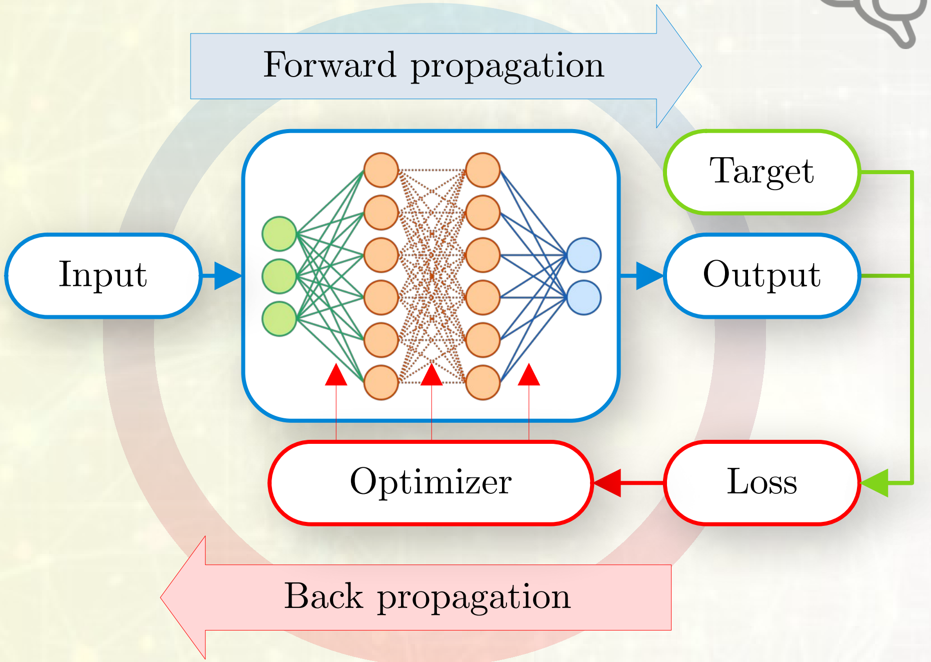


- Gradient Descent Optimizers

Parameters updated via
Optimizers driven by the Loss function

Classic ANN & NQS (minimize)



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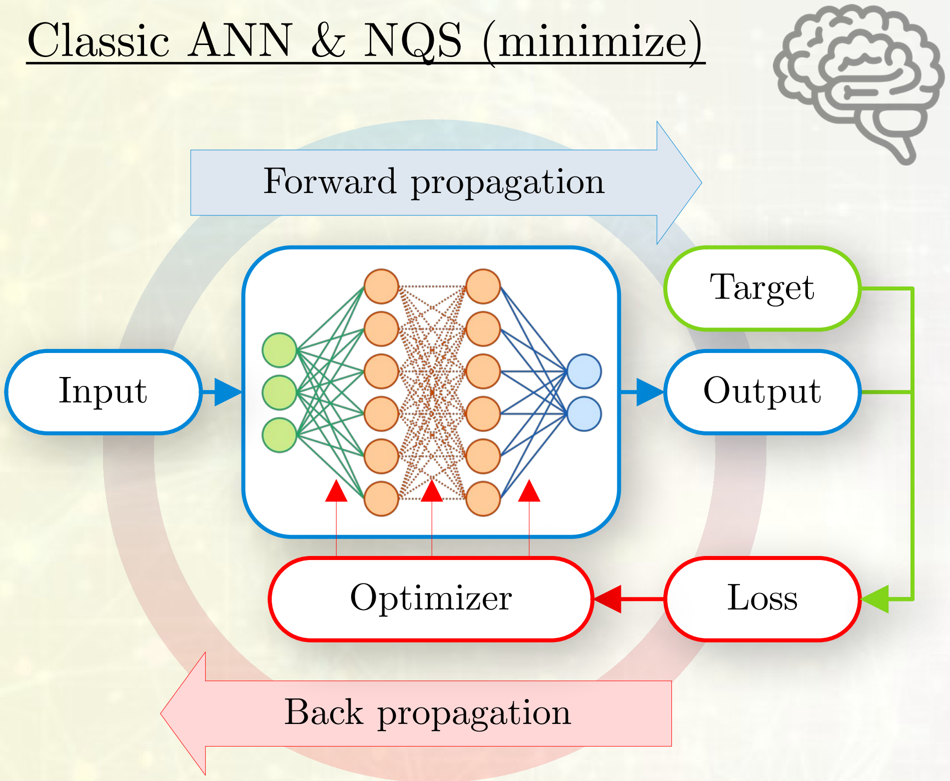

- Gradient Descent Optimizers

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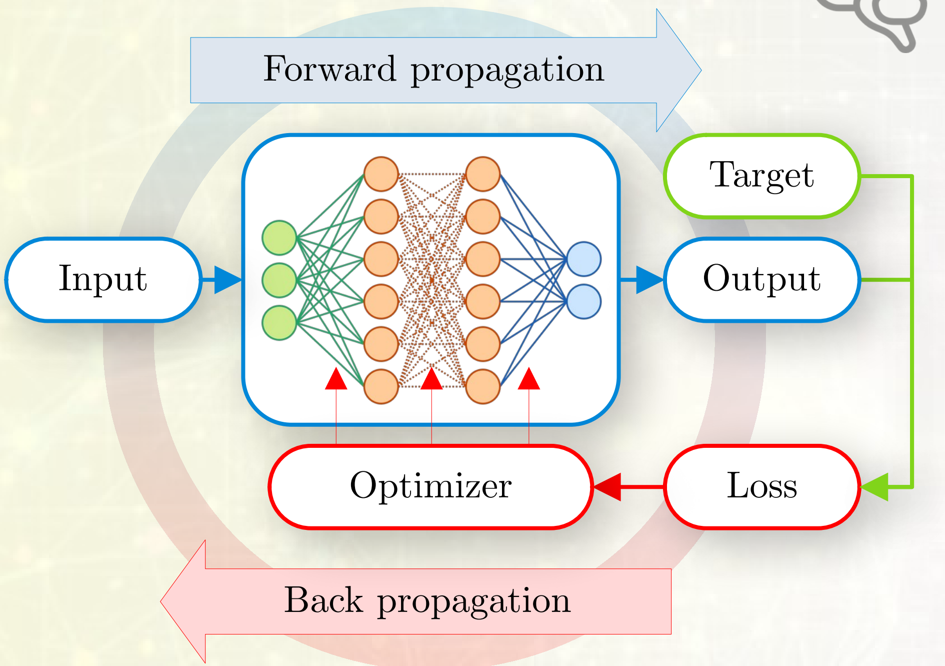
Second-order optimization

Classic ANN & NQS (minimize)



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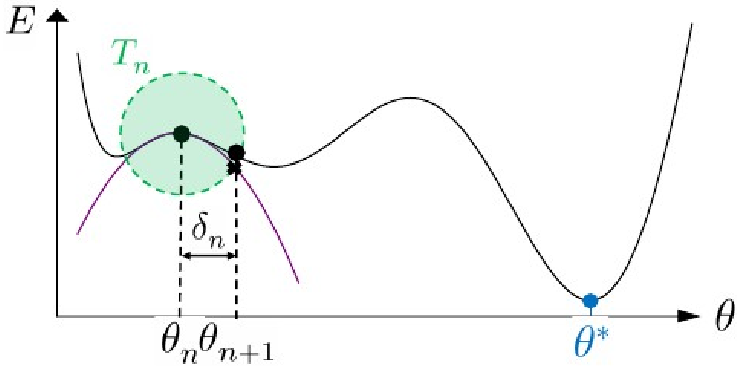

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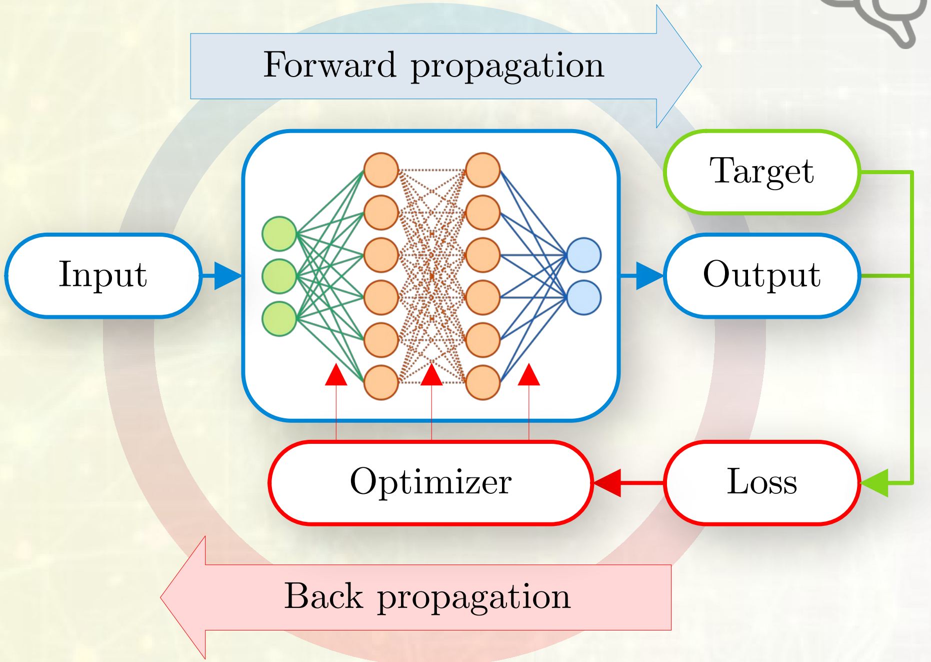

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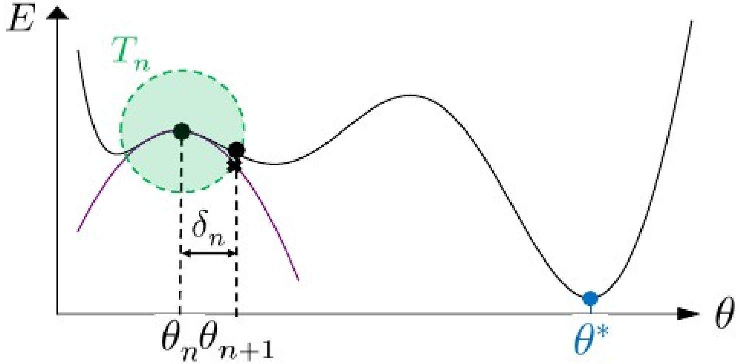
Second-order optimization

Local quadratic model: $M_n(\delta) = \frac{1}{2}\delta^T Q \delta + L^T \delta + C$



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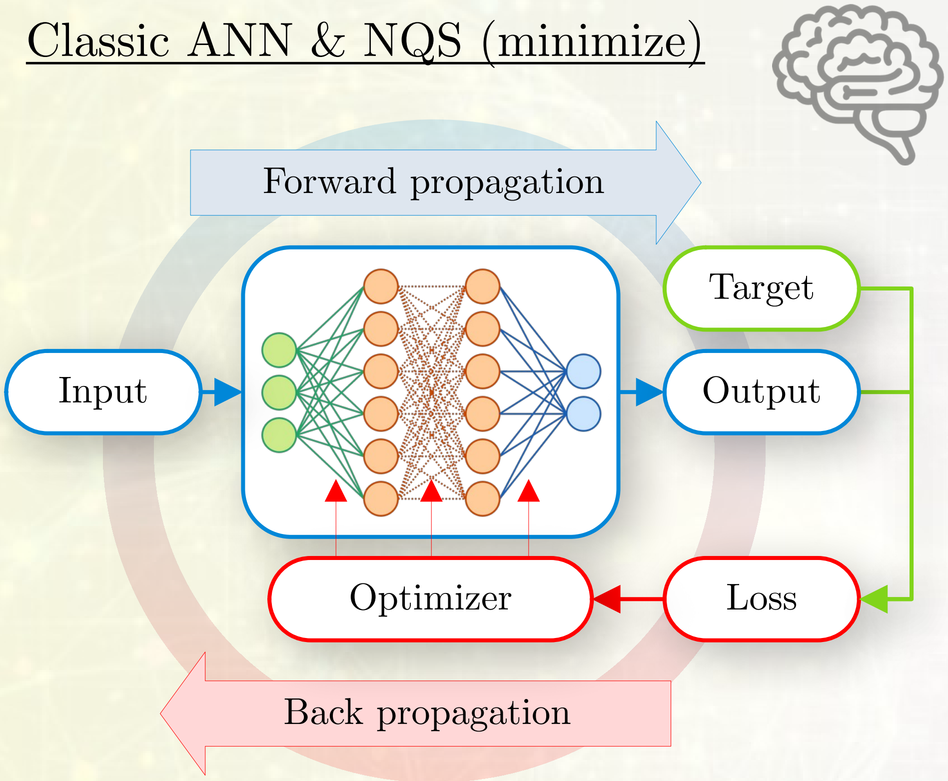

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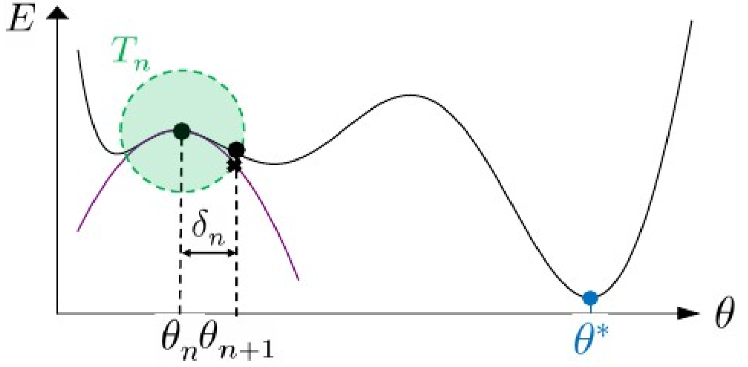
Gradient: $L = \nabla_\theta E$



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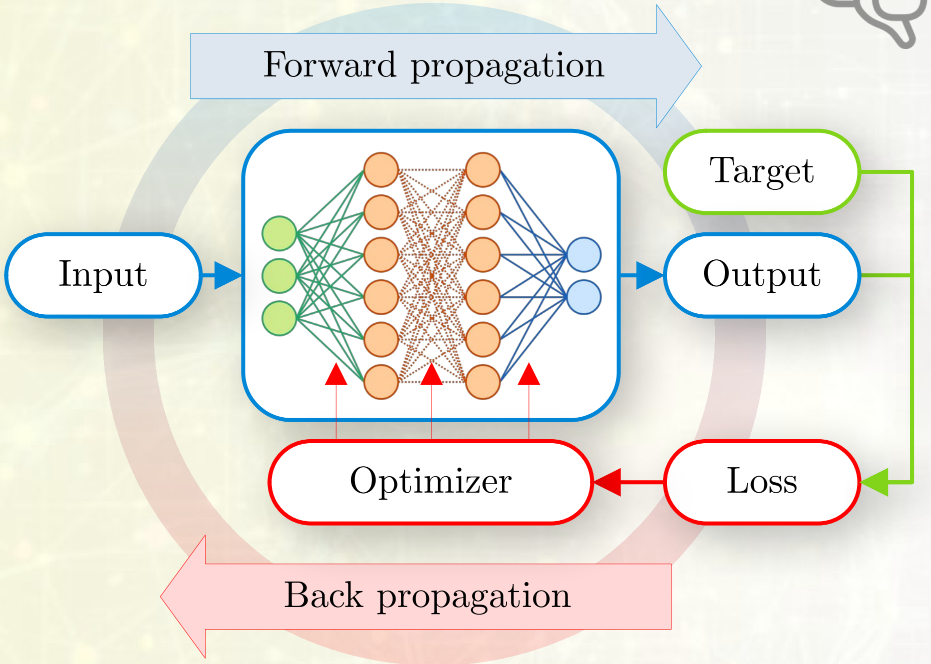

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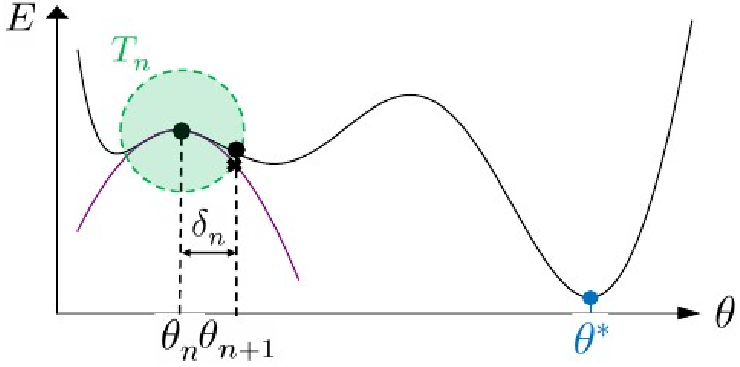
Quantum Geometric Tensor:

$$Q_{ij} = \left\langle \frac{\partial \Psi_\theta}{\partial \theta_i} \middle| \frac{\partial \Psi_\theta}{\partial \theta_j} \right\rangle - \left\langle \frac{\partial \Psi_\theta}{\partial \theta_i} \middle| \Psi_\theta \right\rangle \left\langle \Psi_\theta \middle| \frac{\partial \Psi_\theta}{\partial \theta_j} \right\rangle$$



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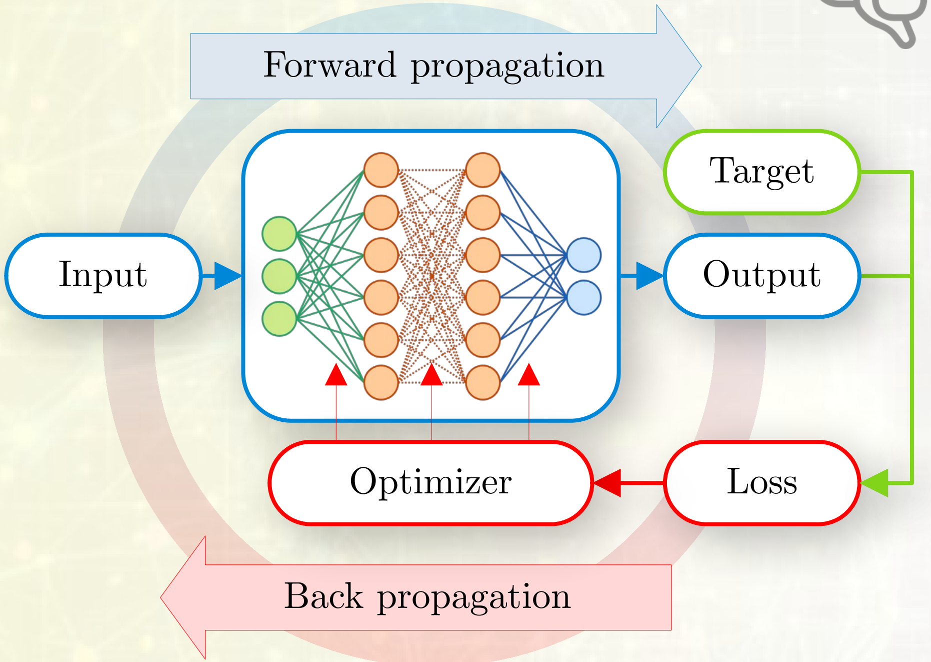

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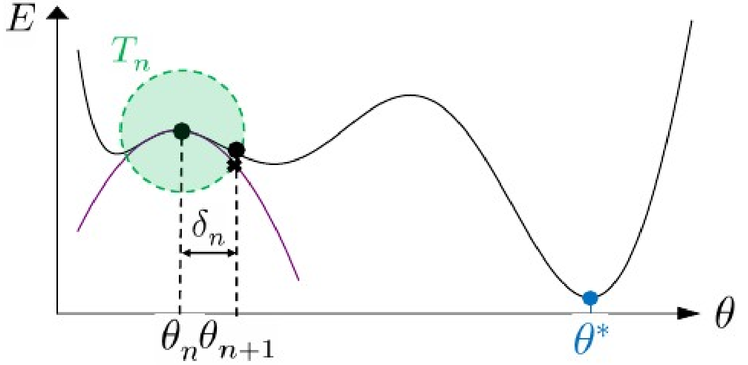
Parameter update:

$$\delta_n = -(Q_n + \lambda_n R_n)^{-1} L_n$$



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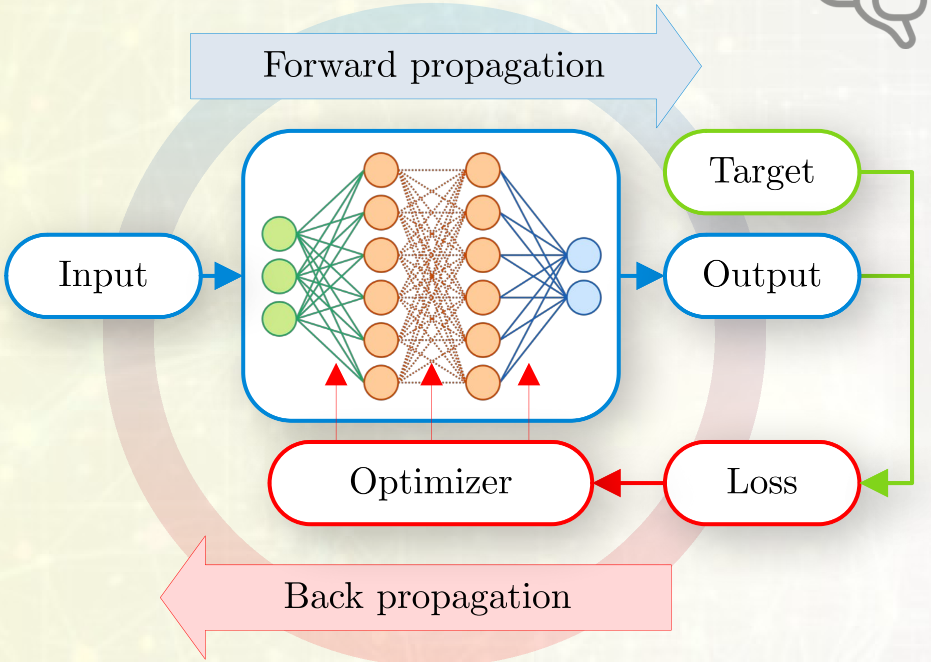

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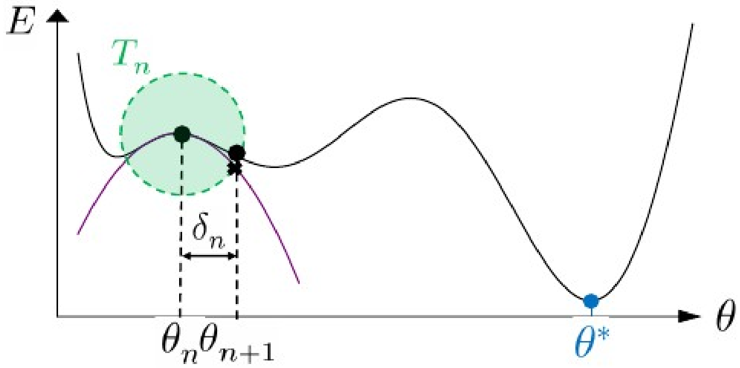

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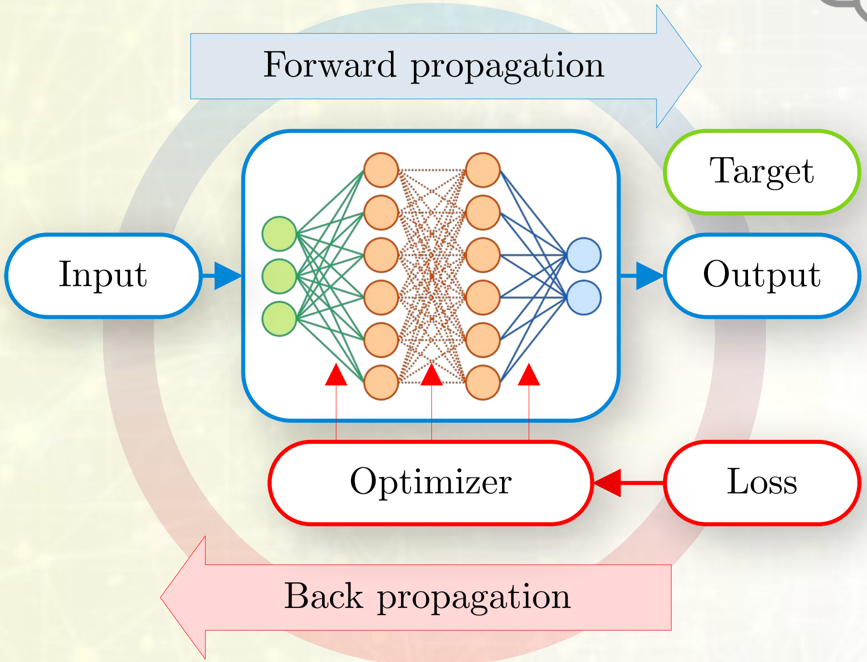

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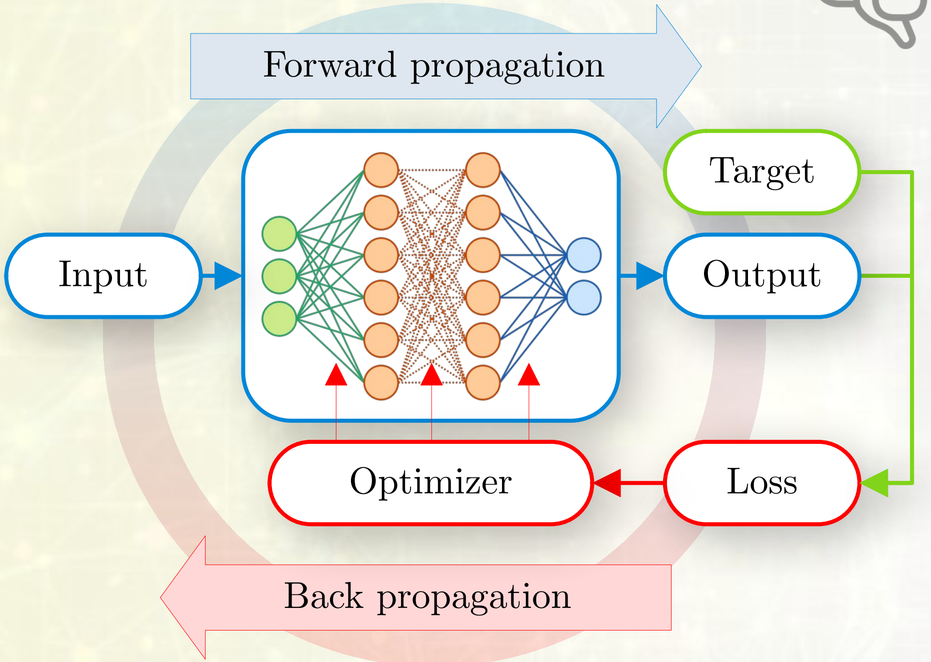
Parameters updated via
Optimizers driven by the Loss function

Time Dependent NQS (evolve)

Classic ANN & NQS (minimize)



- Gradient Descent Optimizers

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Ψ

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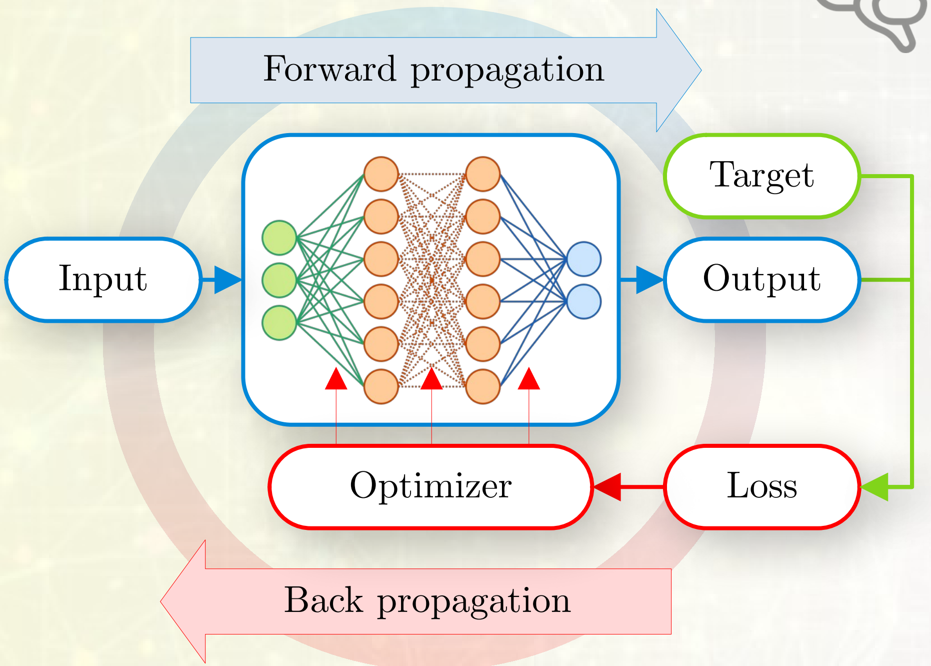

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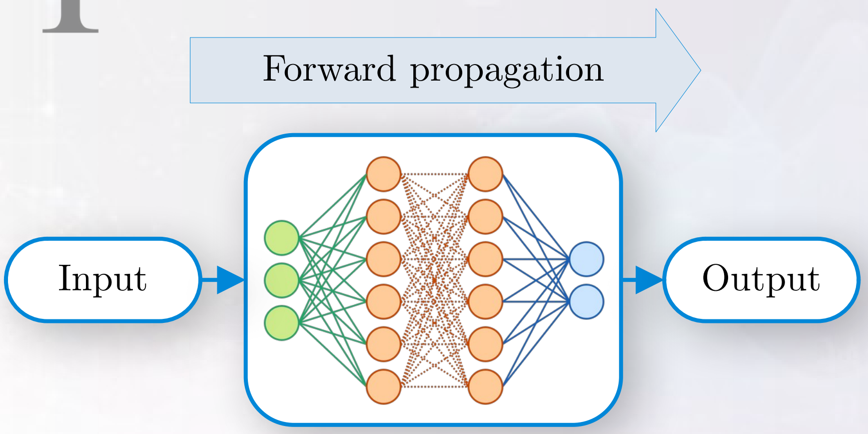

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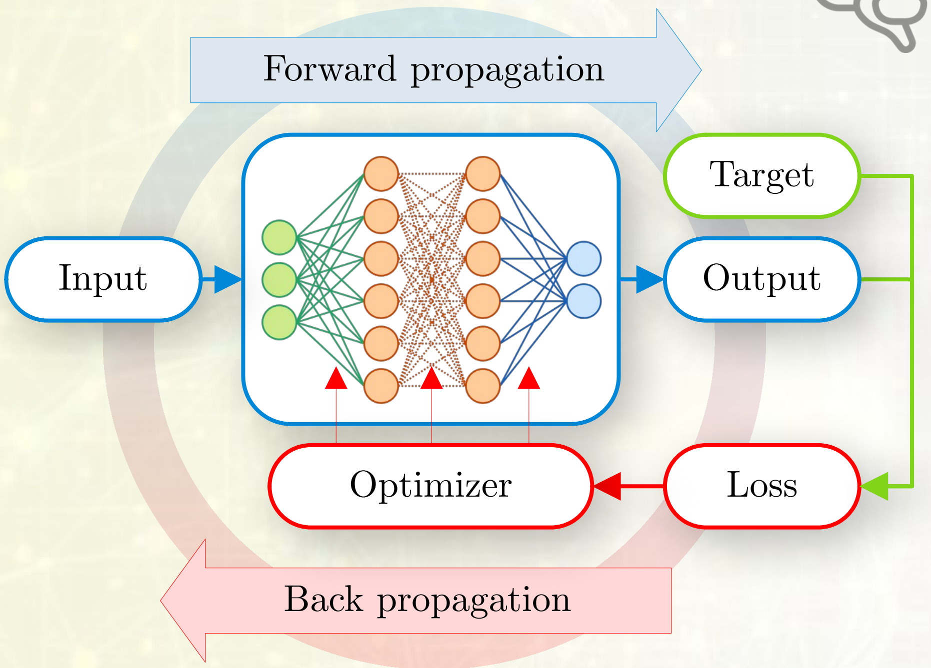

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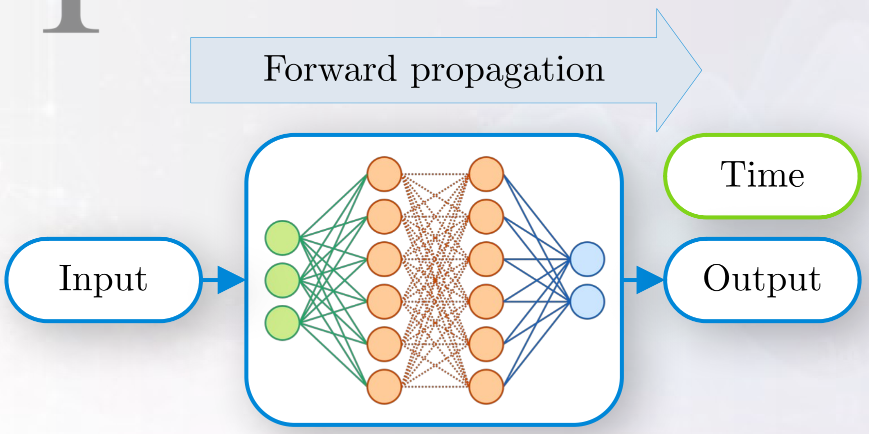

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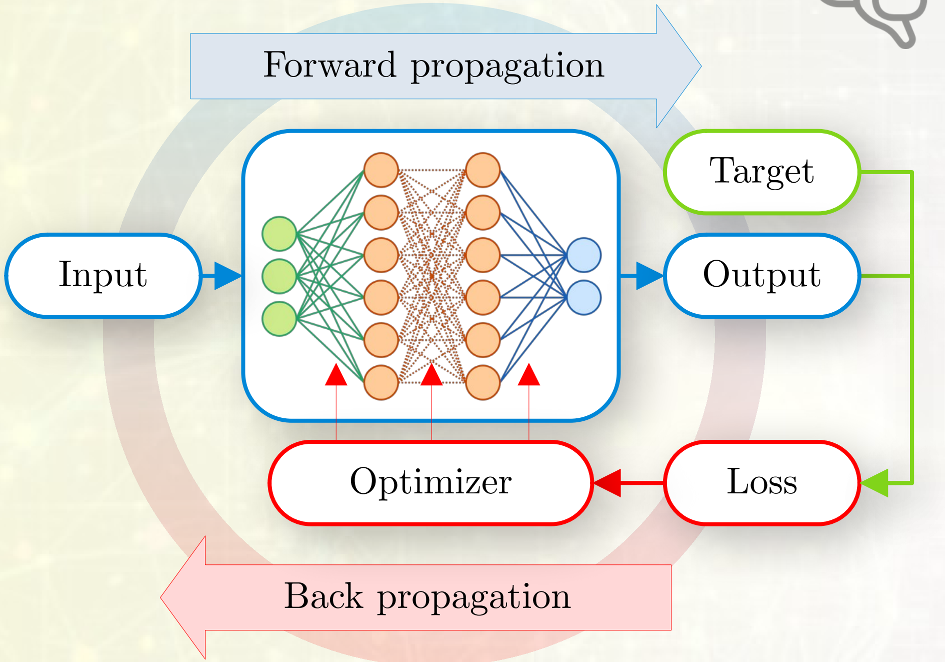

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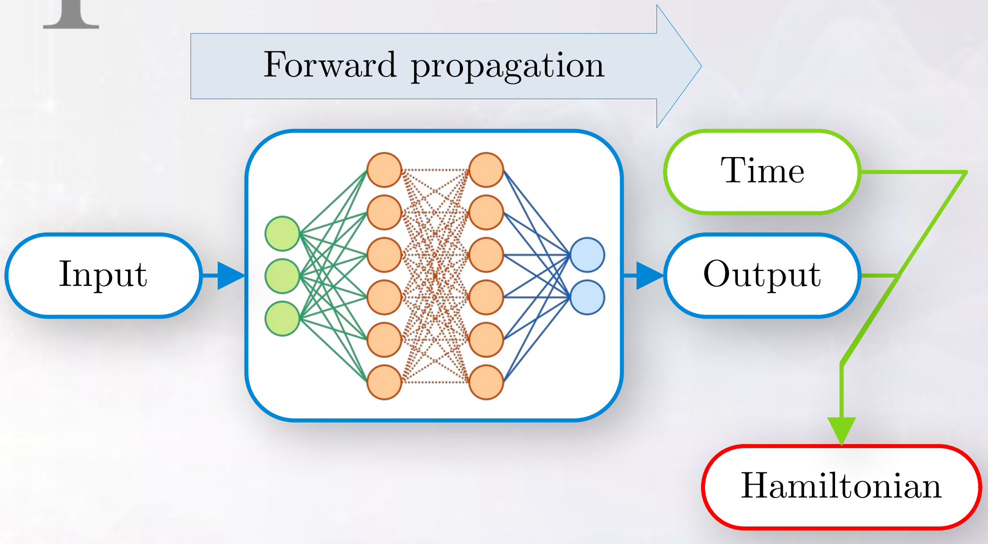

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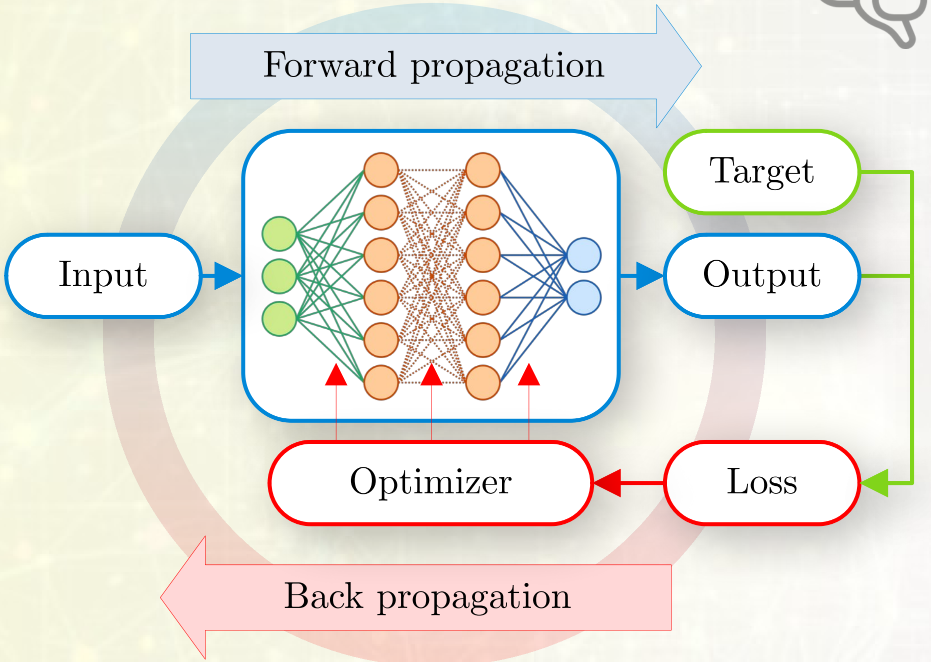

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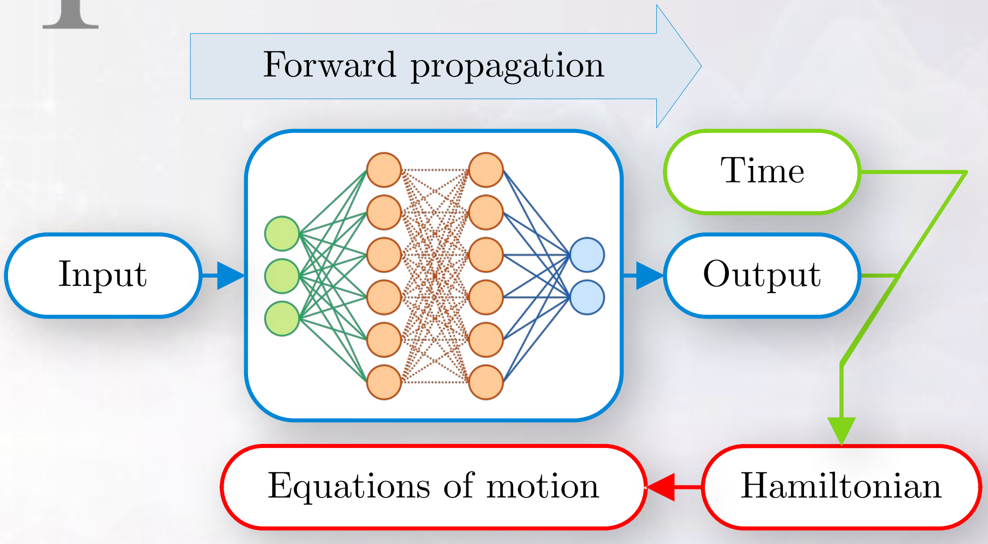

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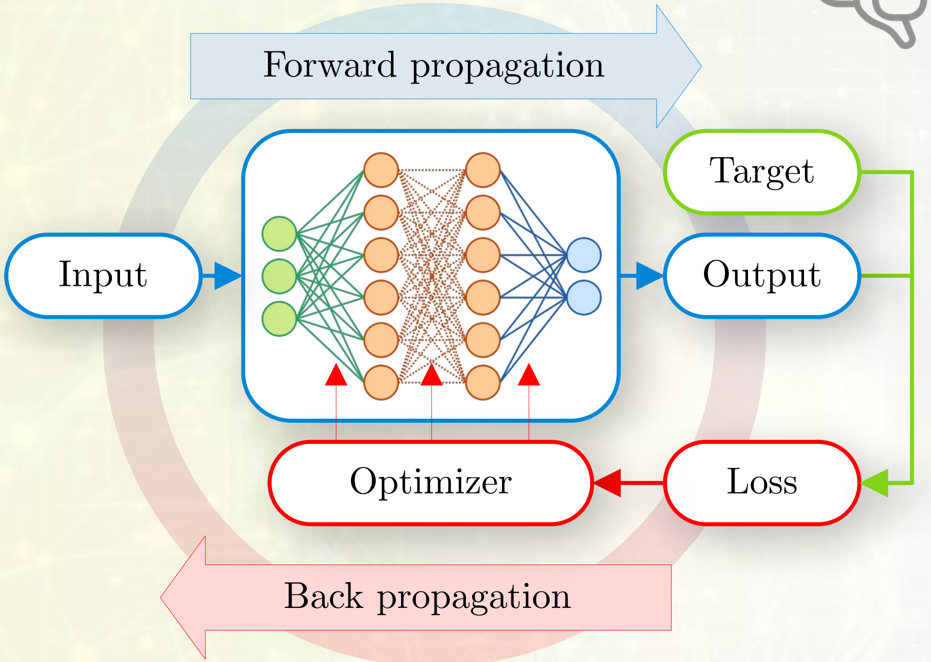

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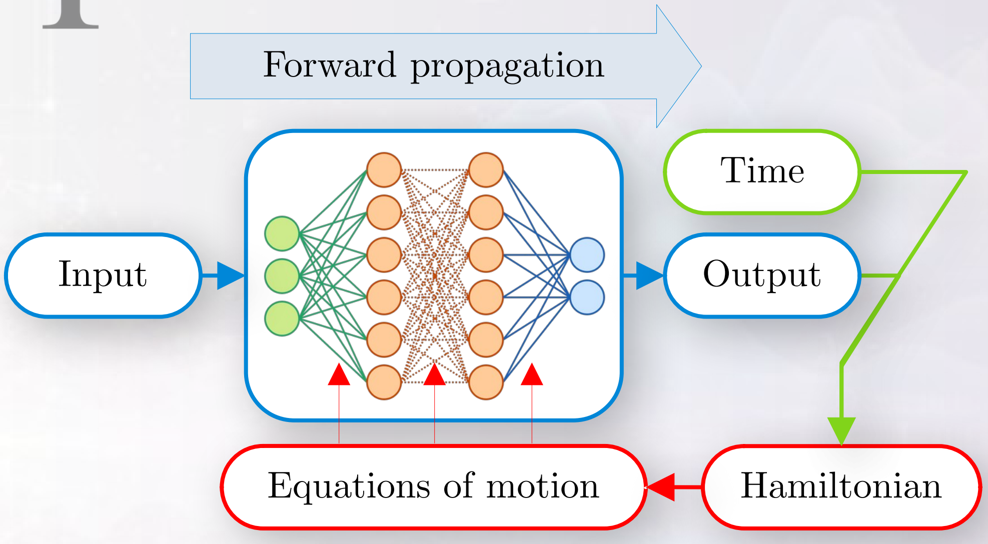

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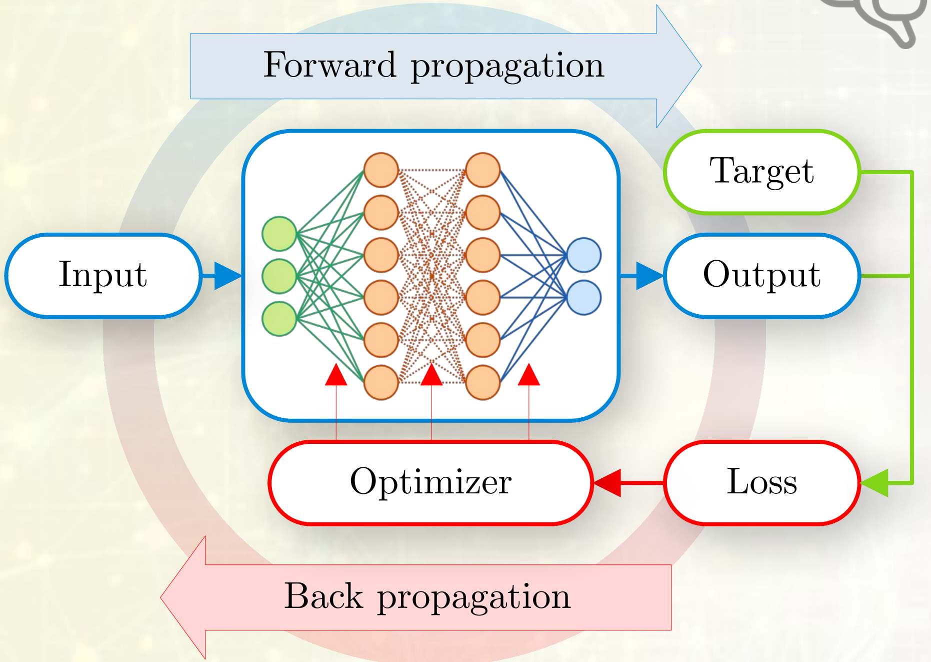

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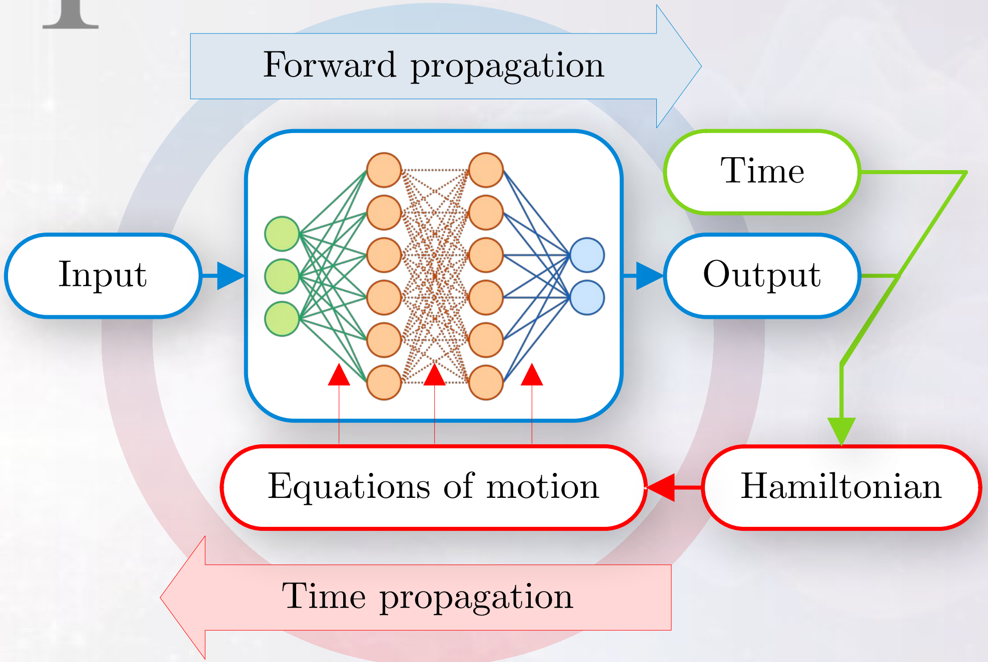

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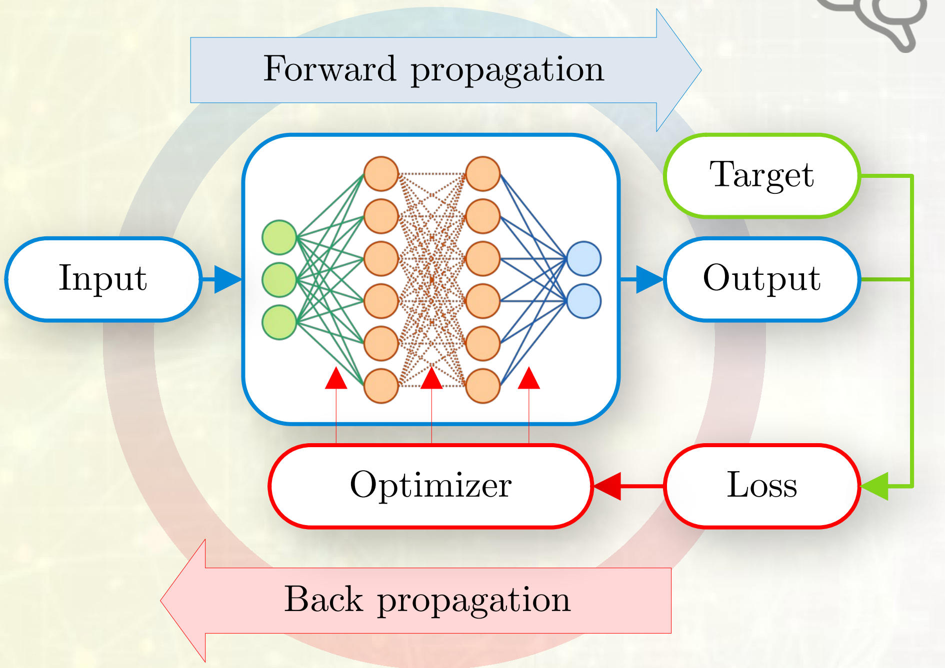

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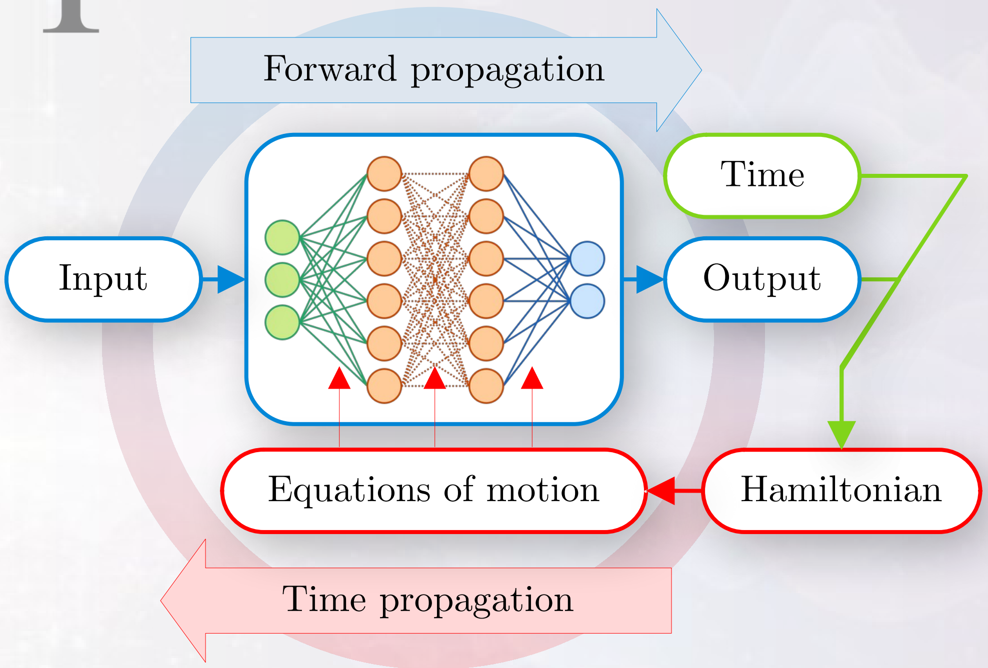

- Time-dependent Variational Principle

Parameters updated via
Equations of motion driven by the Hamiltonian

Time-dependent Variational Principle

Set of parameters:

$$\vec{\theta} = \{\theta_1, \theta_2, \ldots, \theta_m\}$$

Time-dependent Variational Principle

Set of parameters:

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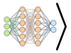
Parametrized wavefunction:

$$|\Psi_{\vec{\theta}}\rangle = |$$  $$\rangle$$

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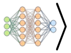
$|\Psi_{\vec{\theta}}\rangle = |$  $\rangle$

Variational manifold:

$$\mathcal{M} = \left\{ |\Psi_{\vec{\theta}}\rangle \in H \mid \vec{\theta} \in \mathbb{C}^m \right\}$$

Time-dependent Variational Principle

Set of parameters:

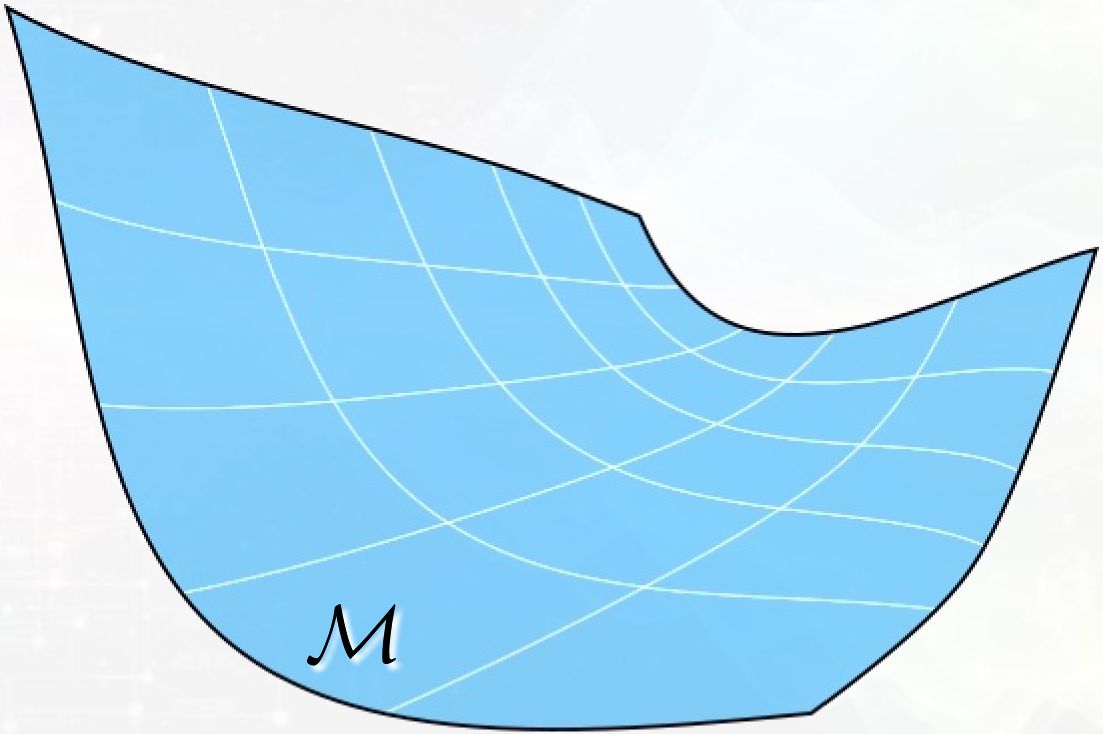
$$\vec{\theta} = \{\theta_1, \theta_2, \ldots, \theta_m\}$$

Parametrized wavefunction:

$$|\Psi_{\vec{\theta}}\rangle = |\text{NN}\rangle$$

Variational manifold:

$$\mathcal{M} = \left\{ |\Psi_{\vec{\theta}}\rangle \in H \mid \vec{\theta} \in \mathbb{C}^m \right\}$$



Time-dependent Variational Principle

Set of parameters:

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Parametrized wavefunction:

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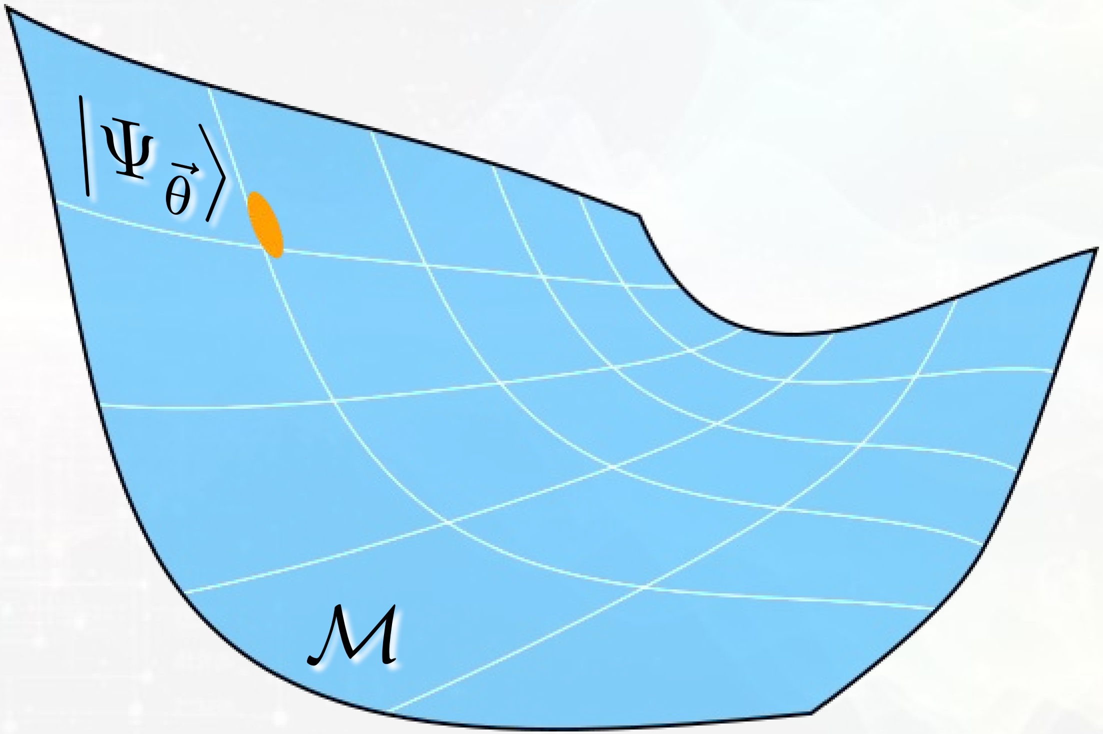

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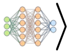
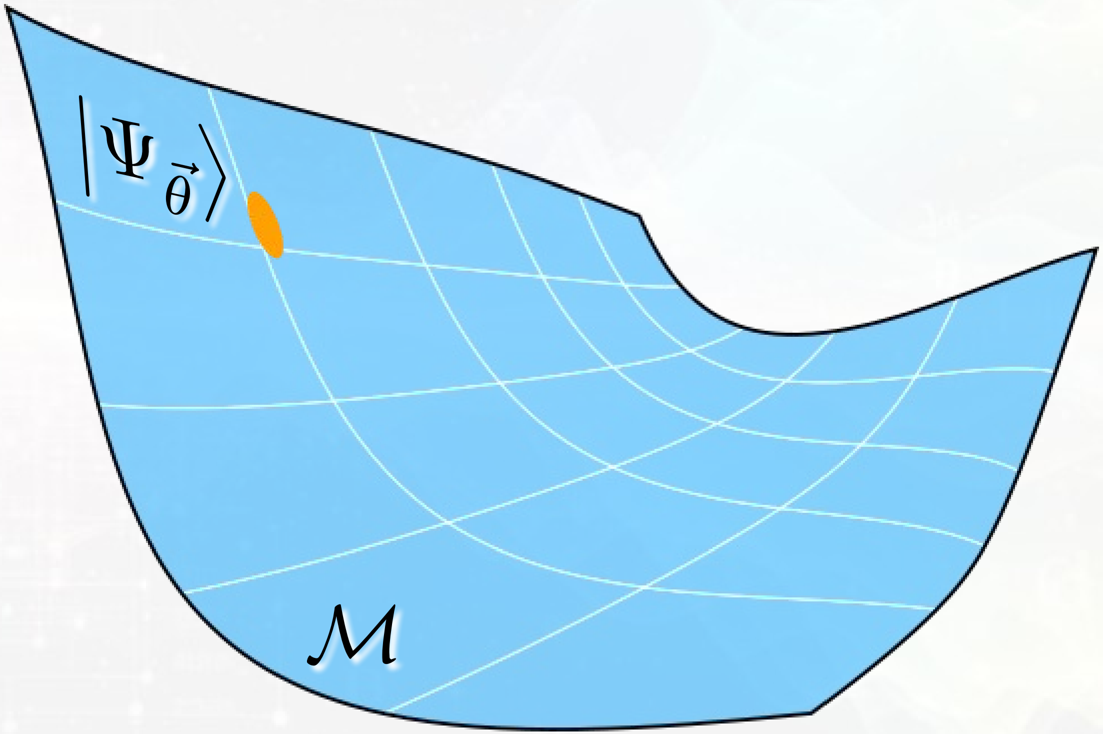
$$|\Psi_{\vec{\theta}}\rangle = |$$  $$\rangle$$

Variational manifold:

$$\mathcal{M} = \left\{ \left|\Psi_{\vec{\theta}}\right\rangle \in H \mid \vec{\theta} \in \mathbb{C}^m \right\}$$

Evolution operator:

$$U(\delta t) = e^{-i\hat{\mathcal{H}}\delta t/\hbar}$$

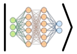


Time-dependent Variational Principle

Set of parameters:

$$\vec{\theta} = \{\theta_1, \theta_2, \ldots, \theta_m\}$$

Parametrized wavefunction:

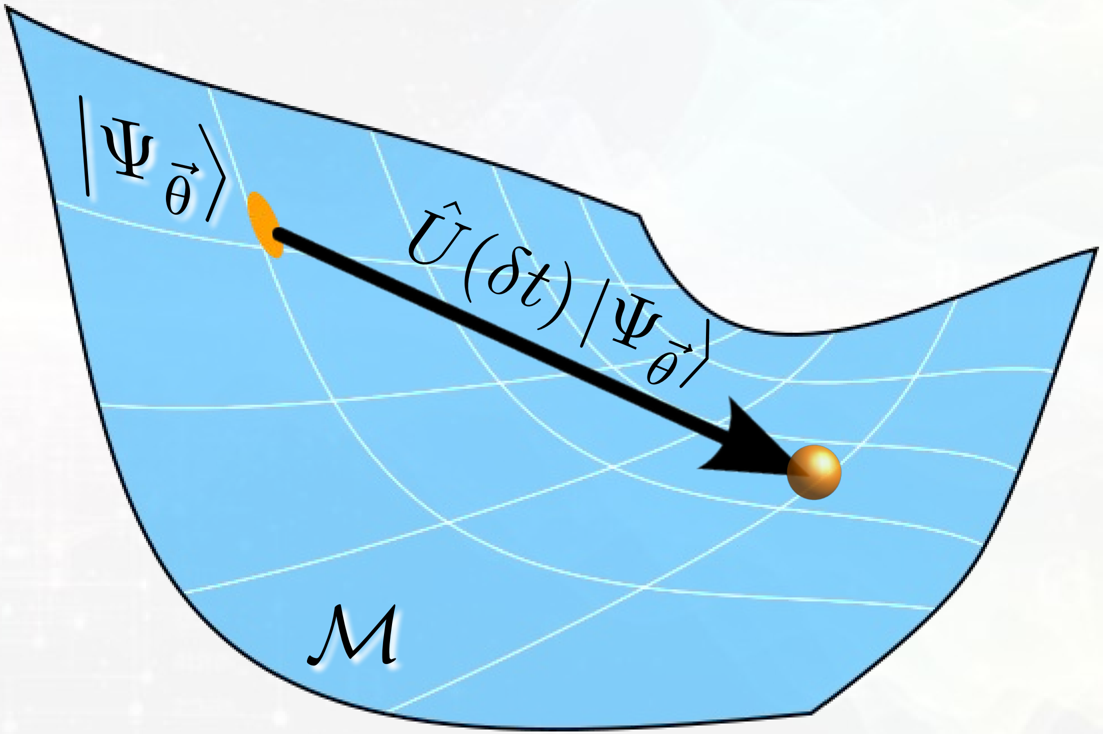
$$|\Psi_{\vec{\theta}}\rangle = |$$  $$\rangle$$

Variational manifold:

$$\mathcal{M} = \left\{ |\Psi_{\vec{\theta}}\rangle \in H \mid \vec{\theta} \in \mathbb{C}^m \right\}$$

Evolution operator:

$$U(\delta t) = e^{-i\hat{\mathcal{H}}\delta t/\hbar}$$

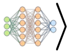


Time-dependent Variational Principle

Set of parameters:

$$\vec{\theta} = \{\theta_1, \theta_2, \ldots, \theta_m\}$$

Parametrized wavefunction:

$|\Psi_{\vec{\theta}}\rangle = |$  $\rangle$

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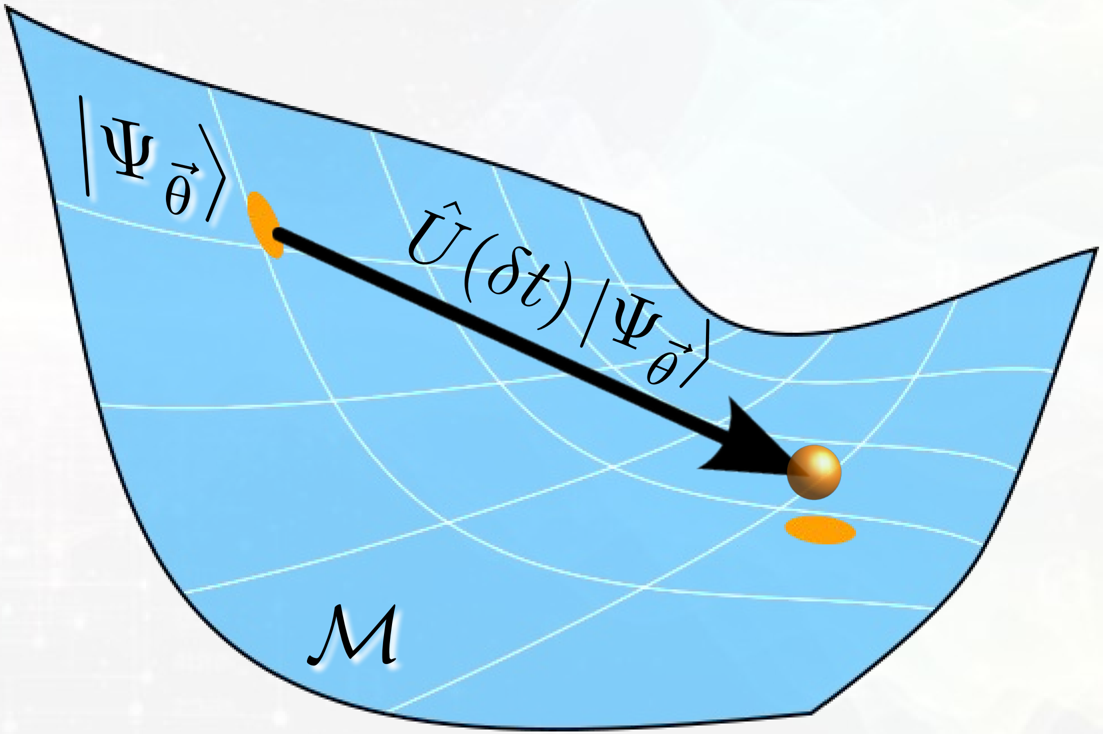

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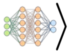
$$|\Psi_{\vec{\theta}}\rangle = |$$  $$\rangle$$

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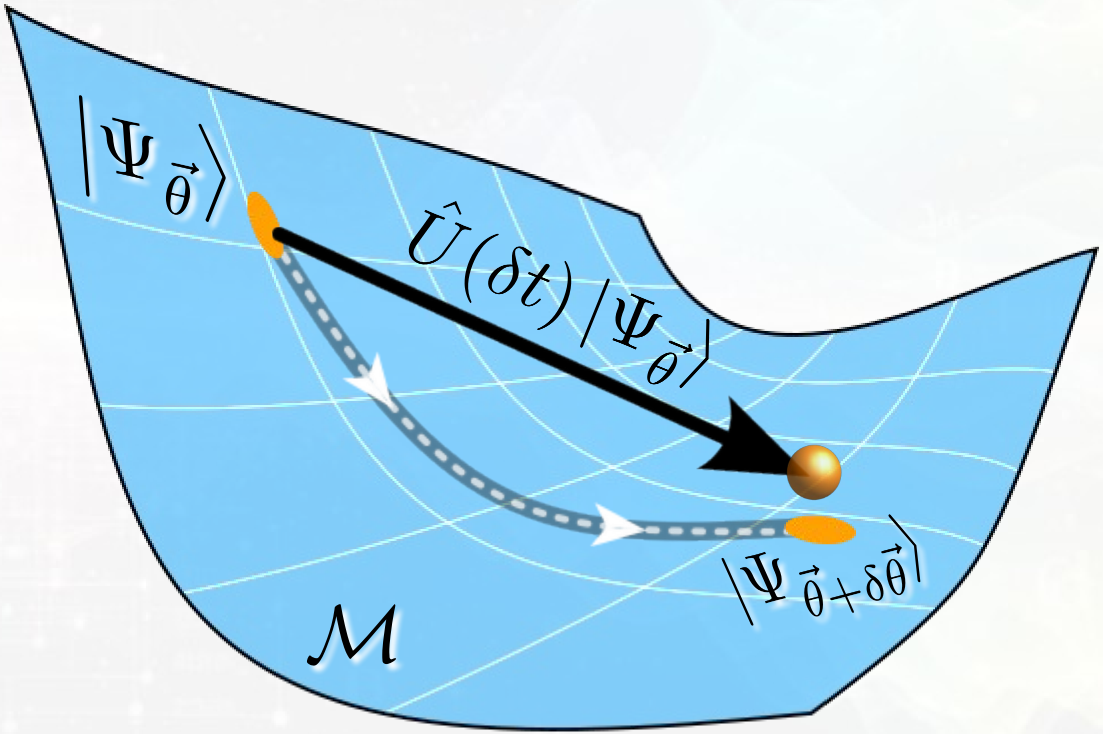


Time-dependent Variational Principle

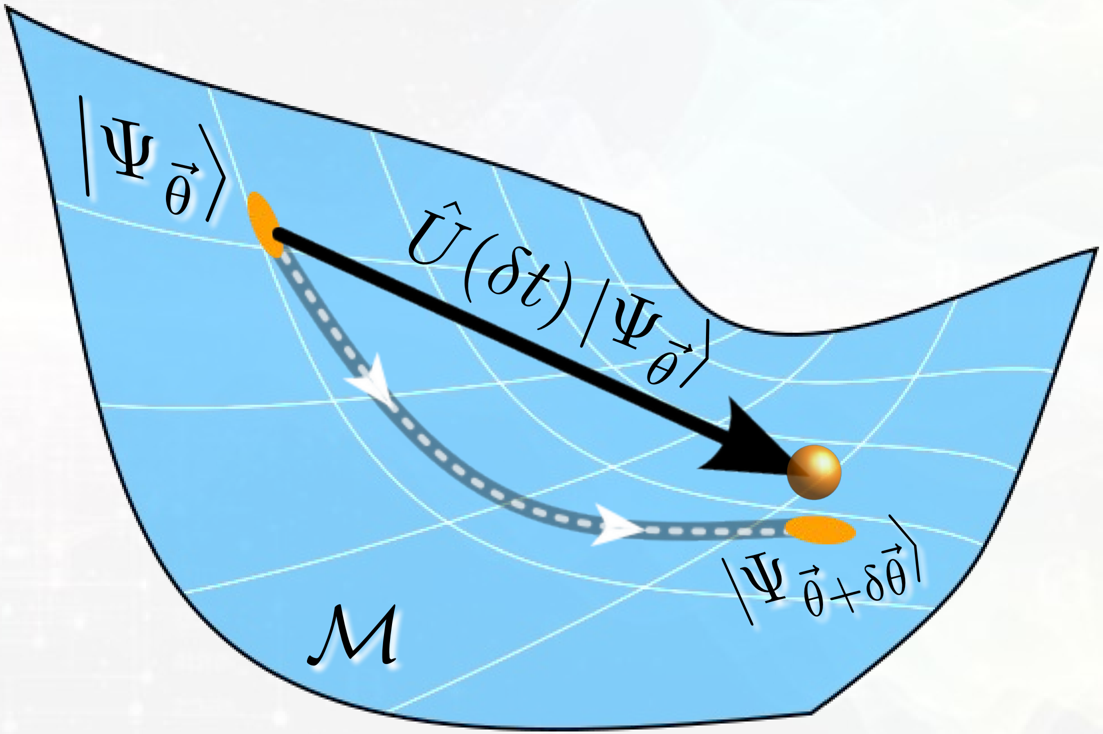
Exact evolution:

$$\hat{U}(\delta t)\left|\Psi_{\vec{\theta}}(t)\right\rangle = \left|\Psi_{\vec{\theta}}(t+\delta t)\right\rangle$$

Parametric evolution:

$$\left|\Psi_{\vec{\theta}+\delta\vec{\theta}}\right\rangle \approx \left|\Psi_{\vec{\theta}}(t+\delta t)\right\rangle$$

with $\vec{\theta} = \vec{\theta}(t)$ and $\delta\vec{\theta} = \dot{\vec{\theta}}(t)\delta t$



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Given a Hamiltonian,
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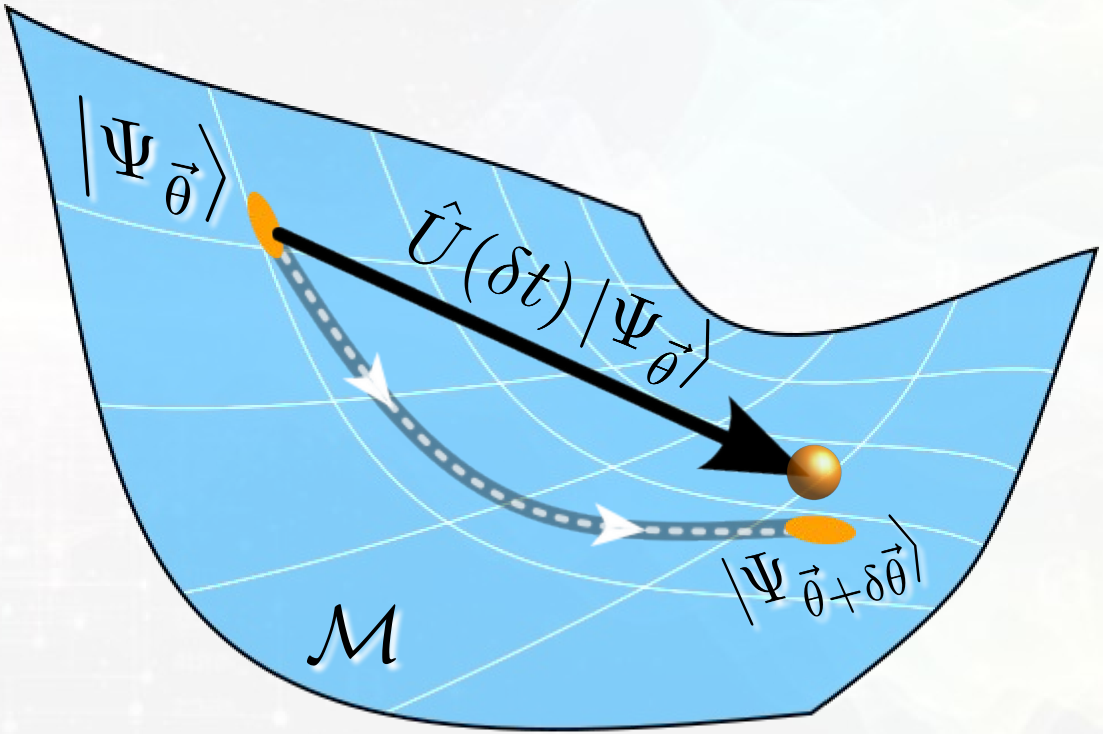

Equations of motion

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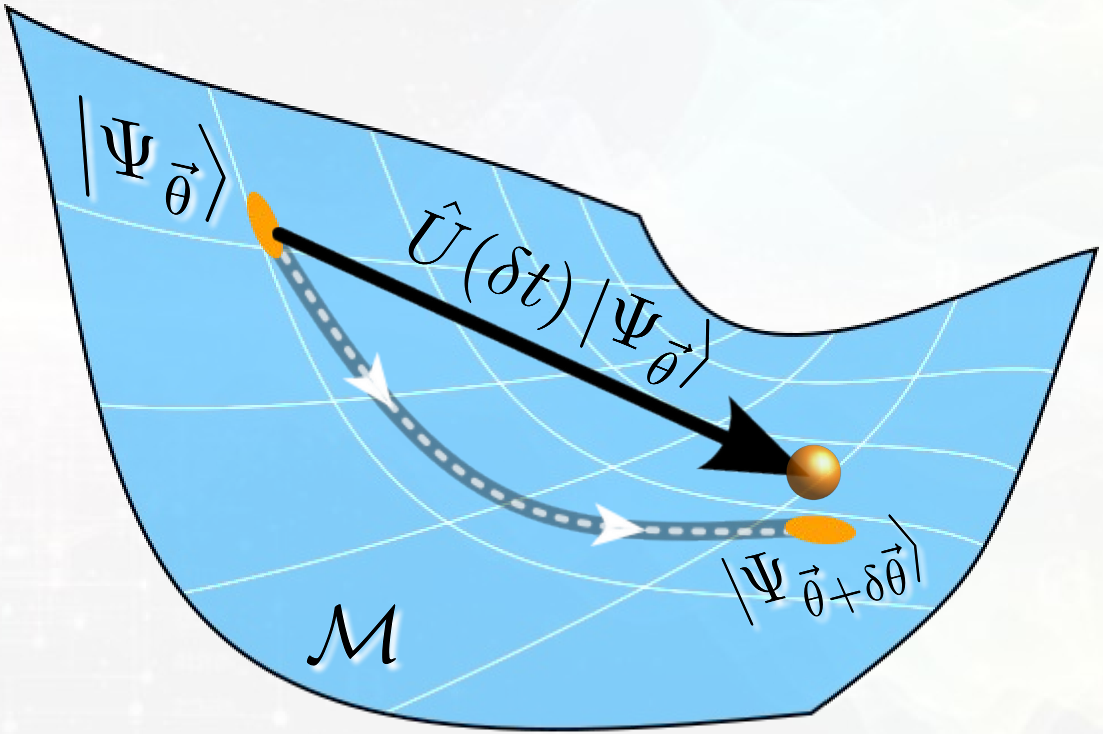

Equations of motion

Given a Hamiltonian,
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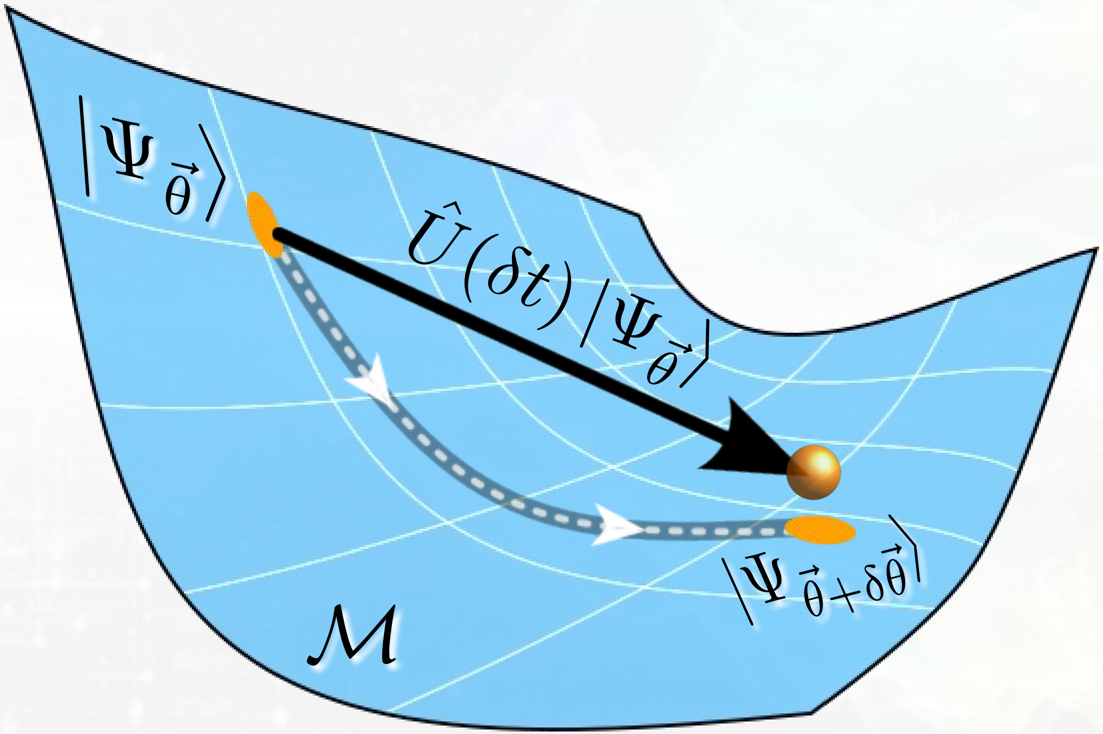
- Optimization problem:

$$\min_{\delta\vec{\theta}} \mathcal{D}\Big(|\Psi_{\vec{\theta}+\delta\vec{\theta}}\rangle \,, \hat{U}(\delta t)\, |\Psi_{\vec{\theta}}\rangle \Big)$$

A. Sinibaldi et al., Quantum **7**, 1131 (2023).



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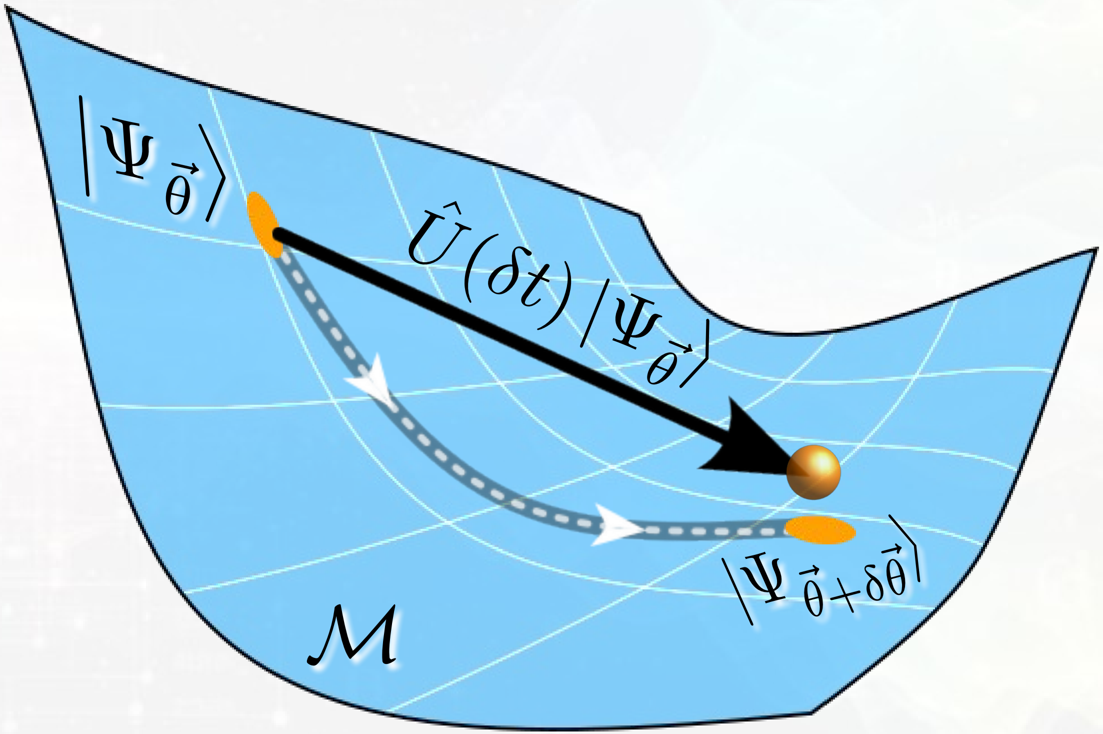

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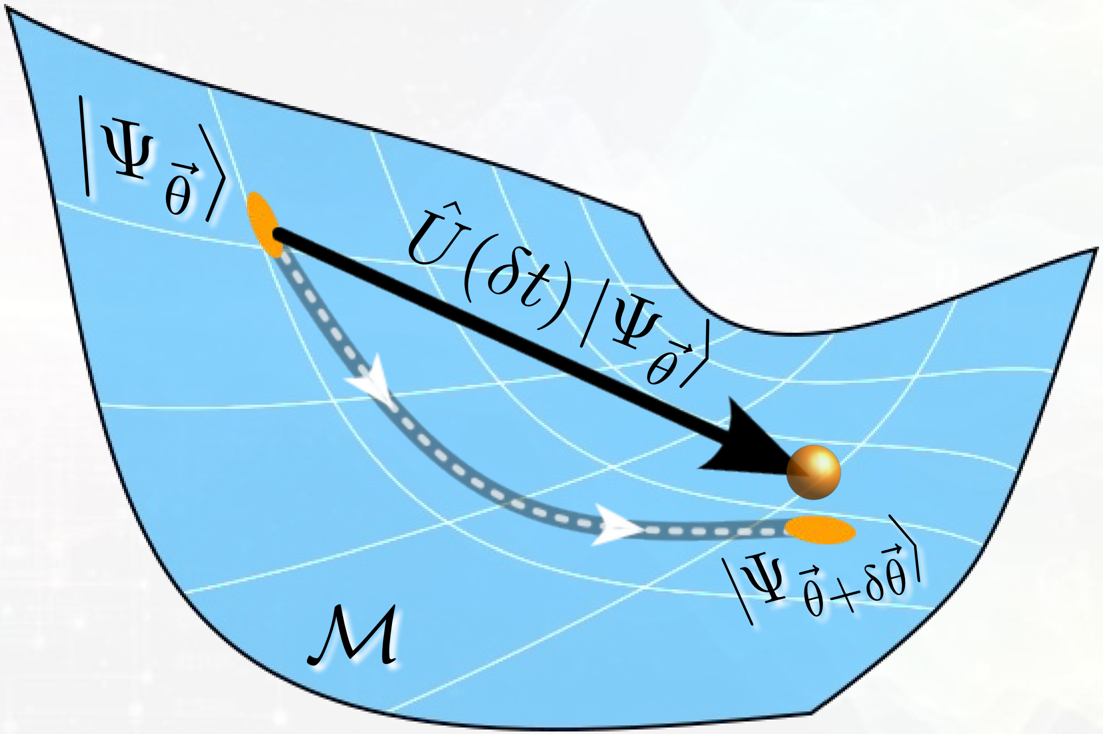
Minimization of the
Fubini-Study Metric



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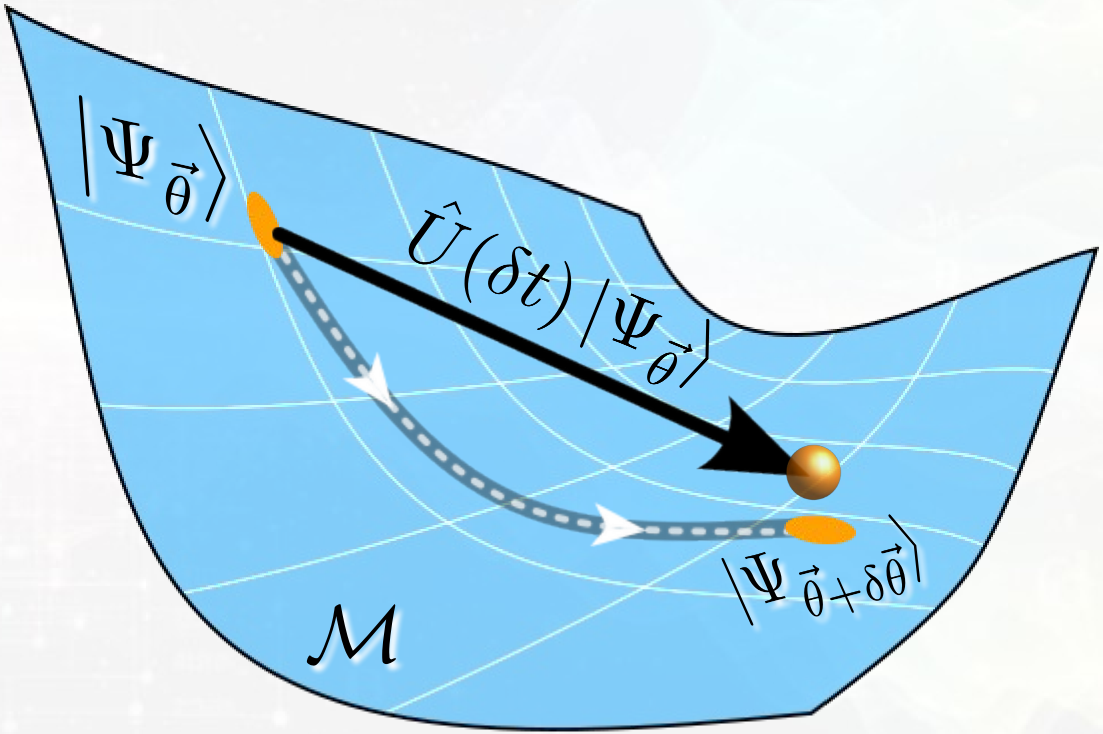
$$\delta\theta_n = -\boldsymbol{i}(Q_n)^{-1} L_n$$



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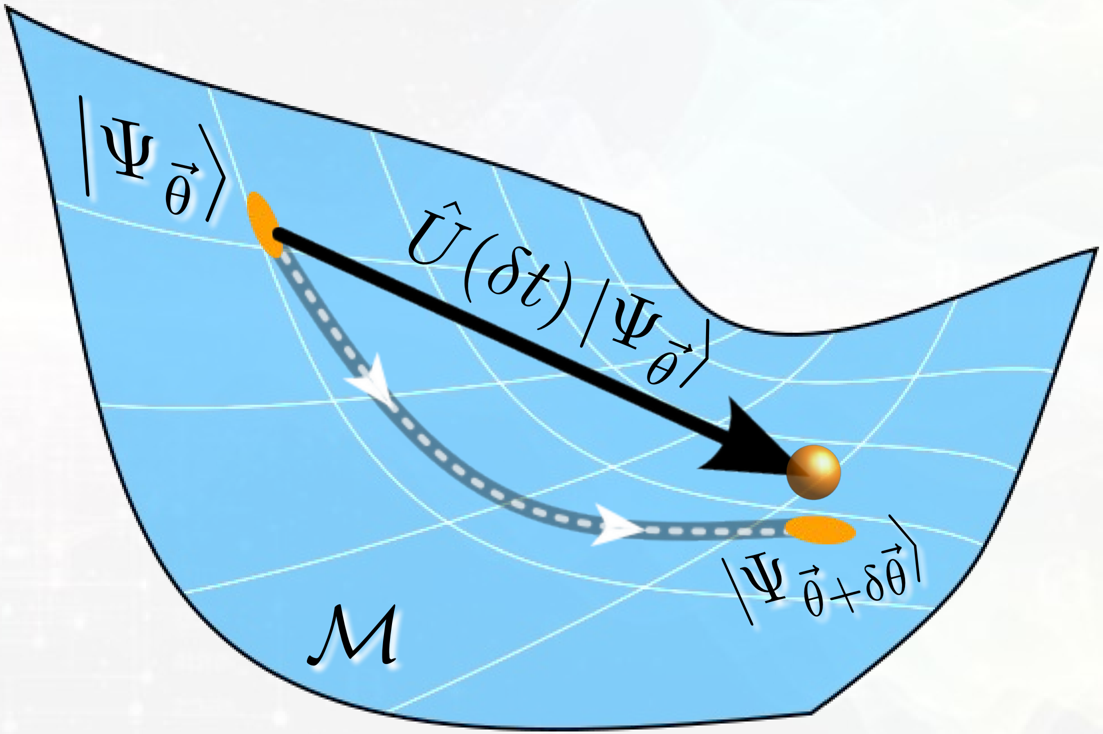

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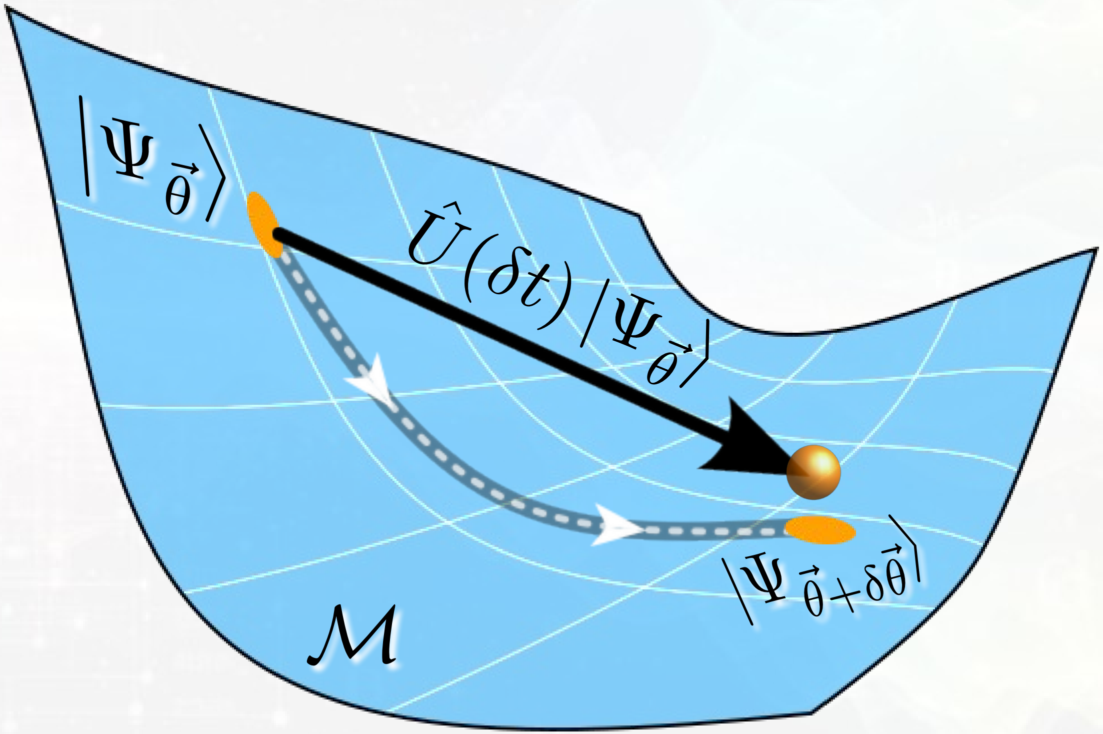

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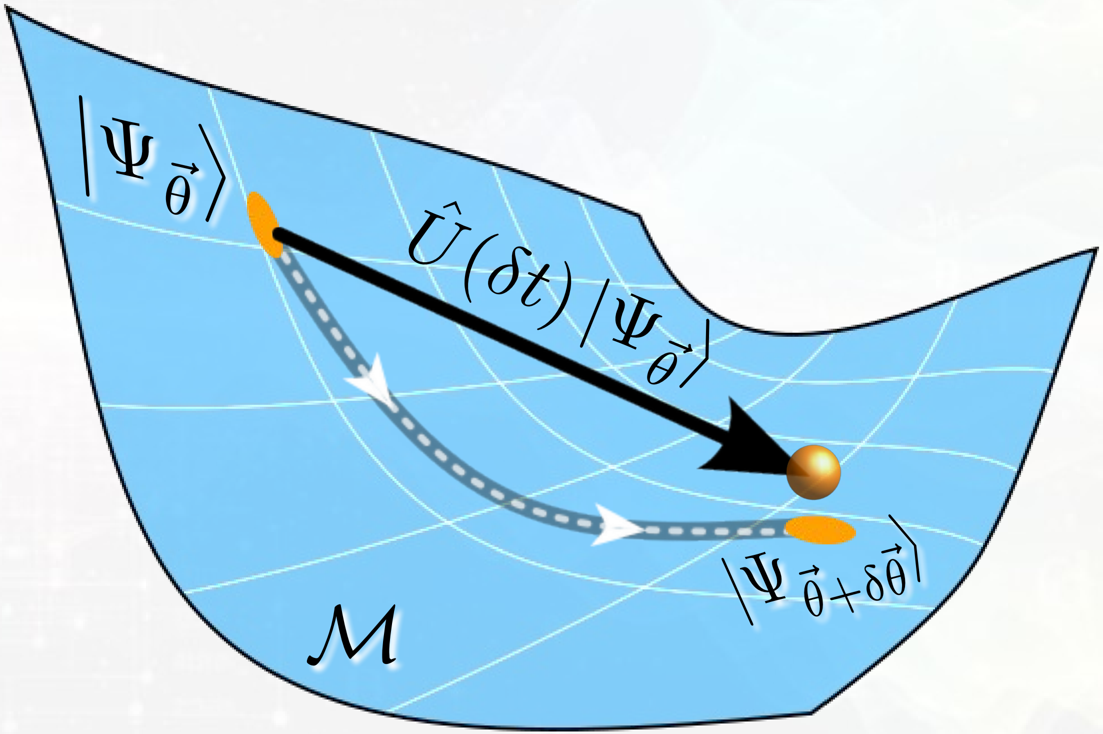

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Minimization of the
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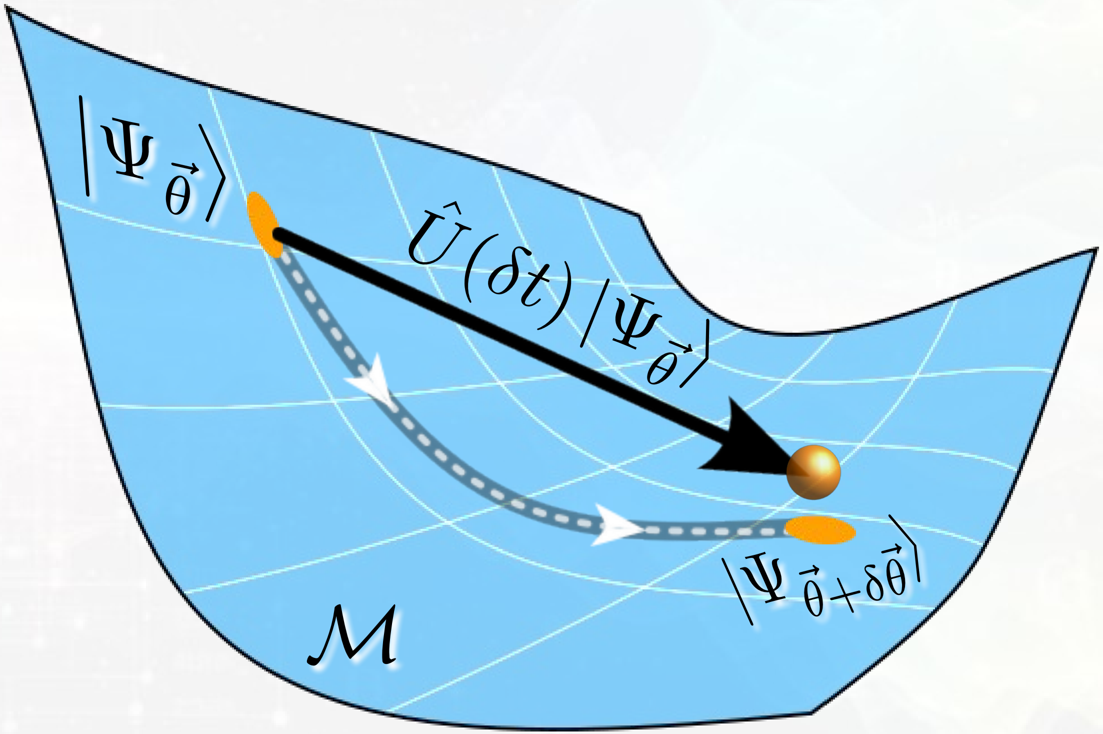
Coarse-grained



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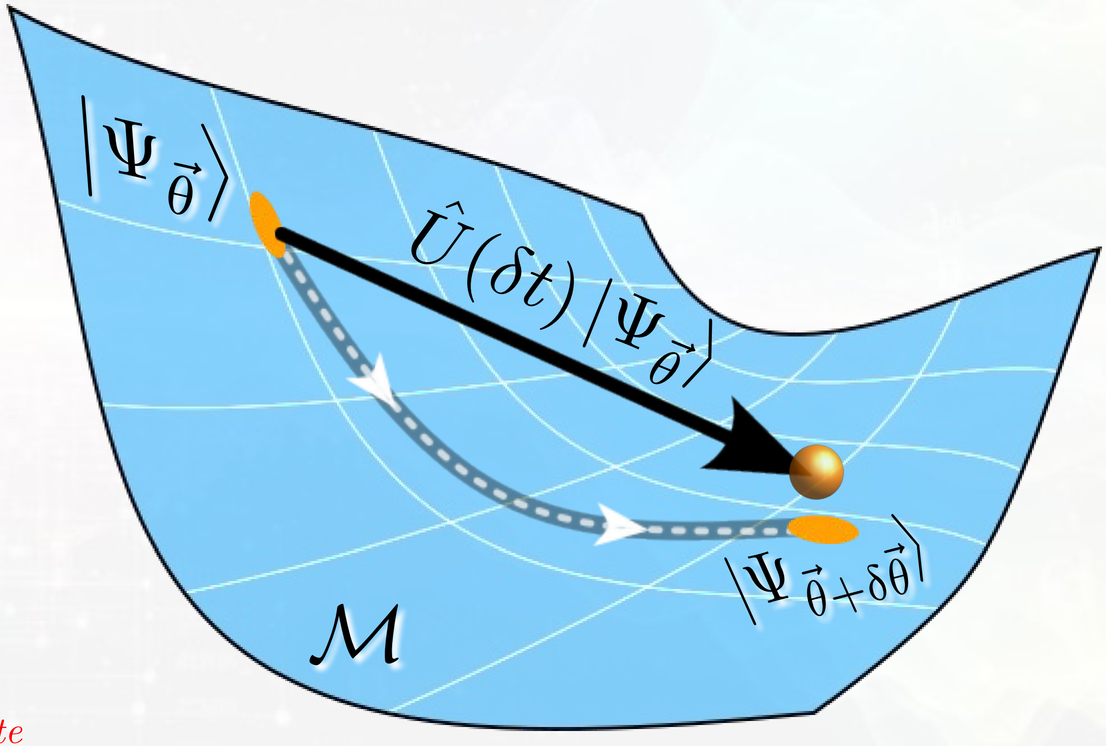

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Incomplete

Equations of motion

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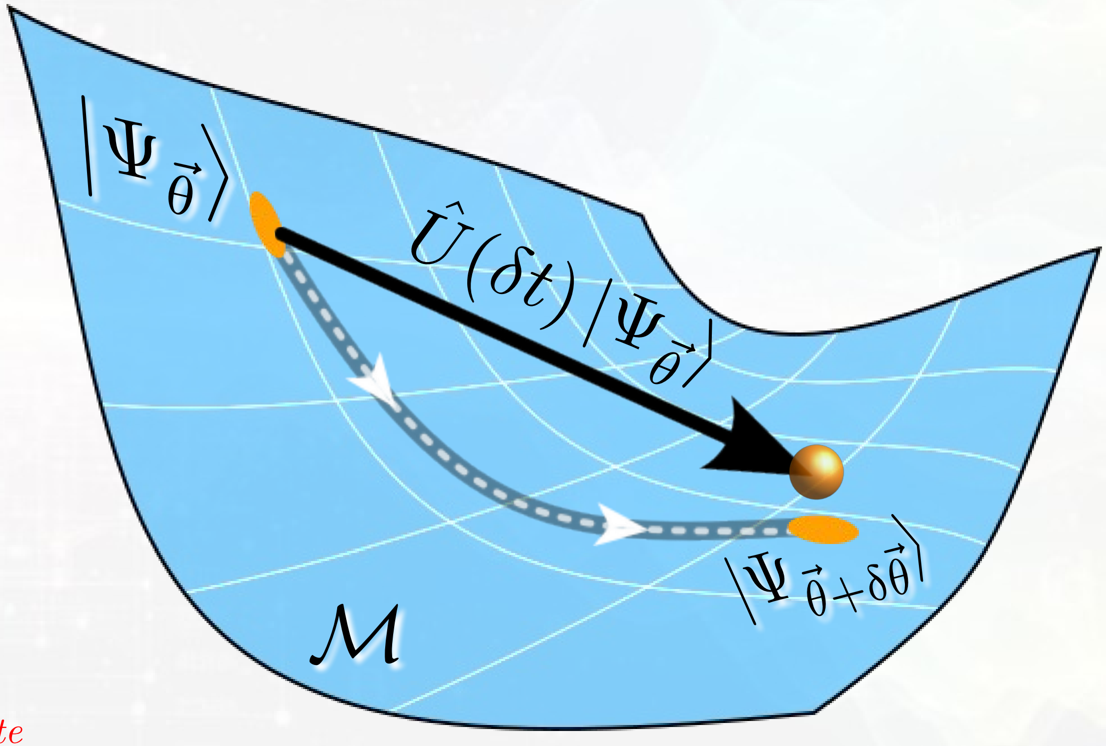

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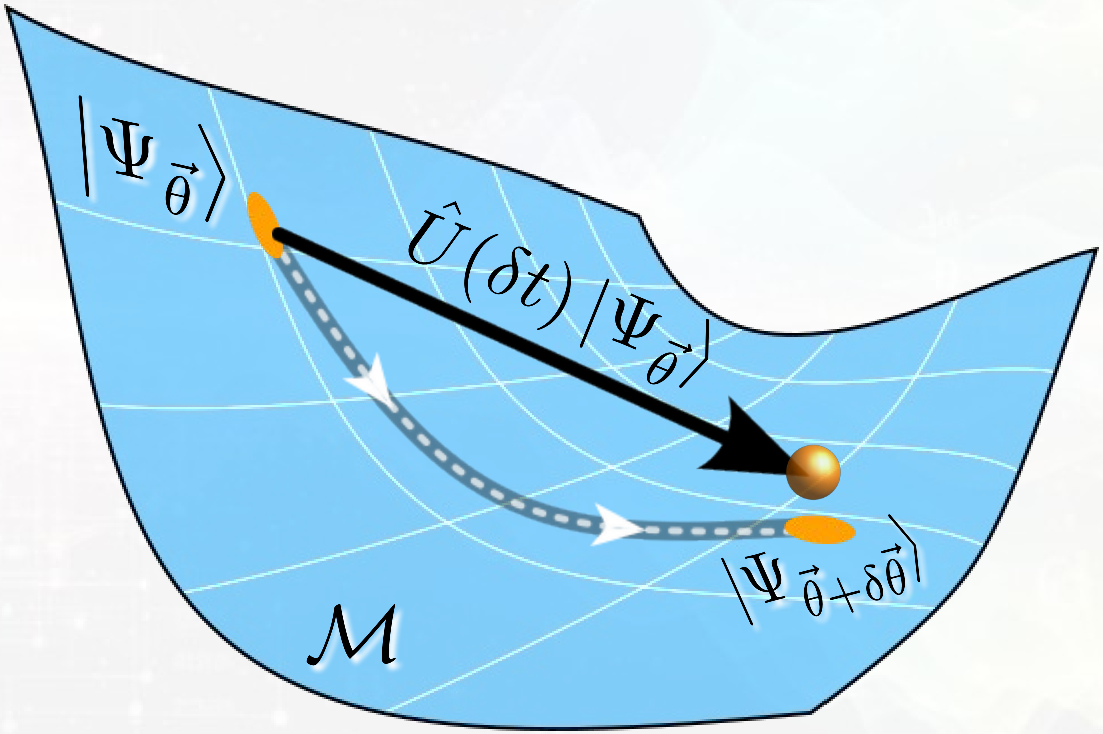

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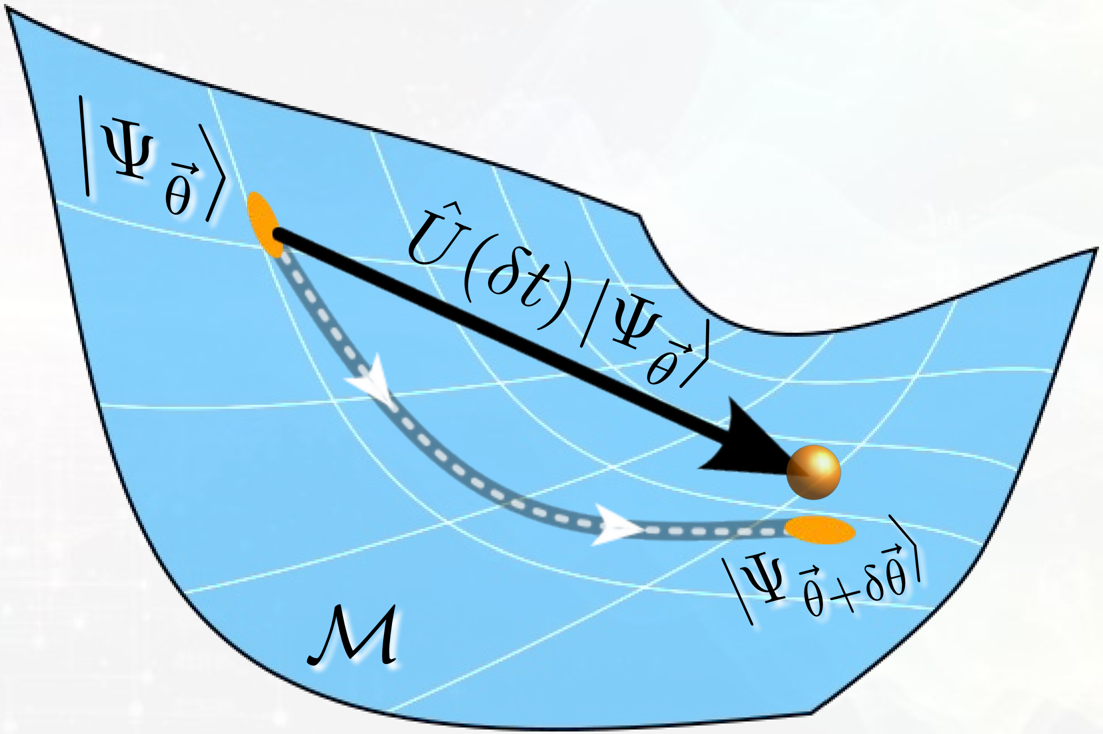
X. Yuan et al., Quantum **3**, 191 (2019).



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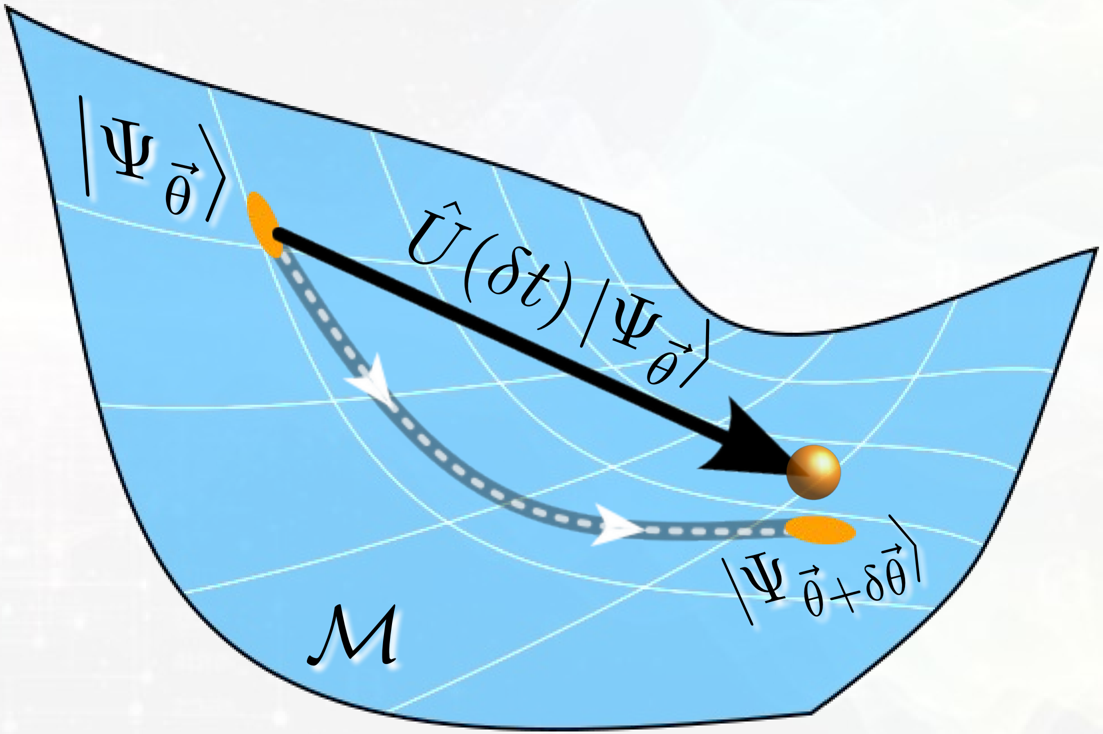

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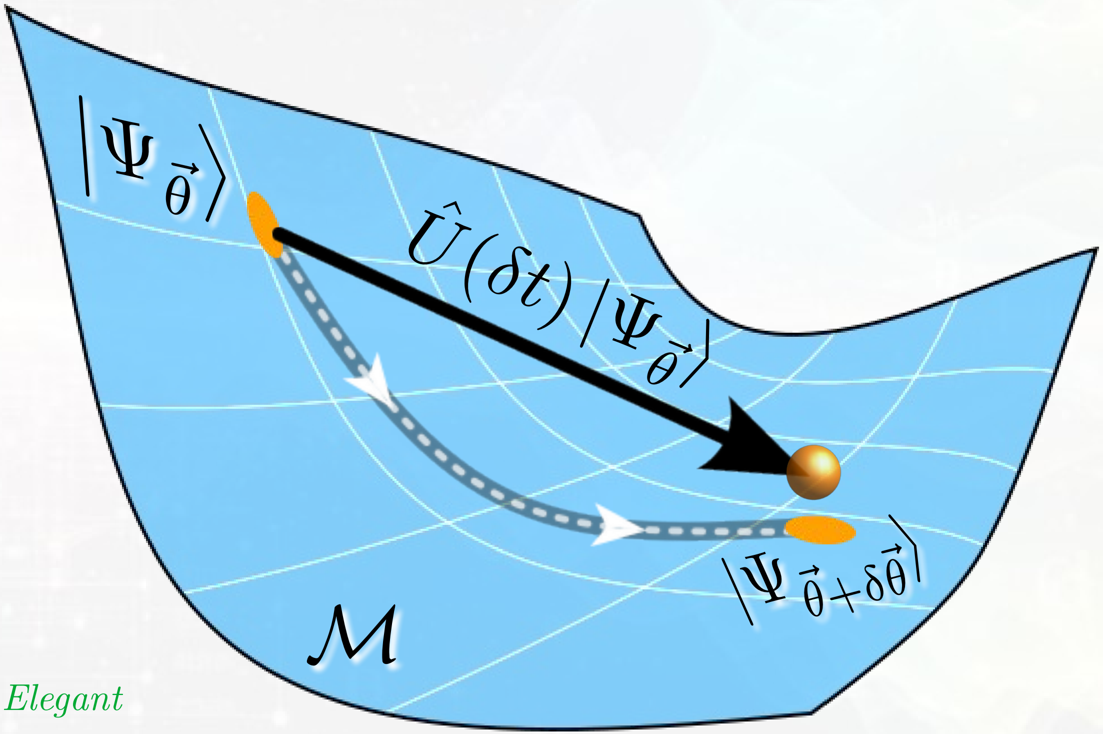
Elegant



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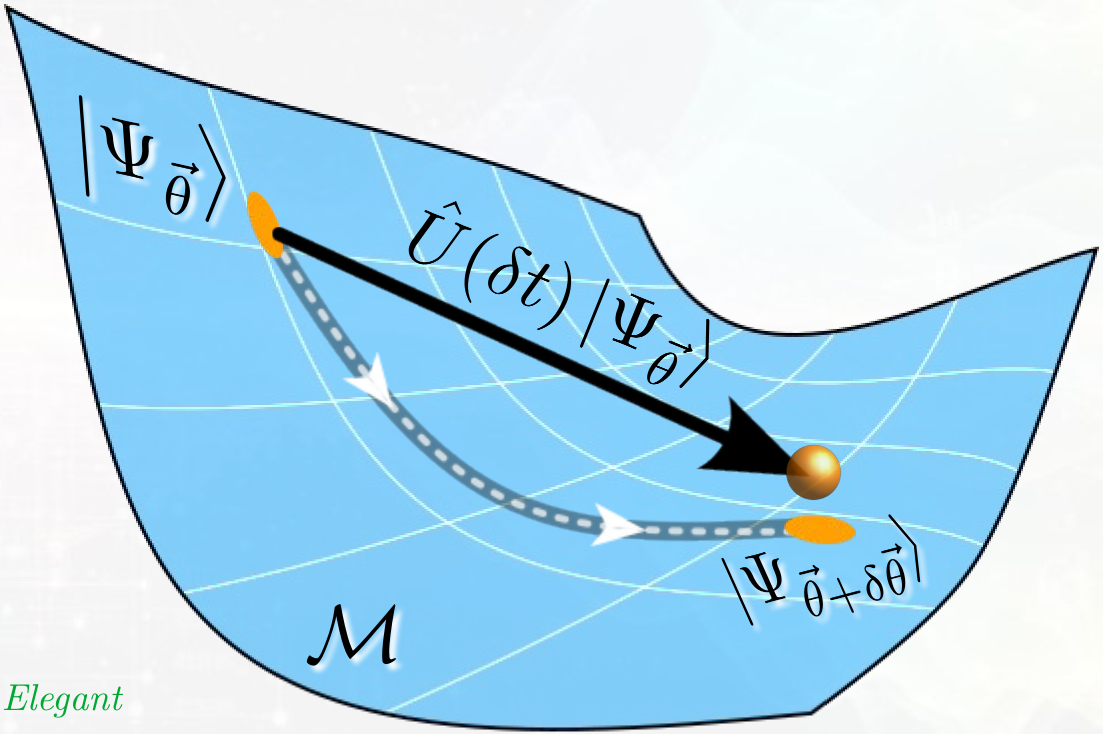

Elegant

Physically relevant

Equations of motion

- First Principles:

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<u>Euler-Lagrange Equations:</u>

$$\frac{\partial \mathcal{L}}{\partial \theta_\mu} - \frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial \mathcal{L}}{\partial \dot{\theta}_\mu} = 0 \quad \text{and} \quad \frac{\partial \mathcal{L}}{\partial \theta^*_\nu} - \frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial \mathcal{L}}{\partial \dot{\theta}^*_\nu} = 0$$

Equations of motion

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Equations of motion:

$$\boldsymbol{\mathcal{S}}\dot{\vec{\Theta}} = -i\vec{\mathcal{F}}$$

$\boldsymbol{\mathcal{S}} \equiv$ Quantum Geometric Tensor

$\vec{\Theta} \equiv$ Vector of parameters

$\vec{\mathcal{F}} \equiv$ Variational Forces

Equations of motion

- First Principles:

$$\mathcal{L}\left(\vec{\theta},\dot{\vec{\theta}},\vec{\theta}^*,\dot{\vec{\theta}}^*\right) = \frac{\langle\Psi_{\vec{\theta}}|\, i\frac{\partial}{\partial t} - \hat{\mathcal{H}}\,|\Psi_{\vec{\theta}}\rangle}{\langle\Psi_{\vec{\theta}}|\Psi_{\vec{\theta}}\rangle}$$

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$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} \dot{\vec{\theta}} \\ \dot{\vec{\theta}}^* \end{pmatrix} = -i \begin{pmatrix} \vec{F} \\ \vec{F}^* \end{pmatrix}$$

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$$\boldsymbol{\nabla}_{\vec{\theta}} E(\vec{\theta}, \vec{\theta}^*) = \vec{F}$$

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$$A_{\mu'\mu} = \frac{\partial_{\mu'} \langle\Psi| \partial_{\mu} |\Psi\rangle}{\langle\Psi|\Psi\rangle} - \frac{\partial_{\mu} \langle\Psi| \partial_{\mu'} |\Psi\rangle}{\langle\Psi|\Psi\rangle} - \left(\frac{\partial_{\mu'} \langle\Psi|\Psi\rangle}{\langle\Psi|\Psi\rangle}\frac{\langle\Psi|\partial_{\mu}|\Psi\rangle}{\langle\Psi|\Psi\rangle} - \frac{\partial_{\mu} \langle\Psi|\Psi\rangle}{\langle\Psi|\Psi\rangle}\frac{\langle\Psi|\partial_{\mu'}|\Psi\rangle}{\langle\Psi|\Psi\rangle}\right)$$

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$$B_{\mu'\nu} = \frac{\partial_{\mu'} \langle\Psi| \partial_\nu |\Psi\rangle}{\langle\Psi|\Psi\rangle} - \frac{\partial_\nu \langle\Psi| \partial_{\mu'} |\Psi\rangle}{\langle\Psi|\Psi\rangle} - \left(\frac{\partial_{\mu'} \langle\Psi|\Psi\rangle}{\langle\Psi|\Psi\rangle} \frac{\langle\Psi|\partial_\nu|\Psi\rangle}{\langle\Psi|\Psi\rangle} - \frac{\partial_\nu \langle\Psi|\Psi\rangle}{\langle\Psi|\Psi\rangle} \frac{\langle\Psi|\partial_{\mu'}|\Psi\rangle}{\langle\Psi|\Psi\rangle} \right)$$

$$F_{\mu'} = \frac{\partial_{\mu'} \langle\Psi| \hat{\mathcal{H}} |\Psi\rangle}{\langle\Psi|\Psi\rangle} + \frac{\langle\Psi| \partial_{\mu'}\hat{\mathcal{H}} |\Psi\rangle}{\langle\Psi|\Psi\rangle} + \frac{\langle\Psi| \hat{\mathcal{H}}\partial_{\mu'} |\Psi\rangle}{\langle\Psi|\Psi\rangle} - \left(\frac{\partial_{\mu'} \langle\Psi|\Psi\rangle}{\langle\Psi|\Psi\rangle} + \frac{\langle\Psi| \partial_{\mu'} |\Psi\rangle}{\langle\Psi|\Psi\rangle} \right) \frac{\langle\Psi|\hat{\mathcal{H}}|\Psi\rangle}{\langle\Psi|\Psi\rangle}$$

Equations of motion

$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} \dot{\vec{\theta}} \\ \dot{\vec{\theta}}^* \end{pmatrix} = -i \begin{pmatrix} \vec{F} \\ \vec{F}^* \end{pmatrix}$$

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$\lvert\Psi(\vec{\theta}, \vec{\theta}^*)\rangle$ non-holomorphic	$A_{\mu'\mu} = -A_{\mu\mu'}$ complex skew-symmetric	$B_{\mu'\nu} = B^*_{\mu\nu'}$ Hermitian	$\boldsymbol{\mathcal{S}}\dot{\vec{\Theta}} = -i\vec{\mathcal{F}}$ $\boldsymbol{\mathcal{S}}$ block matrix
$\lvert\Psi(\vec{\theta})\rangle$ holomorphic	$A_{\mu'\mu} = 0$ null	$B_{\mu'\nu} = B^*_{\mu\nu'}$ Hermitian	$\boldsymbol{S}\dot{\vec{\theta}} = -i\vec{F}^*$ $\boldsymbol{S} = -\boldsymbol{B}^*$
$\lvert\Psi(\vec{\alpha})\rangle$ real parameters	$\boldsymbol{A} = \boldsymbol{B}$ and $A^*_{\alpha'\alpha} = -A_{\alpha'\alpha} = A_{\alpha\alpha'}$ purely imaginary skew-symmetric		$\boldsymbol{S}\dot{\vec{\theta}} = -i\vec{F}$ $\boldsymbol{S} = \boldsymbol{A}$

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Ground state search

$$\delta_n = -(Q_n + \lambda_n R_n)^{-1} L_n \qquad \lambda \in \mathbb{C}$$

Outline

- Introduction
- Methodology

Outline

Introduction

Methodology

Time-dependent Variational Principle

Outline

Introduction

Methodology

Time-dependent Variational Principle

Equations of motion

Outline

- Introduction
- Methodology
- Time-dependent NQS

Time-dependent NQS

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1) Restricted Bolzmann Machine

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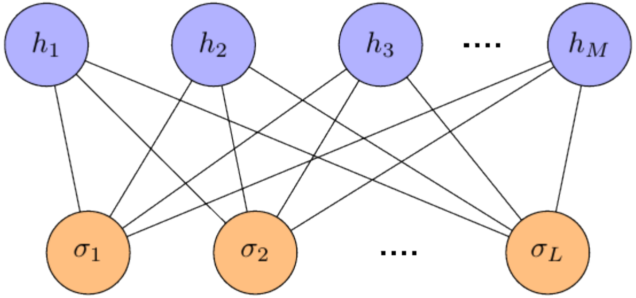
$$\psi(\sigma) = \sum_{\{h_i\}} \mathrm{e}^{\sum_j a_j \sigma_j + \sum_i b_i h_i + \sum_{i,j} w_{ij} h_i \sigma_j}$$



(a) Restricted Boltzmann machine architecture

I. L. Gutiérrez and C. B. Mendl, Quantum **6**, 627 (2022).

Time-dependent NQS

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2) Transverse-field Ising Model

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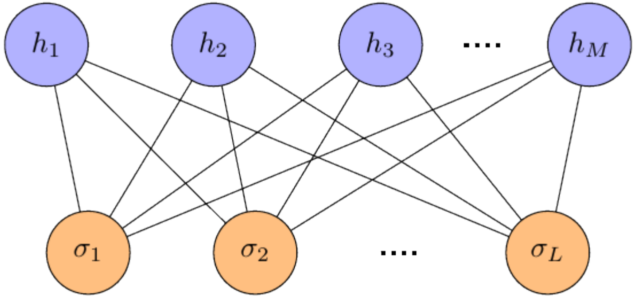

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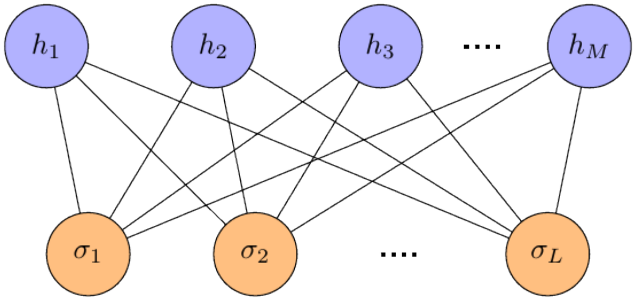

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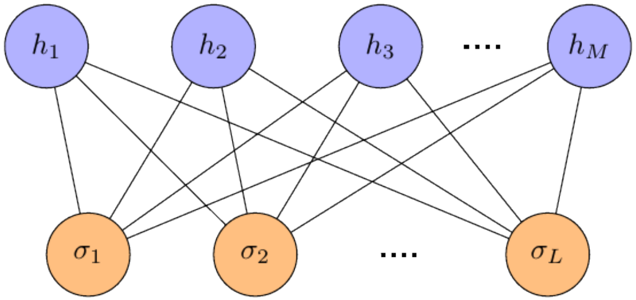

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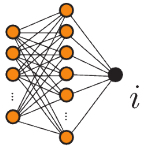
Neural Quantum Galerkin

$$|\Psi_\theta(t)\rangle = \sum_{i=0}^{M} c_i(t) |\phi_i\rangle = \sum_{i=0}^{M} c_i(t)$$



A. Sinibaldi et al., arXiv:2412.11778.

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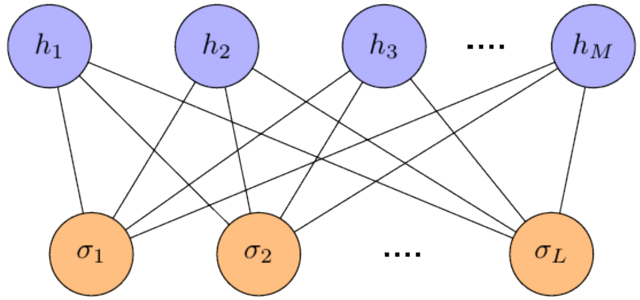

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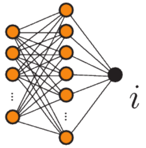

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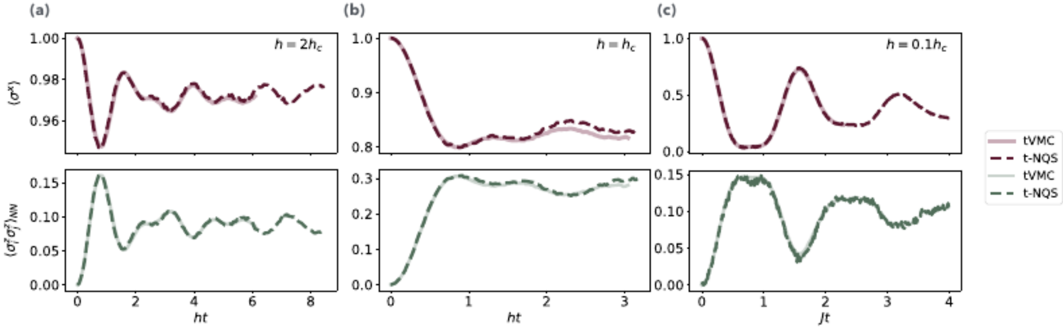

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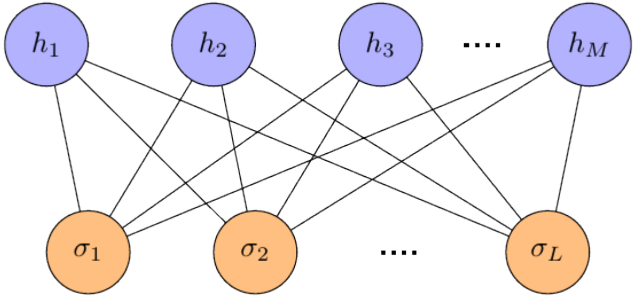

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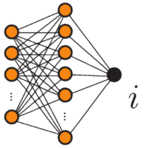

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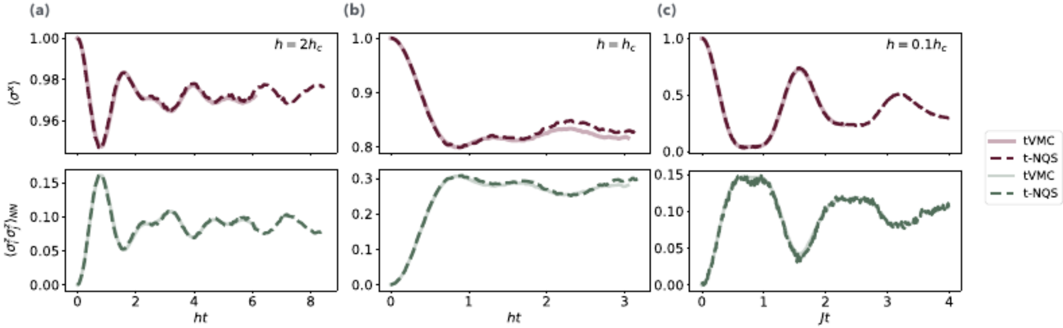

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Most dynamics done for discrete systems!

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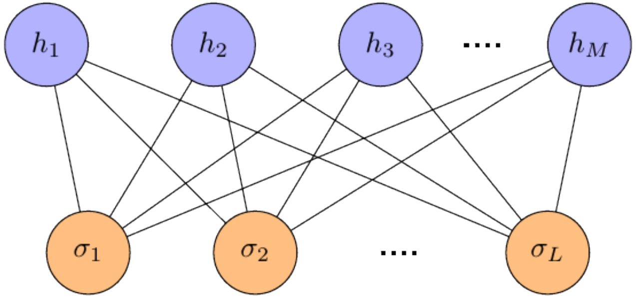

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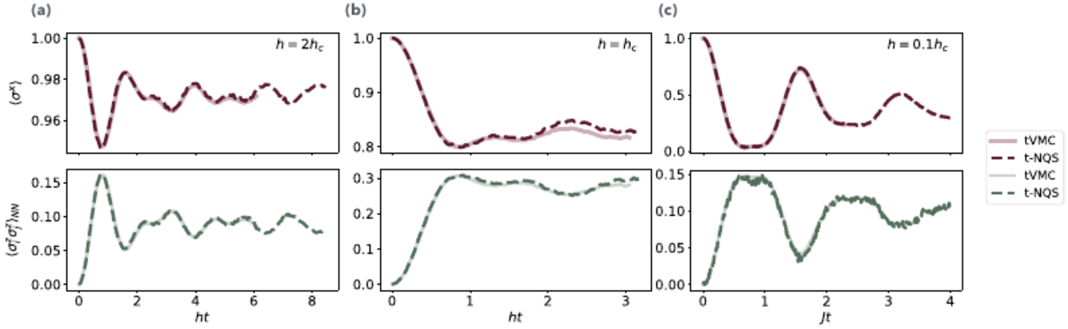

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Most dynamics done for discrete systems!

Outline

- Introduction
- Methodology
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- Introduction
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  - Gross-Pitaevskii Equation

$$\mathcal{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2$$

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Has exact analytical solutions
to benchmark our methods!

Quantum Harmonic Oscillator (HO)

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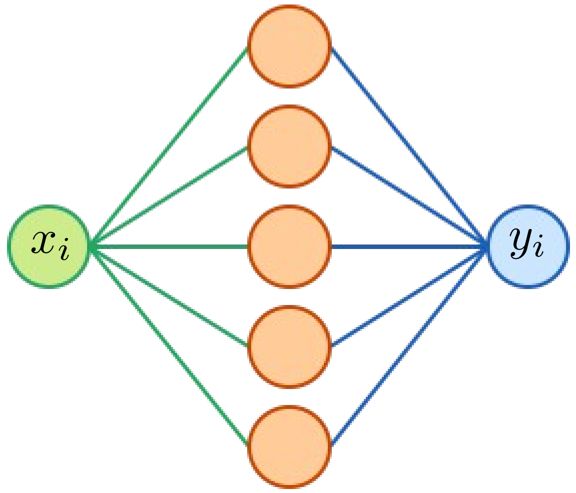

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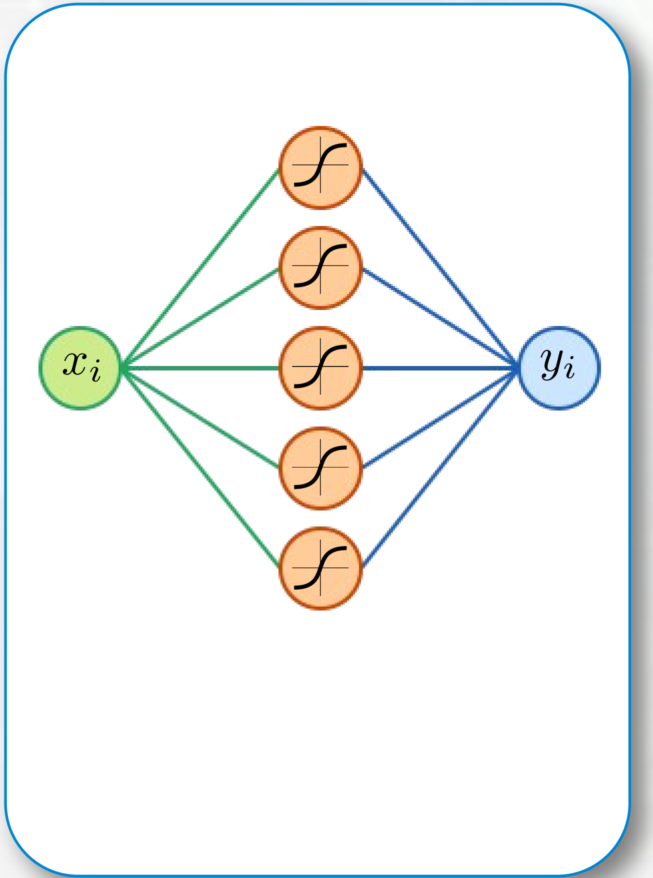

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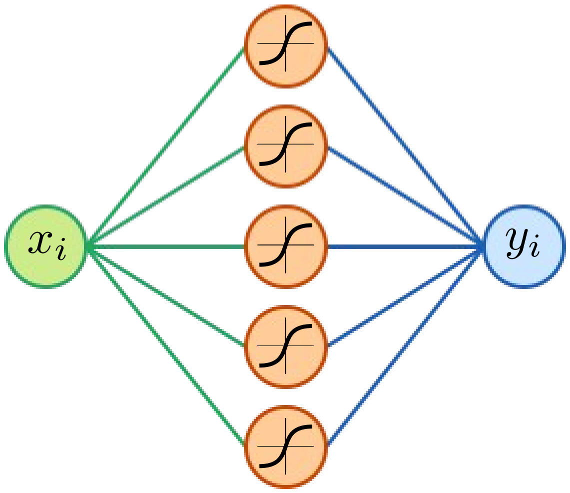
Holomorphic



$\vec{\theta} \in \mathbb{C}^m; m = 16$

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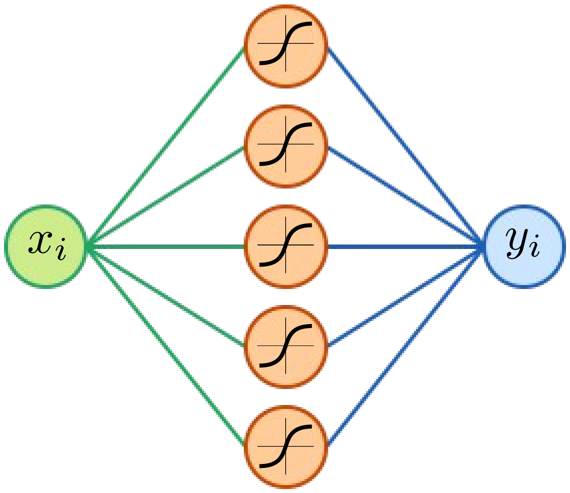

$\vec{\theta} \in \mathbb{C}^m; m = 16$

$\ln \Psi\left(x_i; \vec{\theta}\right) = e^{y_i}$

HO: Breathing dynamics

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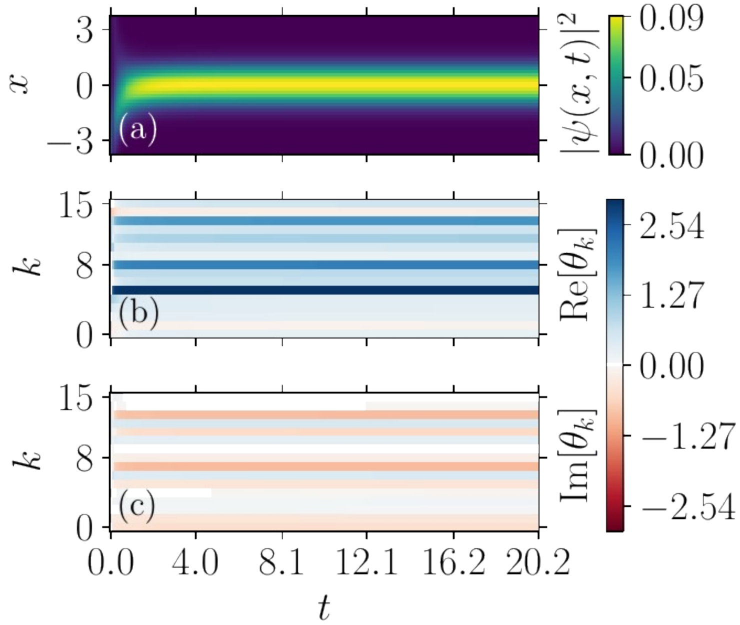
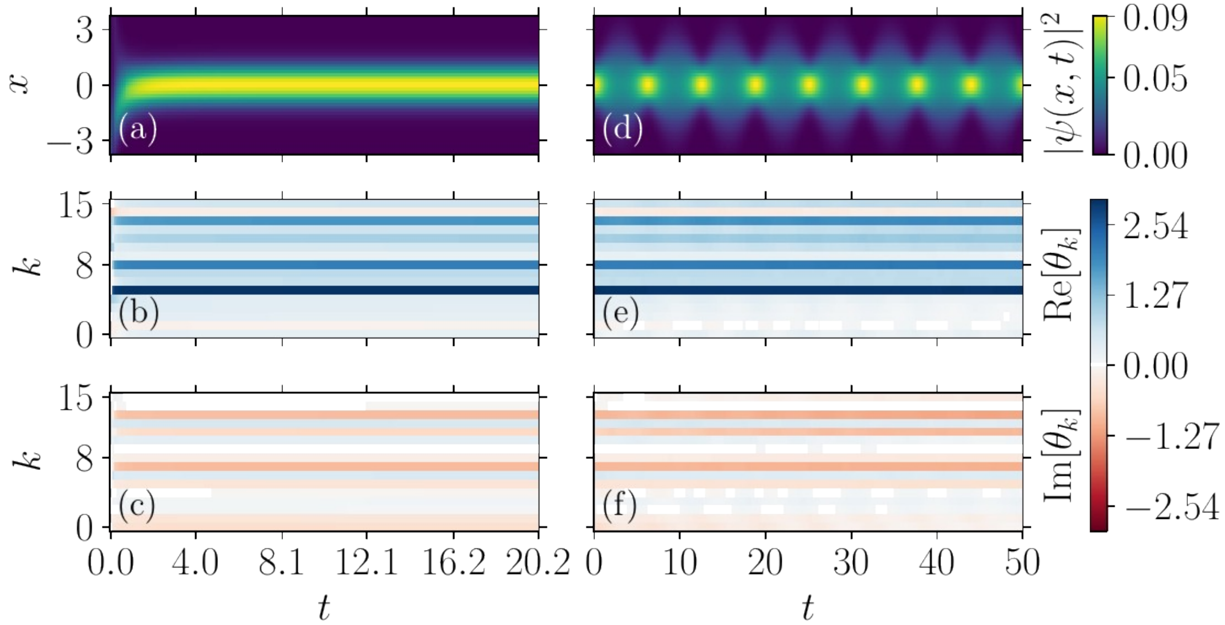
Imaginary time
GS search



Imaginary time
GS search

Real time
Dynamics

$(\omega = 1 \to 0.5)$



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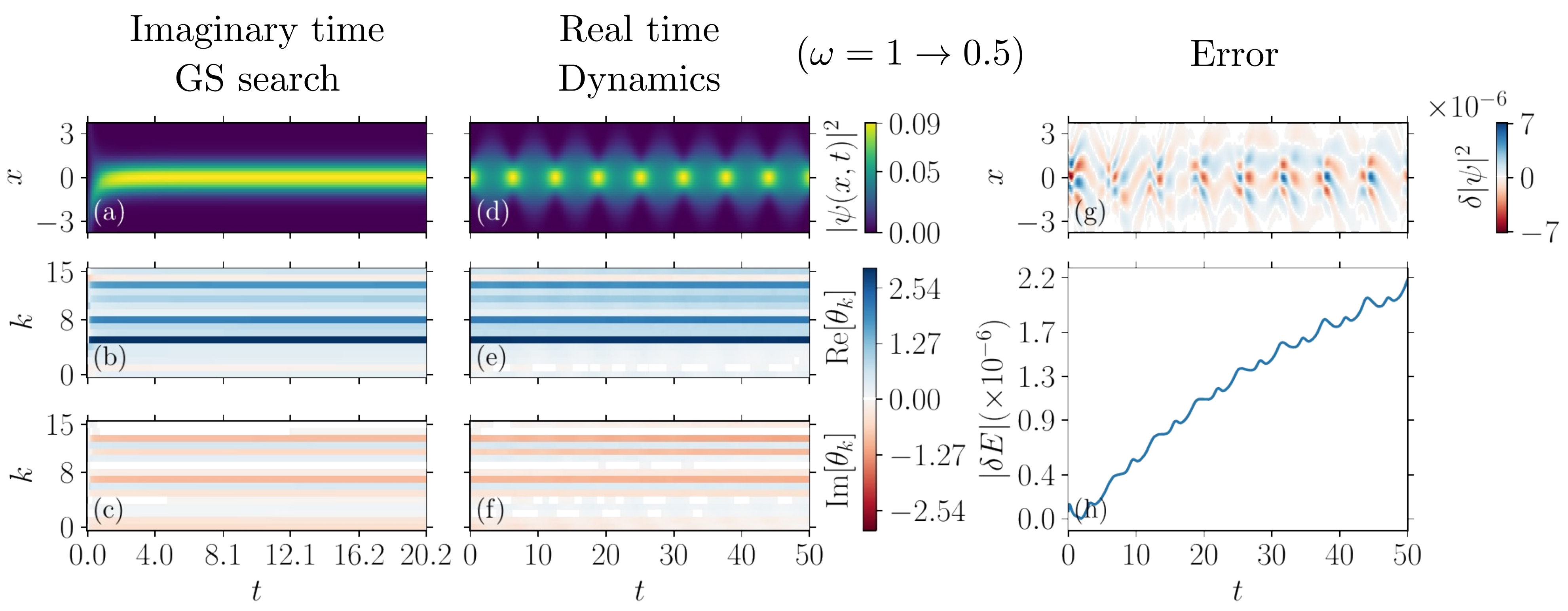

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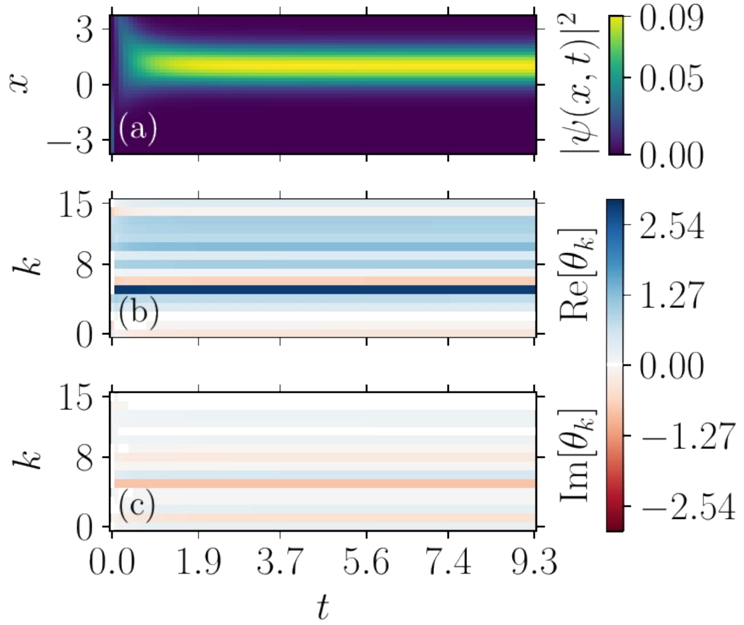
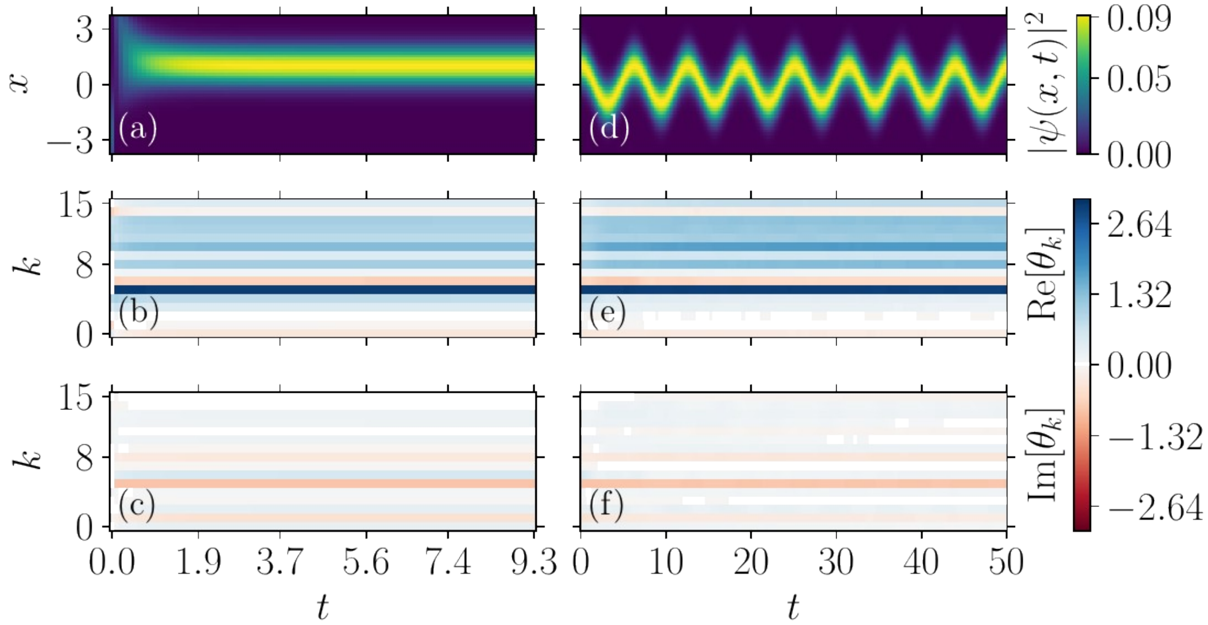


HO: Coherent State

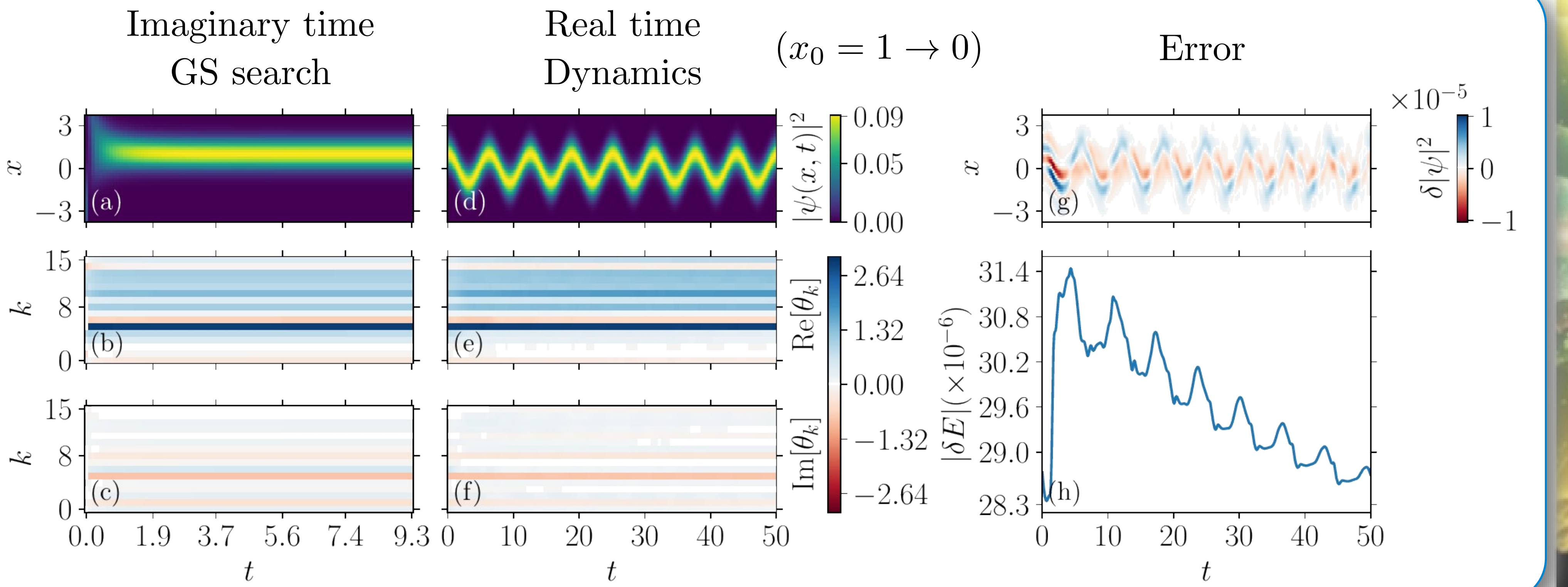
Imaginary time
GS search

Real time
Dynamics

$(x_0 = 1 \to 0)$



HO: Coherent State



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$$\mathcal{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2 + g|\Psi|^2$$

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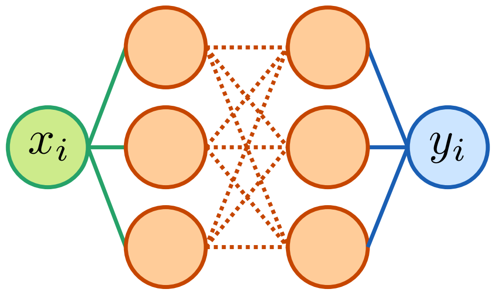

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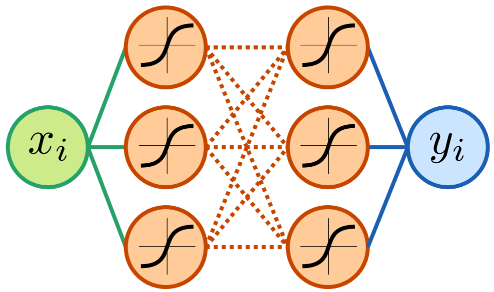

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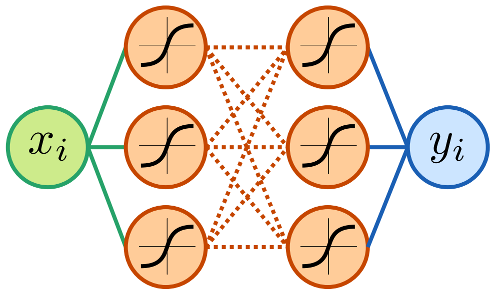
Holomorphic



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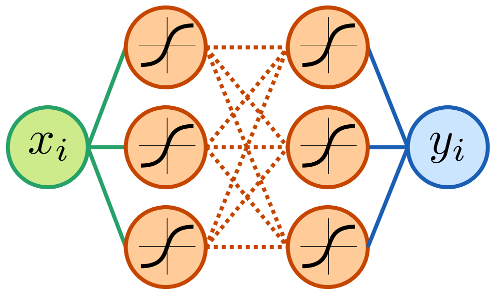

$\vec{\theta} \in \mathbb{C}^m; m = 22$

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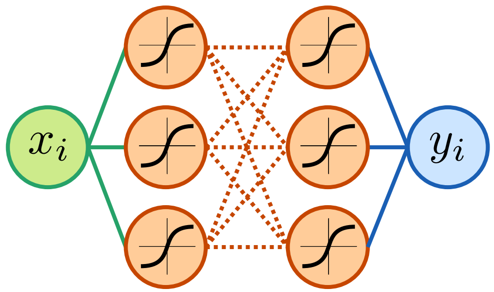

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Gross-Pitaevskii Equation (GPE)

Imaginary time propagation
Ground state search

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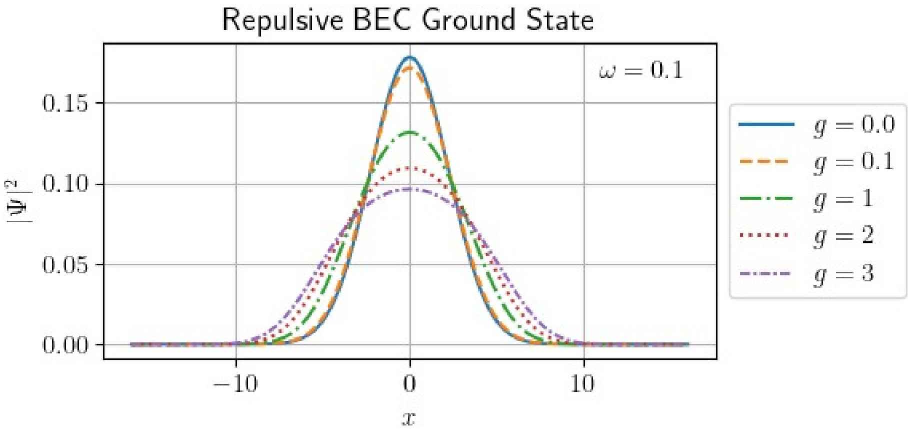
Ground state search

$g > 0$ (repulsive)



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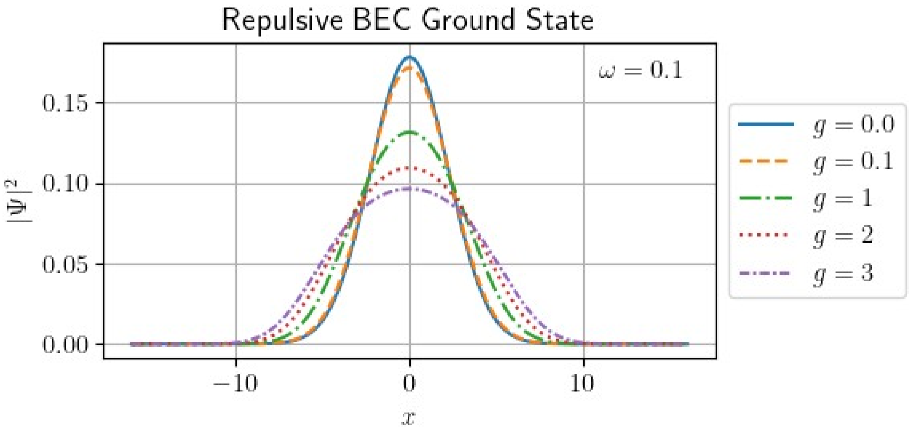

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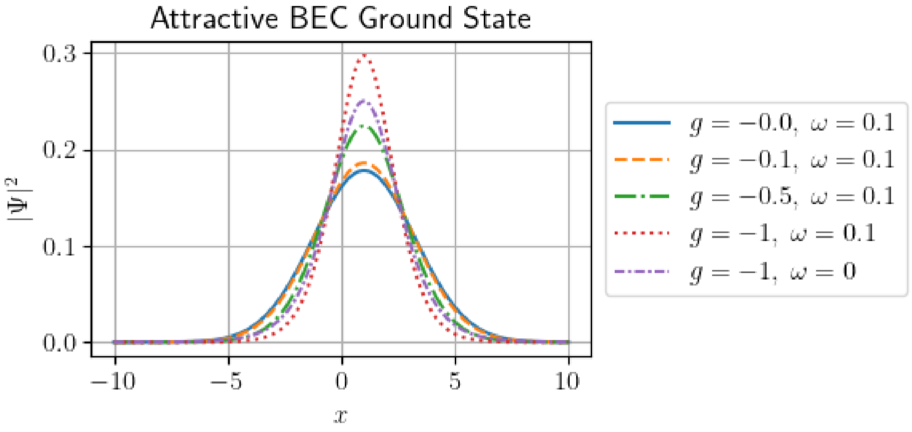

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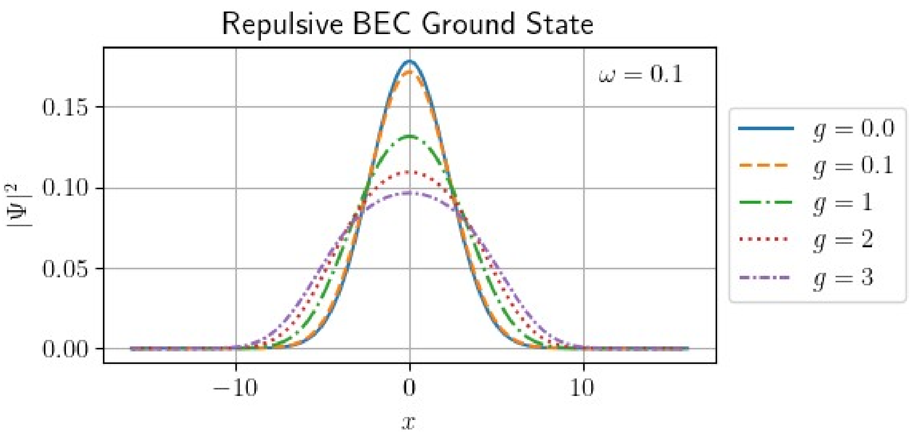

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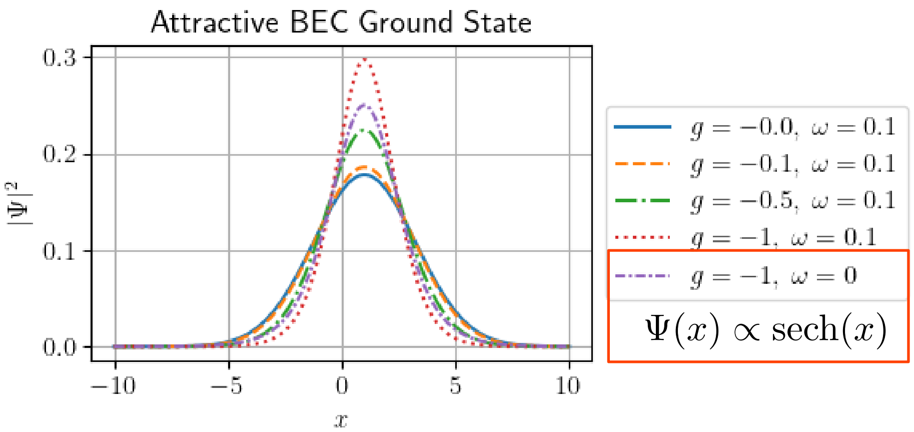

$\Psi(x) \propto \text{sech}(x)$

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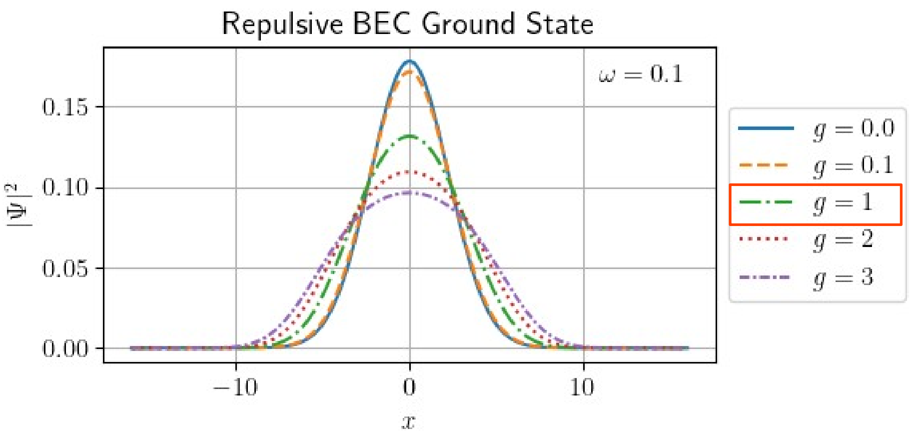

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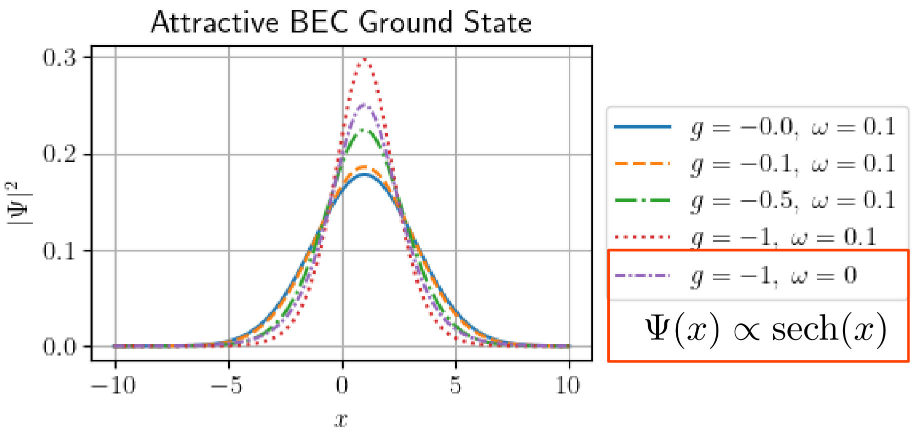

GPE: Breathing dynamics $g = 1$ (repulsive)

Small oscillations: $\omega_0 = \sqrt{3}\omega$

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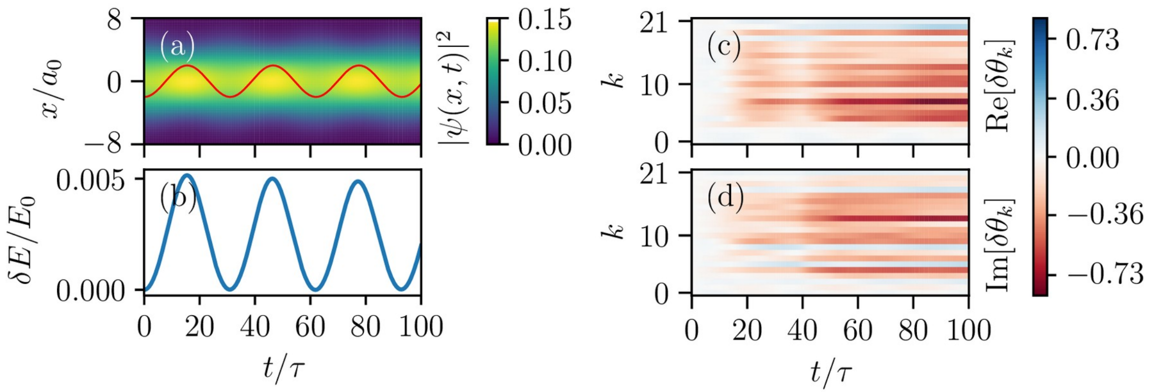

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$\omega = 0.1 \to 0.11$

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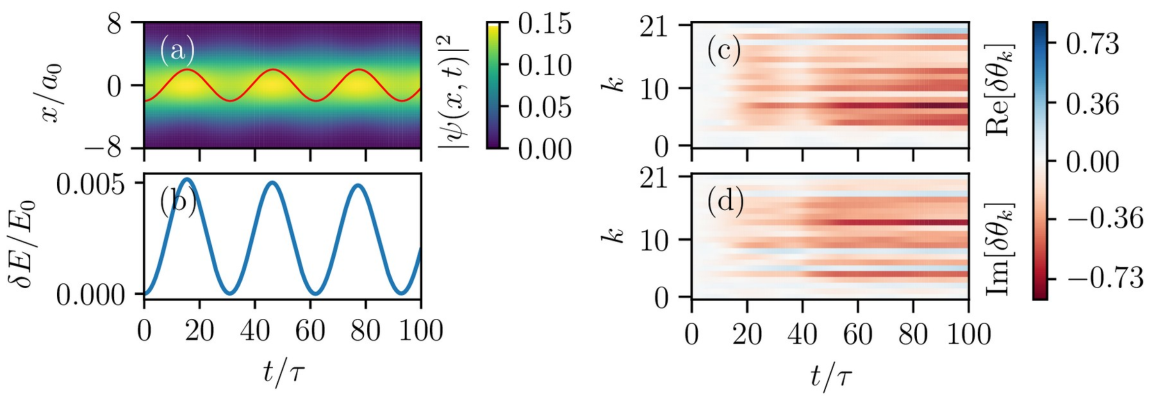

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Comptes Rendus. Physique **24** (S3), 15 (2023)

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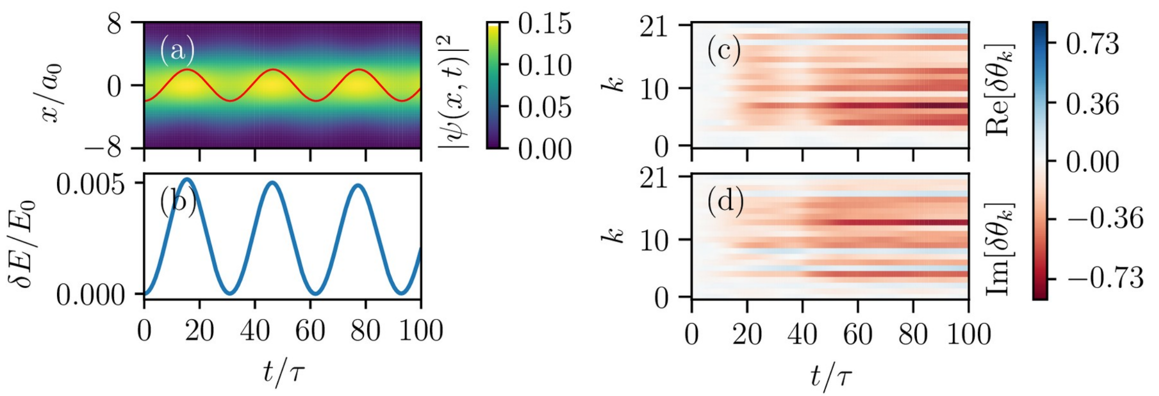

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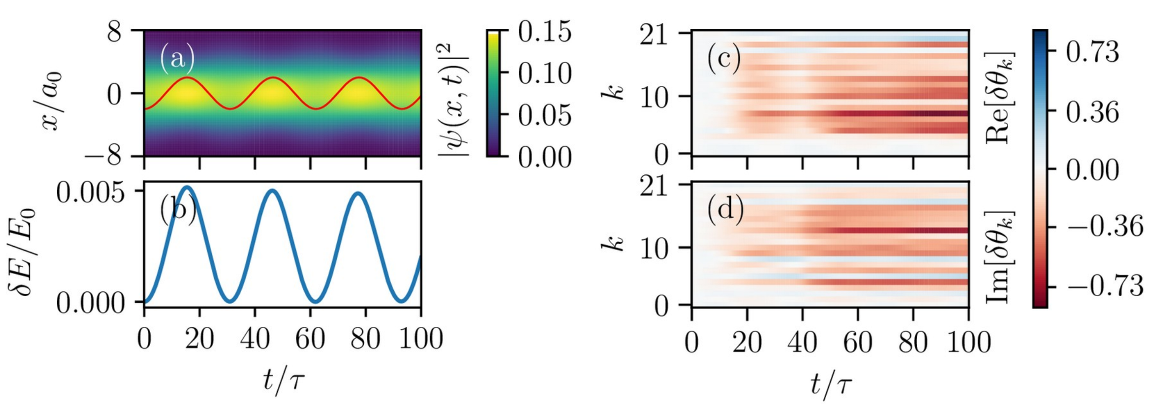

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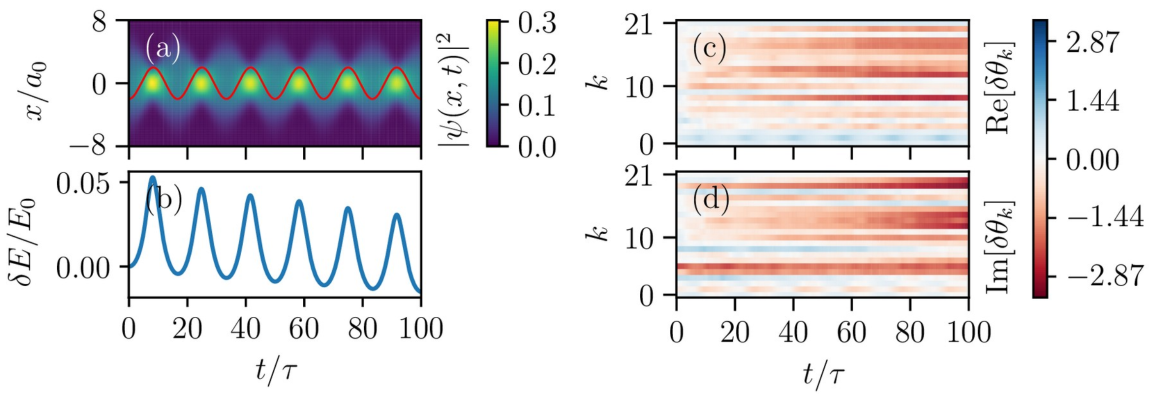

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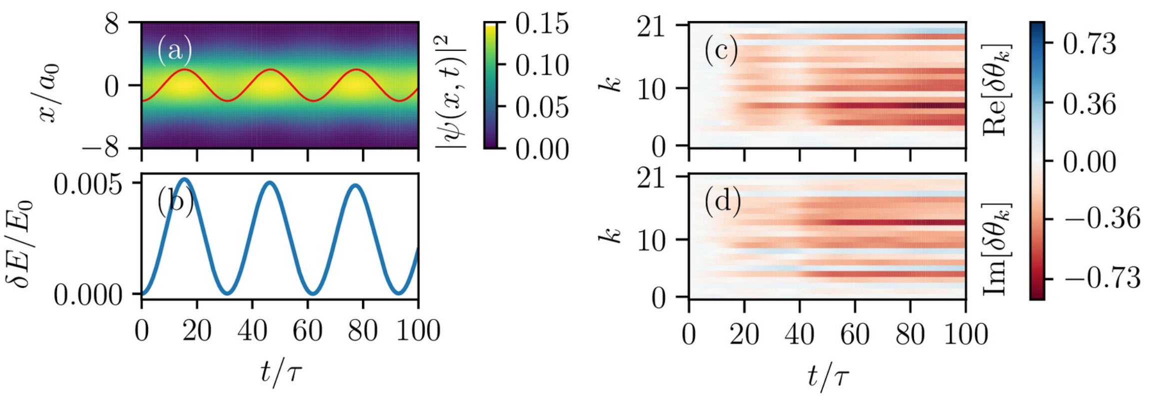

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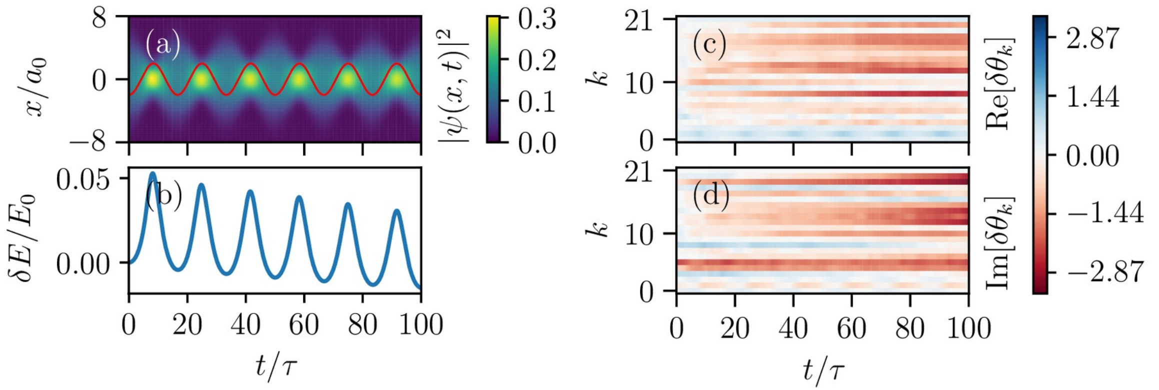

Large oscillations: $\omega_0 = 2\omega$

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Comptes Rendus. Physique **24** (S3), 15 (2023)

GPE: Bright soliton dynamics $g = -1$ (att.)

Brigth soliton solution:

$$\Psi(x,t) = \eta \,\mathrm{sech}\left[\eta(x - x_0(t))\right] e^{-i\phi(t)}$$

L. Khaykovich et al., Science **296**, 1290 (2002).

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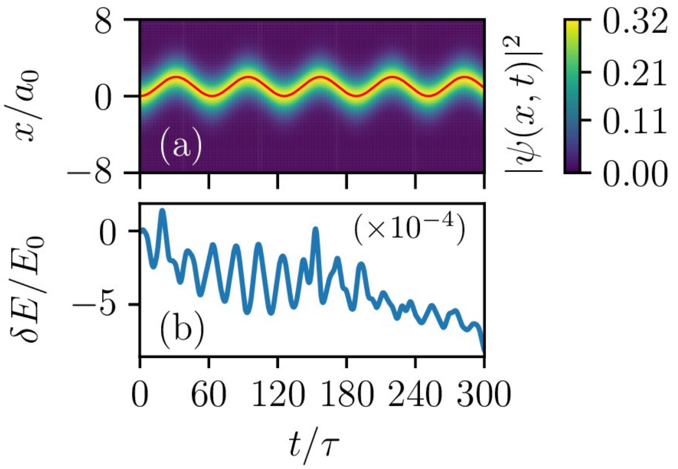

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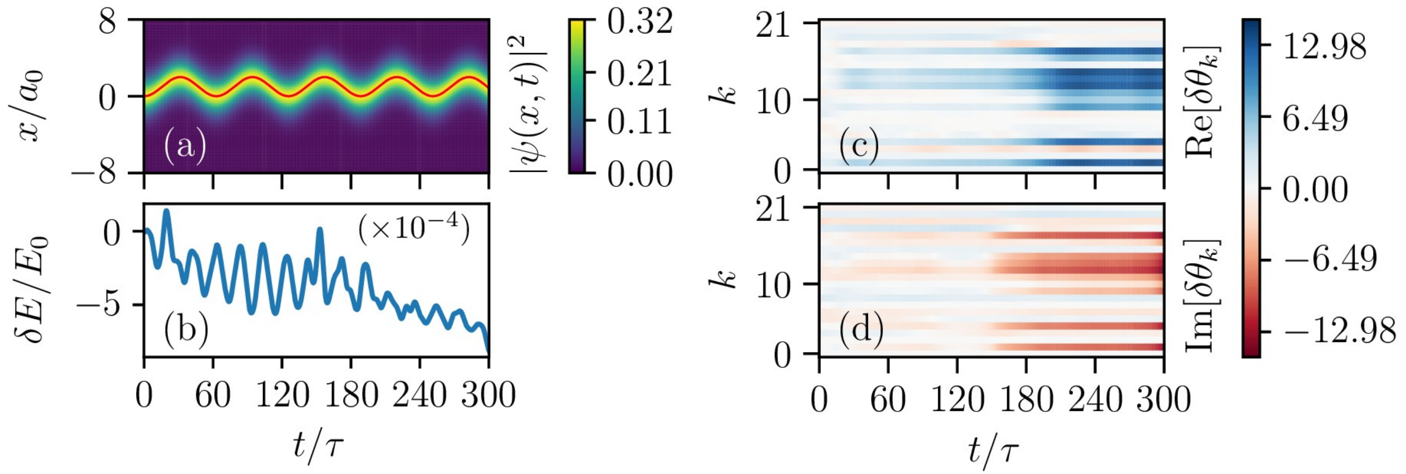
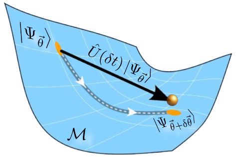


- TD-NQS are a TDV approach



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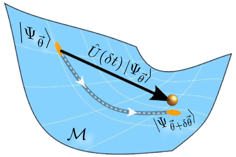
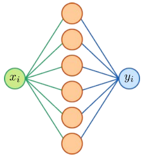
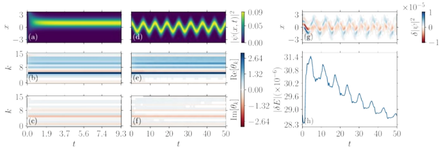


- Small NQS are expressive enough to describe HO dynamics





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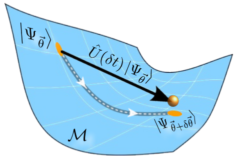

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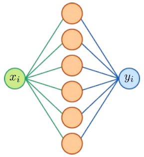

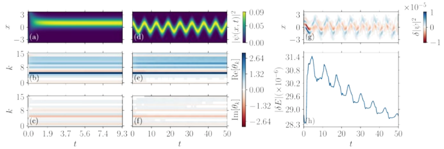

- Small NQS can capture the dynamics of nonlinear systems

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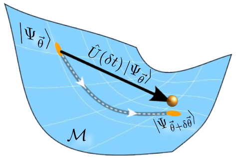

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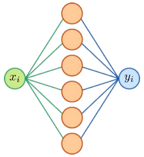
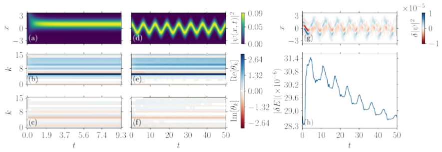


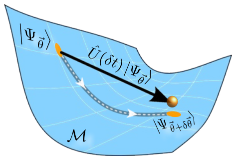


- Small NQS can capture the dynamics of nonlinear systems

- Add generic boundary conditions

Conclusions & Future Perspectives

- TD-NQS are a TDV approach



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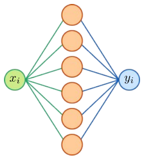

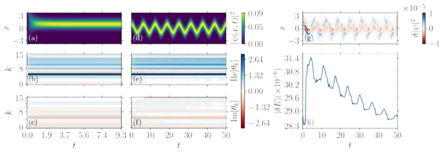

- Small NQS can capture the dynamics of nonlinear systems

- Add generic boundary conditions

- Improve regularization methods

Conclusions & Future Perspectives

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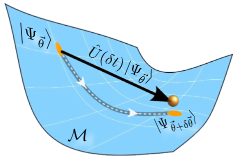

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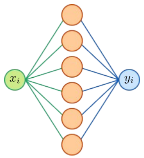

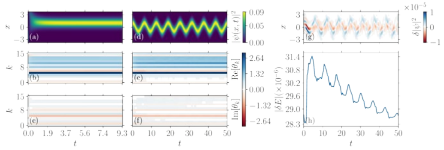

- Small NQS can capture the dynamics of nonlinear systems

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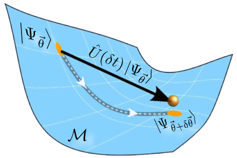
- Extend the NQS for excited states, i.e., dark solitons

Conclusions & Future Perspectives

- TD-NQS are a TDV approach



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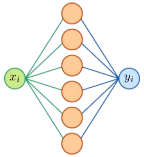
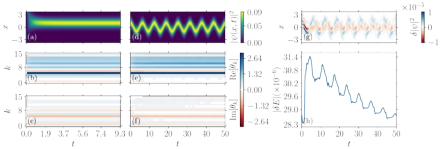
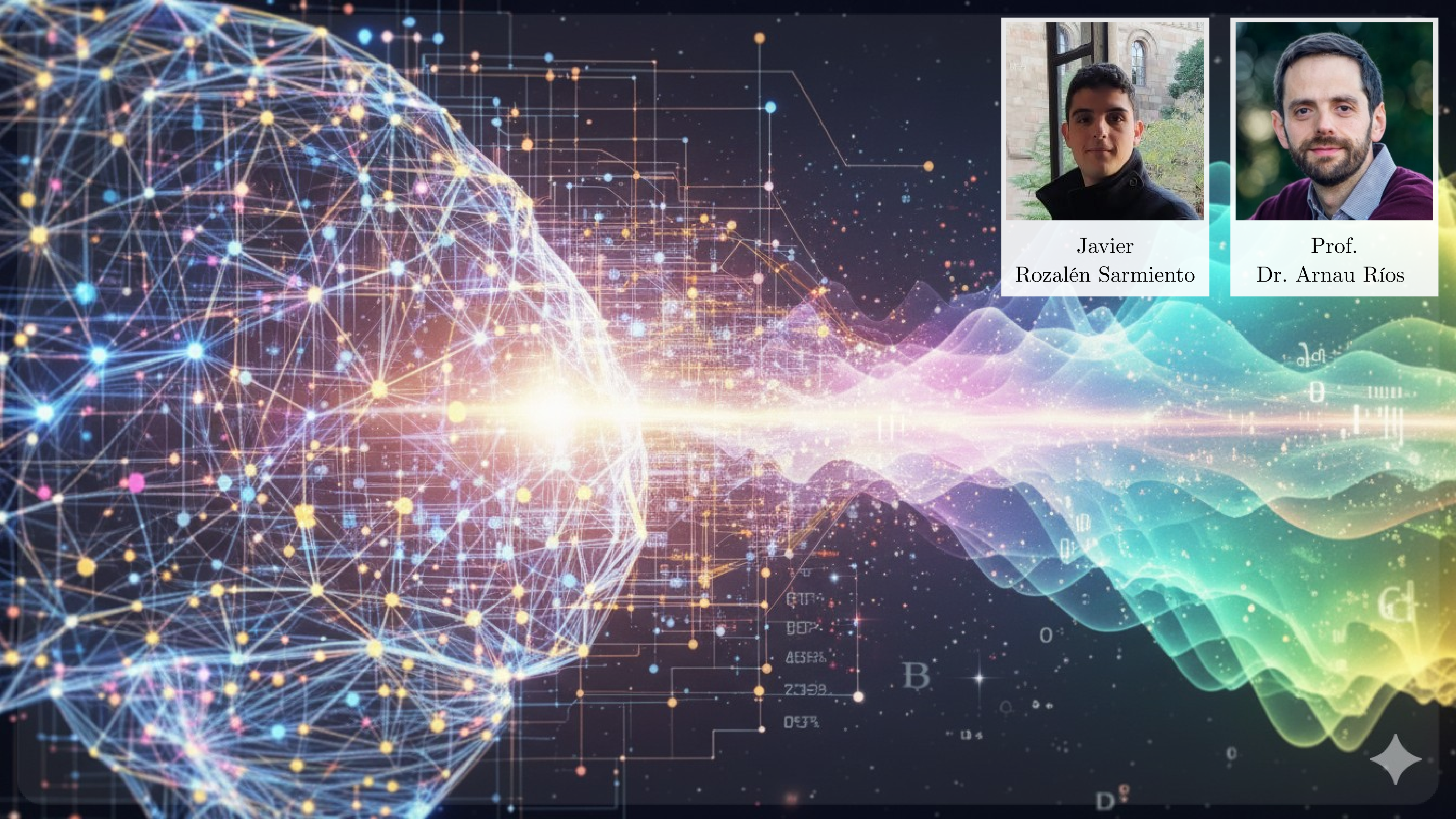




- Small NQS can capture the dynamics of nonlinear systems

- Add generic boundary conditions
- Improve regularization methods
- Extend the NQS for excited states, i.e., dark solitons
- Extend the TD-NQS to few-body interaction problems or higher dimensional problems



Javier
Rozalén Sarmiento

Prof.
Dr. Arnau Ríos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Rozalén Sarmiento

Prof.
Dr. Arnau Ríos

arXiv:2509.24865

GitHub: Alejandro-FQA

THANK YOU!

Alejandro Romero-Ros (alejandro.romero.ros@fqa.ub.edu)
Departament Física Quàntica i Astrofísica, UB

Time-dependent Neural Quantum States

Exploring the quantum chromodynamics phase diagram:
from hadrons and nuclei to matter under extreme conditions

UNIVERSITAT DE BARCELONA

ICCUB
Institut de Ciències del Cosmos
UNIVERSITAT DE BARCELONA

EXCELENCIA MARÍA DE MAEZTU 04/2025-03/2031

MINISTERIO DE CIENCIA, INNOVACIÓN Y UNIVERSIDADES

Financiado por la Unión Europea NextGenerationEU

Plan de Recuperación, Transformación y Resiliencia

AGENCIA ESTATAL DE INVESTIGACIÓN

Technicalities – Code parameters

PyTorch

Integrator: 4th order Runge-Kutta

Quantum Harmonic Oscillator		Gross-Pitaevskii Equation
$x \in [-8, 8]$	Grid size	$x \in [-16, 16]$
$n = 101$	Grid points	$n = 301$
$\mathrm{d}t = 0.1$	Integration step	$\mathrm{d}t = 0.1$
$\epsilon = 10^{-8}$	Convergence error	$\epsilon = 10^{-8}$
$\lambda_{\text{imag}} = 10^{-4}$	Regularization imaginary time	$\lambda_{\text{imag}} = 0$
$\lambda_{\text{real}} = i10^{-6}$	Regularization real time	$\lambda_{\text{real}} = (0.01 + i) \times 10^{-4}$
Direct	Inversion method	Pseudo-inverse

Outline

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Introduction

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Artificial Neural Networks

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Artificial Neural Networks

Neural Quantum States

Outline

- Introduction
- Methodology
- Results
- Conclusions & Future Perspectives

Methodology

Results