Quantum Dynamics with Time-Dependent Neural Quantum States

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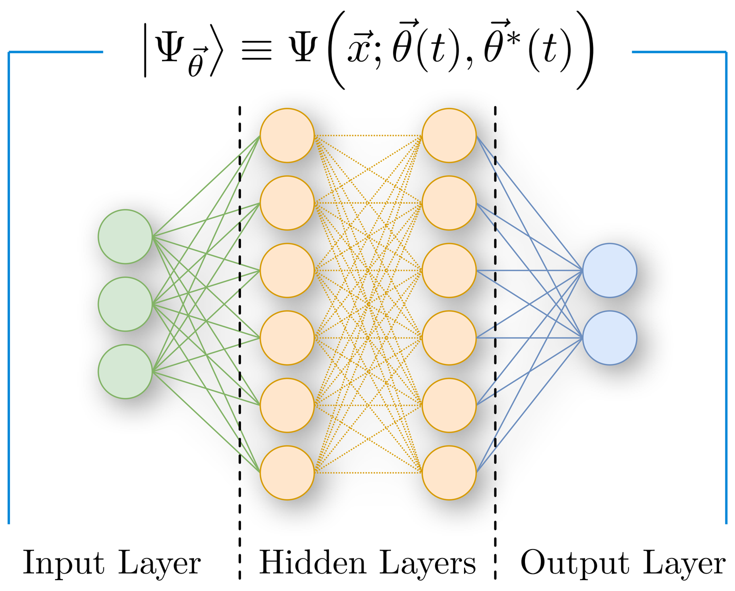
MOTIVATION

Neural Quantum States (NQS) leverage the power of machine learning to reformulate quantum wavefunctions as parameterized neural networks.

NQS offer a scalable framework for solving many-body problems beyond the reach of traditional methods — from spin systems[1] to quantum chemistry[2].

In this poster, we present an introduction to NQS by solving two Quantum Harmonic Oscillator examples.

NEURAL QUANTUM STATES (NQS)



A NQS is a wavefunction ansatz parametrized by the weights and biases of an artificial neural network (NN).

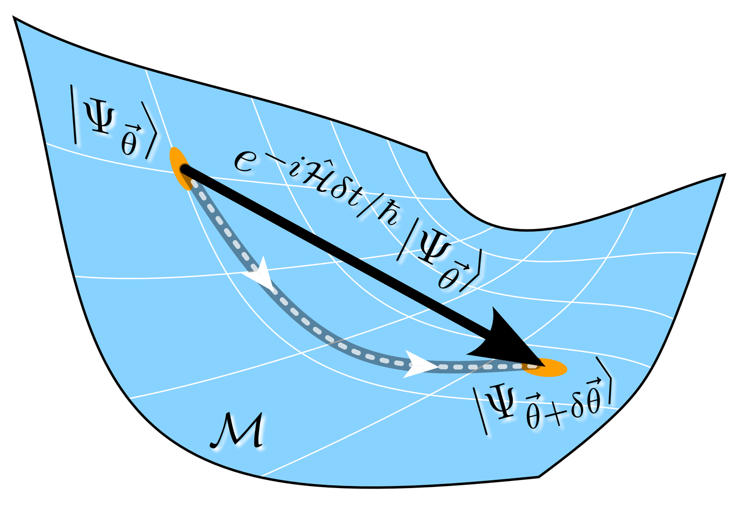
The architecture of the NN needs to be able to efficiently capture the relevant symmetries and physical constrains of the system under consideration[3,4].

The time-dependent variational principle allows to compute the equations of motion of the NN parameters that determine the dynamics of the wavefunction[5].

TIME-DEPENDENT VARIATIONAL PRINCIPLE

The variational manifold $\mathcal{M}$ contains all the possible trial states $|\Psi_{\vec{\theta}}\rangle$.

Our goal is to time evolve the parameters $\vec{\theta}(t)$ so that $|\Psi_{\vec{\theta}+\delta\vec{\theta}}\rangle$ reaches the target state $e^{-i\hat{\mathcal{H}}\delta t/\hbar}|\Psi_{\vec{\theta}}\rangle$ through changes $\delta\vec{\theta}$ within the manifold $\mathcal{M}$.



EQUATIONS OF MOTION

Given the Lagrangian $\mathcal{L}\left(\vec{\theta}, \dot{\vec{\theta}}, \vec{\theta}^*, \dot{\vec{\theta}}^*\right) = \dfrac{\langle\Psi_{\vec{\theta}}| i\frac{\partial}{\partial t} - \hat{\mathcal{H}} |\Psi_{\vec{\theta}}\rangle}{\langle\Psi_{\vec{\theta}}|\Psi_{\vec{\theta}}\rangle}$, the minimization of the action, $\delta\mathcal{S}[\vec{\theta}(t)] = \int \delta\mathcal{L}(\vec{\theta}, \dot{\vec{\theta}}, \vec{\theta}^*, \dot{\vec{\theta}}^*)\mathrm{d}t = 0$, yields the following equations of motion:

$$\begin{pmatrix} \boldsymbol{A} & \boldsymbol{B} \\ -\boldsymbol{B}^* & -\boldsymbol{A}^* \end{pmatrix} \begin{pmatrix} \dot{\vec{\theta}} \\ \dot{\vec{\theta}}^* \end{pmatrix} = -i \begin{pmatrix} \vec{F} \\ \vec{F}^* \end{pmatrix} \qquad \text{with} \quad \partial_\mu = \frac{\partial}{\partial\theta_\mu}, \ \partial_\nu = \frac{\partial}{\partial\theta_\nu^*}$$

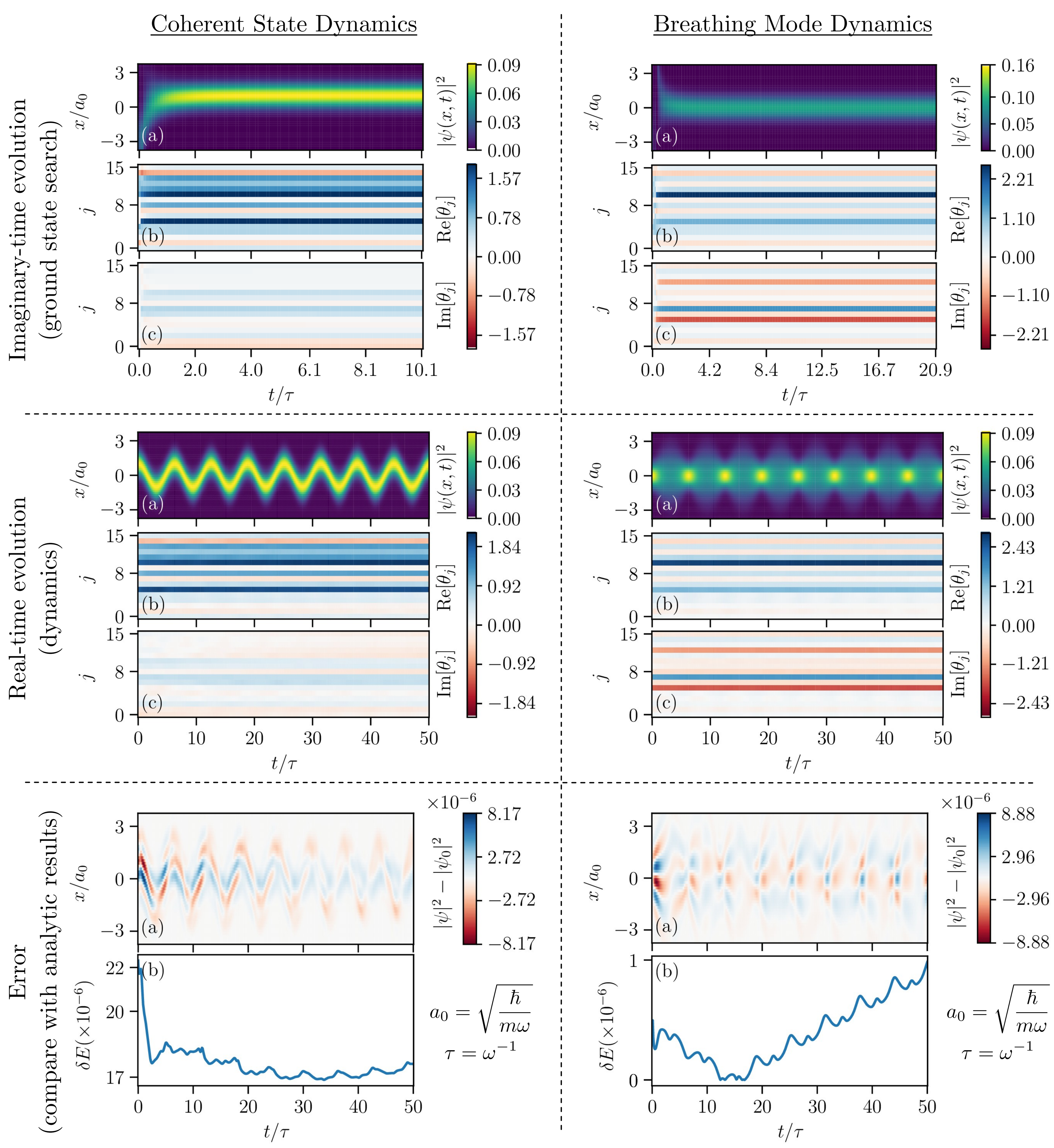
$$A_{\mu'\mu} = \frac{\partial_{\mu'}\langle\Psi|\partial_\mu|\Psi\rangle}{\langle\Psi|\Psi\rangle} - \frac{\partial_\mu\langle\Psi|\partial_{\mu'}|\Psi\rangle}{\langle\Psi|\Psi\rangle} - \left(\frac{\partial_{\mu'}\langle\Psi|\Psi\rangle}{\langle\Psi|\Psi\rangle}\frac{\langle\Psi|\partial_\mu|\Psi\rangle}{\langle\Psi|\Psi\rangle}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

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

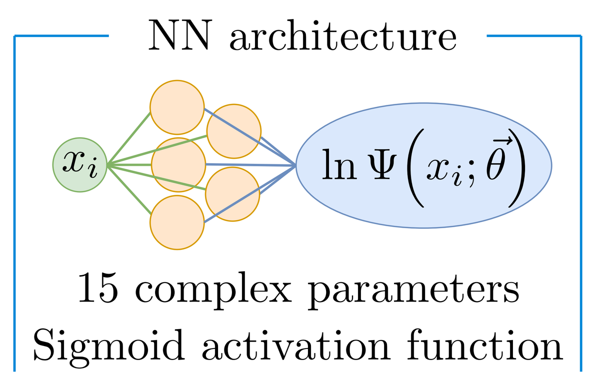
$$F_{\mu'} = \frac{\partial_{\mu'}\langle\Psi|\hat{\mathcal{H}}|\Psi\rangle}{\langle\Psi|\Psi\rangle} + \frac{\langle\Psi|\partial_{\mu'}\hat{\mathcal{H}}|\Psi\rangle}{\langle\Psi|\Psi\rangle} + \frac{\langle\Psi|\hat{\mathcal{H}}\partial_{\mu'}|\Psi\rangle}{\langle\Psi|\Psi\rangle} - \left(\frac{\partial_{\mu'}\langle\Psi|\Psi\rangle}{\langle\Psi|\Psi\rangle}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

$\lvert\Psi_{\vec{\theta}}\rangle \equiv \Psi\left(\vec{x}; \vec{\theta}(t), \vec{\theta}^*(t)\right)$ non-holomorphic	$A_{\mu'\mu} = -A_{\mu\mu'}$ complex skew-symmetric	$B_{\mu'\nu} = B^*_{\mu\nu'}$ Hermitian
$\lvert\Psi_{\vec{\theta}}\rangle \equiv \Psi\left(\vec{x}; \vec{\theta}(t)\right)$ holomorphic	$A_{\mu'\mu} = 0$ null	$B_{\mu'\nu} = B^*_{\mu\nu'}$ Hermitian
$\lvert\Psi_{\vec{\alpha}}\rangle \equiv \Psi(\vec{x}; \vec{\alpha}(t))$ real parameters	$\boldsymbol{A} = \boldsymbol{B}$ and $A^*_{\alpha'\alpha} = -A_{\alpha'\alpha} = A_{\alpha\alpha'}$ purely imaginary skew-symmetric	

QUANTUM HARMONIC OSCILLATOR DYNAMICS $\hat{\mathcal{H}} = -\frac{\hbar^2}{2m}\partial_x^2 + \frac{1}{2}m\omega^2x^2$



METHODS



In our case, $|\Psi_{\vec{\theta}}\rangle$ is holomorphic and the equations of motion read

$$\dot{\vec{\theta}} = -i\boldsymbol{S}^{-1}\vec{F}^*,$$

where $\boldsymbol{S} = -\boldsymbol{B}^*$ is the so-called Quantum Geometric Tensor[6].

In general, $\boldsymbol{S}$ is ill-conditioned. To invert it, we regularize it with a diagonal shift: $\boldsymbol{S} \leftarrow \boldsymbol{S} + \lambda\mathbb{1}$, with $\lambda \in \mathbb{C}$ and $|\lambda| \ll 1$.

The equations of motion are integrated using a 4th order Runge-Kutta method.

The NN is implemented using PyTorch[7].

CONCLUSIONS

- NQS do not require learning nor training.
- NQS evolve in time through the parameters of a NN.
- The equations of motion of the parameters can be integrated using traditional methods.
- Numerical instabilities are an important problem to be addressed.
- For simple systems, small architectures (<100 parameters) are enough to capture quantum dynamics.

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