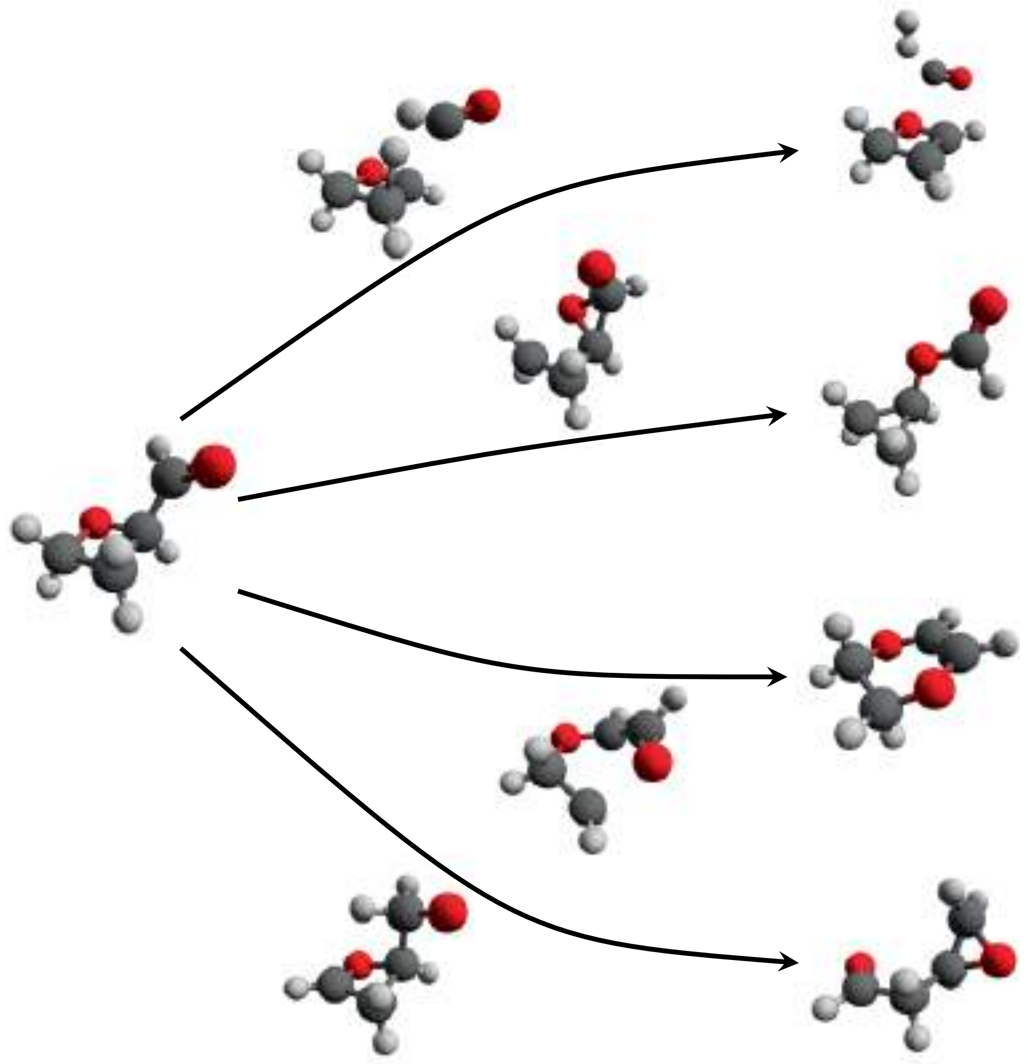
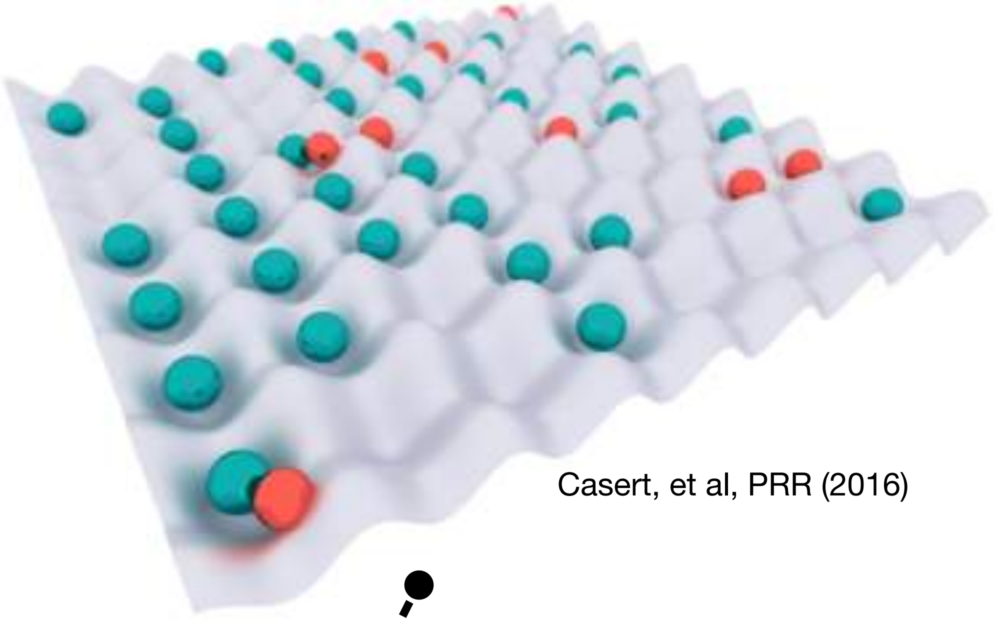
Machine learning fermionic matter

Strongly correlated systems in and out of equilibrium

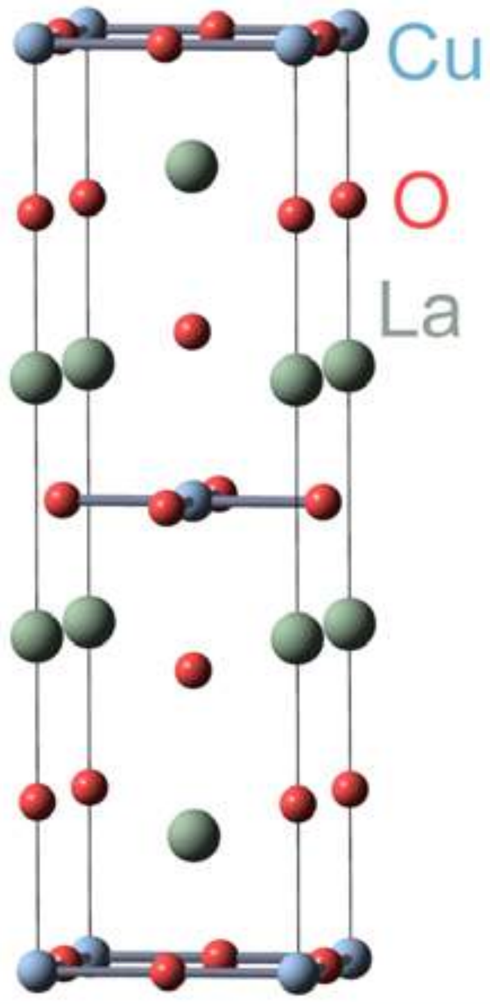
Jannes Nys (ETH Zürich), 14th November 2024



Crambow, et al, Scientific Data (2020)



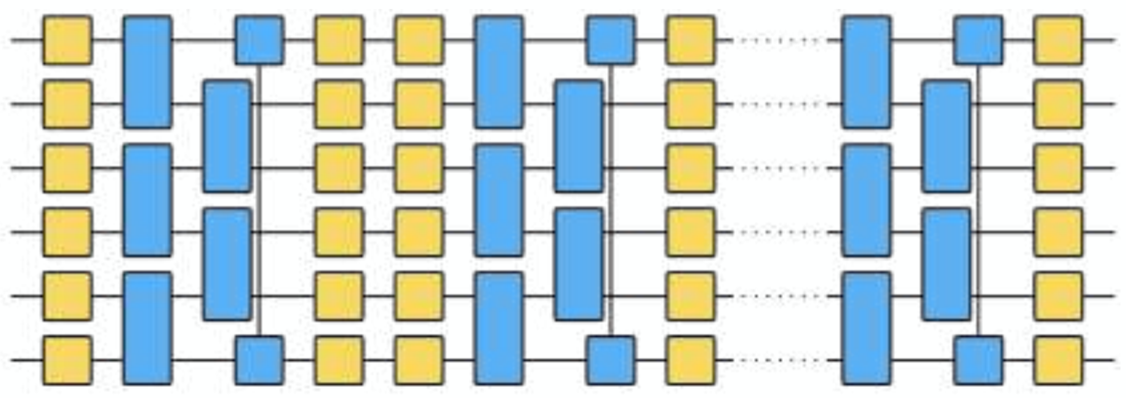
Casert, et al, PRR (2016)

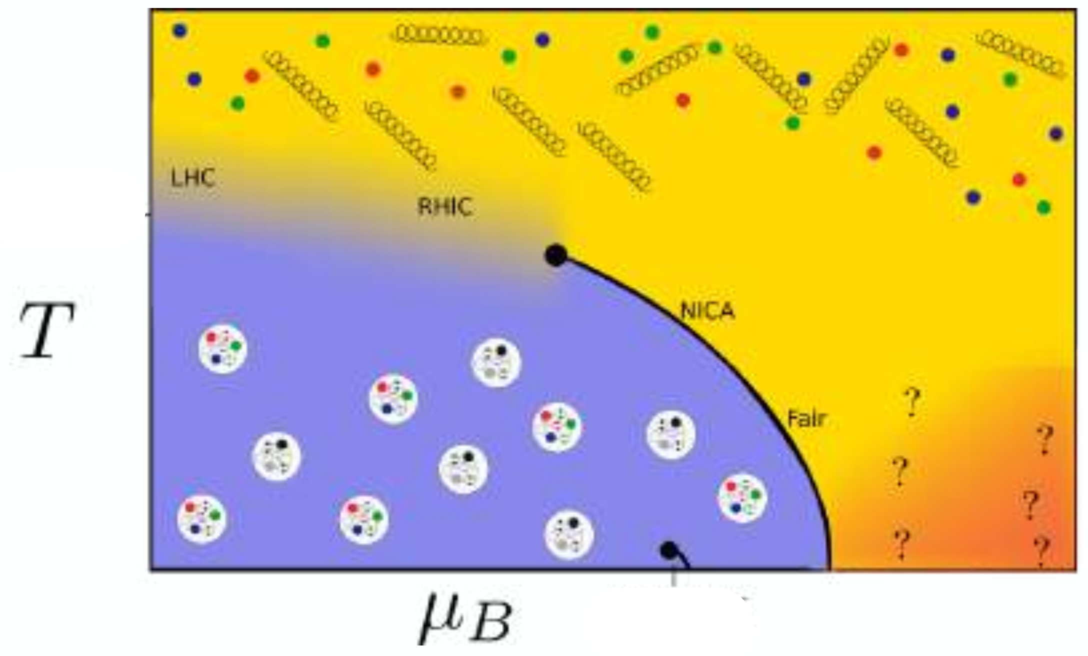


Chen, et al, Rep Prog Phys (2016)

Quantum many-body problem

- Ground states
- Excited states
- Quantum dynamics





Guenther, Eur. Phys. J (2021)

Correlations in many-body systems give rise to emergent collective quantum phenomena

Cannot be described by treating particles independently.

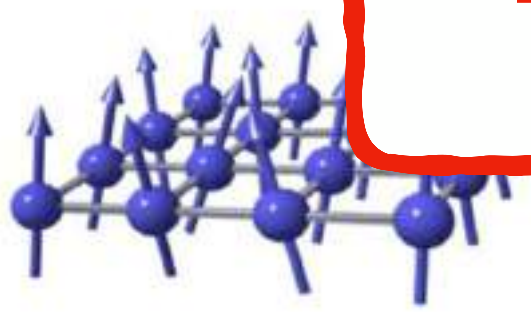
Complexity of quantum physics

Quantum state:
complex vector in Hilbert space: **exponential** (in # particles) = superposition

Entanglement:
no simple factorization into subsystems: consider entire system

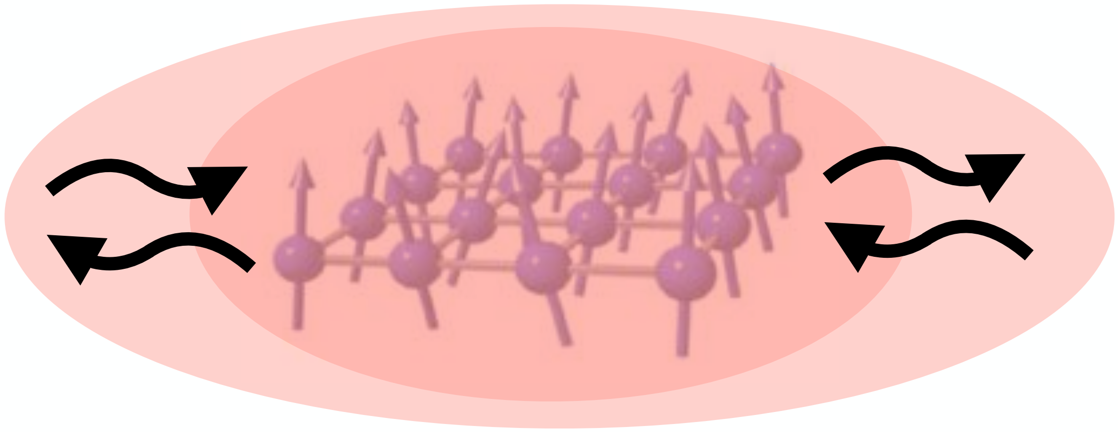
Quantum statistics (Bose-Ei

Numerical methods will play a major role in providing answers!



pins ≈ 16 petabytes

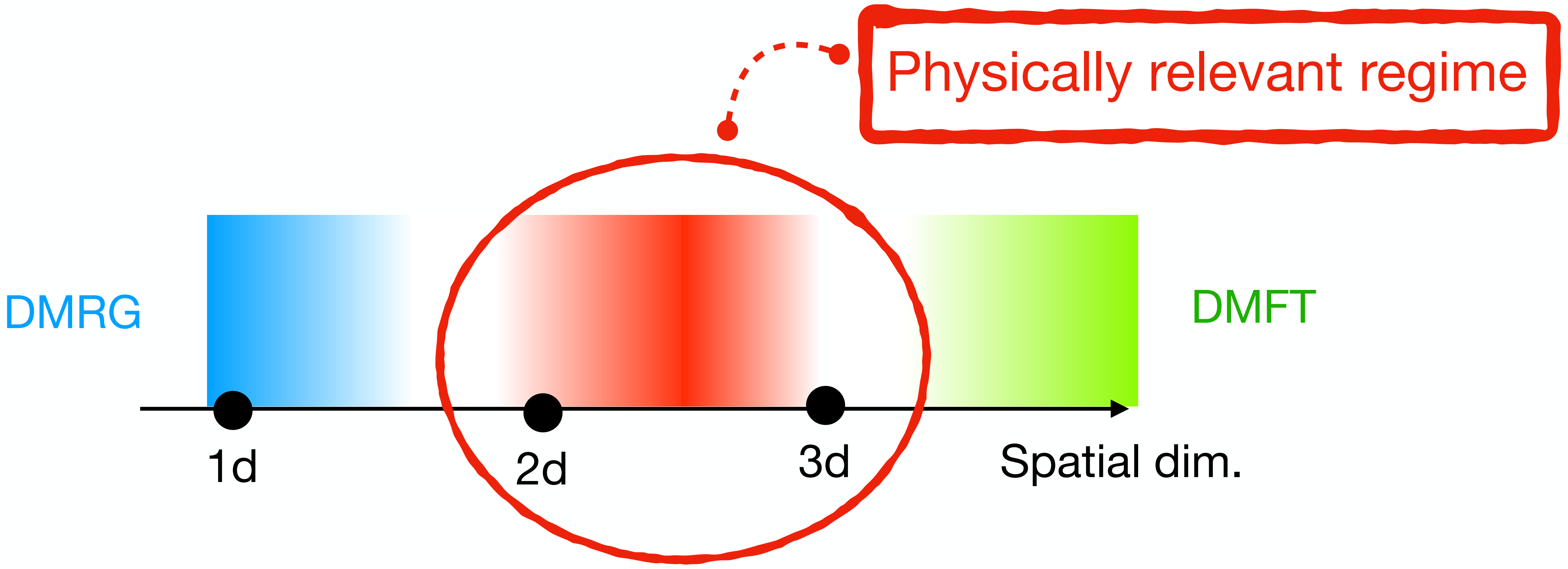
$$s_i \in \{\uparrow,\downarrow\}$$

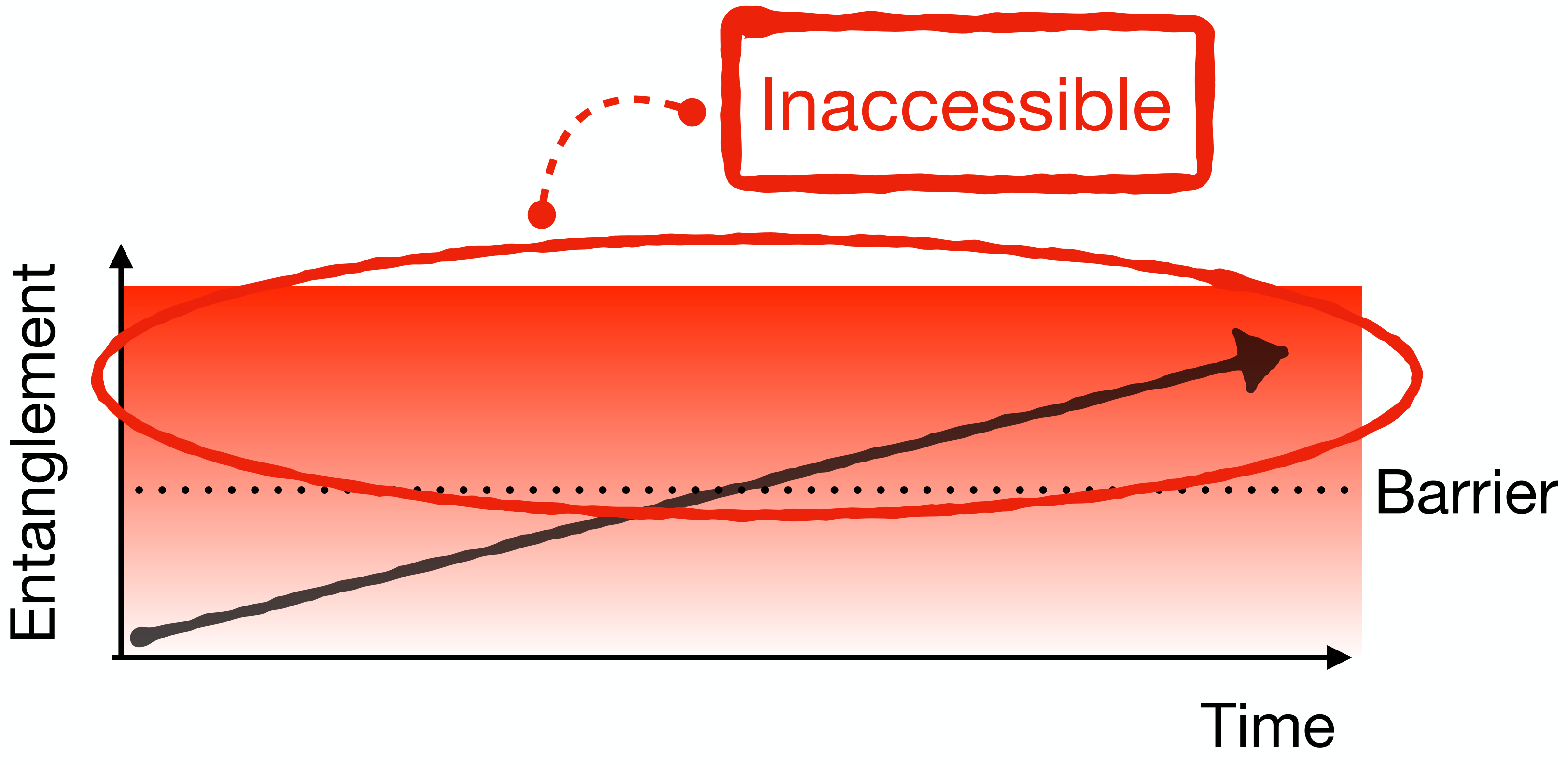


$$\rho = \sum_{s\in\{\uparrow,\downarrow\}^N} \sum_{s'\in\{\uparrow,\downarrow\}^N} \rho(s,s') \left|s\right\rangle \left\langle s'\right| \in \mathbb{C}^{2^N \times 2^N}$$

Fundamental open questions:
- *Dynamics: How do quantum systems thermalize or fail to thermalize?*
- *Phases of matter in the strongly correlated & frustrated regime?*
- *Non-equilibrium dynamics of thermal states and behavior under perturbations?*
- *…*

Strongly correlated quantum systems



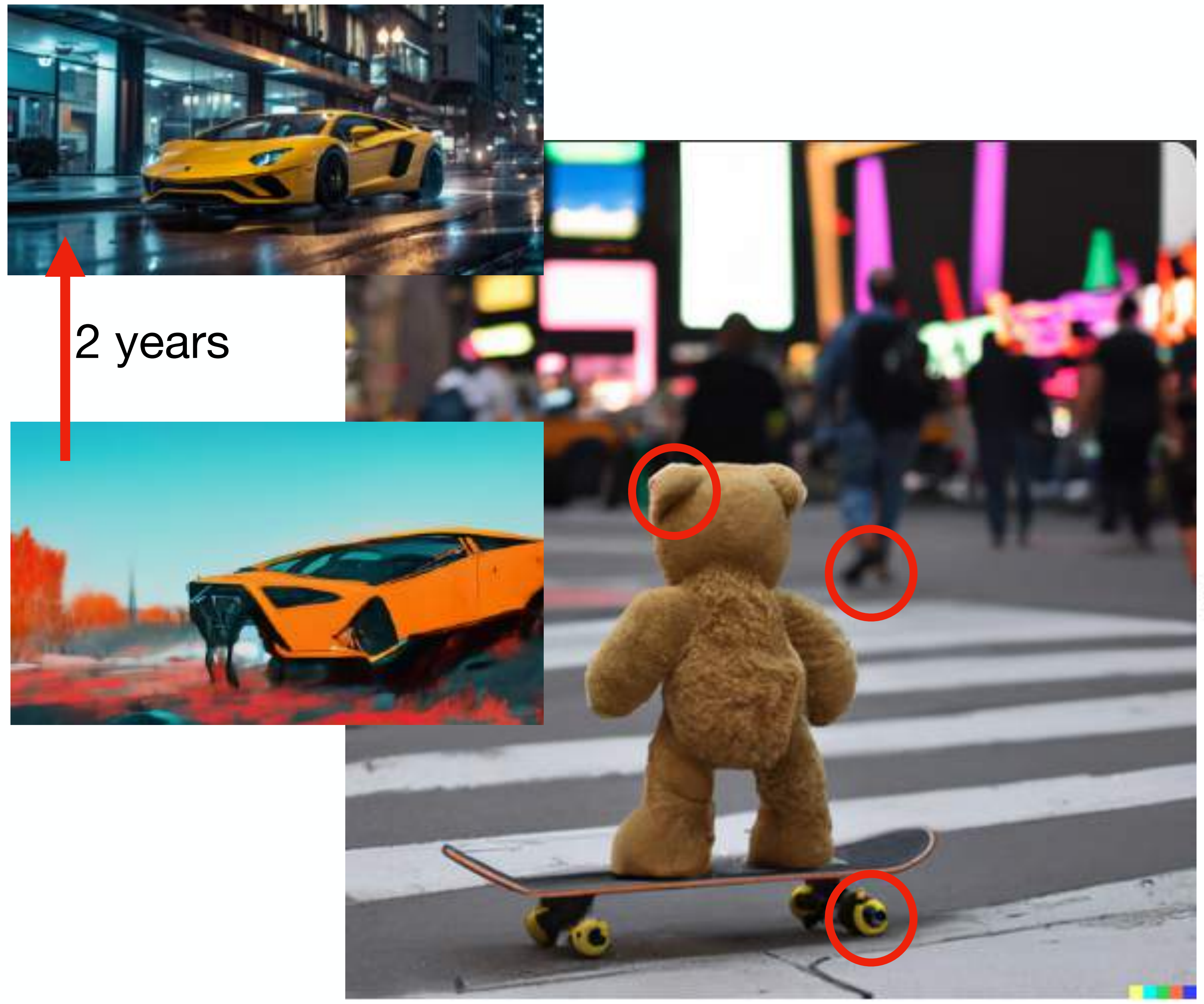


MANY-BODY PHYSICS
Science 386.6719 (2024): 296-301

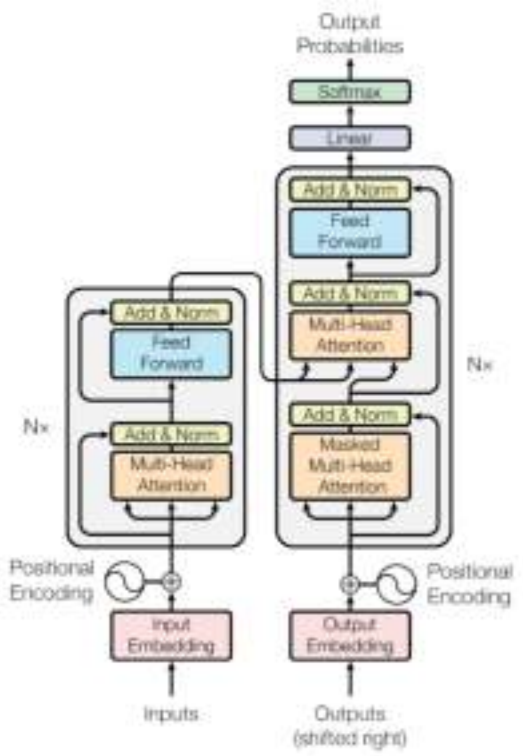
Variational benchmarks for quantum many-body problems

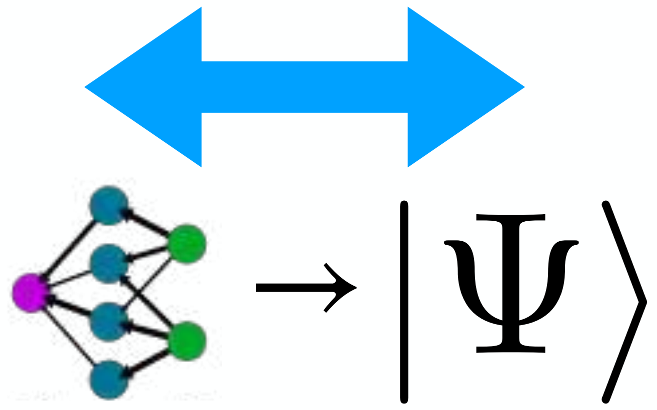
Dian Wu[1,2], Riccardo Rossi[1,3], Filippo Vicentini[2,4,5], Nikita Astrakhantsev[6], Federico Becca[7], Xiaodong Cao[8], Juan Carrasquilla[9,10], Francesco Ferrari[11], Antoine Georges[4,5,8,12], Mohamed Hibat-Allah[9,13,14,15], Masatoshi Imada[16,17,18,19], Andreas M. Läuchli[1,20], Guglielmo Mazzola[21], Antonio Mezzacapo[22], Andrew Millis[8,23], Javier Robledo Moreno[8,24], Titus Neupert[6], Yusuke Nomura[25,26], Jannes Nys[1,2], Olivier Parcollet[8,27], Rico Pohle[17,19], Imelda Romero[1,2], Michael Schmid[17], J. Maxwell Silvester[28], Sandro Sorella[29]†, Luca F. Tocchio[30], Lei Wang[31,32], Steven R. White[28], Alexander Wietek[33], Qi Yang[31,34], Yiqi Yang[35], Shiwei Zhang[8], Giuseppe Carleo[1,2]*

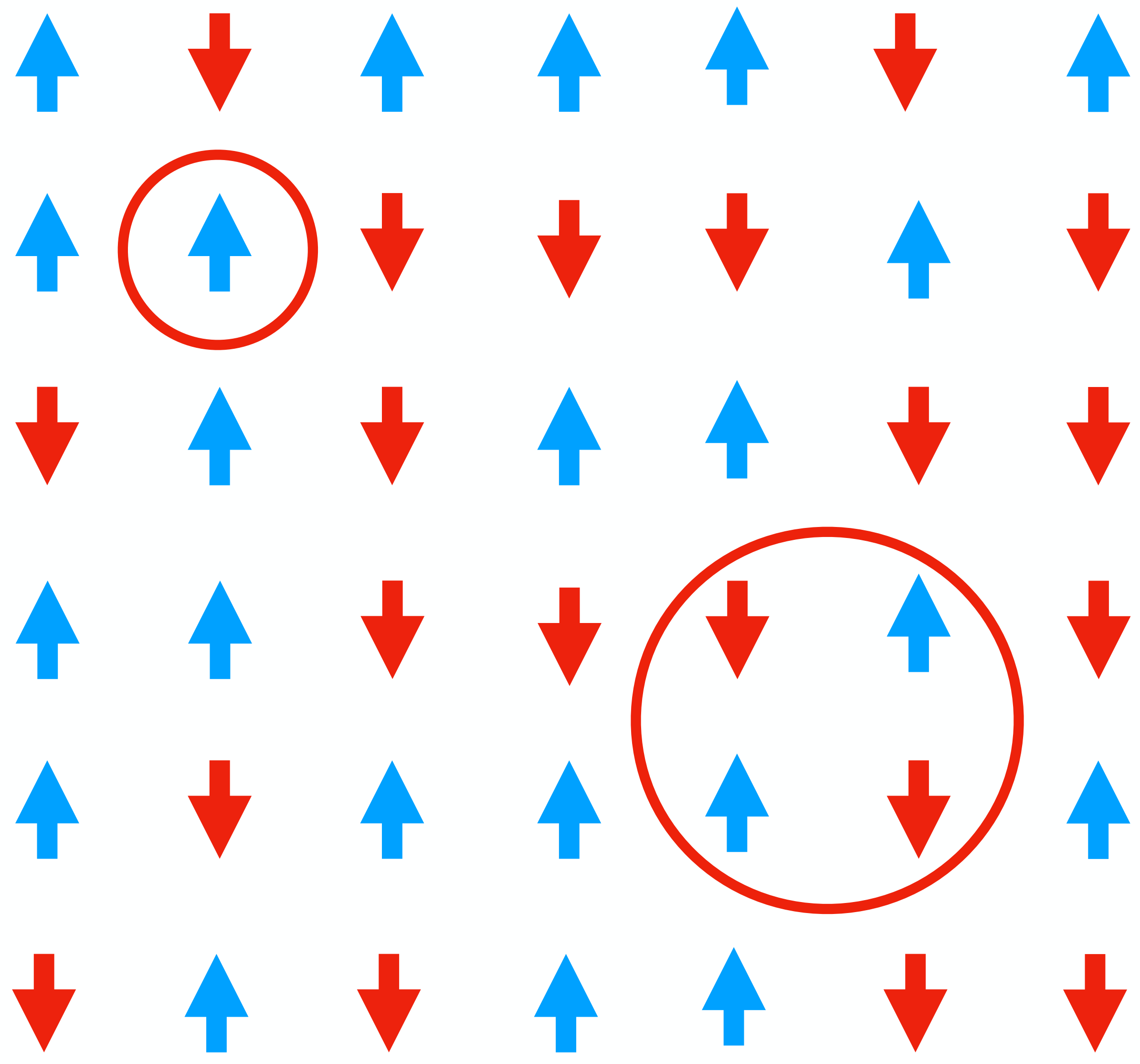
Machine learning & Quantum physics



A photo of a teddy bear on a skateboard in Times Square







Neural networks excel in

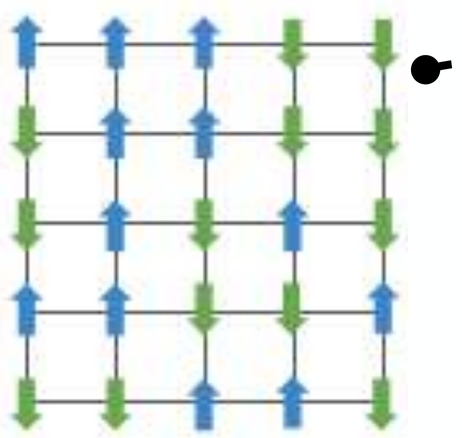
- Compressing high dimensional functions → *large Hilbert space*
- Efficiently representing strong correlations → *strong entanglement*
- Efficient gradients (backprop) → *variational optimization*

Neural representations of quantum states

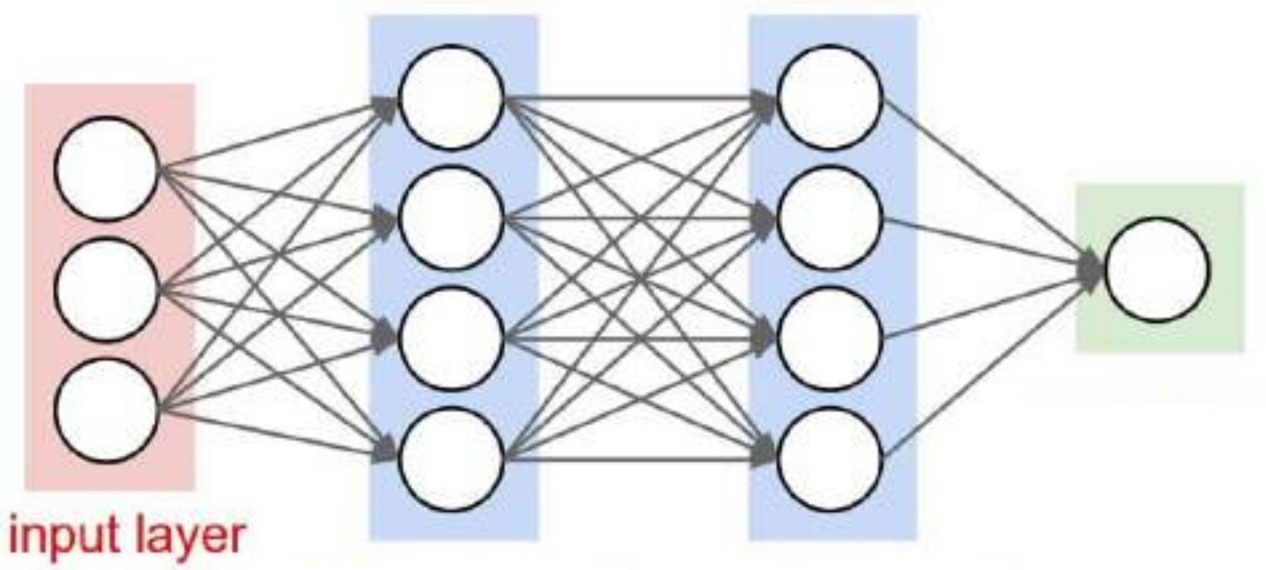
$$|\Psi\rangle = \Psi_{\uparrow,\uparrow,\cdots,\uparrow}|\uparrow,\uparrow,\cdots,\uparrow\rangle + \Psi_{\uparrow,\uparrow,\cdots,\downarrow}|\uparrow,\uparrow,\cdots,\downarrow\rangle + \cdots + \Psi_{\downarrow,\downarrow,\cdots,\downarrow}|\downarrow,\downarrow,\cdots,\downarrow\rangle$$

$\in \mathbb{C}$

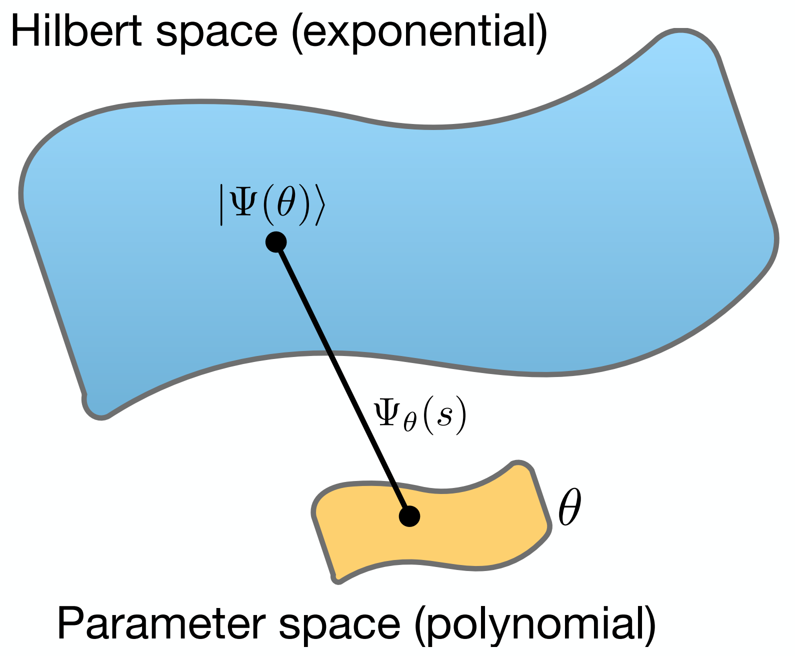
$$|\Psi\rangle = \sum_{s_i \in \{\uparrow,\downarrow\}} \Psi_\theta(s_1, ..., s_N)\,|s_1, ..., s_N\rangle \in \mathbb{C}^{2^N}$$



$(s_1, ..., s_N)$



$\Psi_\theta(s_1, ..., s_N) \in \mathbb{C}$



Neural representations of quantum states

$$|\Psi\rangle = \sum_{s_i \in \{\uparrow,\downarrow\}} \Psi_\theta(s_1, ..., s_N)\, |s_1, ..., s_N\rangle \in \mathbb{C}^{2^N}$$

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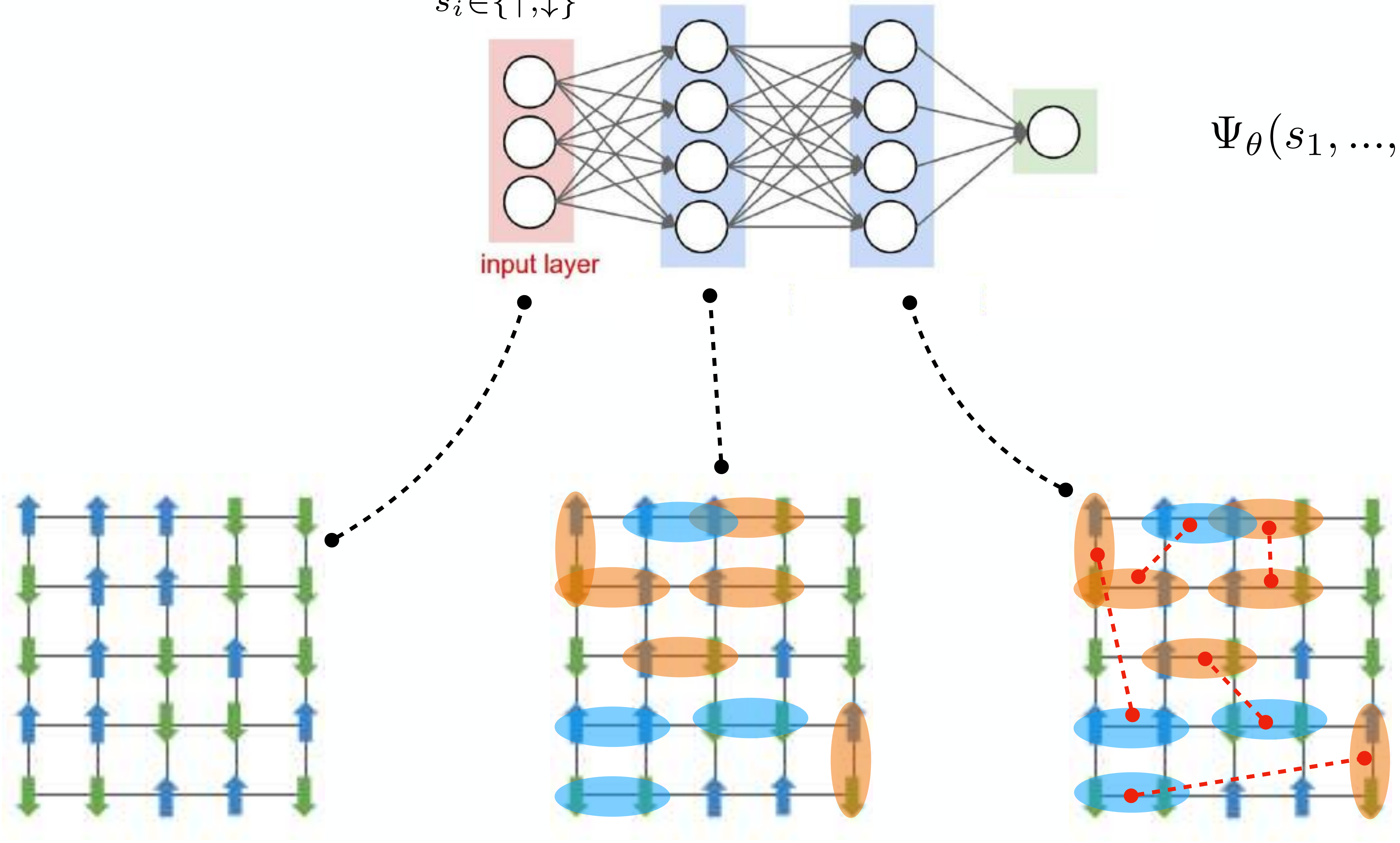


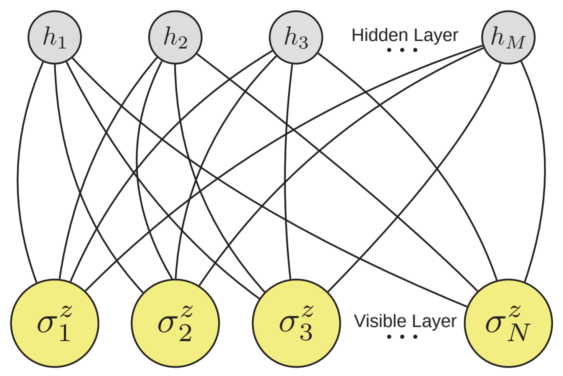
Neural representations of quantum states

$$|\Psi\rangle = \sum_{s_i \in \{\uparrow,\downarrow\}} \Psi_\theta(s_1, ..., s_N)\, |s_1, ..., s_N\rangle \in \mathbb{C}^{2^N}$$

Spin systems: exact for toric code with MLP Carrasquilla & Melko, Nature Physics, 2017

Spin systems: Restricted Boltzmann Machines Carleo & Troyer, Science 2017

$$\Psi_\theta(s_1, ..., s_N) = \frac{1}{Z} \sum_{h_i \in \{\uparrow,\downarrow\}} e^{-E(s,h)}$$



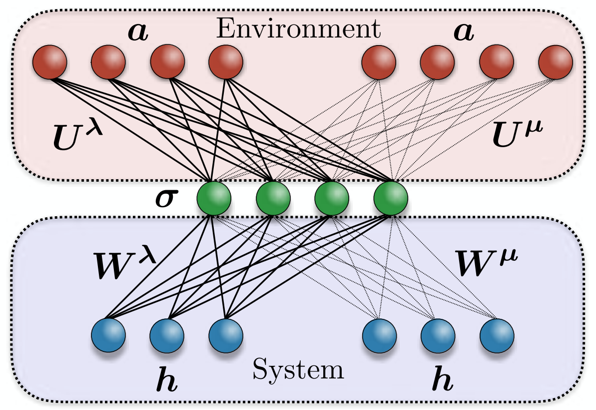
Complex-valued deep neural networks

$$= f_L \circ ... \circ f_1(s_1, ..., s_N) \in \mathbb{C}$$

Density matrices

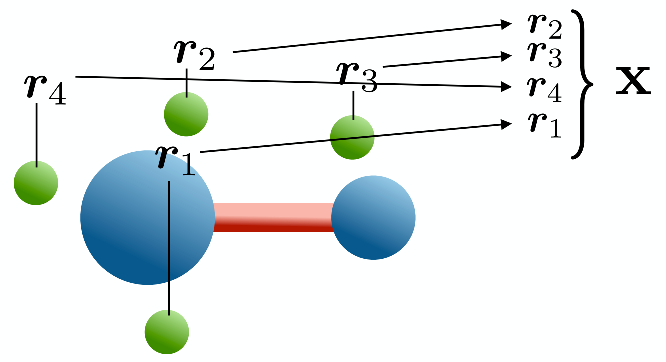
Torlai & Melko, PRL, 2018

$$\rho(s, s') = \sum_{\{h\}} \Psi(s, h)\Psi^*(s', h)$$



Continuous space Pfau, et al, PRR 2020 & Hermann, et al, NatChem (2020)

$$\Psi(\mathbf{r}_1, \cdots, \mathbf{r}_N) = \mathrm{NN}(\mathbf{r}_1, \cdots, \mathbf{r}_N)$$



Schrödinger equation

Part 1

$$\hat{H}\left|\Psi\right\rangle = E\left|\Psi\right\rangle$$

Part 2

$$i\frac{\mathrm{d}}{\mathrm{d}t}\left|\Psi\right\rangle = \hat{H}\left|\Psi\right\rangle$$

Variational optimization

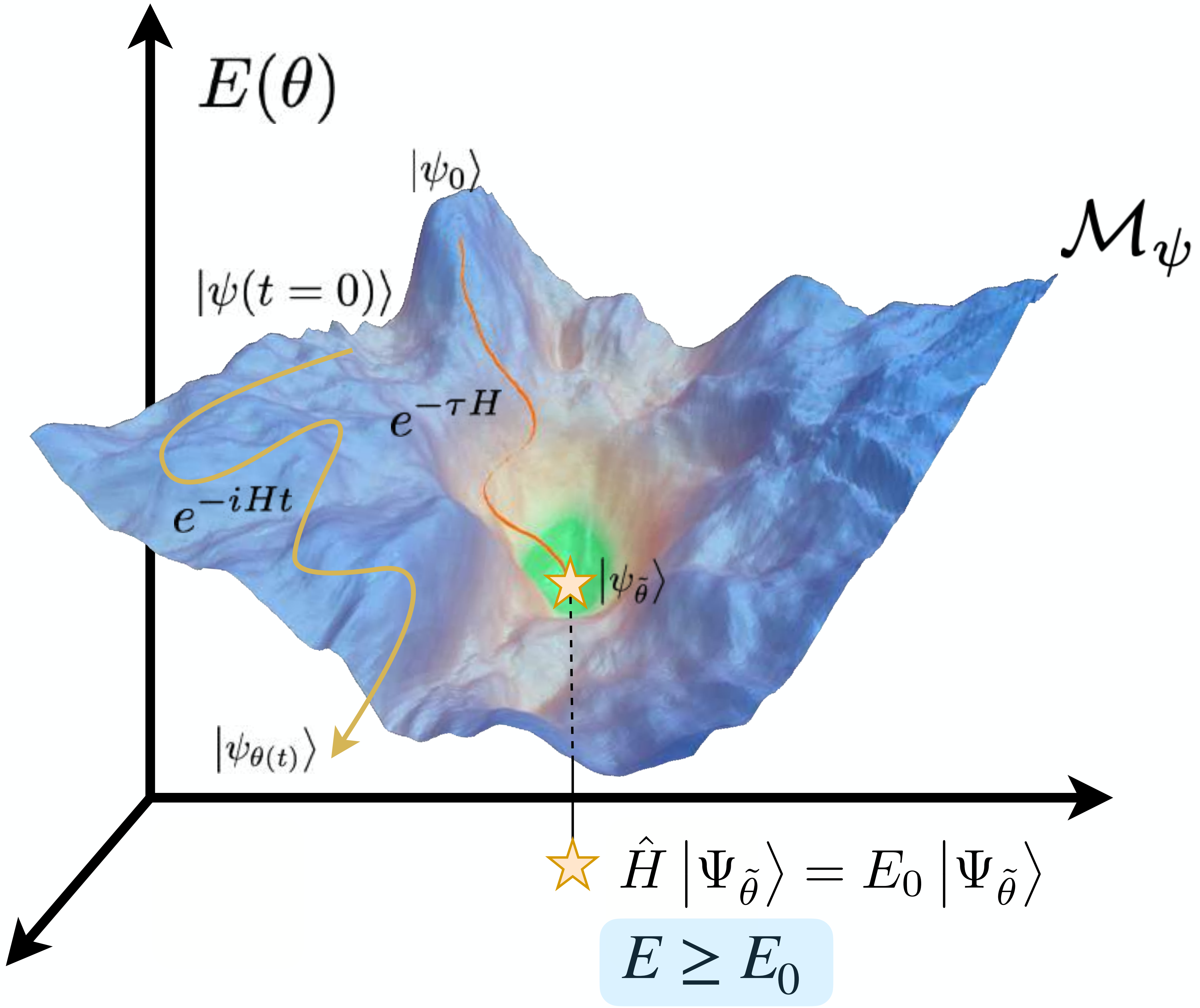
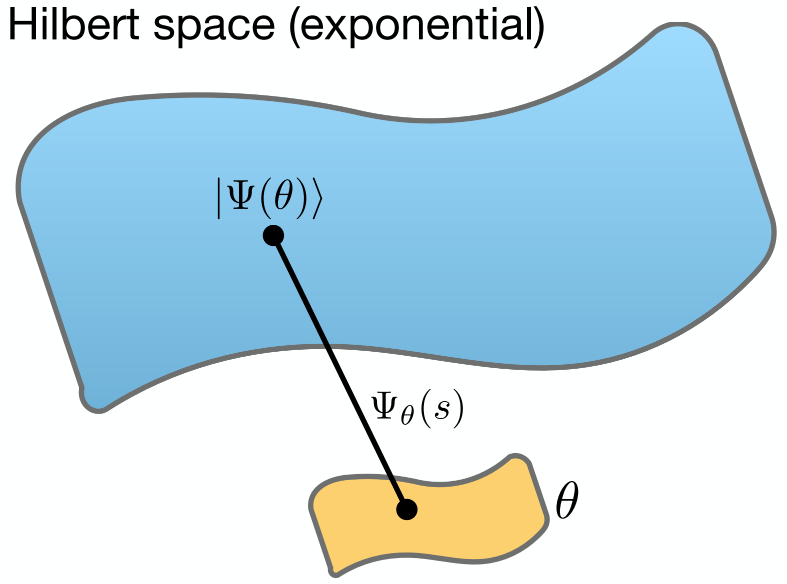


Fig: Medvidović & Moreno, arXiv:2402.11014 (2024)

Ground-state optimization (Ψ_θ)

$$\boxed{\hat{H}\,|\Psi\rangle = E\,|\Psi\rangle}$$



Variational principle: $E \geq E_0$

Energy $\rightarrow$ Loss

$$E = \frac{\langle\Psi|\hat{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle} \quad \rightarrow \quad E = \mathbb{E}_{s\sim|\Psi|^2}\left[\frac{[\hat{H}\Psi](s)}{\Psi(s)}\right]$$

(Markov chain) Monte Carlo

Variational Monte Carlo

Energy gradients

$$F_\theta = \partial_\theta \frac{\langle\Psi|\hat{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle} \quad \rightarrow \quad F_\theta = \mathbb{E}_{s\sim|\Psi|^2}\left[\partial_\theta \log\Psi(s)^* \cdot \left(\frac{[\hat{H}\Psi](s)}{\Psi(s)} - E\right)\right]$$

+ Natural gradients = “Stochastic Reconfiguration”

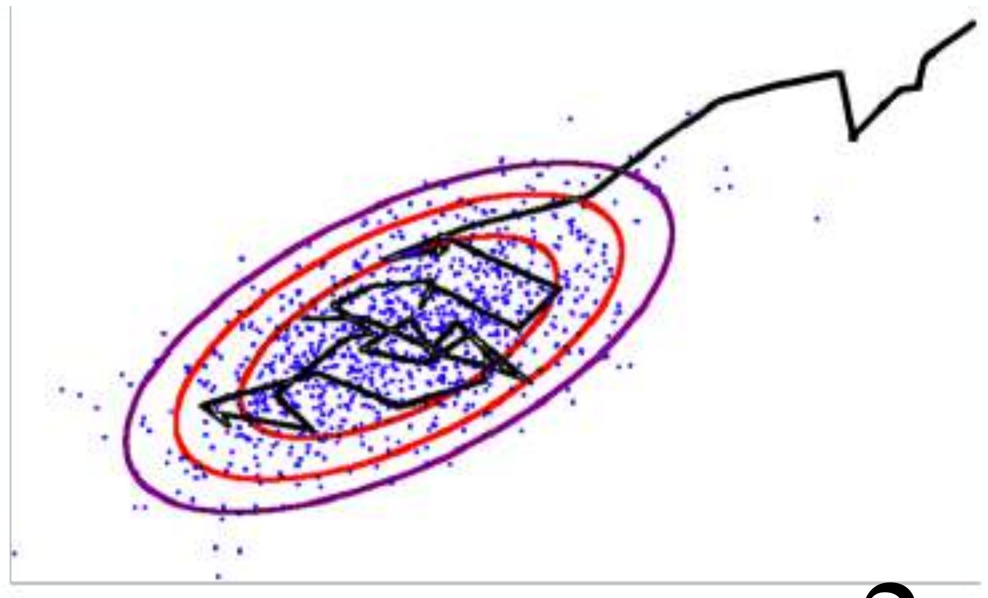
New alternative with better convergence: K.Neklyudov, **J.Nys**, M.Welling, et al., “Wasserstein quantum Monte Carlo”, NeurIPS (2023).

How to “train” neural representations?

Initial parameters θ_0

$$\Psi_{\theta_t}$$

(MC)MC sampling

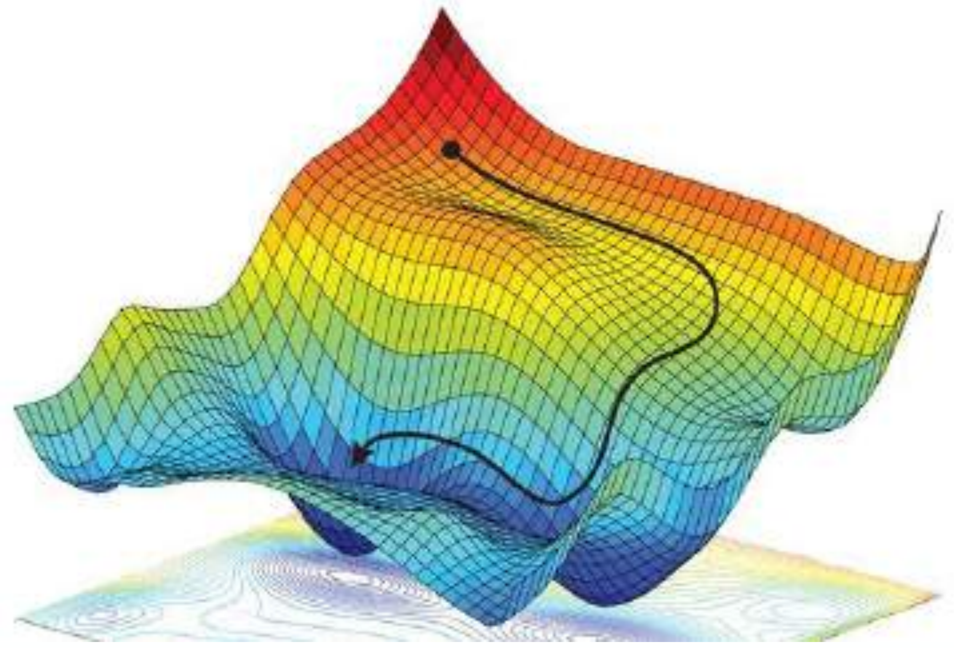


$$x \sim |\Psi_{\theta_t}|^2$$

Expectation value

$$E = \mathbb{E}_{s\sim|\Psi|^2}\left[\frac{[\hat{H}\Psi](s)}{\Psi(s)}\right]$$

Gradient descent: update $\theta_t \rightarrow \theta_{t+1}$



Monte Carlo estimators of energy and gradient

$$
\begin{aligned}
E[\Psi] &= \frac{\langle\Psi|\hat{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle} \\
&= \frac{1}{\langle\Psi|\Psi\rangle} \sum_{x\in\mathcal{H}} \Psi^*(x) \left[\hat{H}\Psi\right](x) \\
&= \sum_{x\in\mathcal{H}} \frac{\left|\Psi(x)\right|^2}{\langle\Psi|\Psi\rangle} \frac{\left[\hat{H}\Psi\right](x)}{\Psi(x)}
\end{aligned}
$$

$$\mathbb{E}_{x\sim|\Psi(x)|^2}$$

Neural representations of quantum states

Theory: representational power

- Volume law entanglement with neural representations *(Deng et al., PRX, 2017)*
- Exact representation of various nonlocal states *(Glasser, et al., PRX 2018)*

Empirical: benchmarked performance

- Neural networks are less affected by:
  - frustration,
  - quantum statistics,
  - high entanglement, and
  - large correlation lengths

  (D.Wu, et al, Science (2024))

$$\hat{H} = J_1 \sum_R \hat{\boldsymbol{S}}_R \cdot \hat{\boldsymbol{S}}_{R+1} + J_2 \sum_R \hat{\boldsymbol{S}}_R \cdot \hat{\boldsymbol{S}}_{R+2}$$

Ground-state energy on the 10×10 square lattice at $J_2/J_1 = 0.5$.

Energy per site	Wave function	Year
-0.48941(1)	NNQS	2023
-0.494757(12)	CNN	2020
-0.4947359(1)	Shallow CNN	2018
-0.49516(1)	Deep CNN	2019
-0.495502(1)	PEPS + Deep CNN	2021
-0.495530	DMRG	2014
-0.495627(6)	aCNN	2023
-0.49575(3)	RBM-fermionic	2019
-0.49586(4)	CNN	2023
-0.4968(4)	RBM ($p = 1$)	2022
-0.49717(1)	Deep CNN	2022
-0.497437(7)	GCNN	2021
-0.497468(1)	Deep CNN	2022
-0.4975490(2)	VMC ($p = 2$)	2013
-0.497627(1)	Deep CNN	2023
-0.497629(1)	RBM+PP	2021
-0.497634(1)	**Deep ViT**	**2023**

Rende et al., Comm Phys (2024)

Overview

- **Fermionic neural network** representations
- **Applications**
  - Phase diagram of homogeneous electron gas
  - Electron dynamics: electrons out of equilibrium
- Future prospects

Fermionic neural networks?

$$\Psi(..., \mathbf{r}_j, ..., \mathbf{r}_i, ...) = -\Psi(..., \mathbf{r}_i, ..., \mathbf{r}_j, ...)$$

✔ **Non-interacting fermions**

$$\Psi(\mathbf{r}_1, ..., \mathbf{r}_N) = \det \begin{bmatrix} \phi_1(\mathbf{r}_1) & \dots & \phi_1(\mathbf{r}_N) \\ \vdots & \ddots & \vdots \\ \phi_N(\mathbf{r}_1) & \dots & \phi_N(\mathbf{r}_N) \end{bmatrix}$$

Neural backflow →

$$f_L \circ \cdots \circ f_1(\mathbf{r}_1, \dots, \mathbf{r}_N) = [\mathbf{q}_1, \dots, \mathbf{q}_N]$$

Luo & Clark, PRL (2019)

✘ **Interacting fermions**

$$\det \begin{bmatrix} \phi_1(\mathbf{q}_1) & \dots & \phi_1(\mathbf{q}_N) \\ \vdots & \ddots & \vdots \\ \phi_N(\mathbf{q}_1) & \dots & \phi_N(\mathbf{q}_N) \end{bmatrix}$$

For second quantization: **J.Nys** & Carleo, “Variational solutions to fermion-to-qubit mappings in 2d”, Quantum, 2022

Backflow as coordinate transformations

- Imaginary time evolution: $\Phi_\tau(\mathbf{X}) = \langle \mathbf{X} | e^{-\tau H} | \Phi_0 \rangle$ $\qquad |\langle \Psi_0 | \Phi_0 \rangle| > 0$
- Representative X' for each X

$$\Phi_\tau(\mathbf{X}) = \int_\Omega d\mathbf{X}' G_\tau(\mathbf{X}, \mathbf{X}') \Phi_0(\mathbf{X}') \qquad = \mathrm{Vol}(\Omega) \times G_\tau\left(\mathbf{X}, \mathbf{Y}(\mathbf{X})\right) \Phi_0(\mathbf{Y}(\mathbf{X}))$$

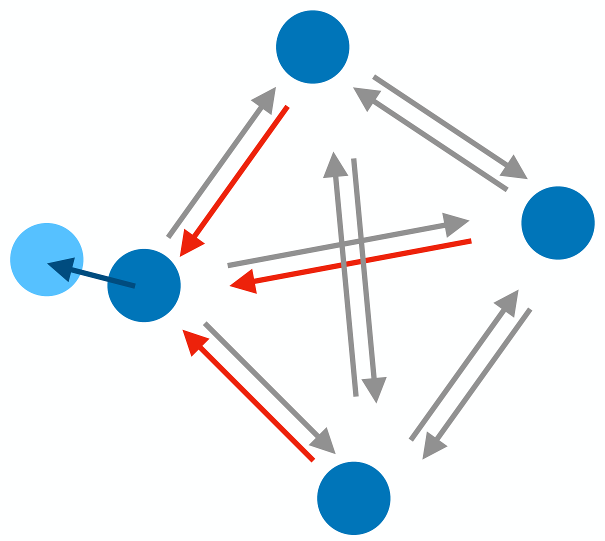
- **Backflow transformation** Y(X):

$$\Phi_\tau(\mathbf{X}) = J(\mathbf{X}) \times \Phi_0(\mathbf{Y}(\mathbf{X}))$$

Interacting fermions $\xrightarrow{\mathbf{Y}(\mathbf{X})}$ Non-interacting fermions

G.Pescia, **J.Nys**, et al., PRB (2024)

Backflow



Feynman & Cohen (1956)

$$\mathbf{q}_i = \mathbf{r}_i + \sum_{j \neq i} f\left(\|\mathbf{r}_i - \mathbf{r}_j\|\right)\left(\mathbf{r}_i - \mathbf{r}_j\right)$$

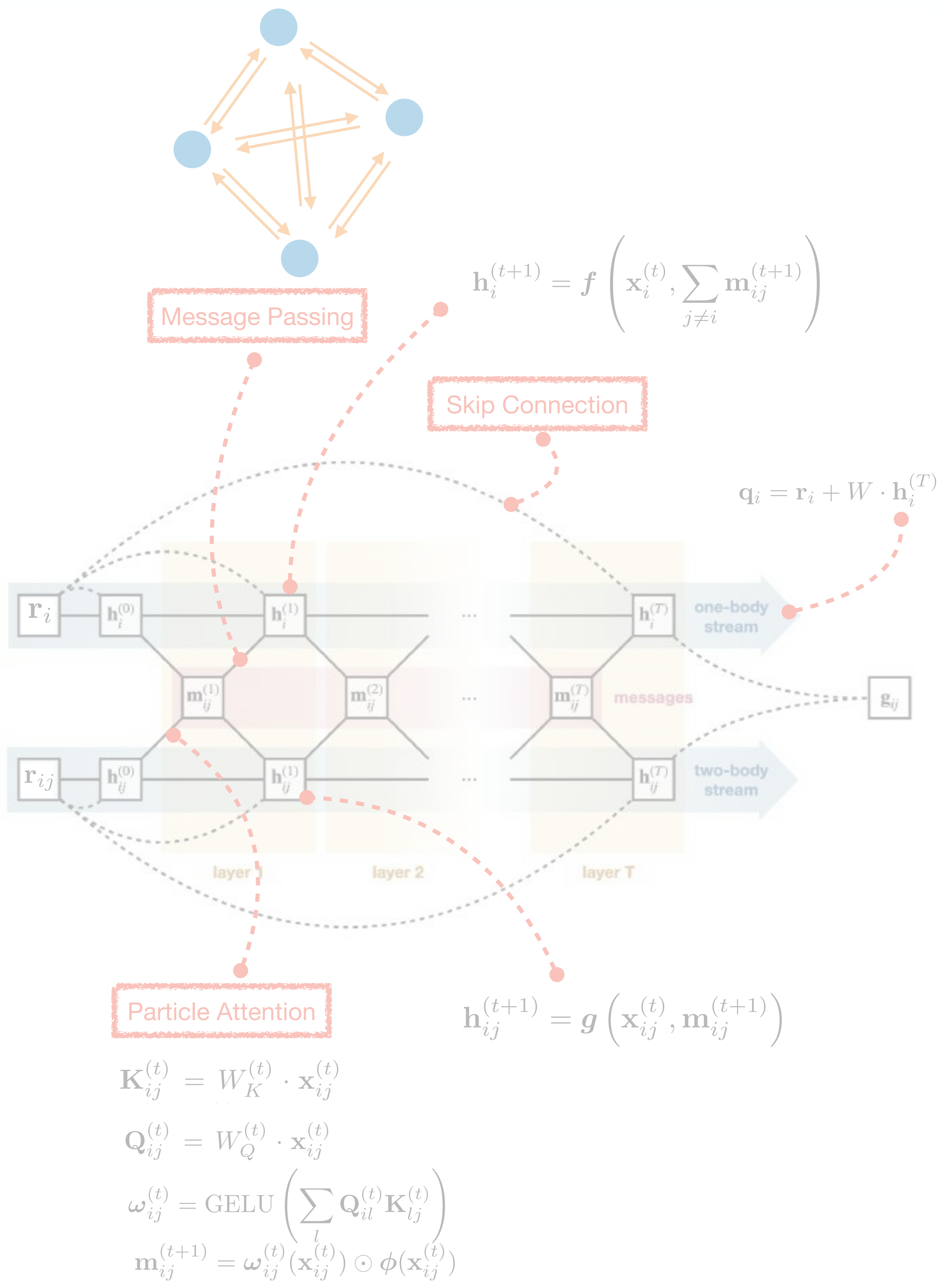
Luo & Clark, PRL (2019)

$$\mathbf{q}_i = \mathbf{r}_i + \mathrm{NN}(\mathbf{r}_1, \ldots, \mathbf{r}_N)$$

Graph neural networks:
permutation equivariance

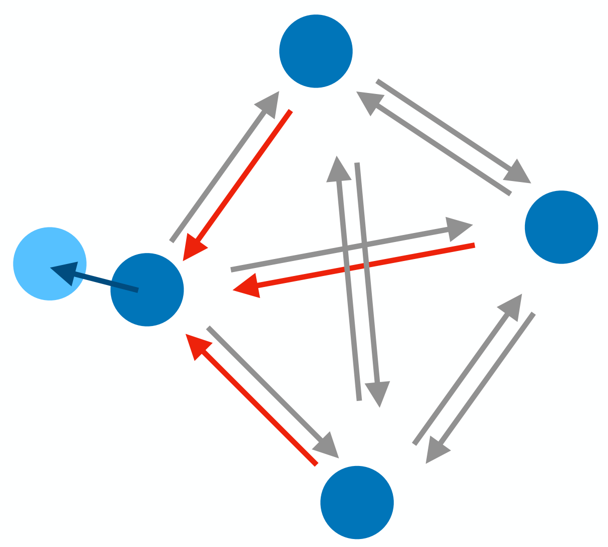
$$[\ldots, \mathbf{q}_j, \ldots, \mathbf{q}_i, \ldots] = f_L \circ \cdots \circ f_1(\ldots, \mathbf{r}_j, \ldots, \mathbf{r}_i, \ldots)$$

$$P_{ij}\mathbf{q} = f(P_{ij}\mathbf{r})$$



G.Pescia, **J.Nys**, et al., PRB (2024)

Particle attention: capturing correlations



$$\mathbf{x}_{ij}^{(0)} = [\mathbf{r}_{ij}, \|\mathbf{r}_{ij}\|, s_i \cdot s_j]$$

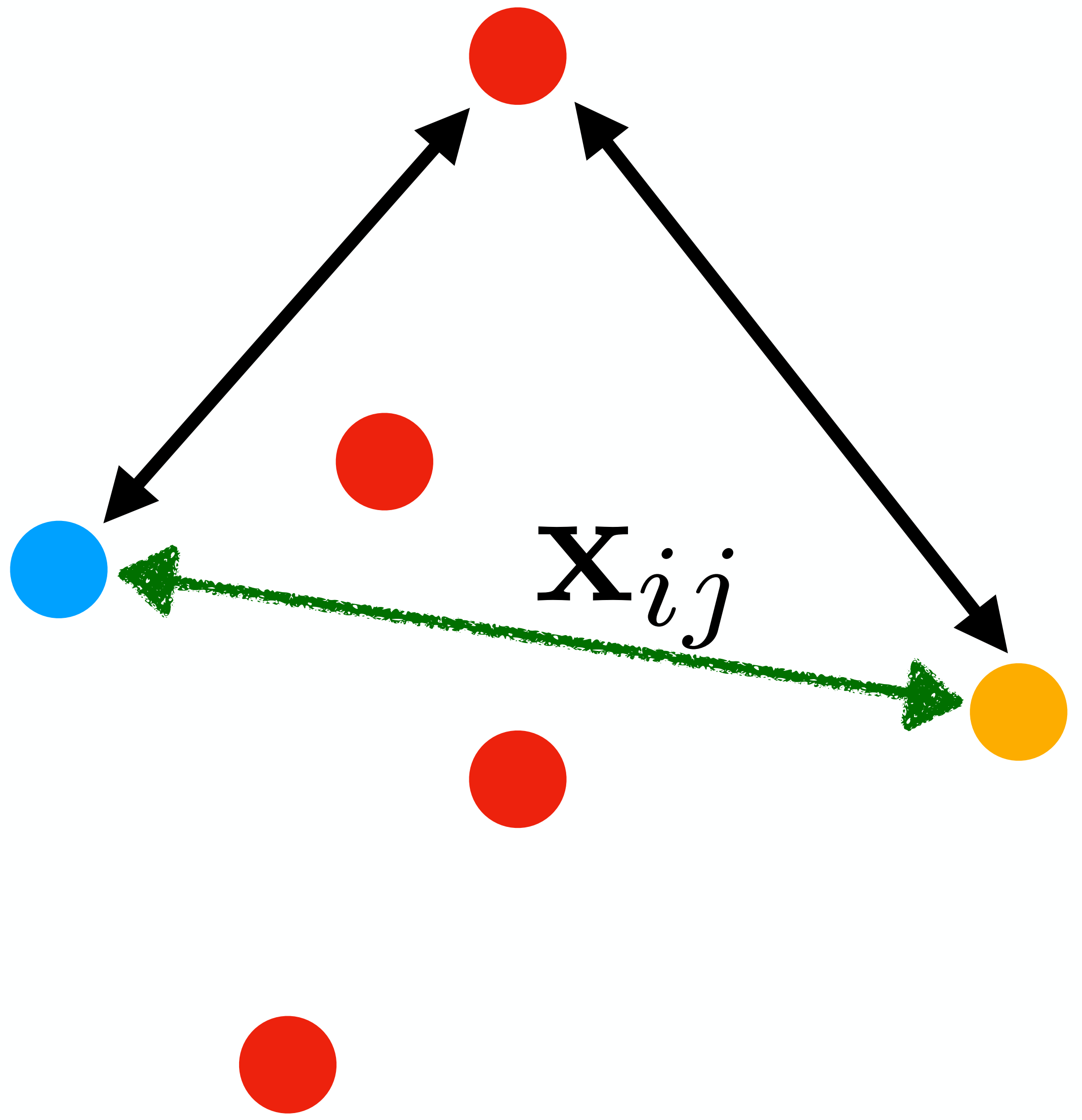
$$\mathbf{Q}_{ij} = Q \cdot \mathbf{x}_{ij} \qquad \mathbf{K}_{ij} = K \cdot \mathbf{x}_{ij}$$

$$\omega_{ij} = \sigma\left(\sum_l \mathbf{Q}_{il} \cdot \mathbf{K}_{lj}\right)$$

$$\mathbf{V}_{ij} = V \cdot \mathbf{x}_{ij}$$

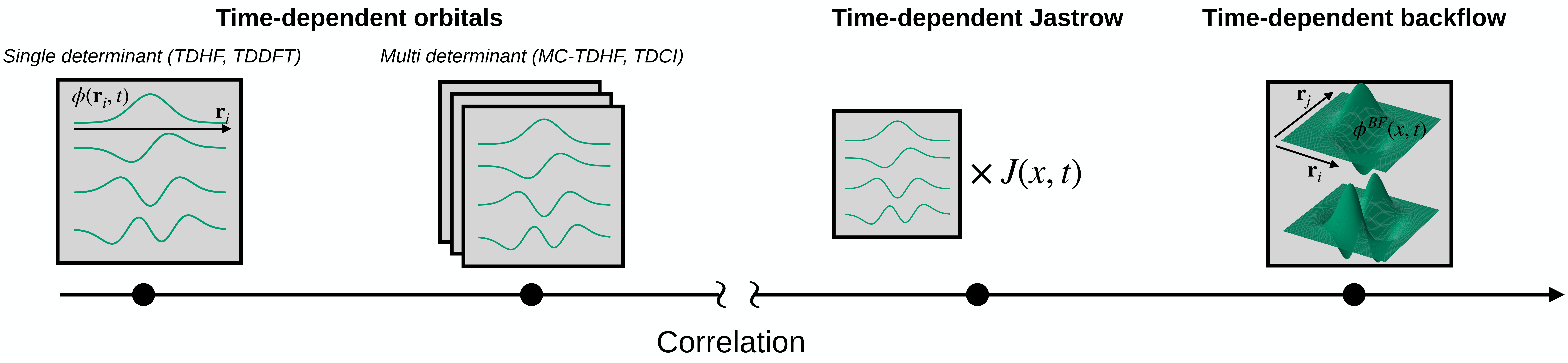
$$\mathbf{m}_{ij} = \omega_{ij} \odot \mathbf{V}_{ij}$$

Permutation equivariance —> message passing



G.Pescia, **J.Nys**, et al., PRB (2024)

(Time-dependent) variational models



Anti symmetry: determinant

$$\Psi(x) = \begin{vmatrix} \phi_1(\mathbf{r}_1) & \dots & \phi_1(\mathbf{r}_N) \\ \vdots & \ddots & \vdots \\ \phi_N(\mathbf{r}_1) & \dots & \phi_N(\mathbf{r}_N) \end{vmatrix}$$

Single-body orbitals

Superconductivity: BCS theory?

Neural backflow Pfaffian

Fermionic pairing

$$\mathbf{x}_i = (\mathbf{r}_i, \sigma_i)$$

$$\phi(\boldsymbol{x}_i, \boldsymbol{x}_j) = \nu(\boldsymbol{x}_i, \boldsymbol{x}_j) - \nu(\boldsymbol{x}_j, \boldsymbol{x}_i)$$

$$\Phi_{PJ}(X) = \mathrm{pf}\begin{bmatrix} 0 & \phi(\boldsymbol{x}_1, \boldsymbol{x}_2) & \cdots & \phi(\boldsymbol{x}_1, \boldsymbol{x}_N) \\ \phi(\boldsymbol{x}_2, \boldsymbol{x}_1) & 0 & \cdots & \phi(\boldsymbol{x}_2, \boldsymbol{x}_N) \\ \vdots & \vdots & \ddots & \vdots \\ \phi(\boldsymbol{x}_N, \boldsymbol{x}_1) & \phi(\boldsymbol{x}_N, \boldsymbol{x}_2) & \cdots & 0 \end{bmatrix}$$

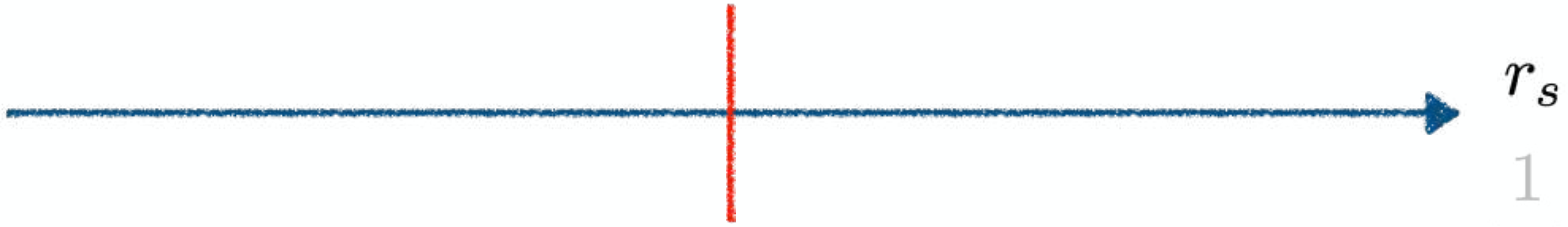
J Kim, **J.Nys**, et al. Comm Phys, "Neural-network quantum states for ultra-cold Fermi gases" (2023)

Homogeneous Electron Gas (3D)

$$H = -\frac{1}{2r_s^2}\sum_i \nabla_i^2 + \frac{1}{r_s}\sum_{i<j}\frac{1}{\|\mathbf{r}_i - \mathbf{r}_j\|} + \text{background}$$

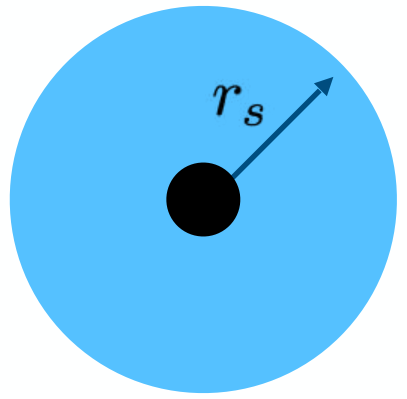
High density:
Fermi liquid

Low density:
Floating Wigner Crystal?



$$-\frac{1}{2r_s^2}\sum_i \nabla_i^2$$

$$\frac{1}{r_s}\sum_{i<j}\frac{1}{\|\mathbf{r}_i - \mathbf{r}_j\|}$$

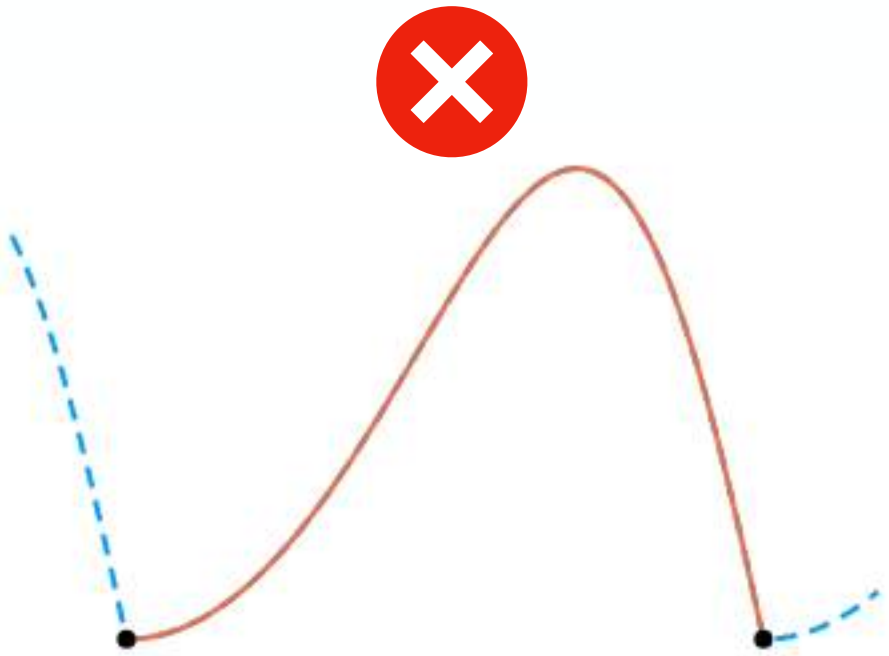


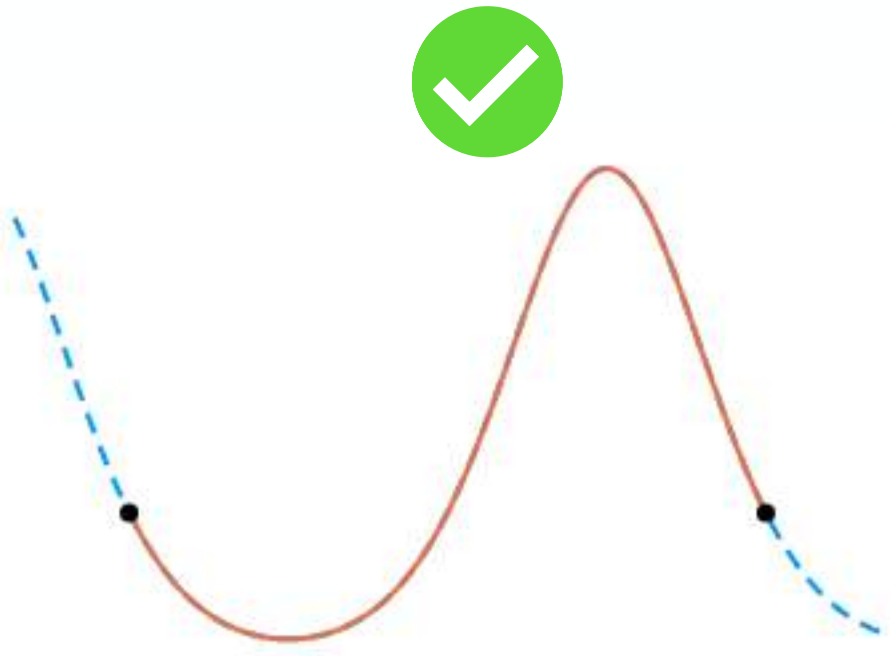
Periodic neural networks

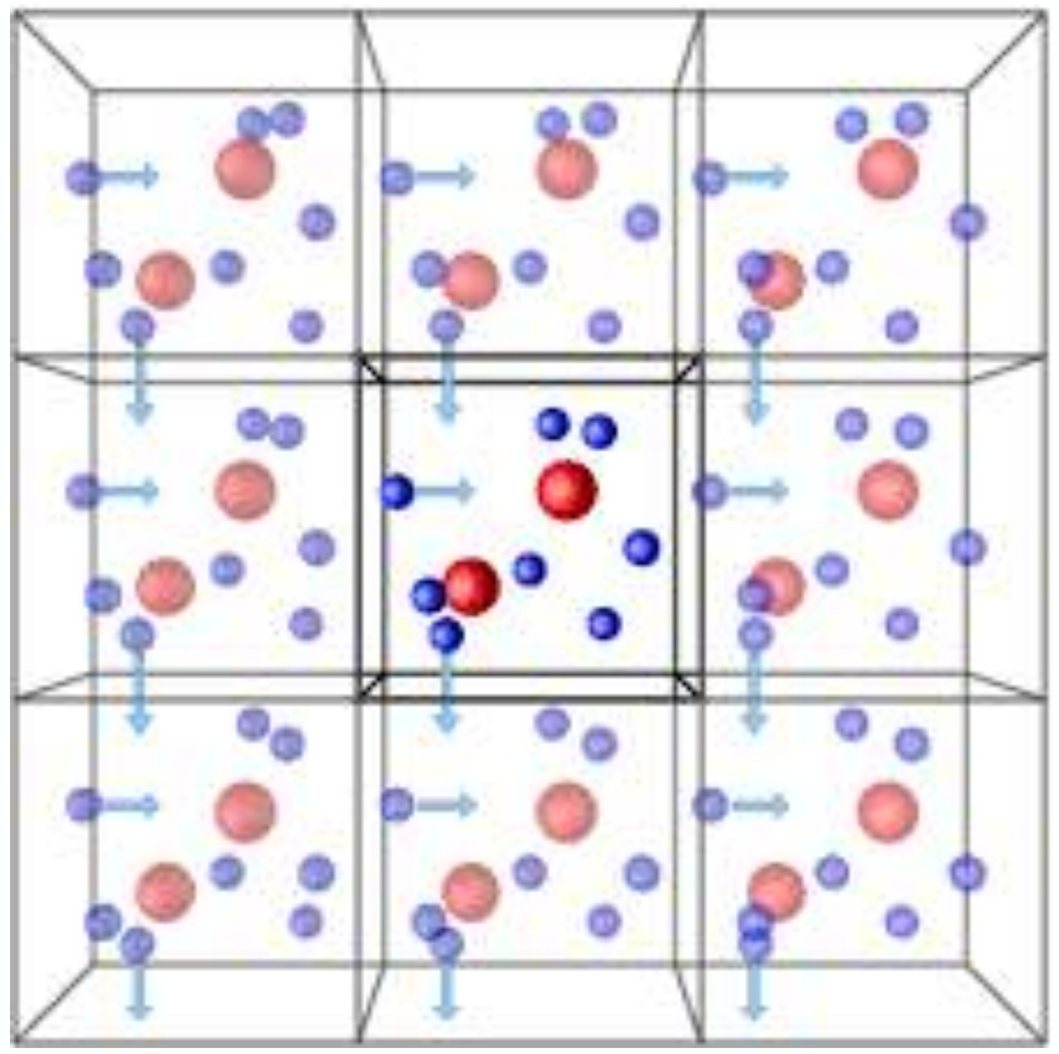
$$\hat{H}(t) = -\frac{1}{2}\sum_{i=1}^{N} \nabla^2_{\mathbf{r}_i} + V(x,t)$$

$$\boldsymbol{r}_{ij} \mapsto (\cos(2\pi \boldsymbol{r}_{ij}/L), \sin(2\pi \boldsymbol{r}_{ij}/L))$$

$$\|\boldsymbol{r}_{ij}\| \mapsto \|\sin(\pi \boldsymbol{r}_{ij}/L)\|,$$

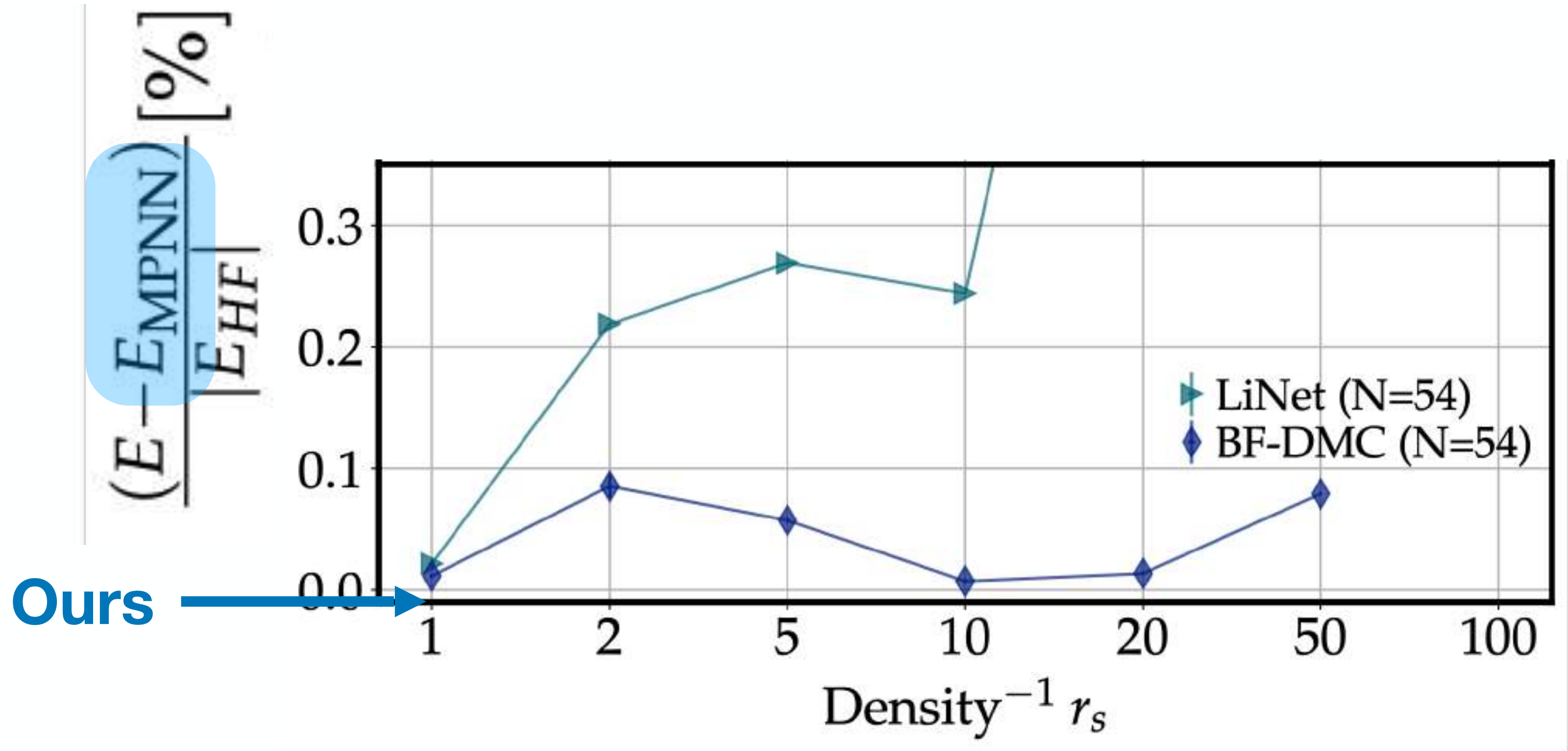




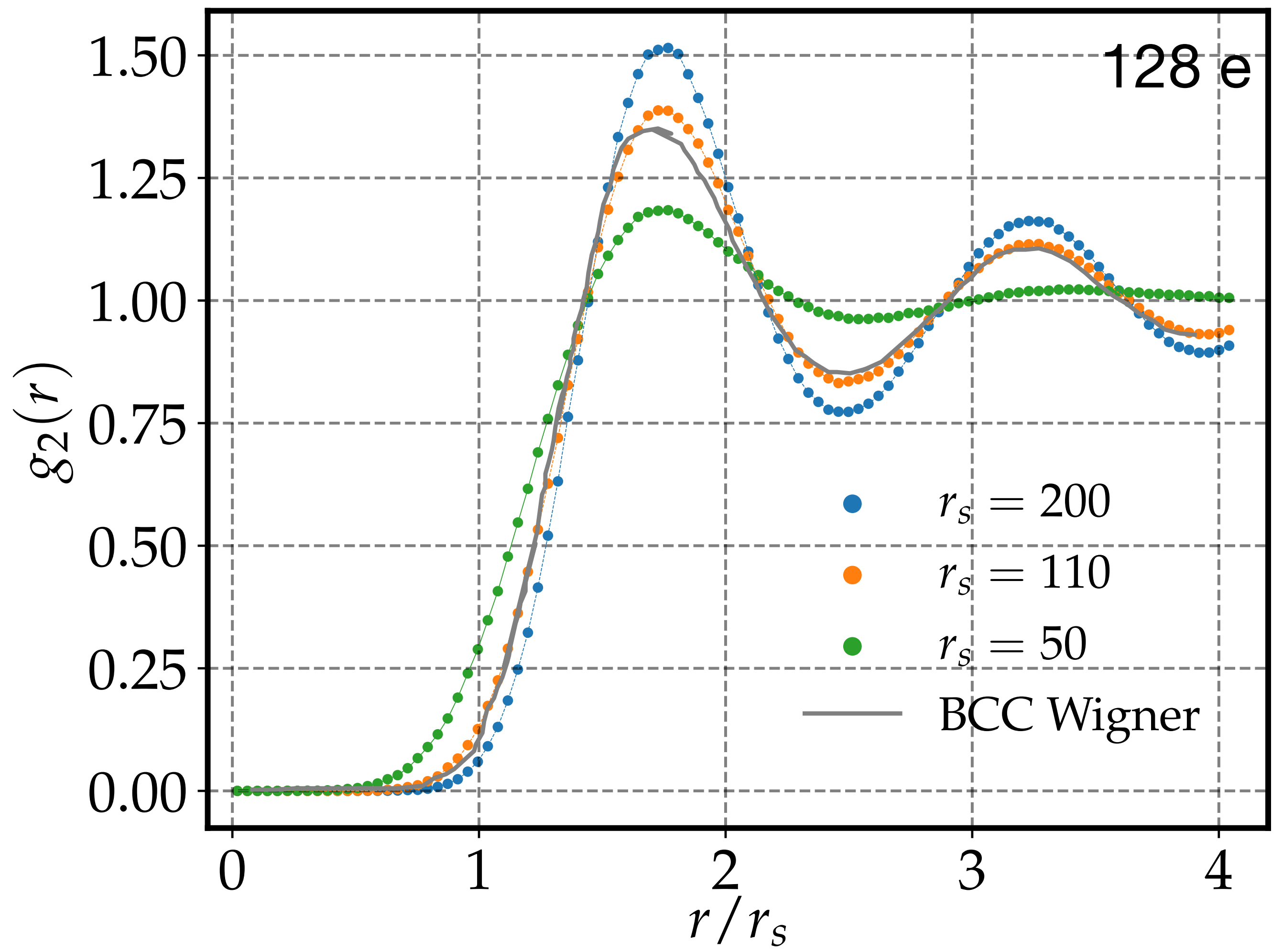


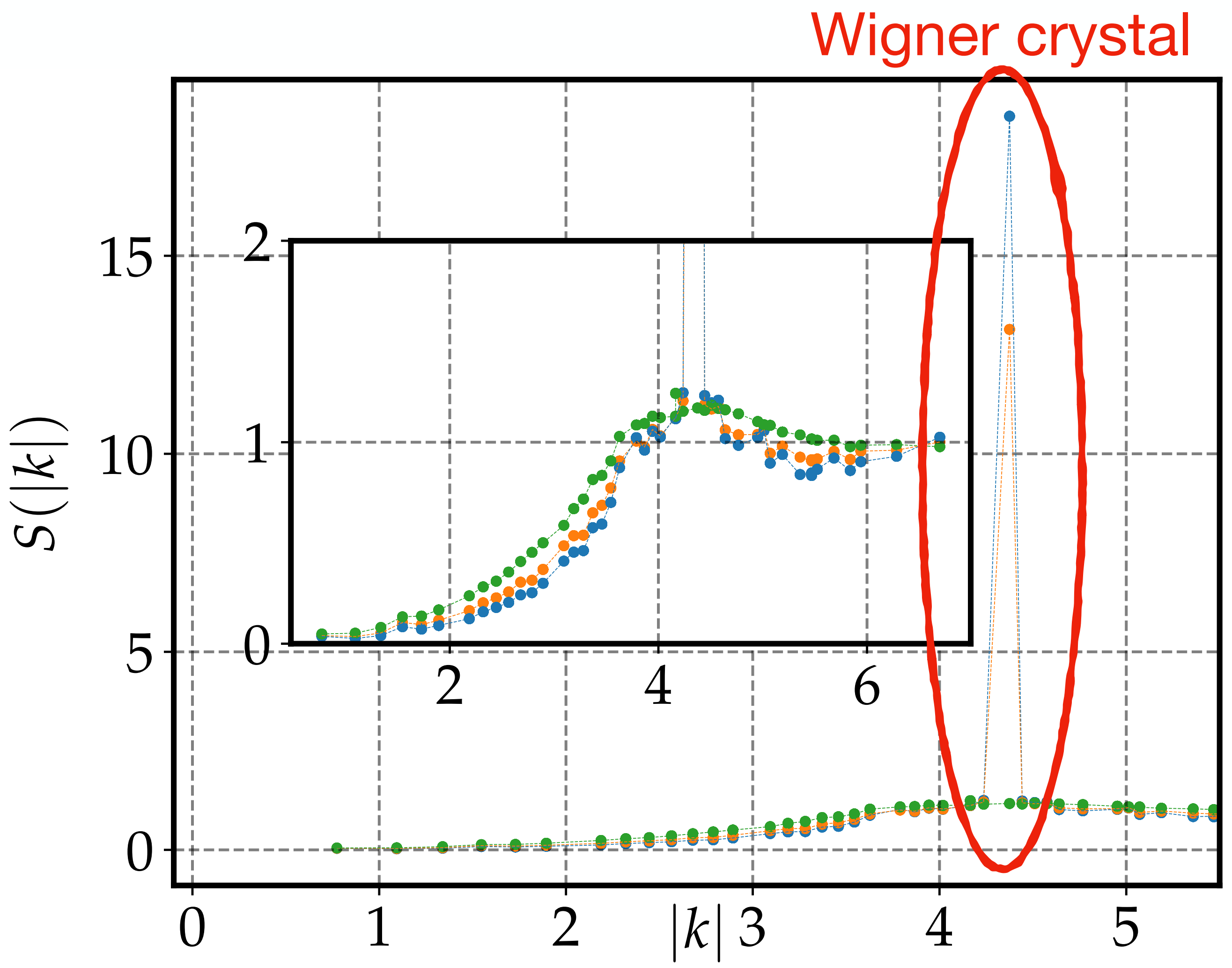
Pescia, Han, Lovato, Lu, & Carleo PRR (2022)

Homogeneous Electron Gas

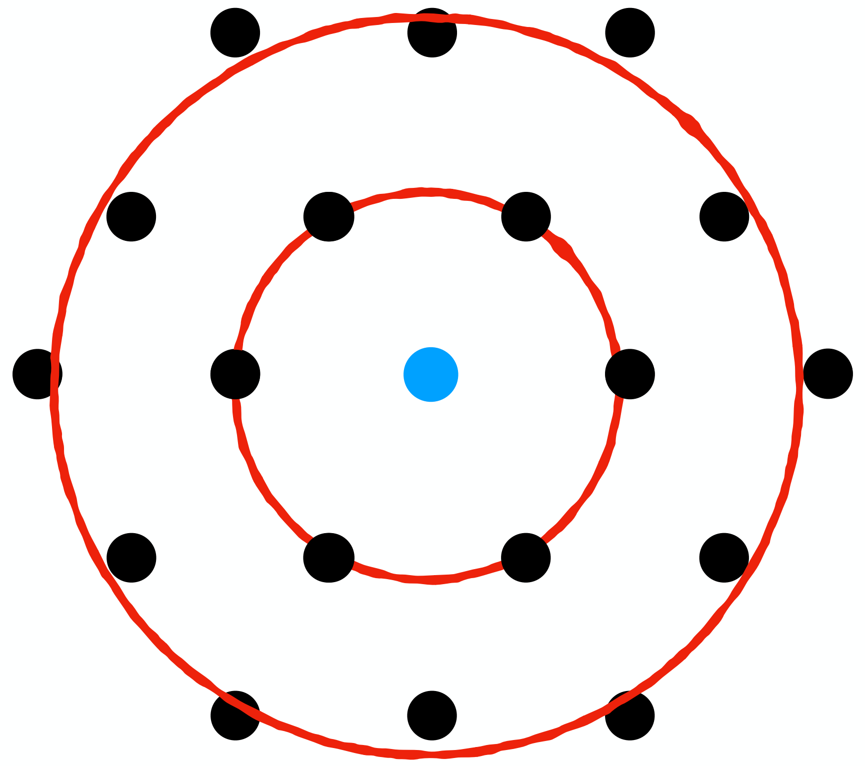


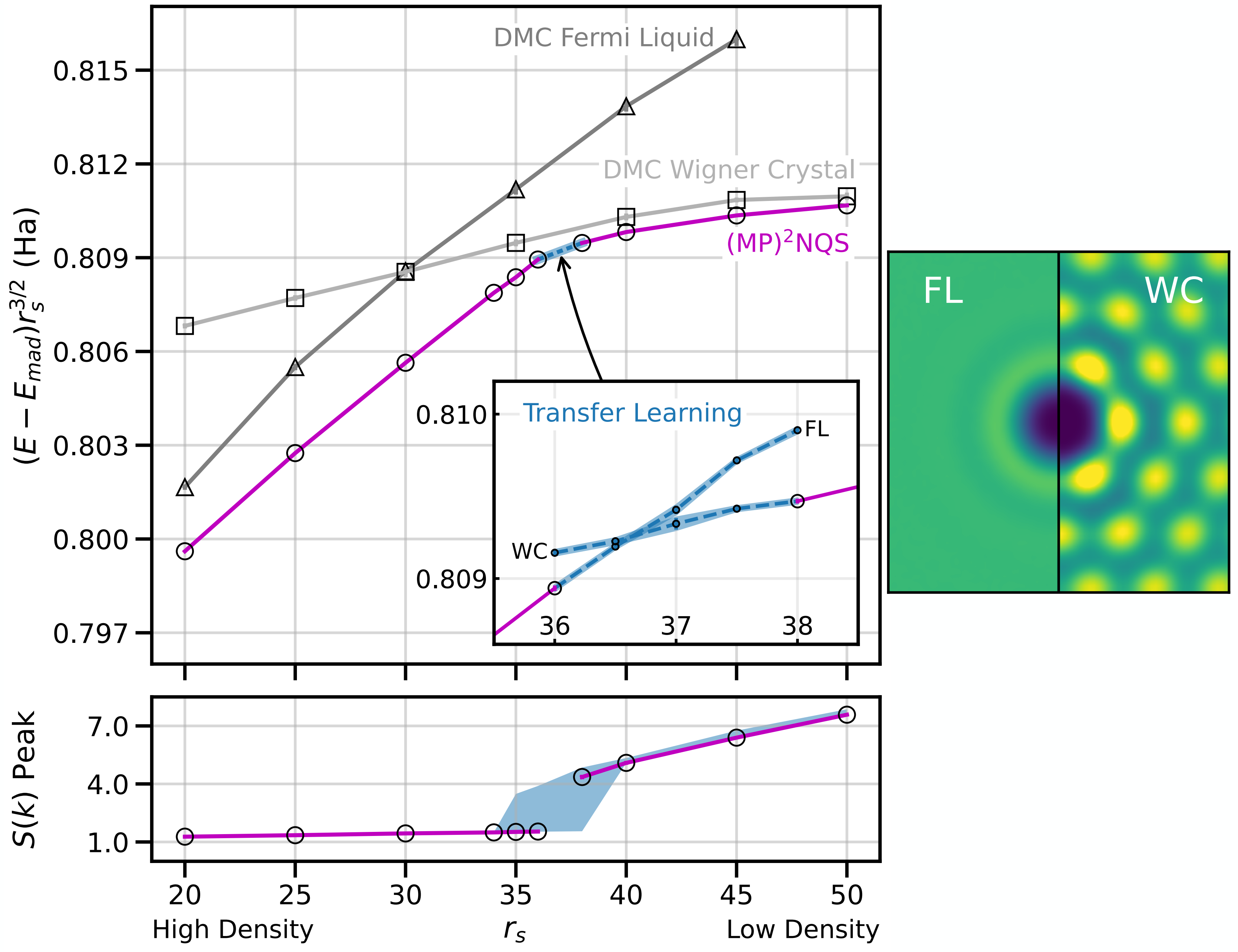
- Many-body correlations: efficient encoding
- **Unbiased** phase diagram
- Accurate representation of the ground state
- Low number of parameters (10k)
- Better optimization (natural gradients)





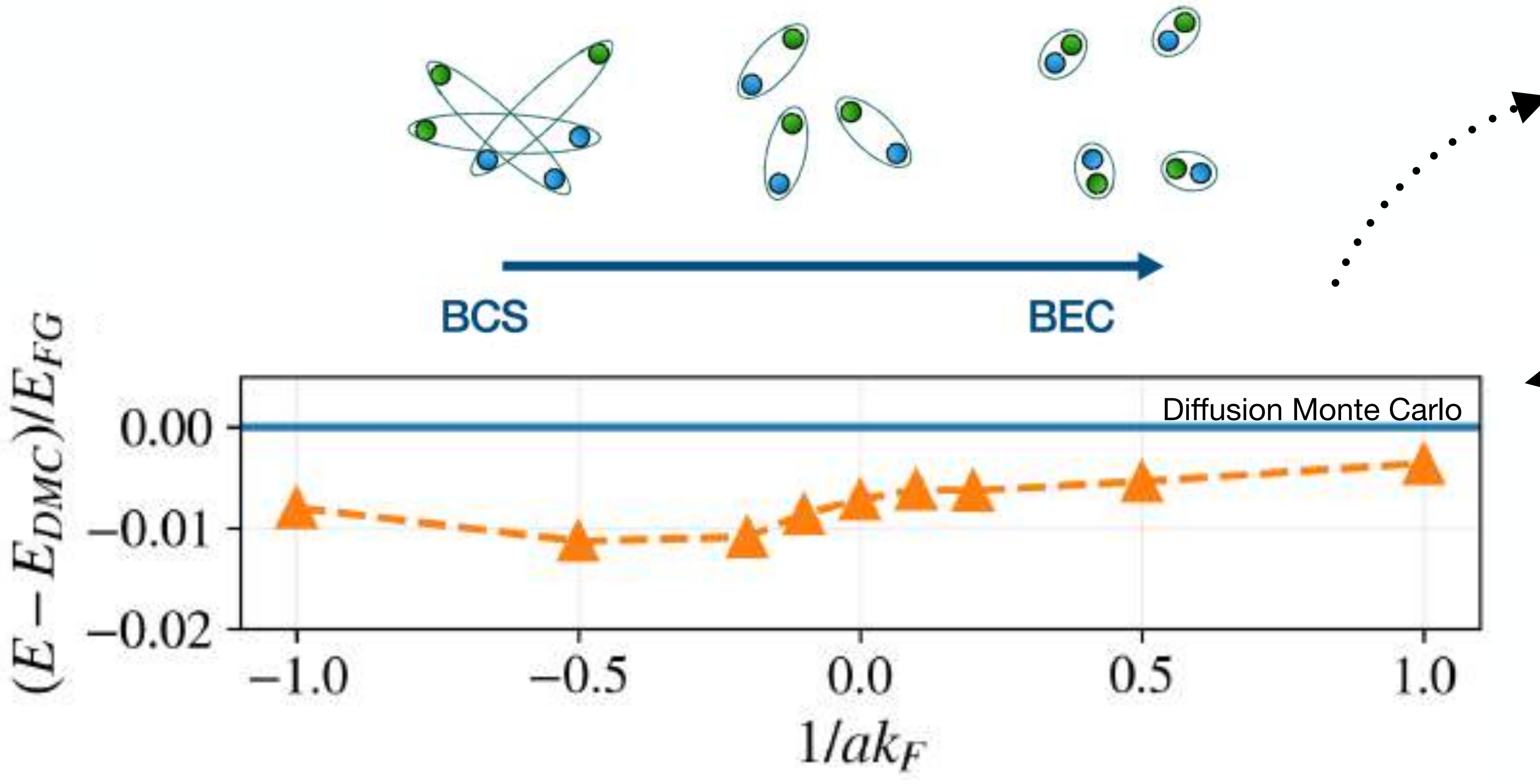
3D: G.Pescia, **J.Nys**, et al., PRB (2024)





2D: C. Smith, et al., 2405.19397 (2024)

Correlated fermionic wave functions



Ultra-cold Fermi gas (BCS - BEC crossover)

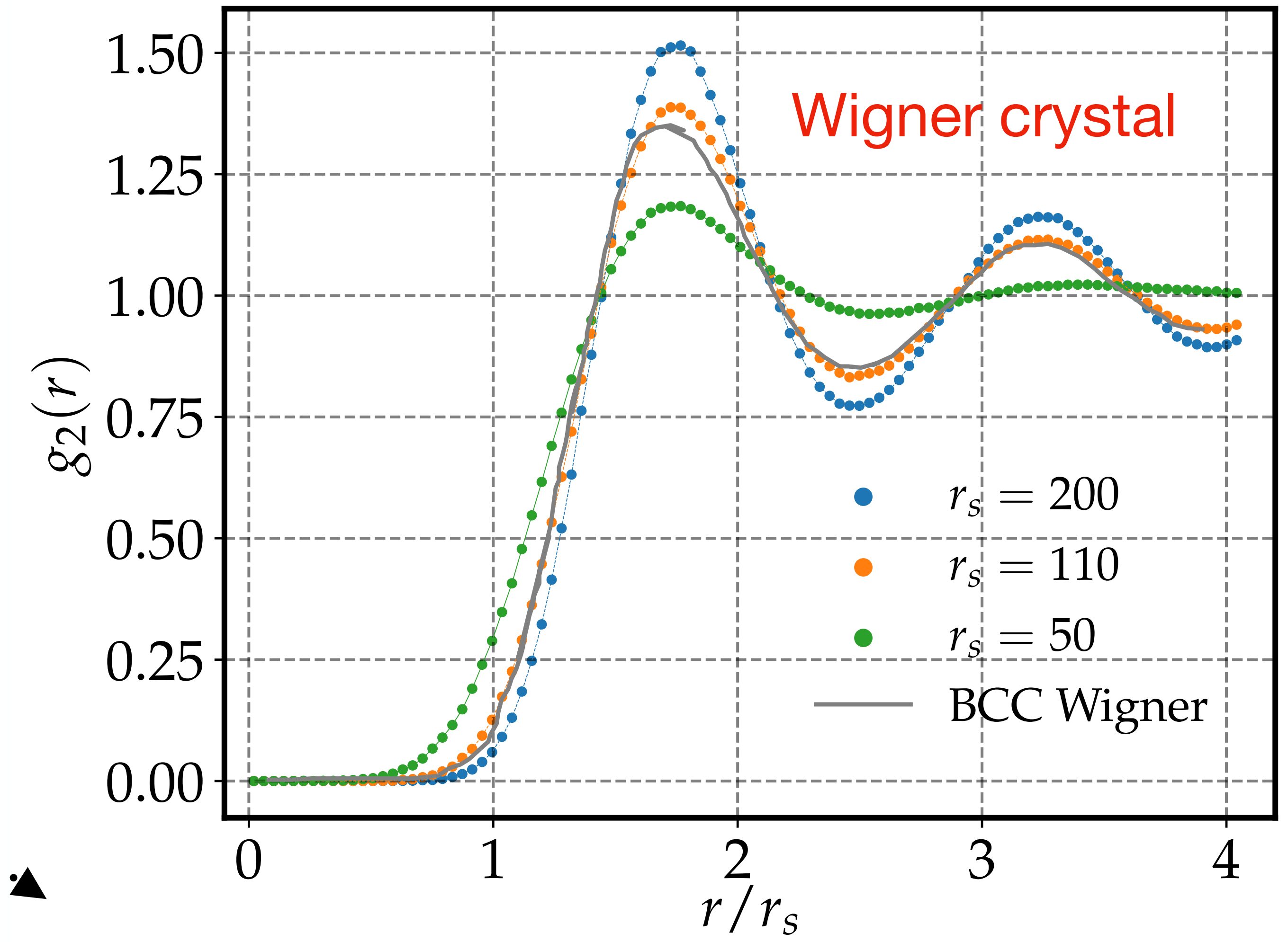
J.Kim, **J.Nys**, et al. Comm. Phys. (2024)

Ionization energies of molecules

Gao, et al., arXiv:2405.14762 (2024)

Bilayer (moiré) materials

Di Luo, et al., arXiv:2311.02143 (2023)



3D Homogenous electron gas

G.Pescia, **J.Nys**, et al., PRB (2024)

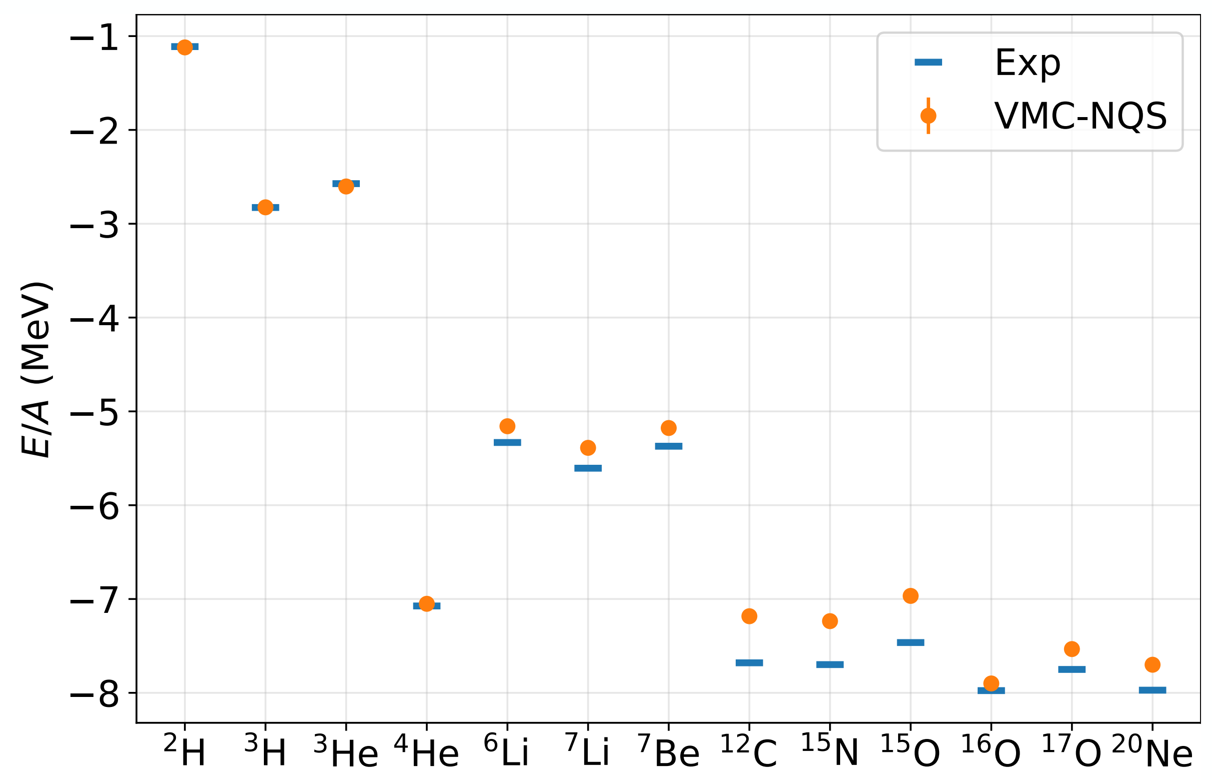
G.Pescia, **J.Nys**, et al., PRB (2024)
- Largest (128 e) & most accurate
- **Based on SOTA neural networks**
- **Strong & efficient correlations**

In all applications: **competitive or better** than existing methods

2D Electron gas

C.Smith, *et al,* 2405.19397 (2024)

Bosonic systems (^{4}He), D.Linteau, **J.Nys**, et al., to appear

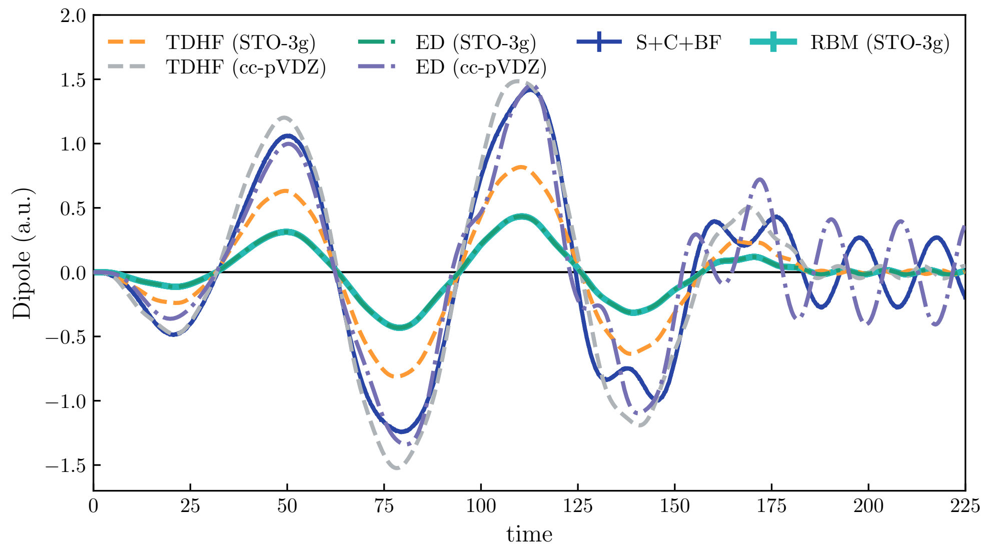


Nuclear physics: nuclear binding

Gnech, et al, PRL (2023)

Quantum dots & diatomic molecules

J.Nys, et al, Nat Comm (2024)

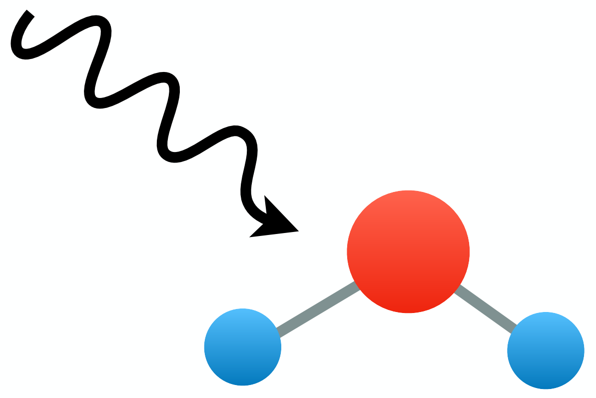


Real-time quantum dynamics

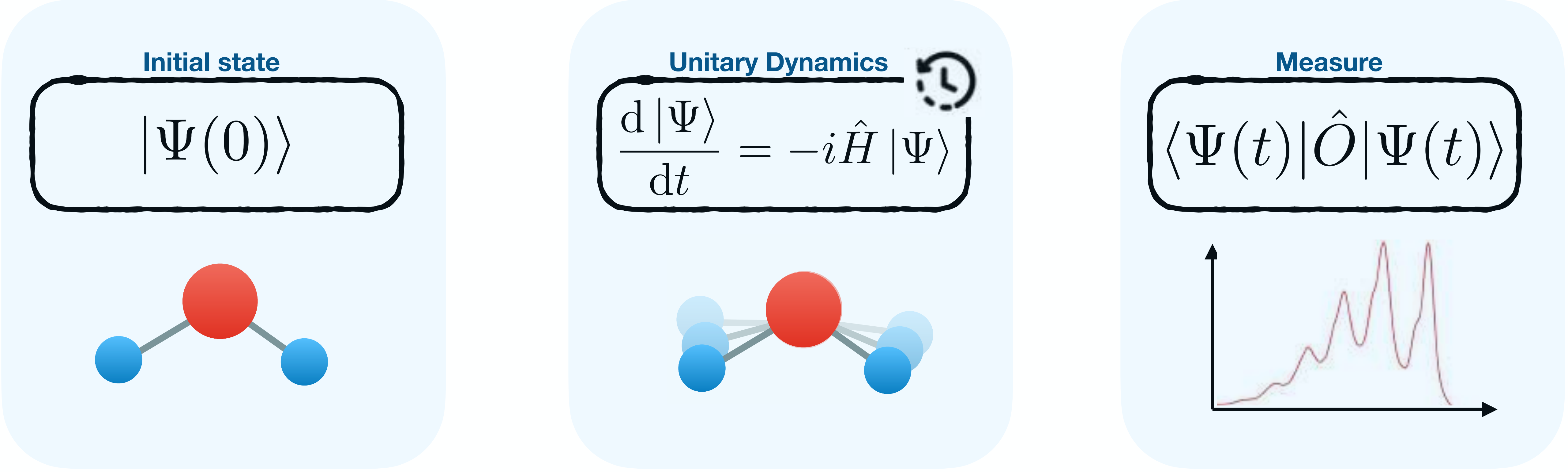
- One of the most significant problems of modern quantum physics
- No reliable classical methods available: approximations for ground states break down
- Quantum dynamics = flagships application of quantum computing

Examples:

- Excited states information
- Spectroscopic experiments
- Nonlinear responses
- Relaxation
- …



$$|\Psi(0)\rangle \xrightarrow{e^{-i\hat{H}t}} |\Psi(t)\rangle$$



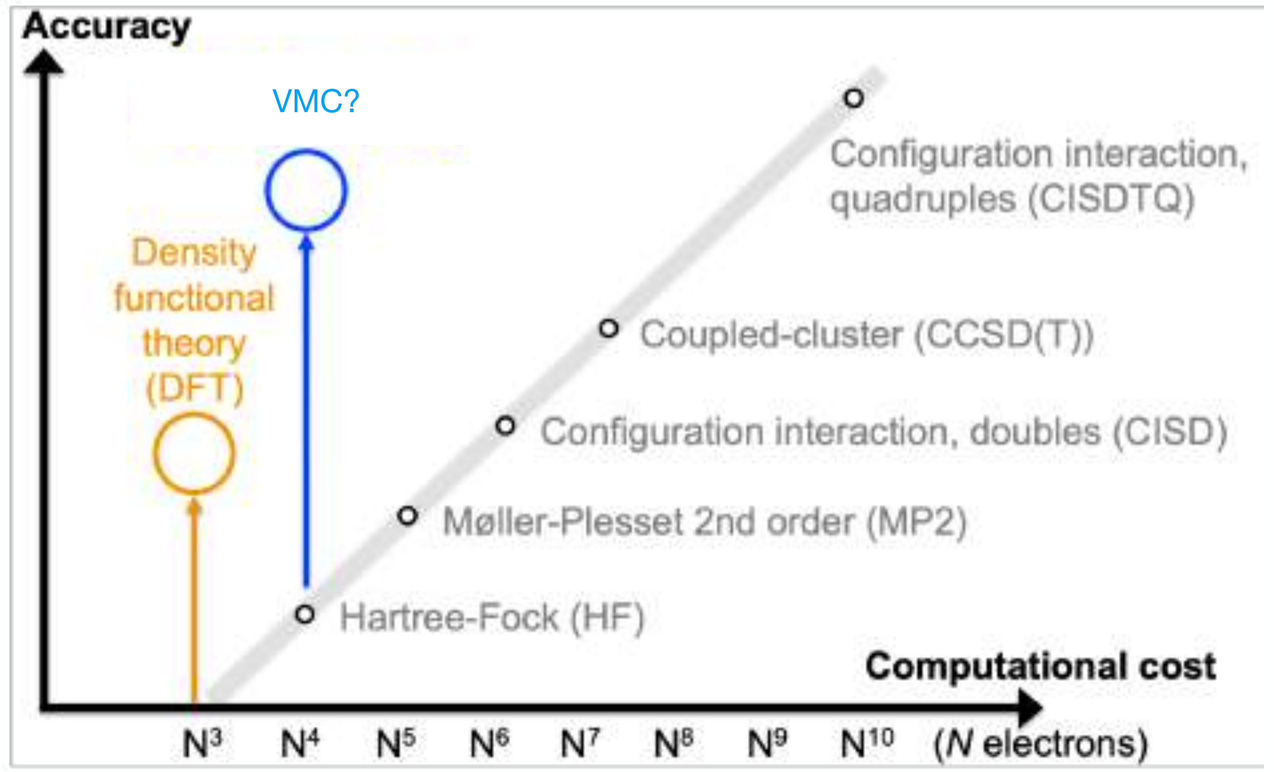
State of the art: classical methods

Quantum chemistry & mat
- TD-HF
- MC-TDHF
- RT-TDDFT
- TD-Configuration Interacti… (CI)
- TD-Coupled cluster (CC)

How can we go beyond DFT and HF to properly account for electron correlation in real time?

Li, et al, Chem Rev (2020)

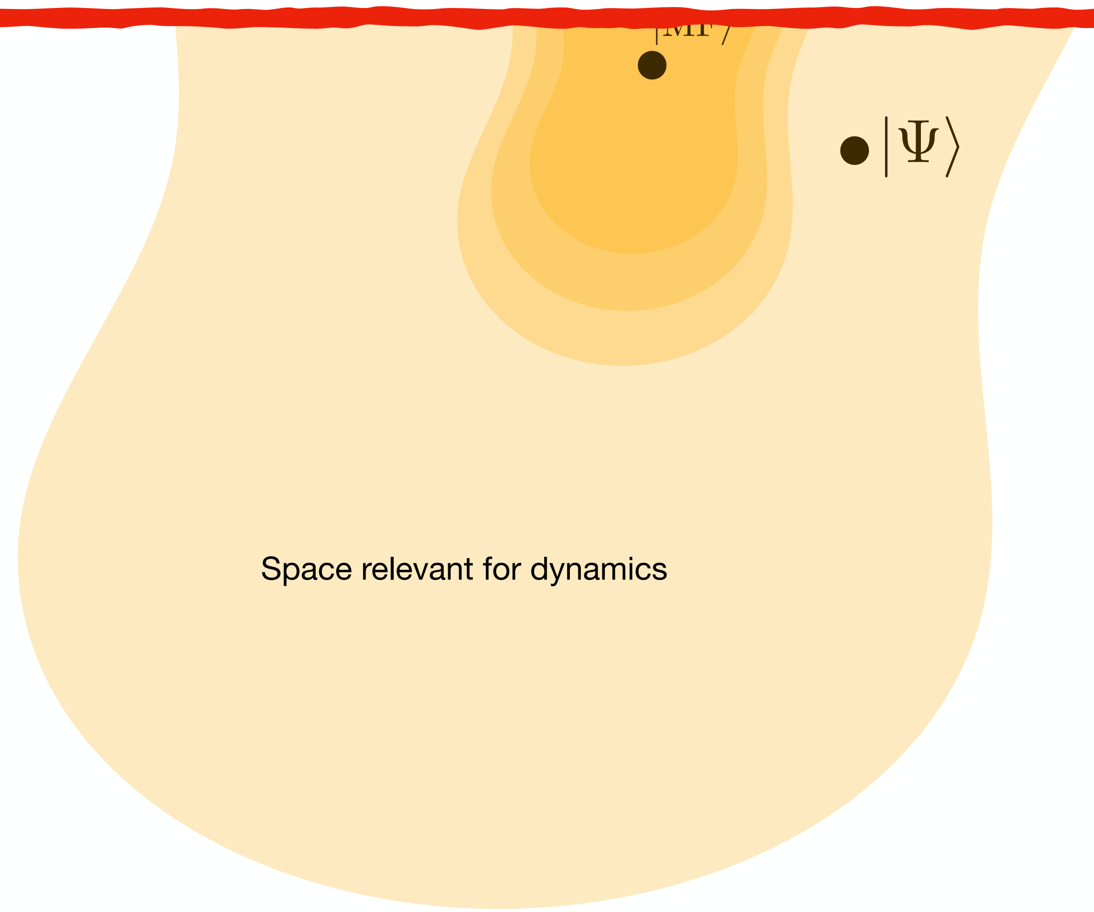
J. Hermann, *Nature Reviews Chemistry* (2023)



Need for new methods to account for strong correlations in real-time dynamics!

Condensed matter
- Exact diagonalization
- Tensor networks

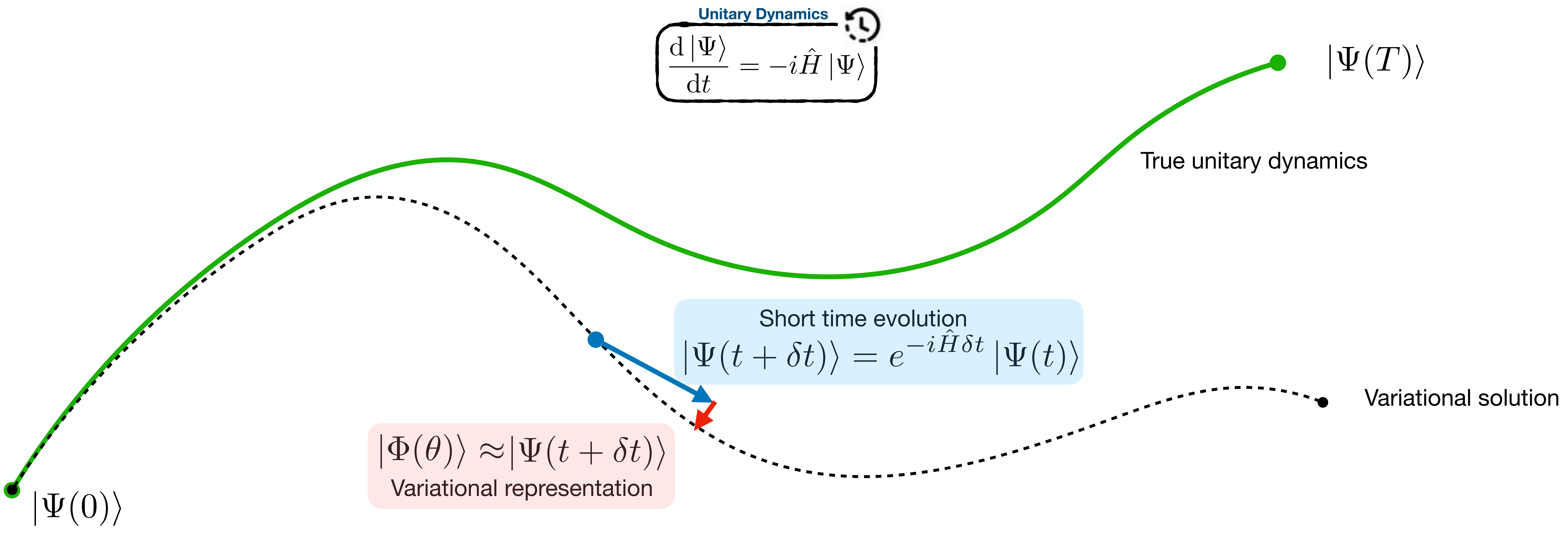
Idea: close to ground states with area law
Challenge: scaling with entanglement



Given recent progress in variational methods for ground-state problems with strong correlations:

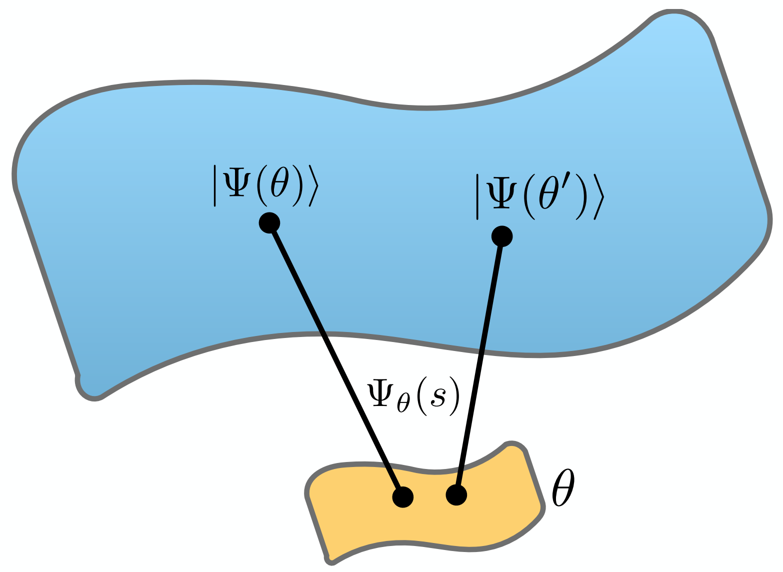
Can we transform them into accurate methods to solve real-time quantum dynamics problems?

Variational dynamics



J.Nys, G.Pescia, A.Sinibaldi, G.Carleo, Nature Communications (2024)

Dynamics: approach 1



Real-time evolution

G. Carleo, et al., PRX, (2017)

$$\frac{\mathrm{d}\,|\Psi\rangle}{\mathrm{d}t} = -i\hat{H}\,|\Psi\rangle \quad \rightarrow \quad G \cdot \dot{\theta} = -iF \qquad \mathcal{O}(N_p^3 N_s)$$

Energy

$$E = \frac{\langle\Psi|\hat{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle} \quad \rightarrow \quad E = \mathbb{E}_{s\sim|\Psi|^2}\left[\frac{[\hat{H}\Psi](s)}{\Psi(s)}\right]$$

Energy forces

$$F_\theta = \partial_\theta \frac{\langle\Psi|\hat{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle} \quad \rightarrow \quad F_\theta = \mathbb{E}_{s\sim|\Psi|^2}\left[\partial_\theta \log\Psi(s)^* \cdot \left(\frac{[\hat{H}\Psi](s)}{\Psi(s)} - E\right)\right] \qquad \in \mathbb{C}^{N_p}$$

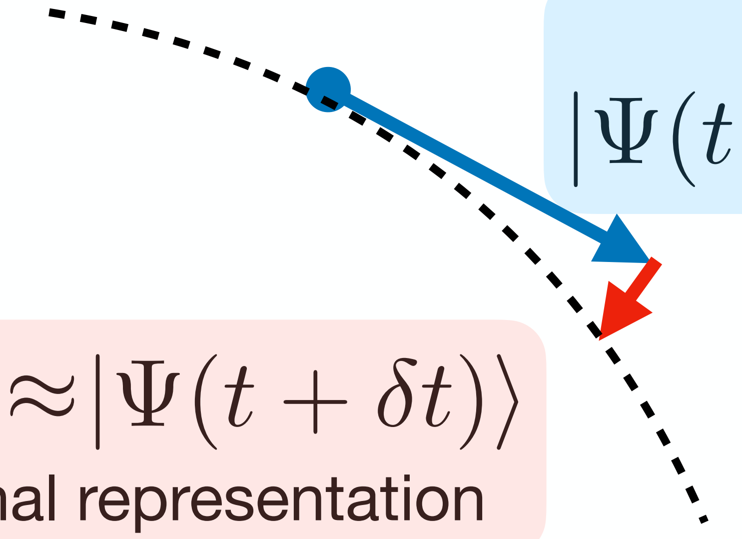
Quantum Geometric Tensor

$$G_{\theta,\theta'} = \frac{\langle\partial_\theta\Psi|\partial_{\theta'}\Psi\rangle}{\langle\Psi|\Psi\rangle} - \frac{\langle\partial_\theta\Psi|\Psi\rangle\,\langle\Psi|\partial_{\theta'}\Psi\rangle}{\langle\Psi|\Psi\rangle^2} \quad \rightarrow \quad G_{\theta,\theta'} = \mathbb{E}_{s\sim|\Psi|^2}\left[\partial_\theta \log\Psi(s)^* \cdot \Delta\partial_{\theta'}\log\Psi(s)\right] \qquad \in \mathbb{C}^{N_p\times N_p}$$

Dynamics: approach 2

Projected tVMC: maximize the overlap between [Gutiérrez & Mendl, Quantum, 6, 627 (2022)]

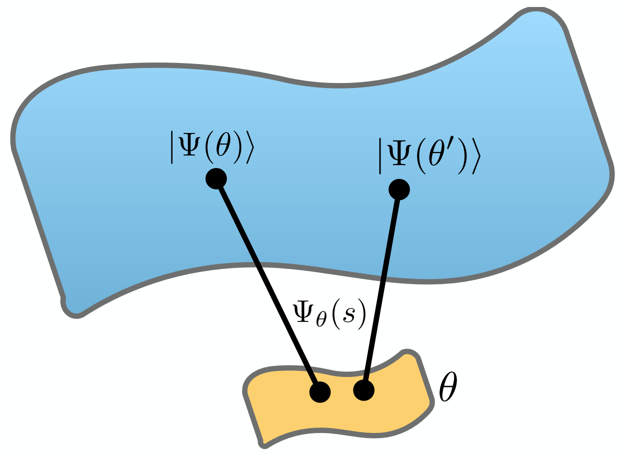
- time evolved state
- variational state



Short time evolution
$$|\Psi(t+\delta t)\rangle = e^{-i\hat{H}\delta t}\,|\Psi(t)\rangle$$

$$|\Phi(\theta)\rangle \approx |\Psi(t+\delta t)\rangle$$
Variational representation

$$G^{-1}\dot{\theta} = -iF \quad \rightarrow \quad \mathcal{D}\left[\,|\Psi(\theta)\rangle,\; e^{-i\hat{H}\delta t}\,|\Psi(t)\rangle\,\right]$$



Fidelity: Sinibaldi et al, Quantum (2023)

Novel propagator product expansion: Taylor-root expansion:
Higher orders at low computational cost

J.Nys, G.Pescia, A.Sinibaldi, G.Carleo, Nature Communications (2024)

Novel time propagator expansions

$$e^{-i\delta t\hat{H}} = \prod_{k=1}^{K} \hat{R}_k + \mathcal{O}\left(\delta t^{K+1}\right)$$

$$\hat{R}_k = 1 - ic_k\delta t\hat{H}$$

Example: Taylor expansion matching

"Taylor root expansion"

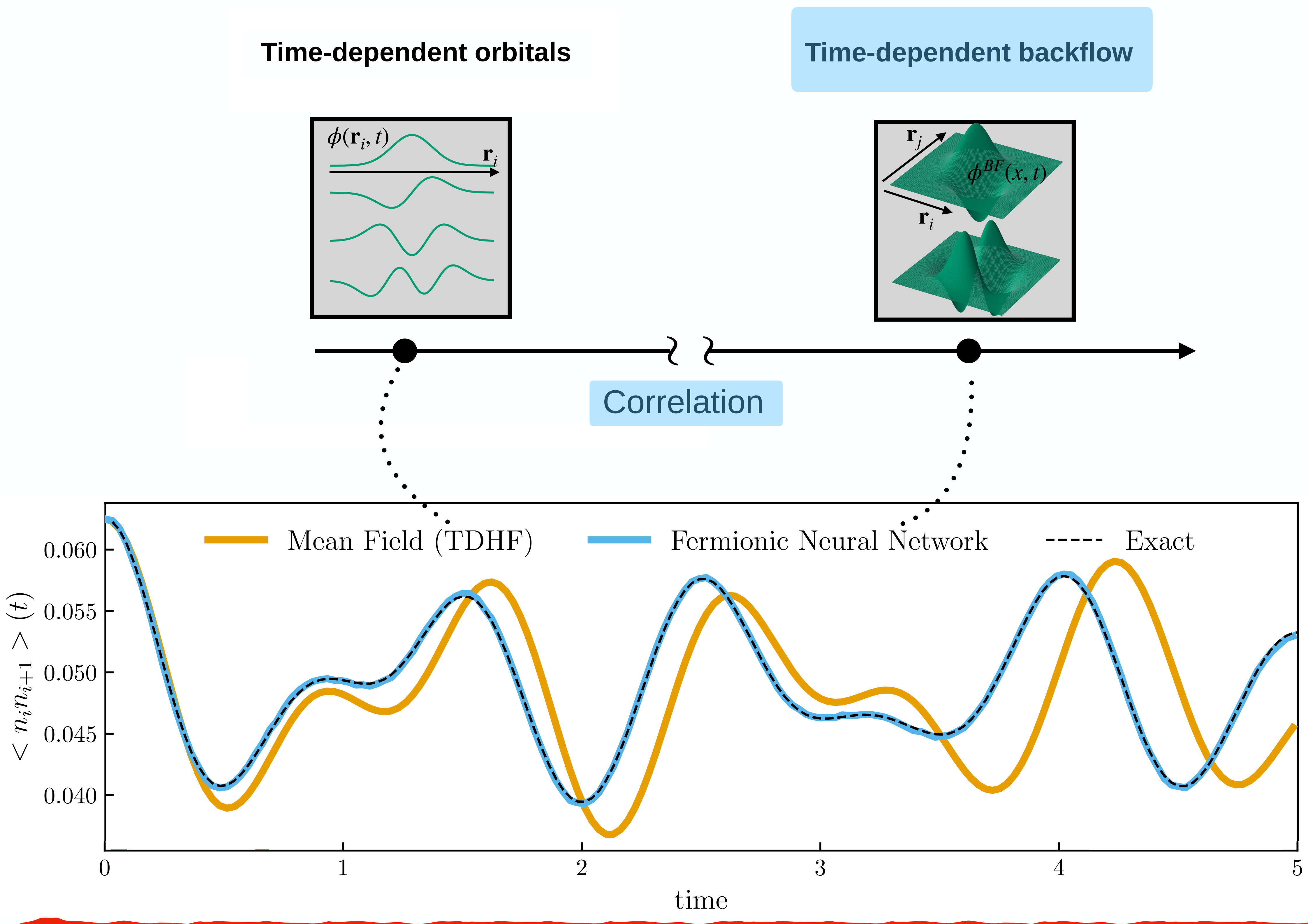
$$\hat{R}_1\hat{R}_2 = \mathbb{I} - i\hat{H}\delta t(c_1 + c_2) - \hat{H}^2\delta t^2 c_1 c_2 \quad \Rightarrow \quad U_{\text{Taylor}} = \mathbb{I} - i\hat{H}\delta t - \hat{H}^2\delta t^2\frac{1}{2}$$

$$c_1 = \frac{1 \pm i}{2}$$
$$c_2 = \frac{1 \mp i}{2}$$

J.Nys, G.Pescia, A.Sinibaldi, G.Carleo, Nature Communications (2024)

Electrons out of equilibrium

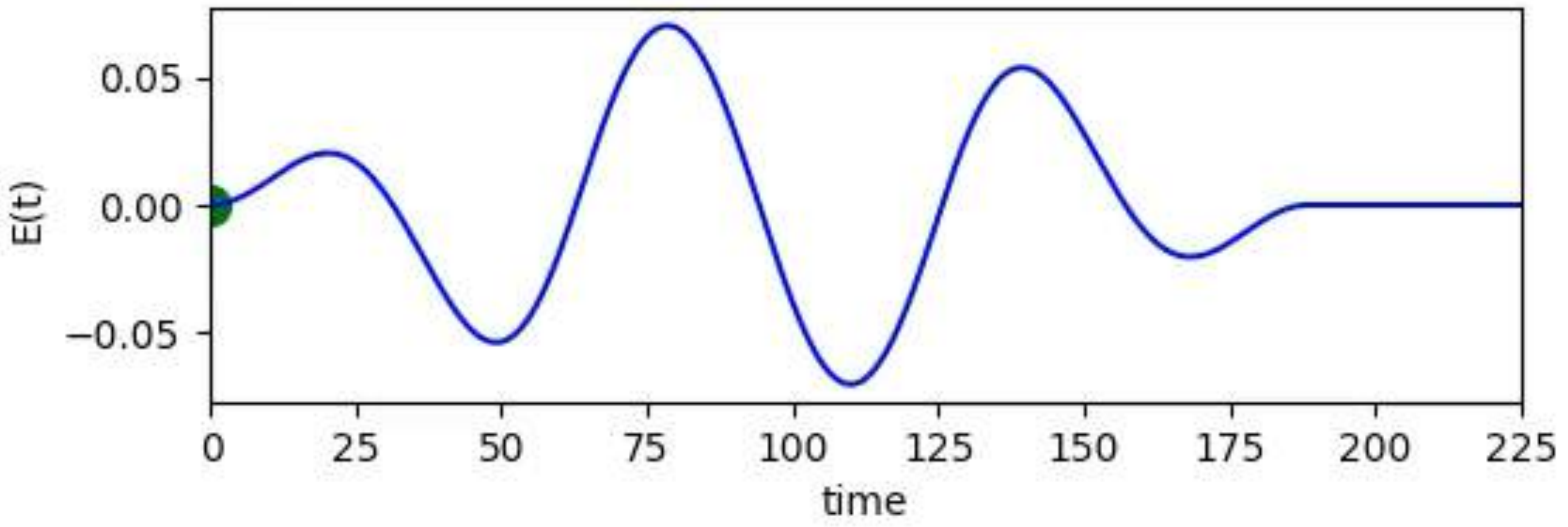
Time-dependent variational wave functions for electronic systems

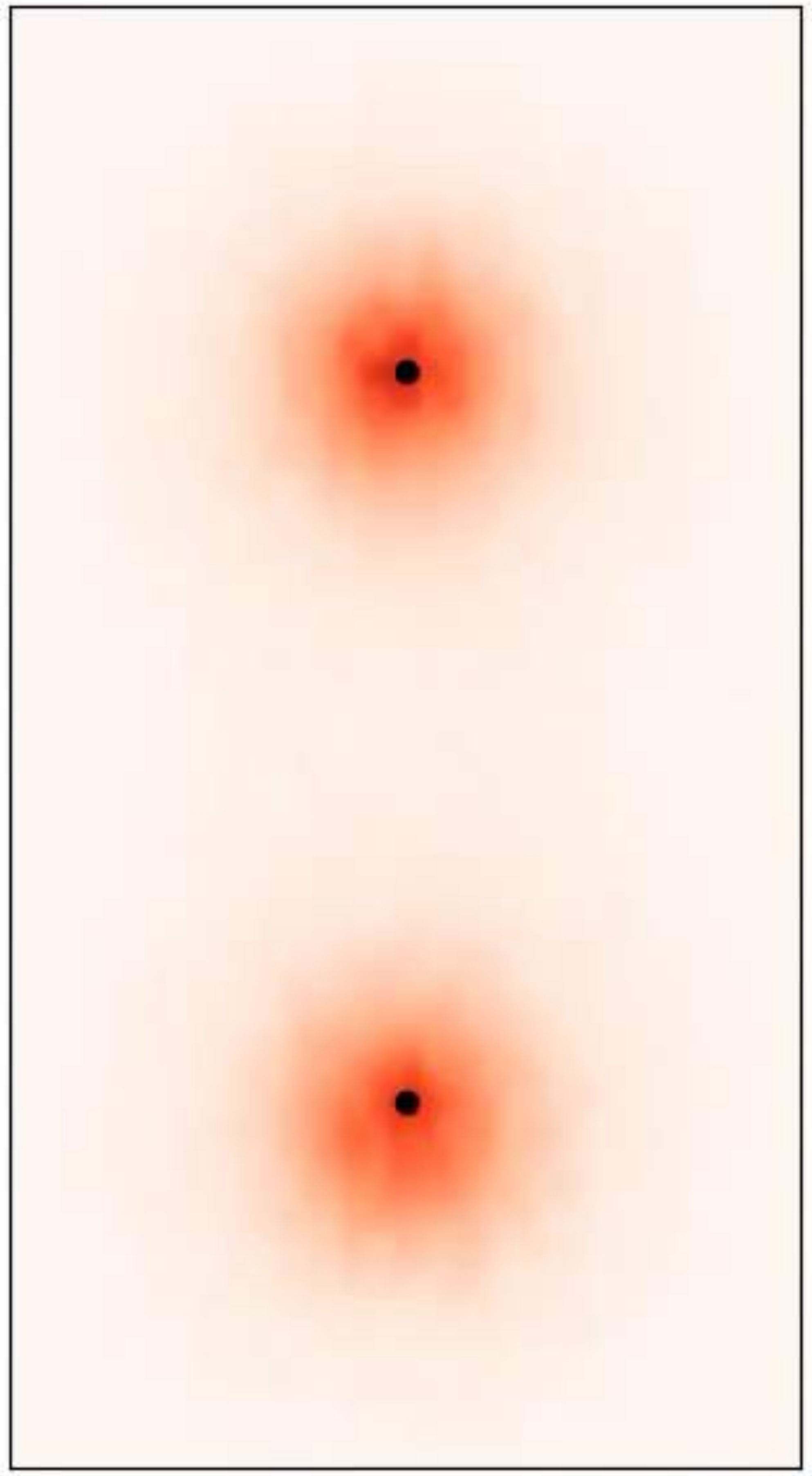


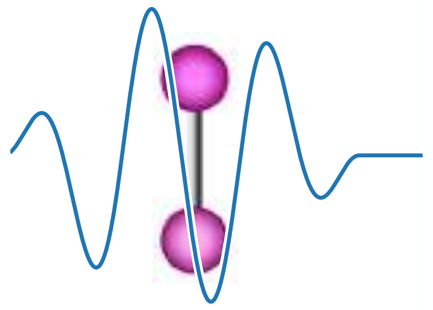
Time-dependent fermionic neural networks efficiently represent **long-range correlations** & **strong entanglement**

J.Nys, G.Pescia, A.Sinibaldi, G.Carleo, Nature Communications (2024)

Ab-initio variatior ... ıantum dynamics



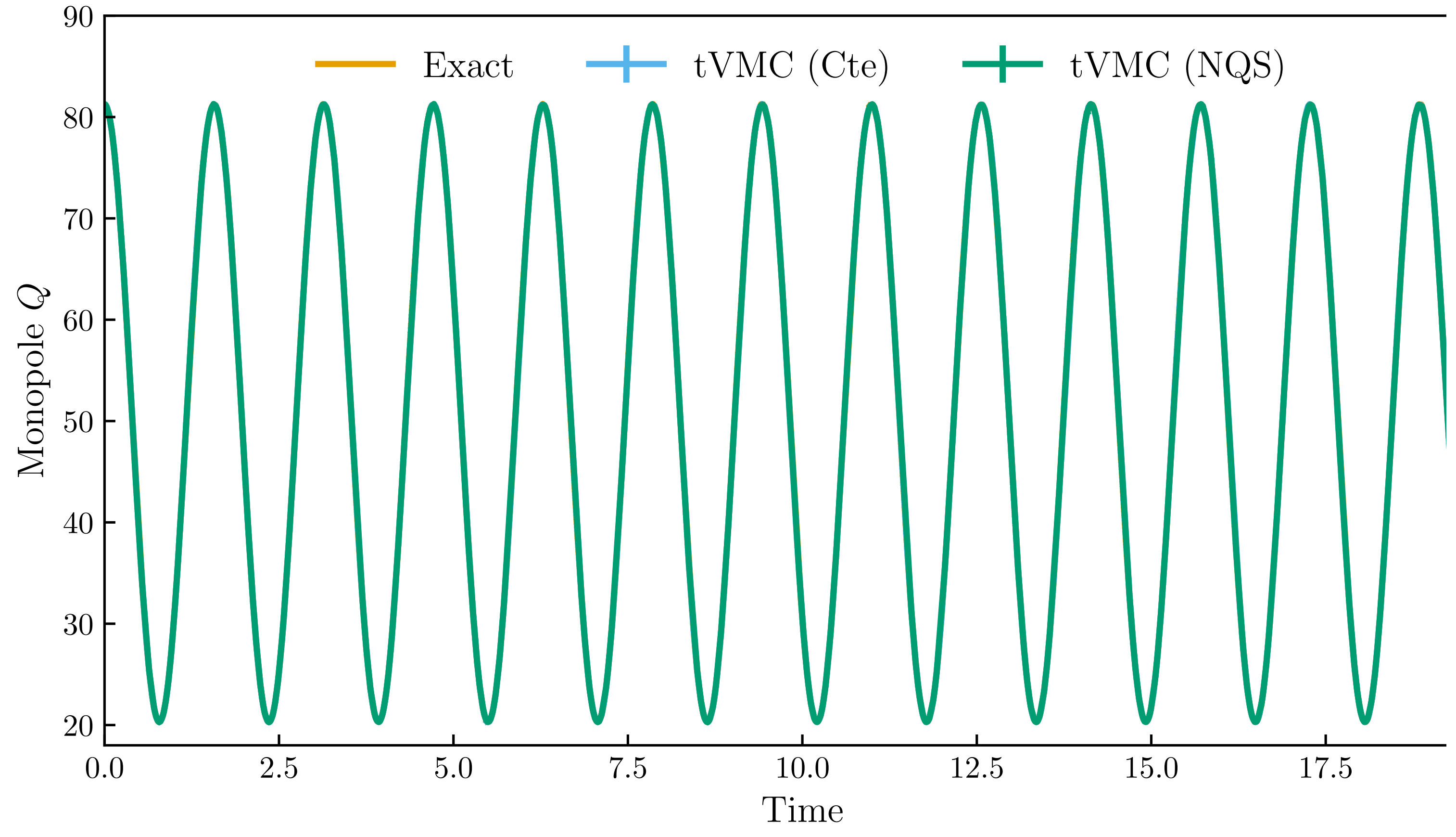




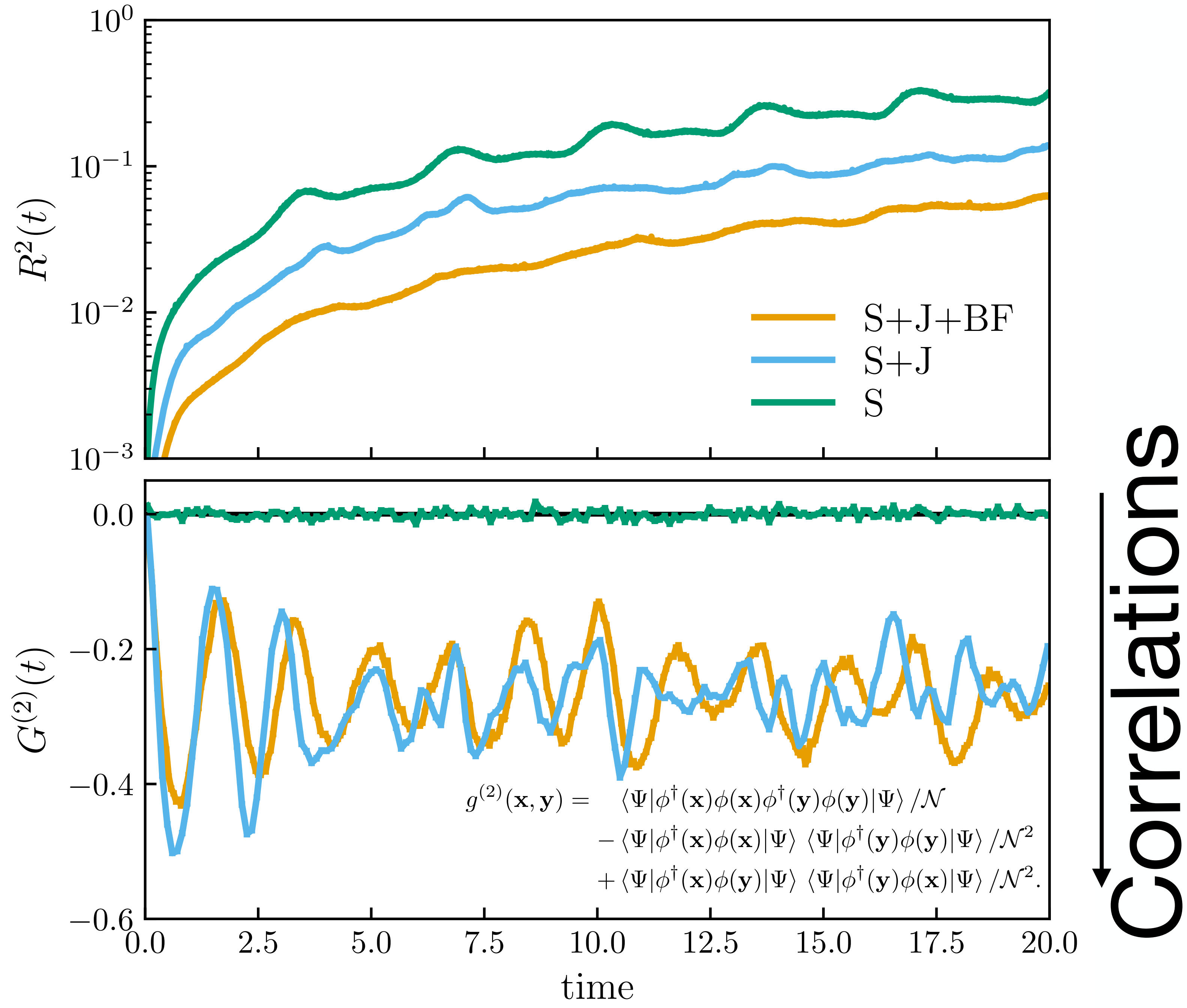
$$\left\| \frac{\mathrm{d}}{\mathrm{d}t} |\Psi(t)\rangle + iH |\Psi(t)\rangle \right\|^2$$

$$V(x,t) = \sum_{i=1}^{N} \frac{1}{2}\omega^2 \mathbf{r}_i^2 + \sum_{i<j}^{N} \frac{\kappa(t)}{\|\mathbf{r}_i - \mathbf{r}_j\|}$$

$$V(x,t) = \sum_{i=1}^{N} \left[\frac{1}{2}\omega(t)^2 \mathbf{r}_i^2 + \frac{g(t)}{2} \sum_{i>j}^{N} (\mathbf{r}_i - \mathbf{r}_j)^2 \right]$$



1D harmonic interaction (solvable

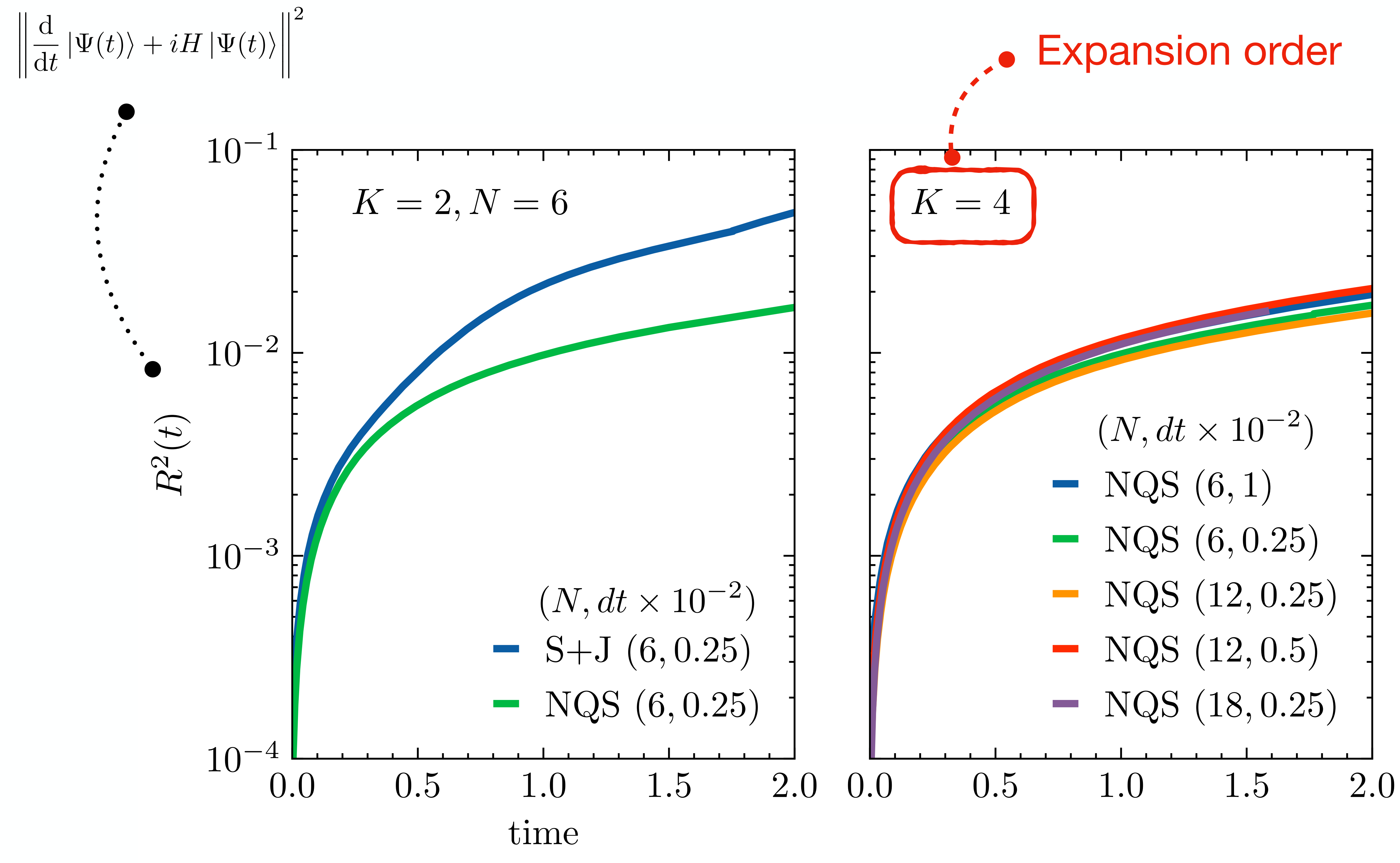


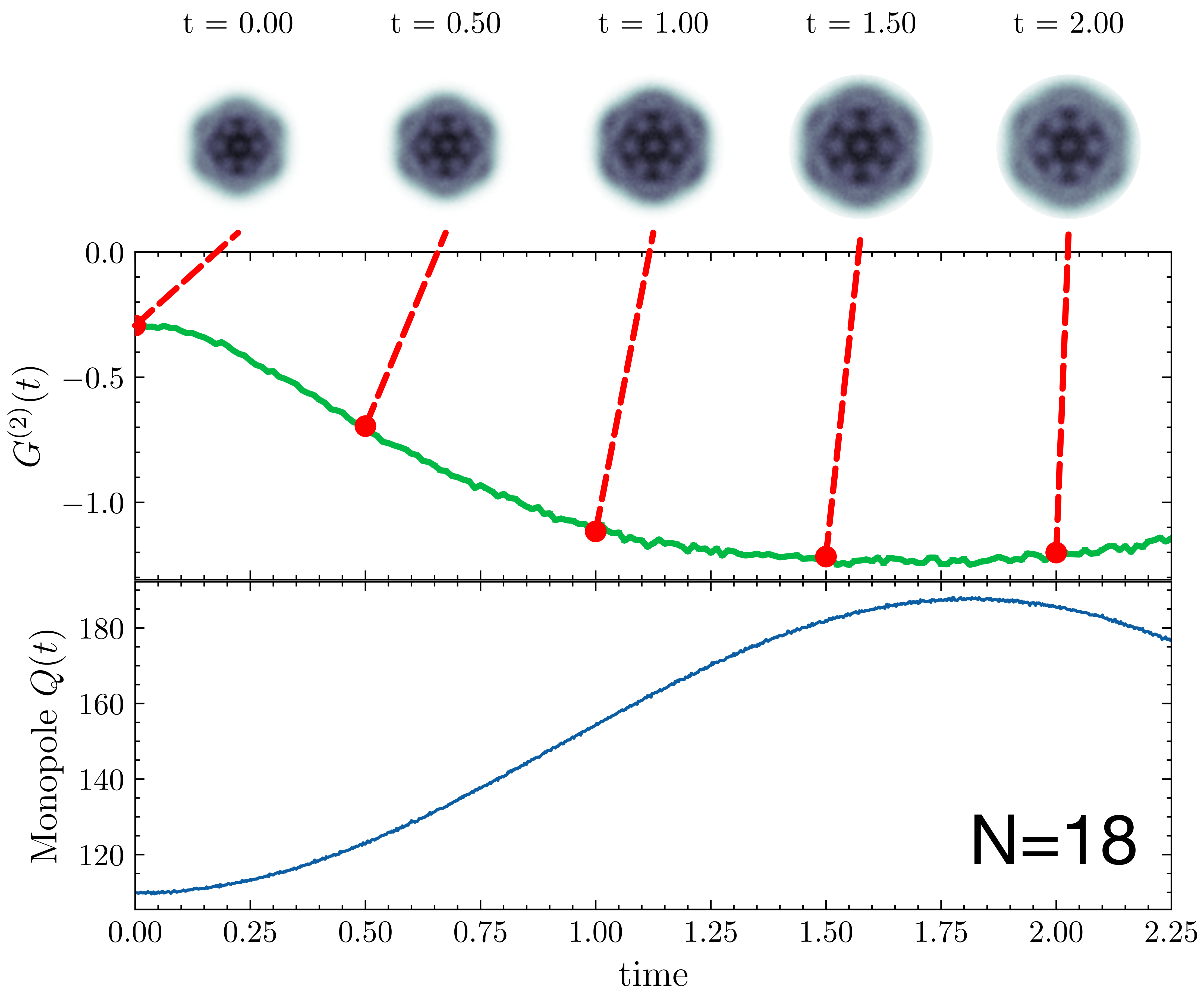
$$g^{(2)}(\mathbf{x},\mathbf{y}) = \langle\Psi|\phi^\dagger(\mathbf{x})\phi(\mathbf{x})\phi^\dagger(\mathbf{y})\phi(\mathbf{y})|\Psi\rangle/\mathcal{N} - \langle\Psi|\phi^\dagger(\mathbf{x})\phi(\mathbf{x})|\Psi\rangle\langle\Psi|\phi^\dagger(\mathbf{y})\phi(\mathbf{y})|\Psi\rangle/\mathcal{N}^2 + \langle\Psi|\phi^\dagger(\mathbf{x})\phi(\mathbf{y})|\Psi\rangle\langle\Psi|\phi^\dagger(\mathbf{y})\phi(\mathbf{x})|\Psi\rangle/\mathcal{N}^2.$$

2D quantum dot

ıs, G.Pescia, A.Sinibaldi, G.Carleo, Nature Communications (2024)

2D Quantum dot quench





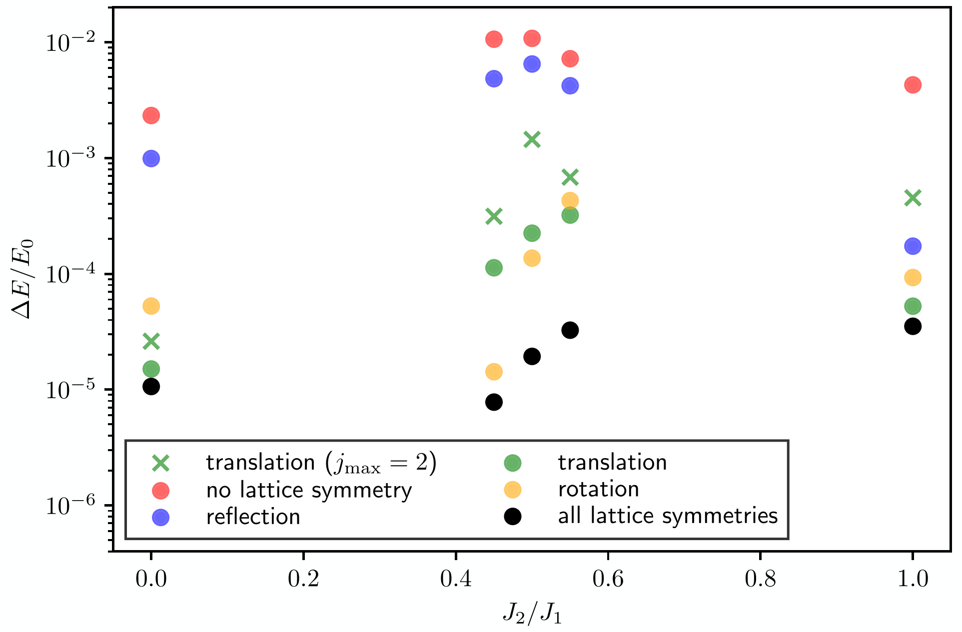
J.Nys, G.Pescia, A.Sinibaldi, G.Carleo, Nature Communications (2024)

Overview of recent progress

New variational methods to capture strongly correlated systems

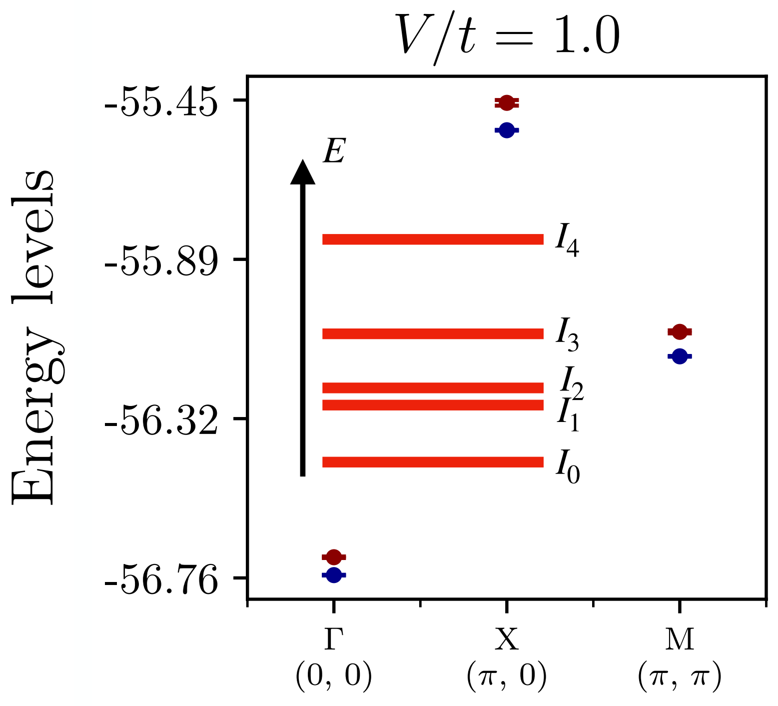
(Non-Abelian) symmetries

SU(2) + lattice symmetries in 2D



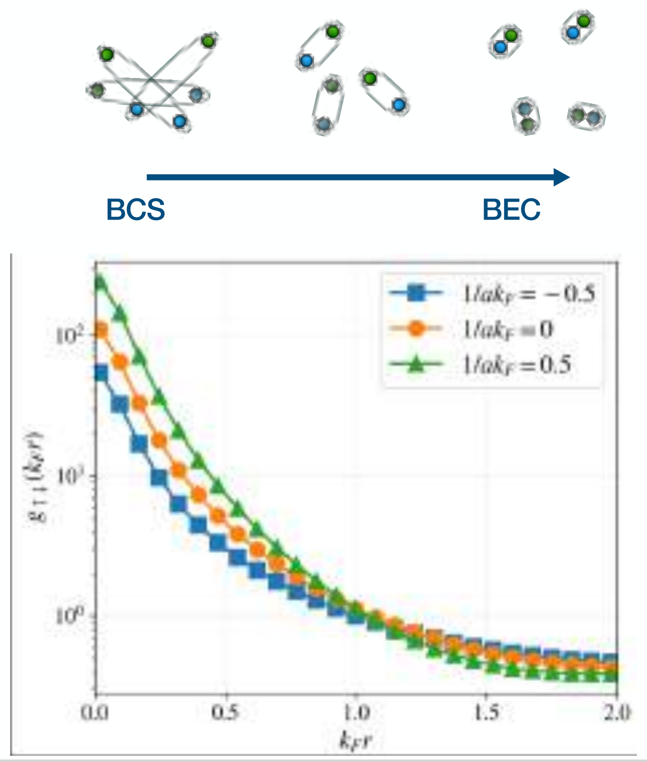
T.Vieijra, JN, et al. PRL (2020)
T.Vieijra, JN, PRB (2021)

Electron spectroscopy



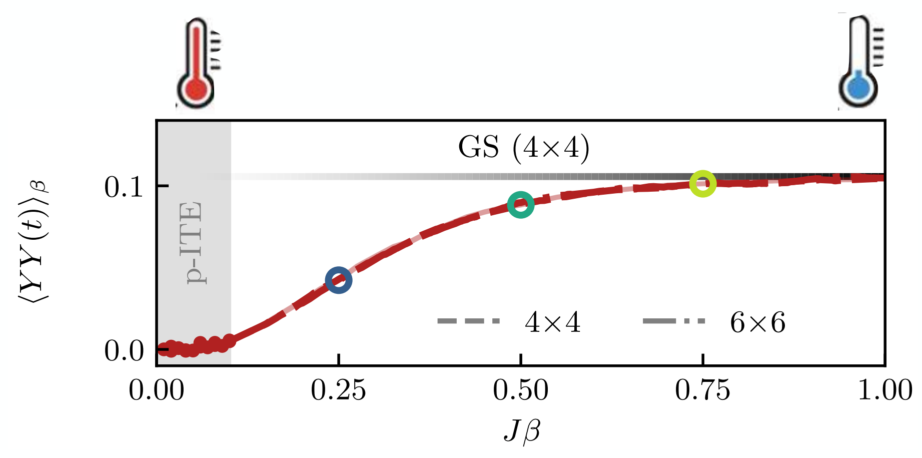
I.Romero, JN, et al, arxiv (2024)

Fermion pairing: BEC-BCS cross.



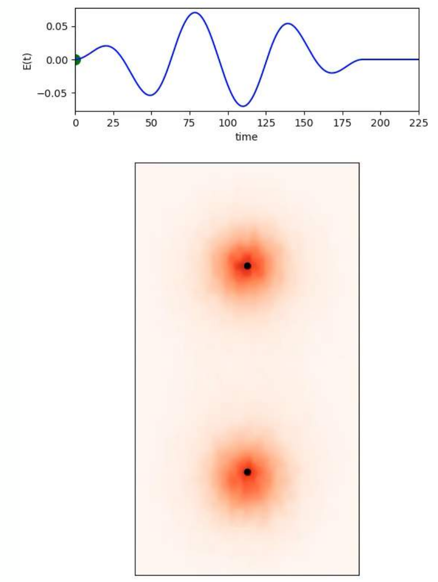
J.Kim, JN, et al, CommPhys (2023)

Thermal spins



JN, et al, PRB (2024)

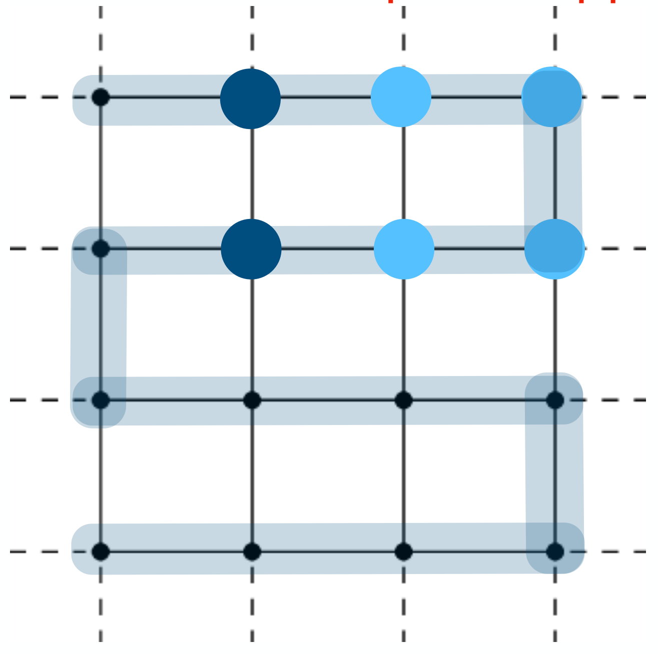
Electron dynamics



JN, et al, Nat Comm (2024)

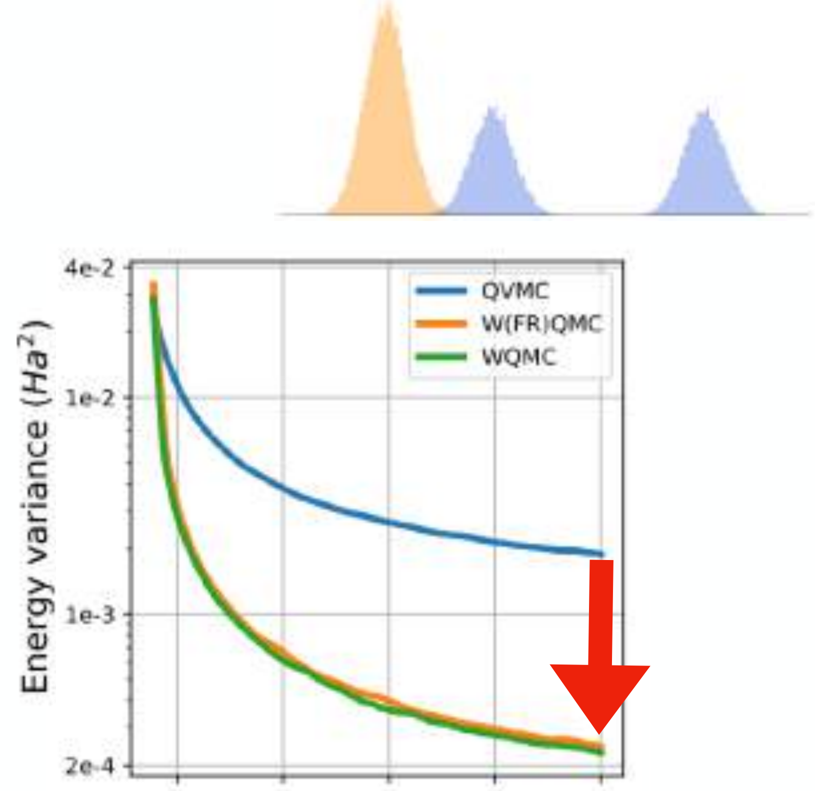
Representing fermions

Exact solutions of bosonization &
local fermion-to-qubit mappings



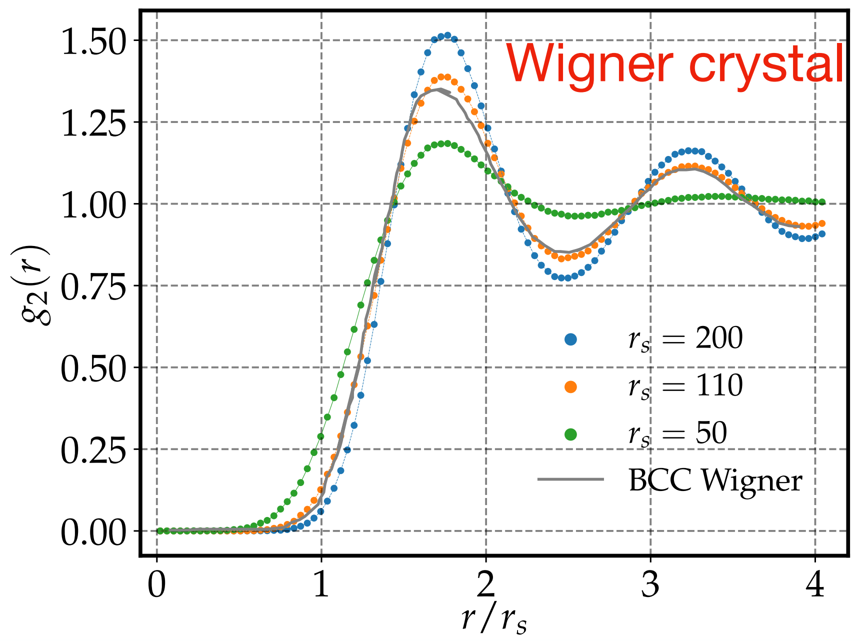
JN & Carleo, Quantum (2022)
JN & Carleo, Quantum (2023)

Advanced optimization in VMC



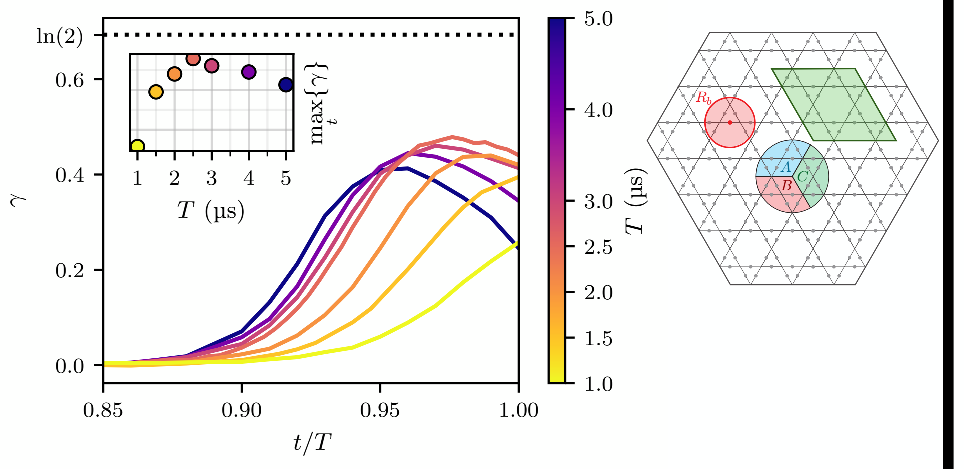
K.Neklyudov, JN, et al. NeurIPS (2024)

Bulk corr. electrons: 3D HEG



G.Pescia, JN, et al., PRB (2024)

Validation: analog simulators



L.Mauron, JN, et al, arxiv (2024)

Open Source VMC

Spins —> Fermions

NetKet.org, SciPost (2022)