Machine-Learning Universal Bosonic Functionals

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Joint work with:

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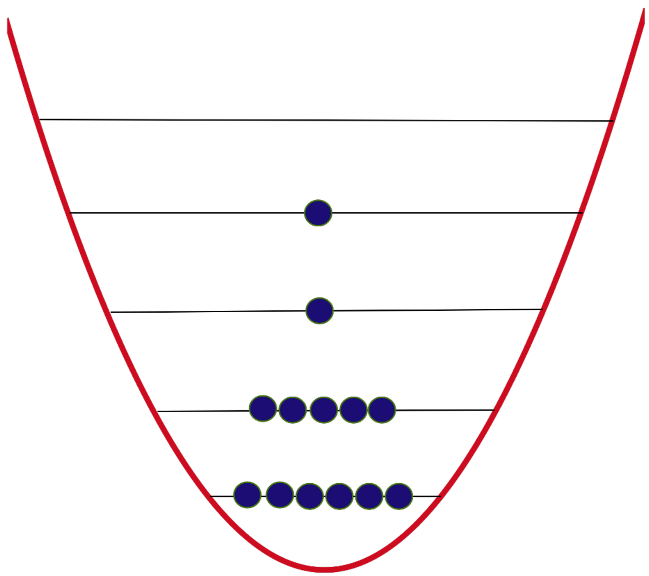
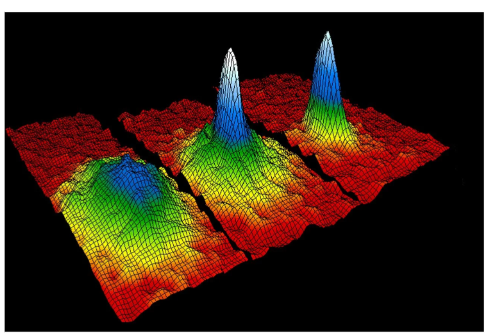
Ground-state problem





Science (1995)

$$H|\Psi_0\rangle = E_0|\Psi_0\rangle$$

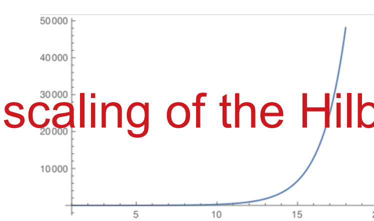
$$E_0 = \min_{\Psi\in\mathcal{H}}\langle\Psi|H|\Psi\rangle$$

$$= \min_{\Psi\in\mathcal{H}}\langle\Psi|h + W|\Psi\rangle$$

1-particle term comprising local potentials.

fixed 2-body Hamiltonian: Coulomb repulsion, on site interaction...

$$\Psi(x_1,\ldots,x_N)$$



Exponential scaling of the Hilbert space!

One-body Reduced Density Matrix

$$\gamma_{ij} = \langle \Psi | b_i^\dagger b_j | \Psi \rangle$$

- It is a **positive semidefinite matrix**.

- It is a crucial variable for the accurate description of Bose-Einstein
- condensates (BEC) and strongly correlated bosonic systems.

occupation numbers

$$\gamma = \sum_i n_i |\varphi_i\rangle\langle\varphi_i|$$

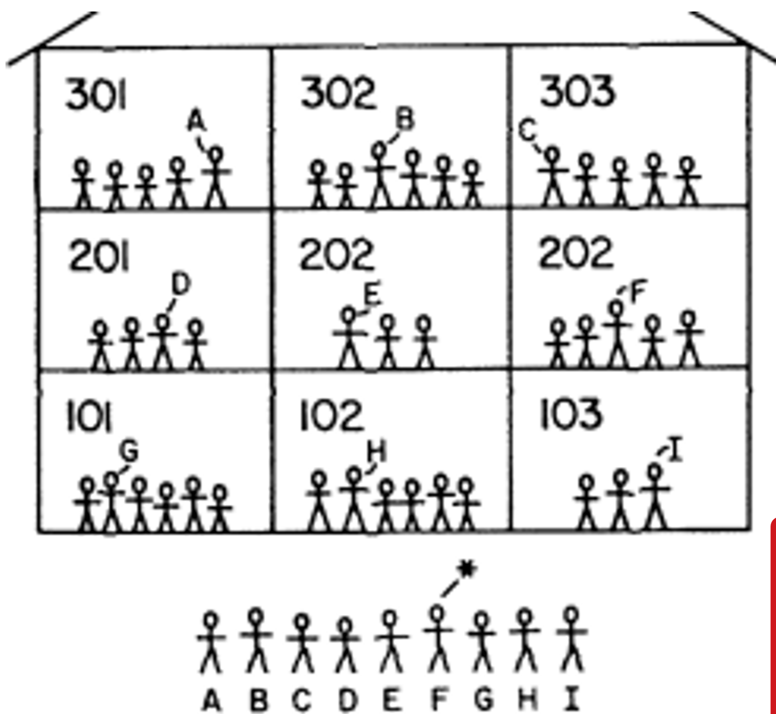
- BEC: $n_1 \approx O(N)$
-

- The information contained in the 1RDM can also be sufficient to
- investigate multipartite quantum correlations in those systems and
- even many-body localization.

S. Bera et al. PRL **115**, 046603 (2015).

Universal functionals

Who is the tallest child?



$$E_0 = \min_{\Psi \in \mathcal{H}} \langle \Psi | H | \Psi \rangle$$

$$= \min_\gamma \min_{\Psi \to \gamma} \langle \Psi | h + W | \Psi \rangle)$$

$$= \min_\gamma (\mathrm{Tr}[h\gamma] + \mathcal{F}_W[\gamma])$$

$$\mathcal{F}_W[\gamma] = \min_{\Psi \in \mathcal{H} \to \gamma} \langle \Psi | W | \Psi \rangle$$

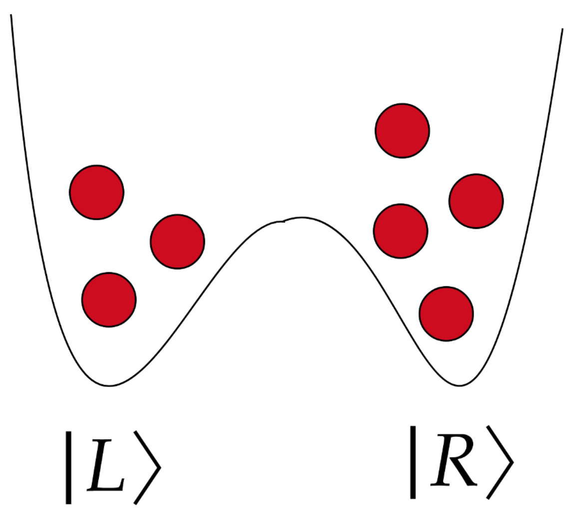
Parr and Yang, famous book on DFT, 1989.

Bose-Hubbard dimer

The Bose-Hubbard dimer describes N bosons in an optical lattice of 2 sites.

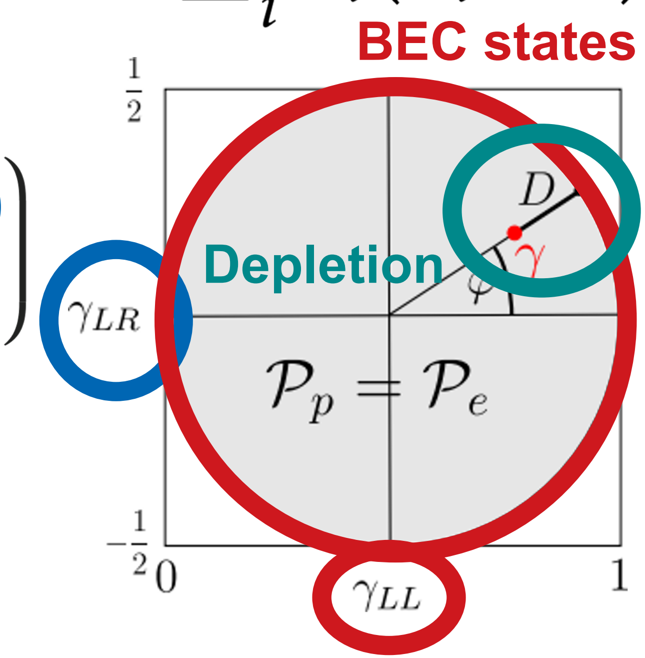
The Hamiltonian reads:

$$H = -t\left(b_L^\dagger b_R + b_R^\dagger b_L\right) + \sum_i v_i n_i + U \sum_i n_i(n_i - 1)$$



$$\gamma = \begin{pmatrix} \gamma_{LL} & \gamma_{LR} \\ \gamma_{LR} & N - \gamma_{LL} \end{pmatrix}$$

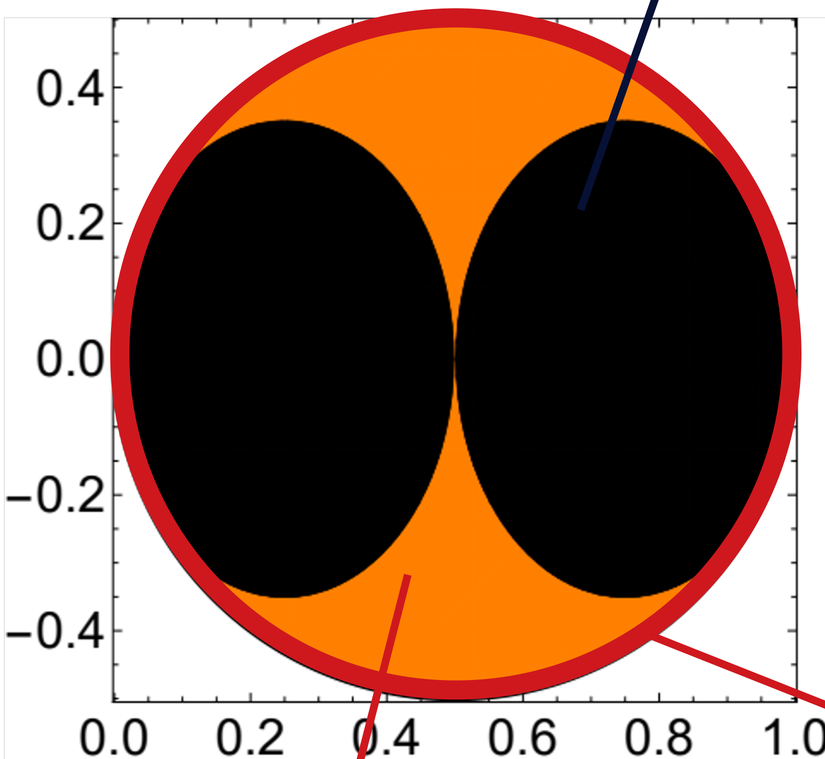
$$\gamma \succcurlyeq 0, \quad \mathrm{Tr}[\gamma] = 1$$

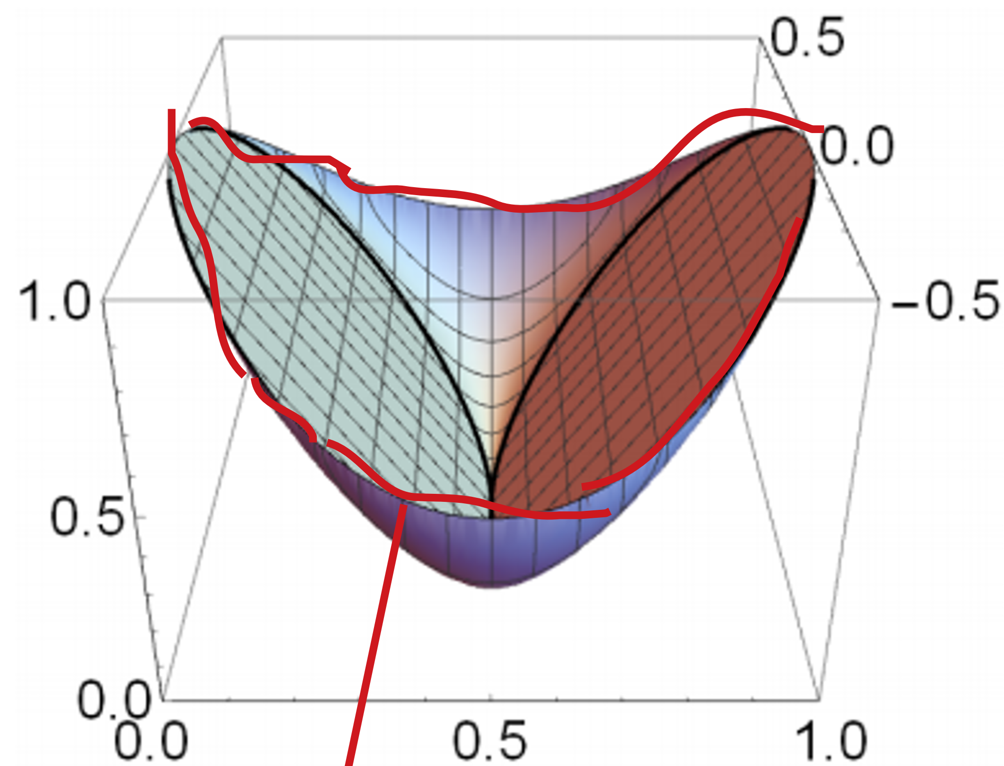


N = 2

non-ground states

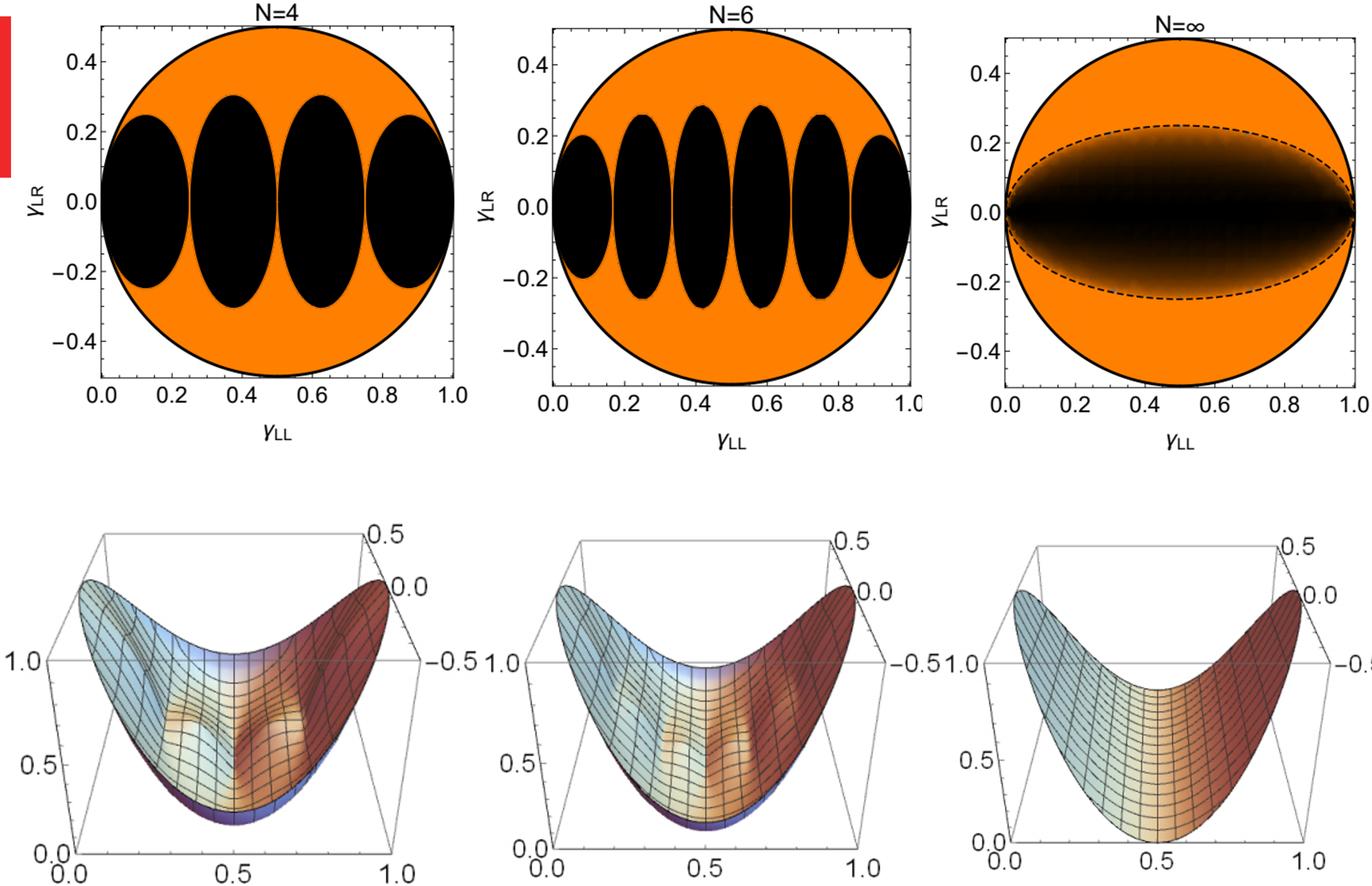
$\mathcal{F}[\gamma_{LL}, \gamma_{LR}]$





ground states

BEC states



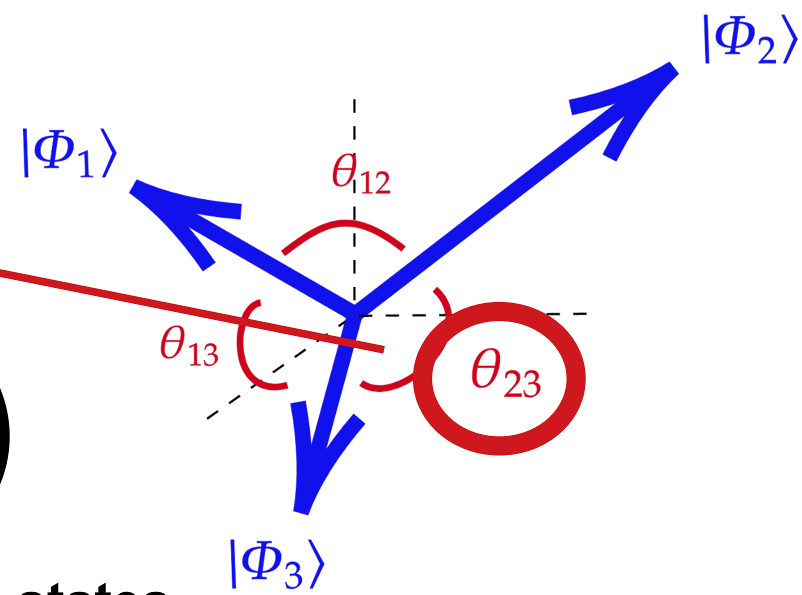
CLBR, J. Wolff, M. A. L. Marques, and C. Schilling, Phys Rev Lett **124**, 180603 (2020).

Machine-Learning Universal Functionals

Is it really possible to use this theory for ground states?

Yes!

$$\gamma_{ij} = \langle \Psi | b_i^\dagger b_j | \Psi \rangle$$



$$|\Phi_j\rangle = b_j|\Psi\rangle = \sum_v c_{j,v}|v\rangle$$

N-1 particle states

This is a Schmidt decomposition of 1 + (N-1) bosons!

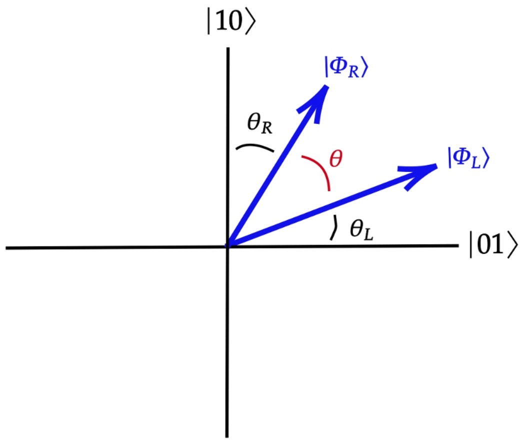
Trivialization map

$$c = U\Sigma V$$

Singular value decomposition!

$$\gamma = cc^{\dagger} = U\Sigma\Sigma^{\dagger}U^{\dagger}$$

$$\mathcal{F}[\gamma] = \min_{V\in SO(M)} \sum_{\alpha\beta} \sqrt{n_\alpha n_\beta}\Delta_{\alpha\beta}(U_\gamma, V)$$



Trivialization map: $\phi:\ \mathbb{R}^M \to SO(M)$

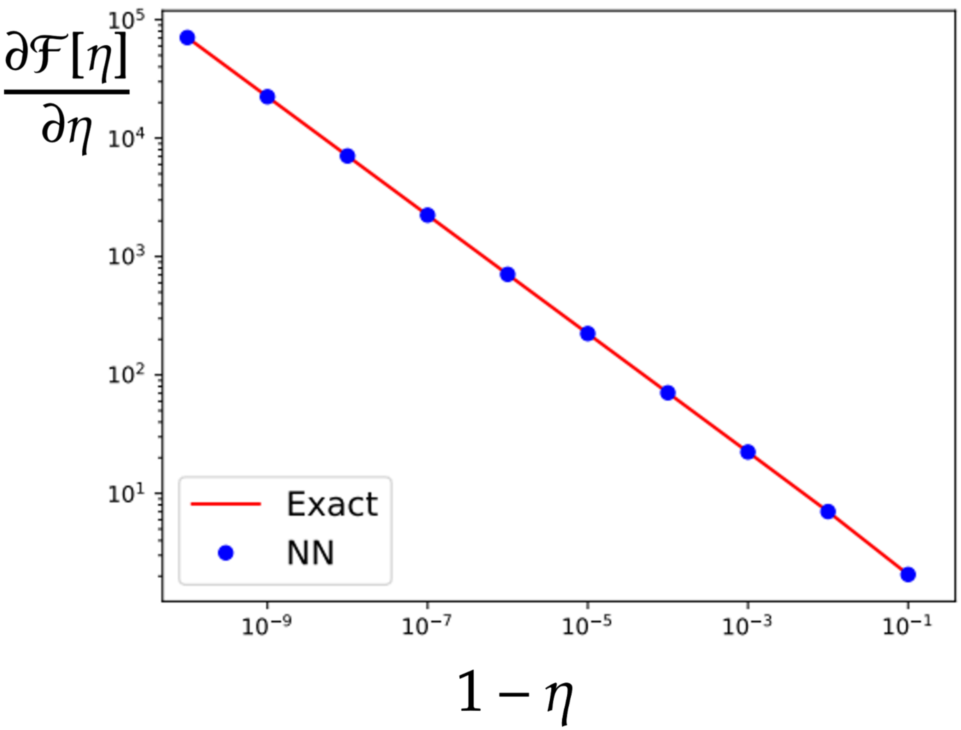
$$\mathcal{F}[\gamma] = \min_{y\in R^M} \sum_{\alpha\beta} \sqrt{n_\alpha n_\beta}\Delta_{\alpha\beta}(U_\gamma, \phi(y))$$

M. Lezcano-Casado, “Trivializations for gradient-based optimization on manifolds,” in Advances in Neural Information Processing Systems, NeurIPS (2019).

J. Siegel, “Accelerated Optimization with Orthogonality Constraints”, J. Comp. Math. **39** 207 (2021).

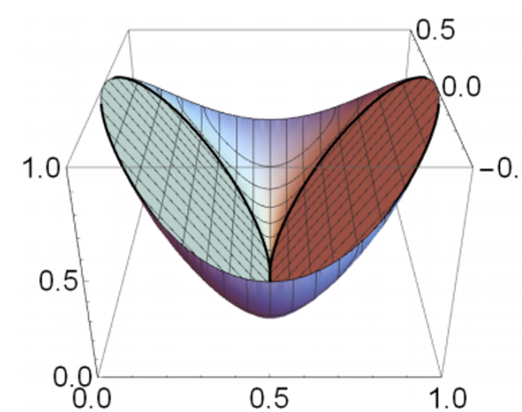
Bose-Hubbard dimer

We trained a fully connected neural network to output the matrix ***V*** using the PyTorch



$$\mathrm{FCNN}_{N,M,\theta}(\eta, \eta^2, \mathbf{US}) \to \mathrm{V} \to \mathcal{F}_{N,M,\theta}[\gamma]$$

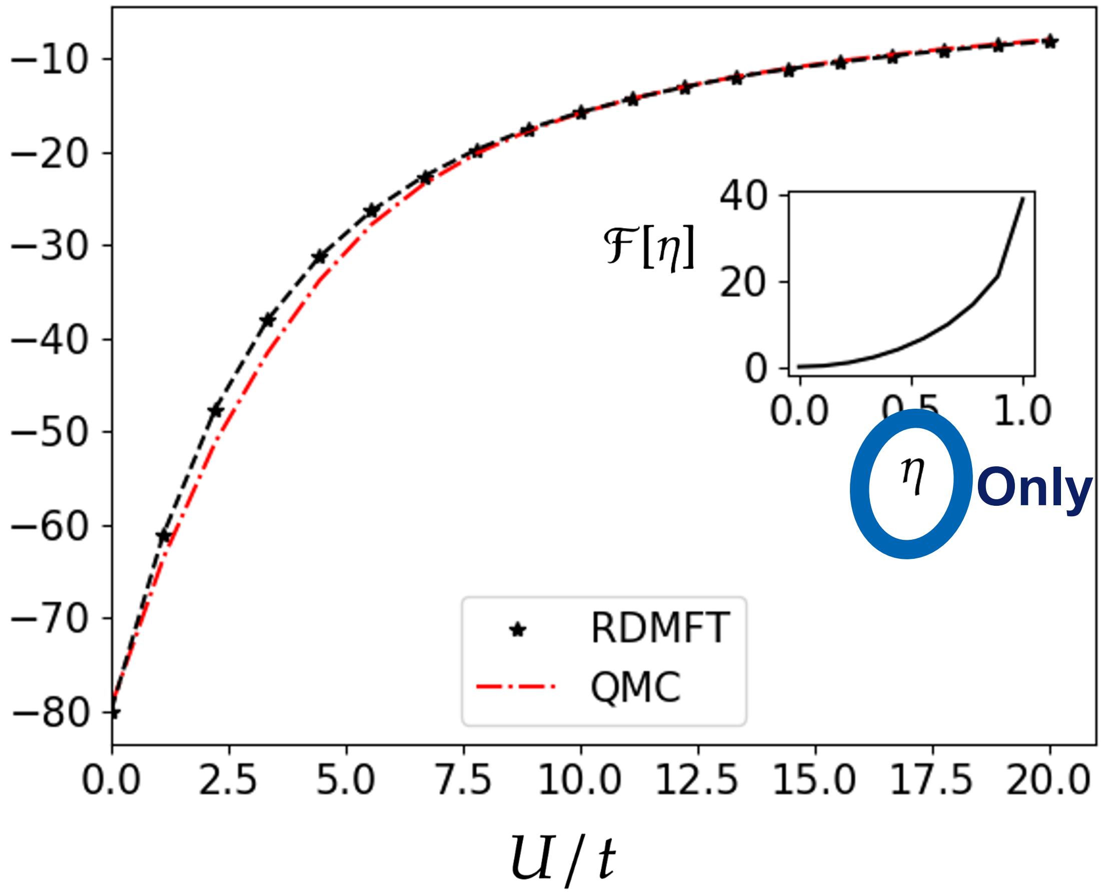
$$\eta = \langle b_i^\dagger b_{i+1} \rangle$$



J. Schmidt, M. Fadel, and **CLBR**, Phys Rev Research (Letter) **3**, L032063 (2021).

Bose-Hubbard Hamiltonian (N = 40, M = 40)

dim = 5 × 10^{22}



$$\eta = \langle b_i^\dagger b_{i+1} \rangle$$

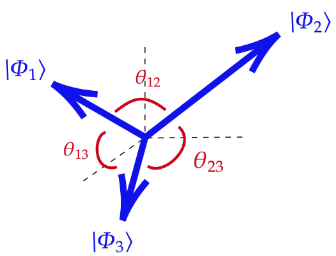
Only one parameter!

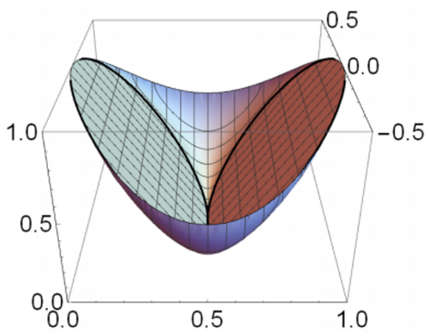
J. Schmidt, M. Fadel, and **CLBR**, Phys Rev Research (Letter) **3**, L032063 (2021).

Take-home messages

Based on a decomposition of γ, we have developed a method to design

$$\gamma_{ij} = \langle \Psi | b_i^\dagger b_j | \Psi \rangle$$





$$\mathrm{FCNN}_{N,M,\theta}(\eta, \eta^2, \mathrm{US}) \rightarrow \mathrm{V} \rightarrow \mathcal{F}_{N,M,\theta}[\gamma]$$

Many thanks!

“Bose Einstein force” I

At the border of the 1-RDM domain, the derivative of the universal funct

$$\nabla_\gamma \mathcal{F}[\gamma] \propto \frac{1}{\sqrt{N - N_{\mathrm{BEC}}}}$$

This is a **repulsive** “force” in the sense that it prevents the system to ful

It is **universal: it does not depend on the form of the external potentials.** As a con

CLBR, J. Wolff, M. A. L. Marques, and C. Schilling, Phys Rev Lett **124**, 180603 (2020).