
Machine Learning Universal Functionals

Trento, Italy, 12.10.22

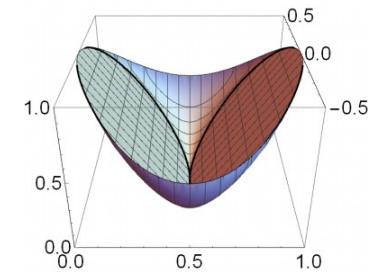
Joint with

Jonathan Schmidt (Halle), Johannes Gedeon (Hannover), Matt Hodgson (York),
Jack Wetherell (Palaiseau), Mateo Fadel (Zürich), and MAL Marques (Halle).

what?

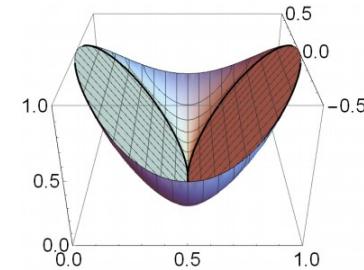
what?

$$\mathcal{F}(\gamma)$$



what?

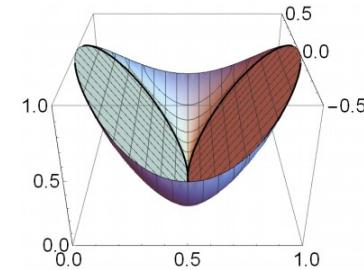
$$\mathcal{F}(\gamma)$$



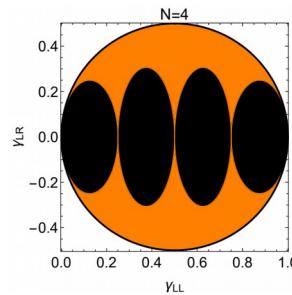
where?

what?

$$\mathcal{F}(\gamma)$$

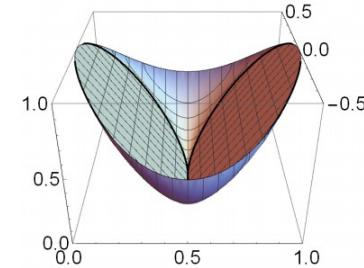


where?

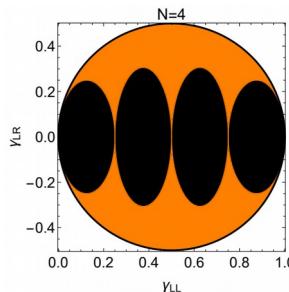


what?

$$\mathcal{F}(\gamma)$$



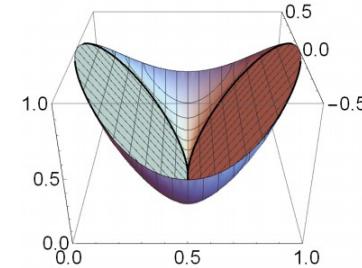
where?



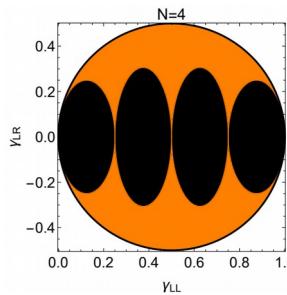
how?

what?

$$\mathcal{F}(\gamma)$$



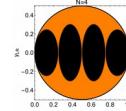
where?



how?

$$E(\hat{h}) = \min[\langle \hat{h}, \gamma \rangle + \mathcal{F}(\gamma)]$$

$$\gamma \in$$



1. ML DFT

2. ML the derivate discontinuity of DFT

3. ML 1-RDMFT

Hohenberg-Kohn map $v_{\text{ext}}(\vec{r}) \leftrightarrow n_{\text{gr}}(\vec{r})$

Kohn-Sham equations:

$$\left(-\frac{\nabla^2}{2} + v_s(\vec{r}) \right) \phi_i(\vec{r}) = \epsilon_i \phi_i(\vec{r})$$

Hohenberg-Kohn map $v_{\text{ext}}(\vec{r}) \leftrightarrow n_{\text{gr}}(\vec{r})$

Kohn-Sham equations:

$$\left(-\frac{\nabla^2}{2} + v_s(\vec{r}) \right) \phi_i(\vec{r}) = \epsilon_i \phi_i(\vec{r})$$

$$v_s(\vec{r}) = v_{\text{ext}}(\vec{r}) + v_{\text{H}}(\vec{r}) + v_{\text{xc}}(\vec{r})$$

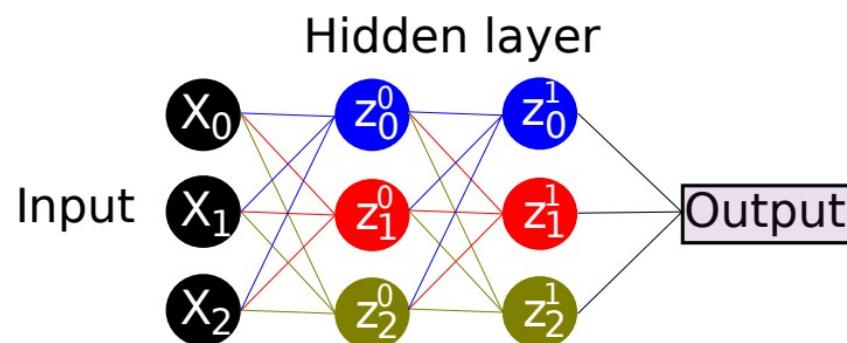
$$v_{\text{xc}}(\vec{r}) = \frac{\delta E_{\text{xc}}}{\delta n(\vec{r})}$$

ML approaches to DFT

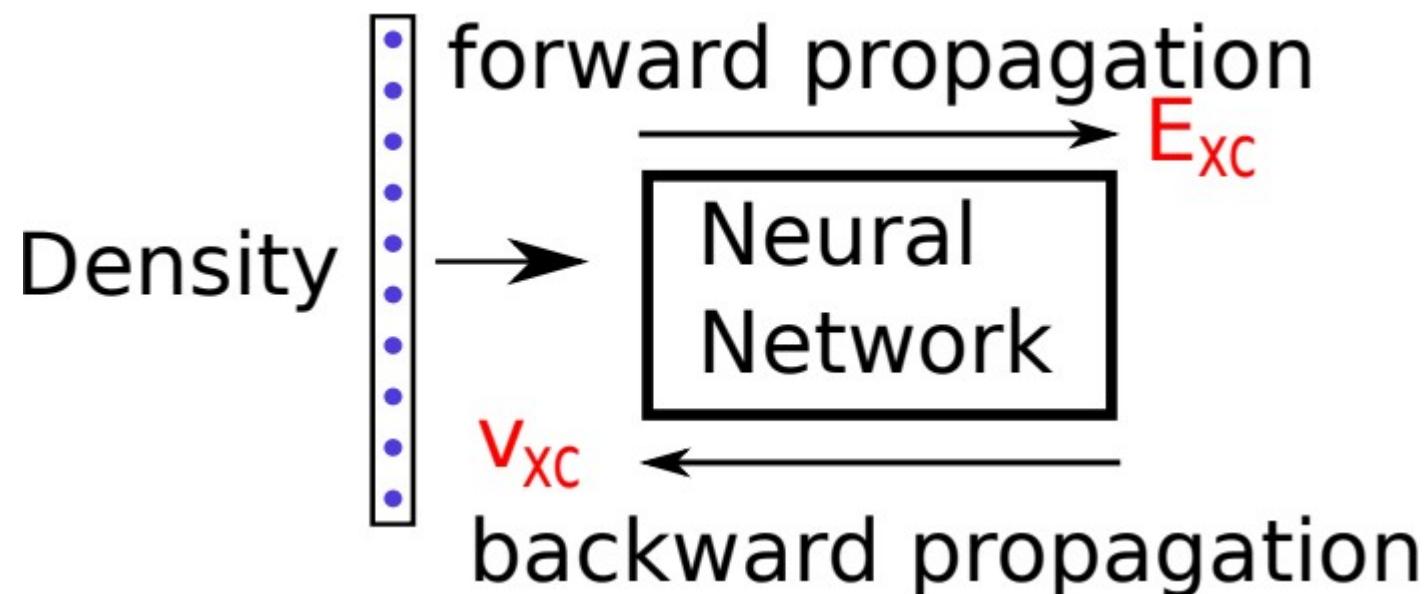
Learning strong non-local functionals

Learn the exchange correlation potential

Learning the non-interacting kinetic energy functional

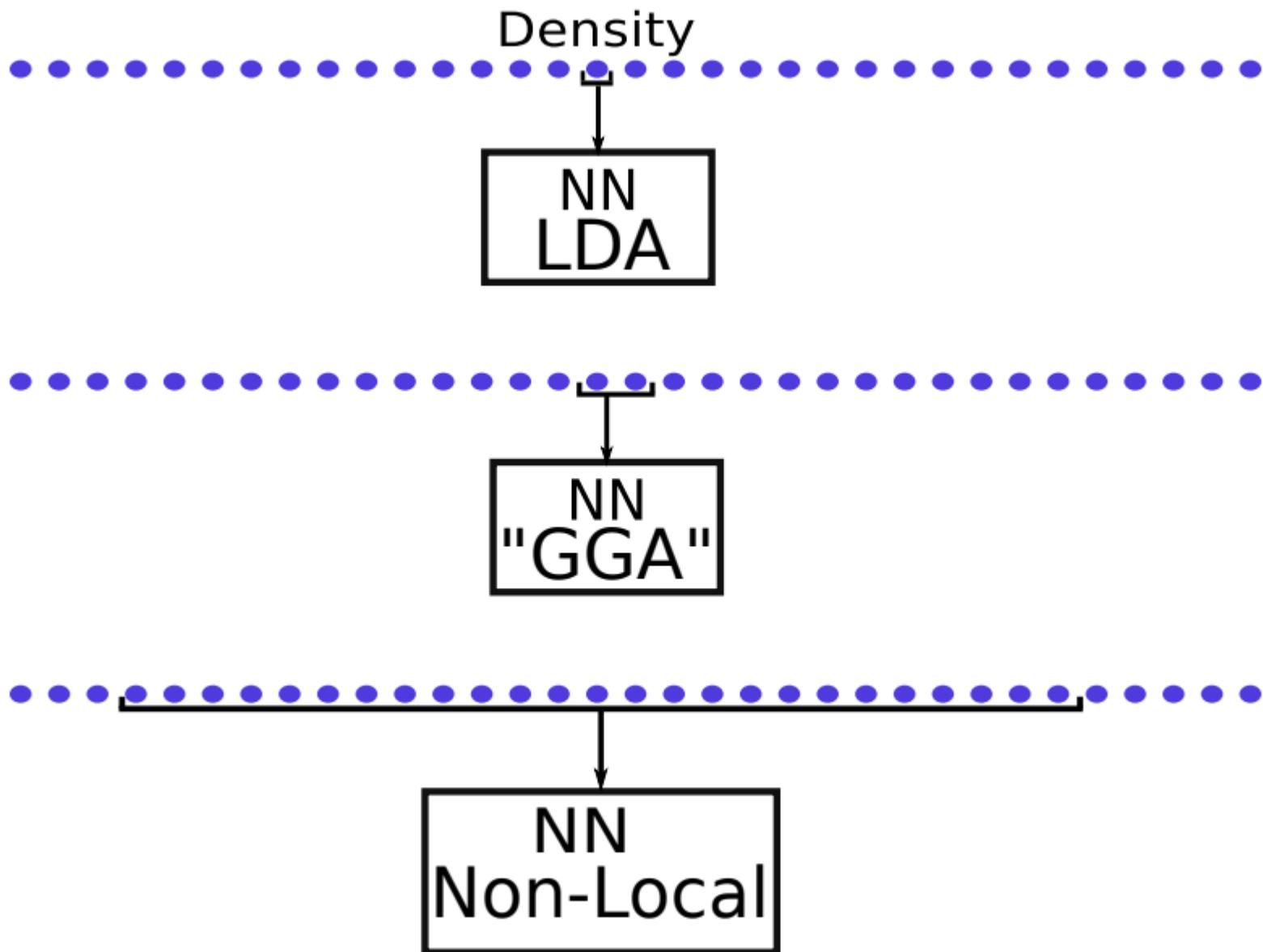


ML the physical non-local xc functional of DFT



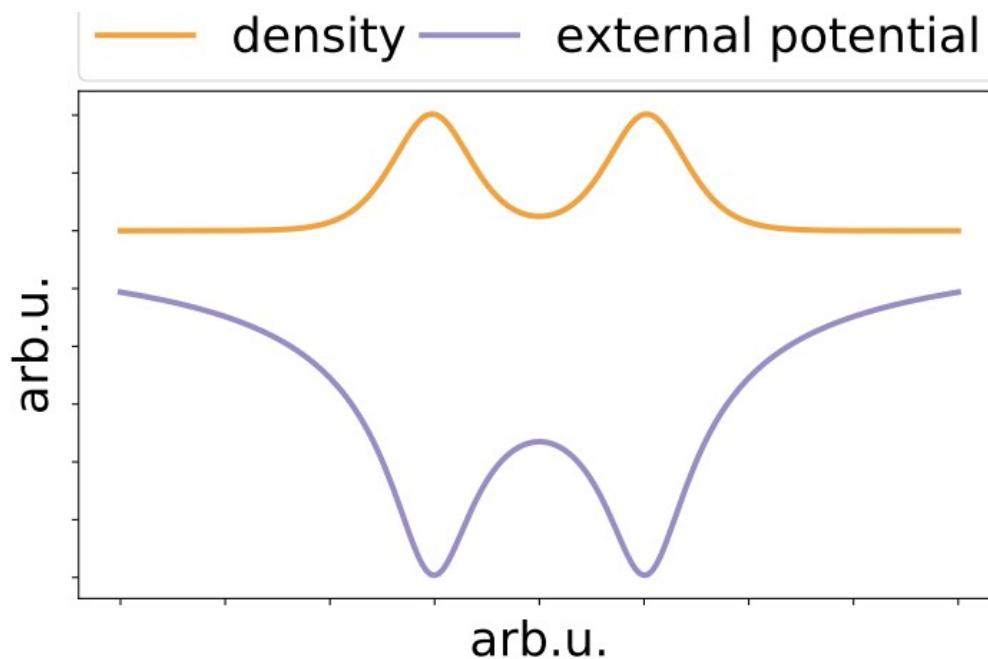
J Schmidt, **CLBR**, and MAL Marques, JCPL 2019

Locality



Data and loss function

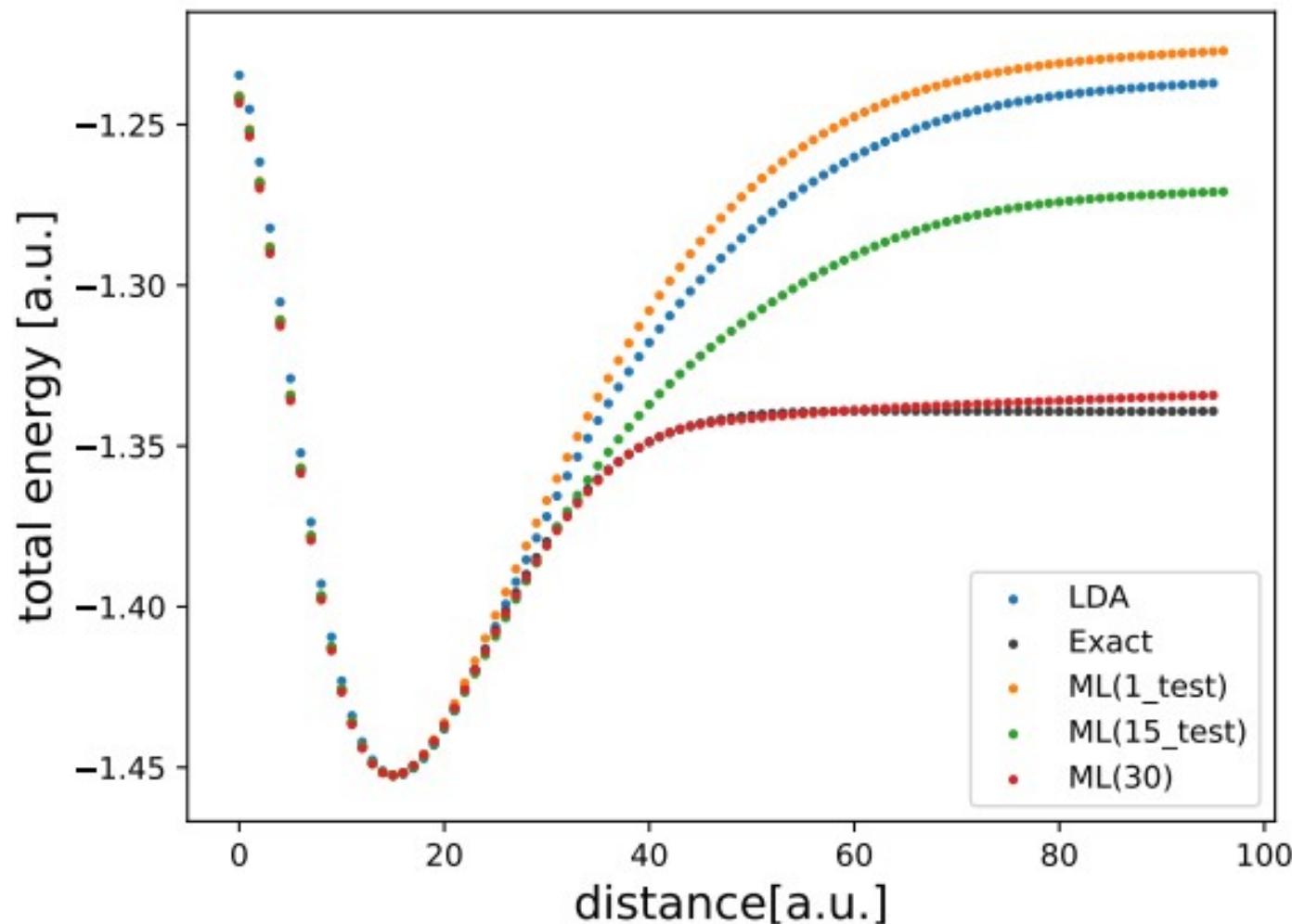
- Exact calculations with 2 electrons in randomized 1D-external potentials
- Inversion of the Kohn-Sham system leads to E_{xc} and v_{xc} which is used for training



loss function

$$L(\theta, n_i) = \alpha \text{MSE}(E_{xc}) + \beta \text{MSE}(v_{xc}) + \gamma \text{MSE}\left(\frac{dv_{xc}(r)}{dr}\right) + \delta \text{MSE}\left(E_{xc} - \int v_{xc}(r)n(r)dr\right)$$

H₂ dissociation



Inserting exact conditions

ML-DFT functionals are mostly trained in Hilbert spaces with **integer N** unable to reproduce the derivative discontinuity of the xc functional (crucial to describe electronic bandgaps or charge-transfer excitations).

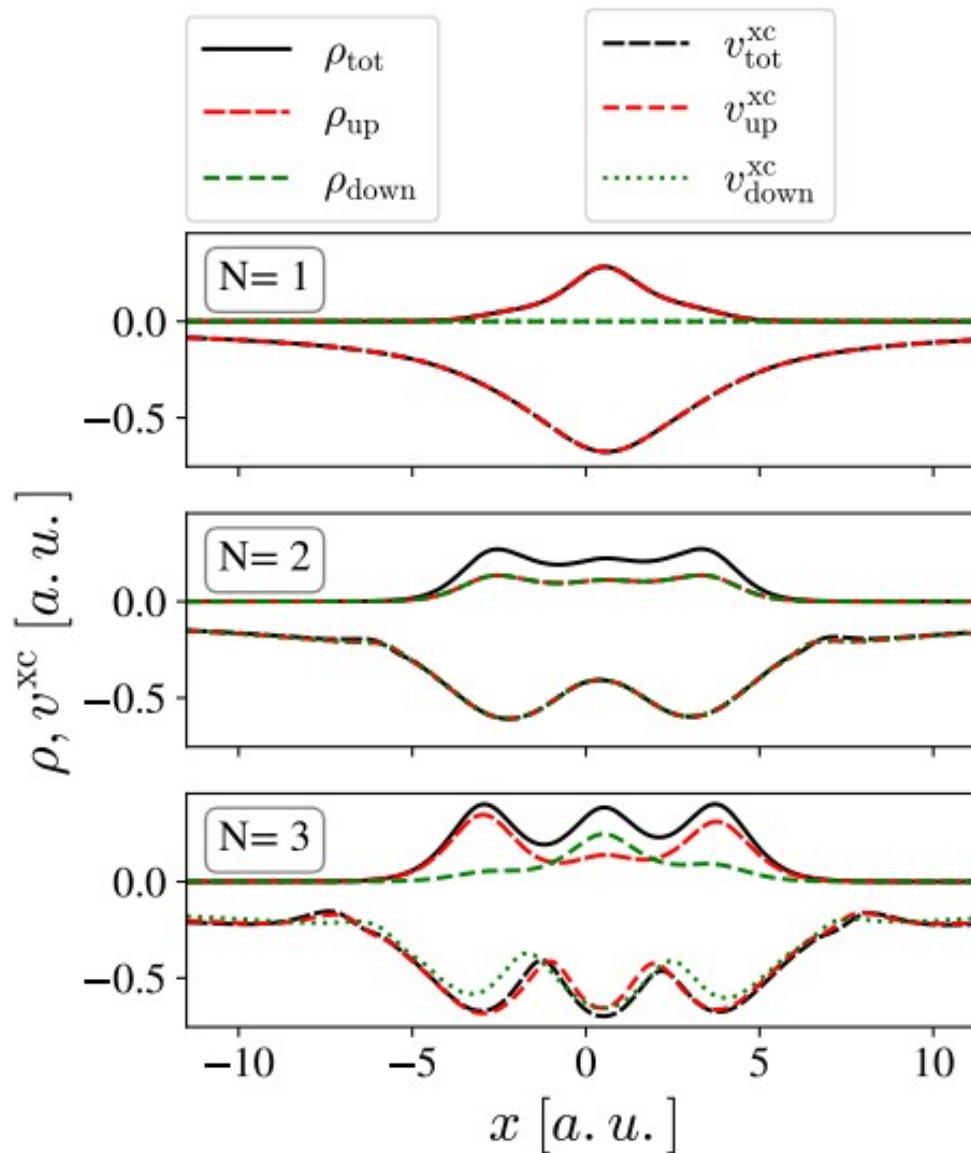
Inserting exact conditions

ML-DFT functionals are mostly trained in Hilbert spaces with **integer N** unable to reproduce the derivative discontinuity of the xc functional (crucial to describe electronic bandgaps or charge-transfer excitations).

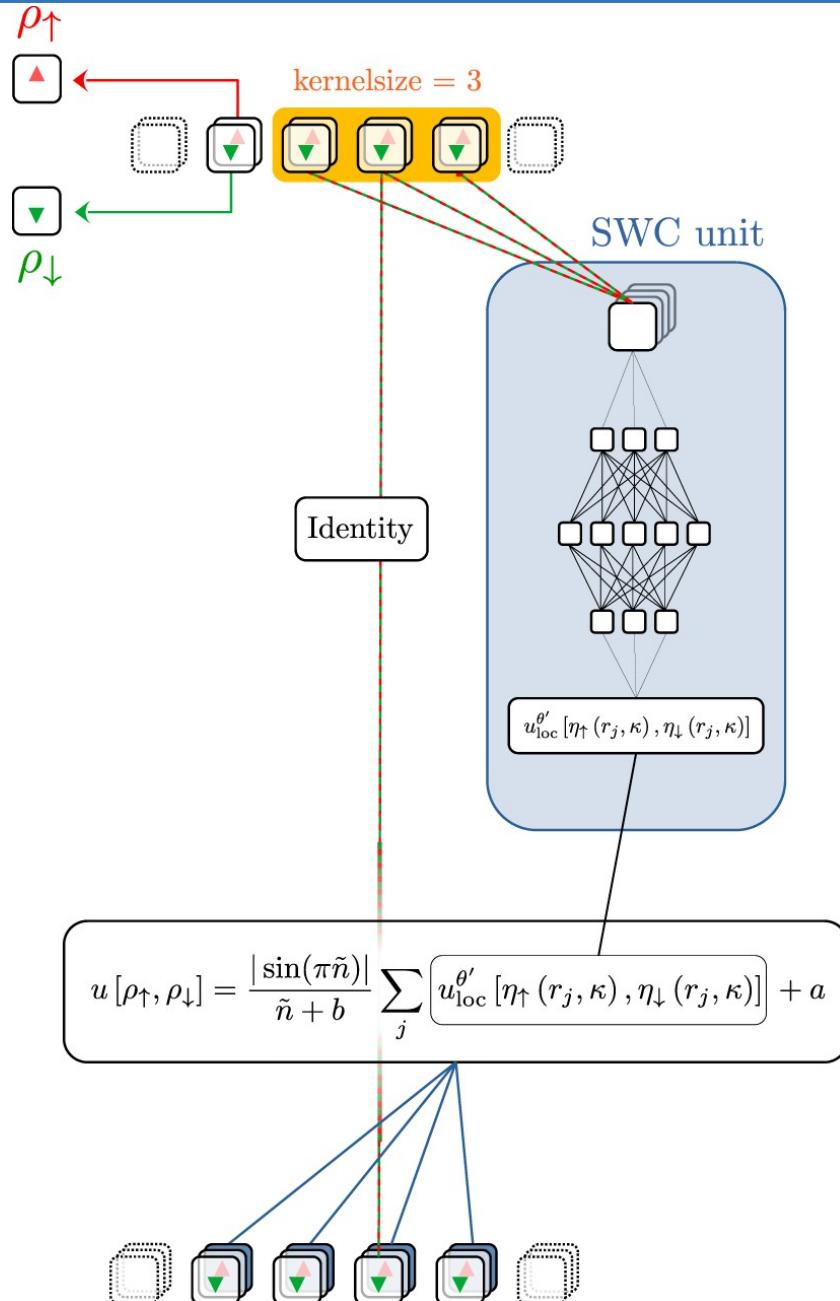
$$n_{N+\epsilon}(\vec{r}) = (1 - \epsilon)n_N + \epsilon n_{N+1}(\vec{r})$$

$$E(N + \epsilon) = (1 - \epsilon)E(N) + \epsilon E(N + 1)$$

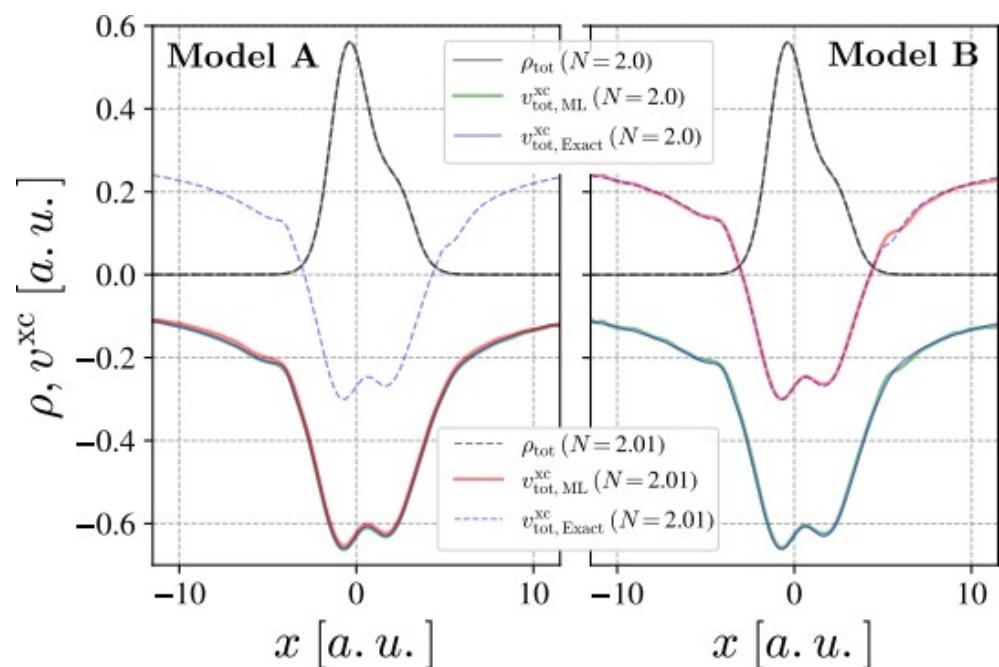
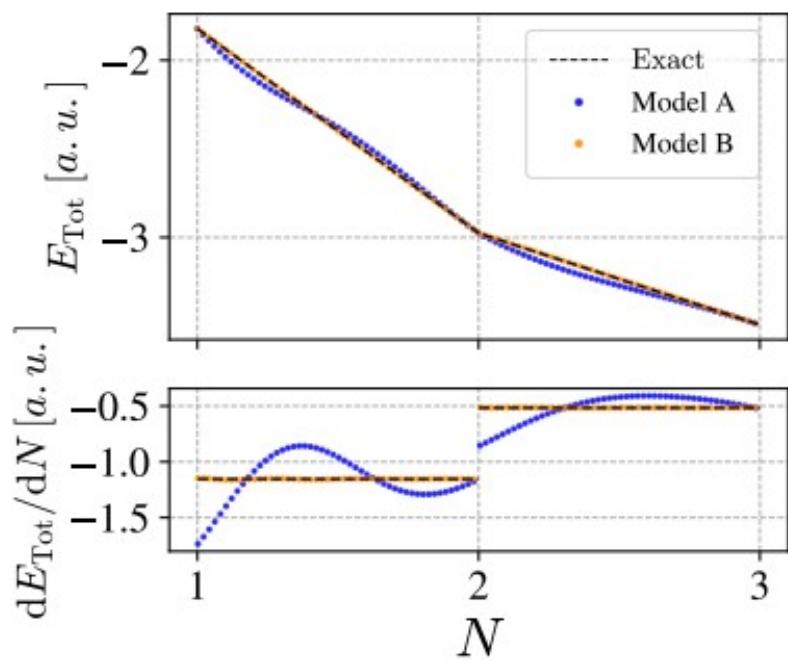
Training with fractional number of electrons



Training with fractional number of electrons

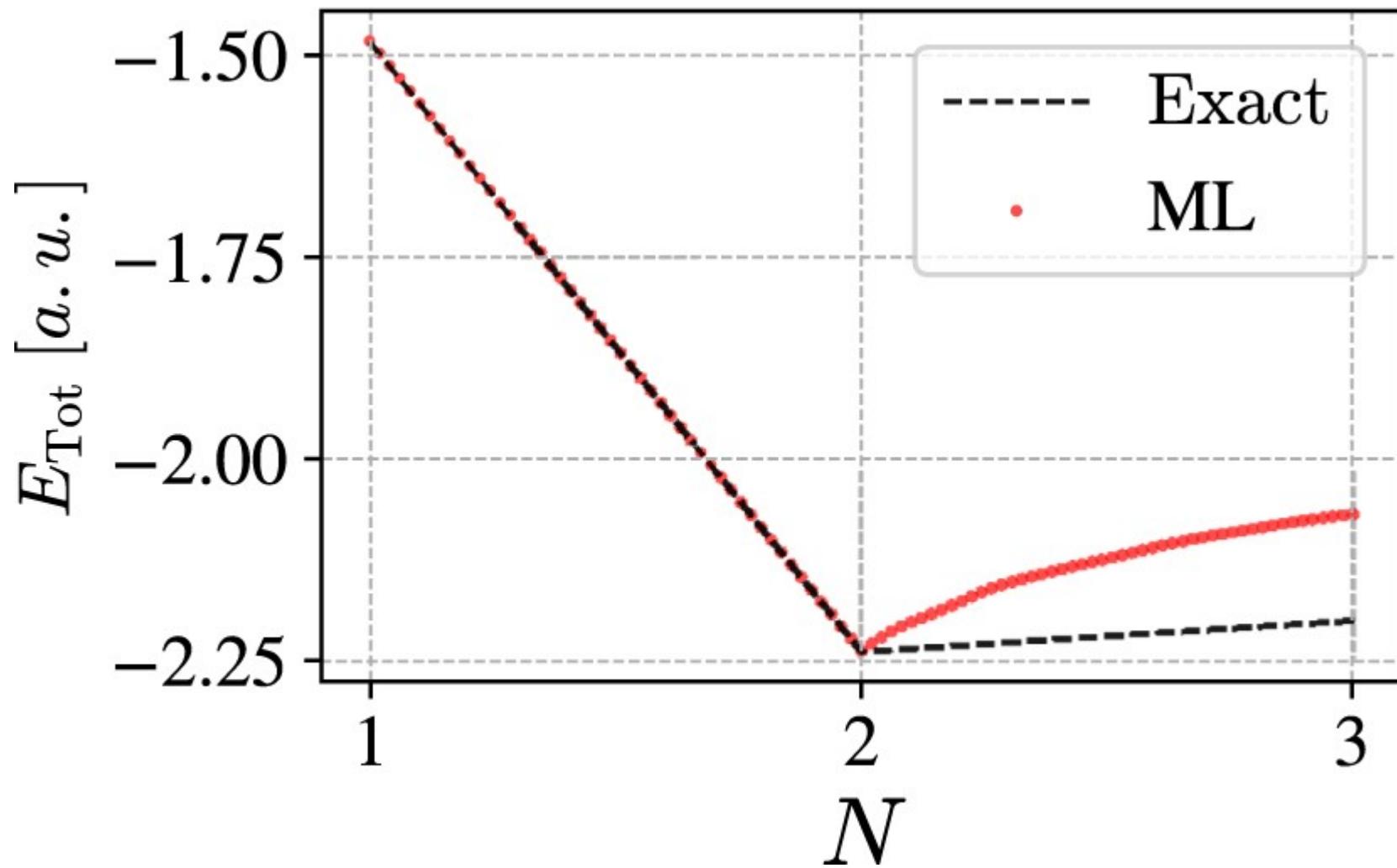


ML the derivative discontinuity of DFT



J Gedeon, J Schmidt, M Hodgson, J Wetherell, **CLBR**, and MAL Marques, MLST 2022

ML the derivative discontinuity of Helium



J Gedeon, J Schmidt, M Hodgson, J Wetherell, **CLBR**, and MAL Marques, MLST 2022

Bose-Hubbard model

$$\hat{H} = -t \sum_j (b_j^\dagger b_{j+1} + b_{j+1}^\dagger b_j) + U \sum_j n_j(n_j - 1)$$

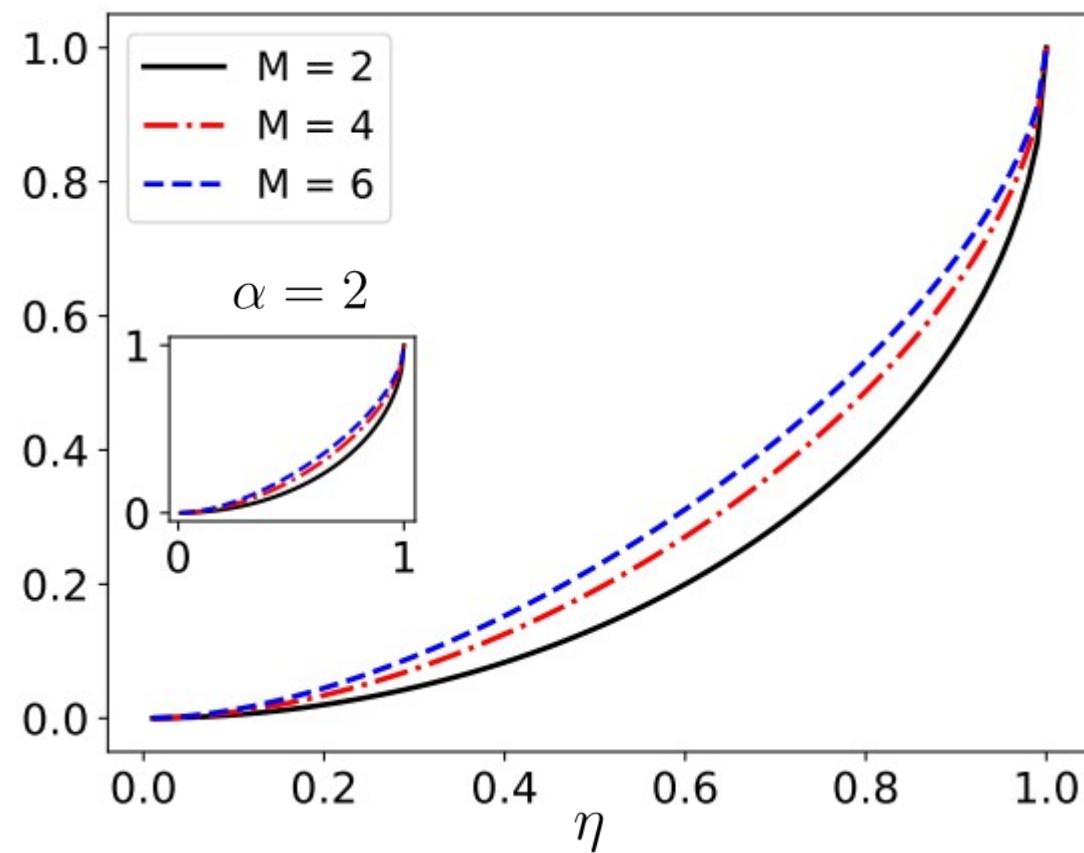
Bose-Hubbard model

$$\hat{H} = -t \sum_j (b_j^\dagger b_{j+1} + b_{j+1}^\dagger b_j) + U \sum_j n_j(n_j - 1)$$

$$\eta = \langle b_j^\dagger b_{j+1} \rangle$$

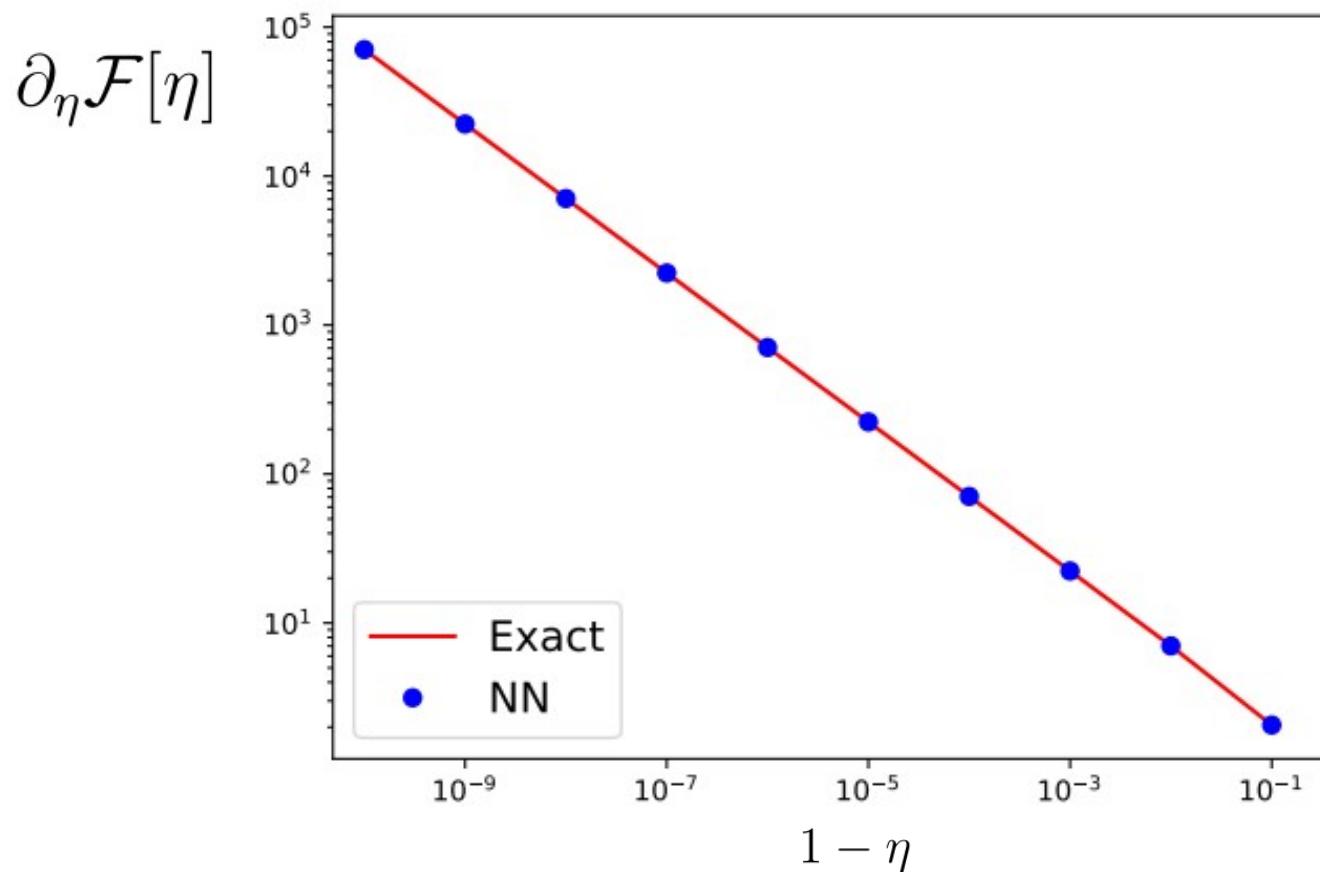
$$\alpha = 1$$

$$\alpha = \langle b_j^\dagger b_j \rangle$$



Universal bosonic functionals

$$\eta, US, N, M \rightarrow \mathcal{F}_{N,M,\theta}[\gamma]$$



J Schmidt, M Fadel, and CLBR, PRR 2021

Universal bosonic functionals

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

J Schmidt, M Fadel, and **CLBR**, PRR 2021

Universal bosonic functionals

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

J Schmidt, M Fadel, and **CLBR**, PRR 2021

Universal bosonic functionals

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

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

J Schmidt, M Fadel, and **CLBR**, PRR 2021

Universal bosonic functionals

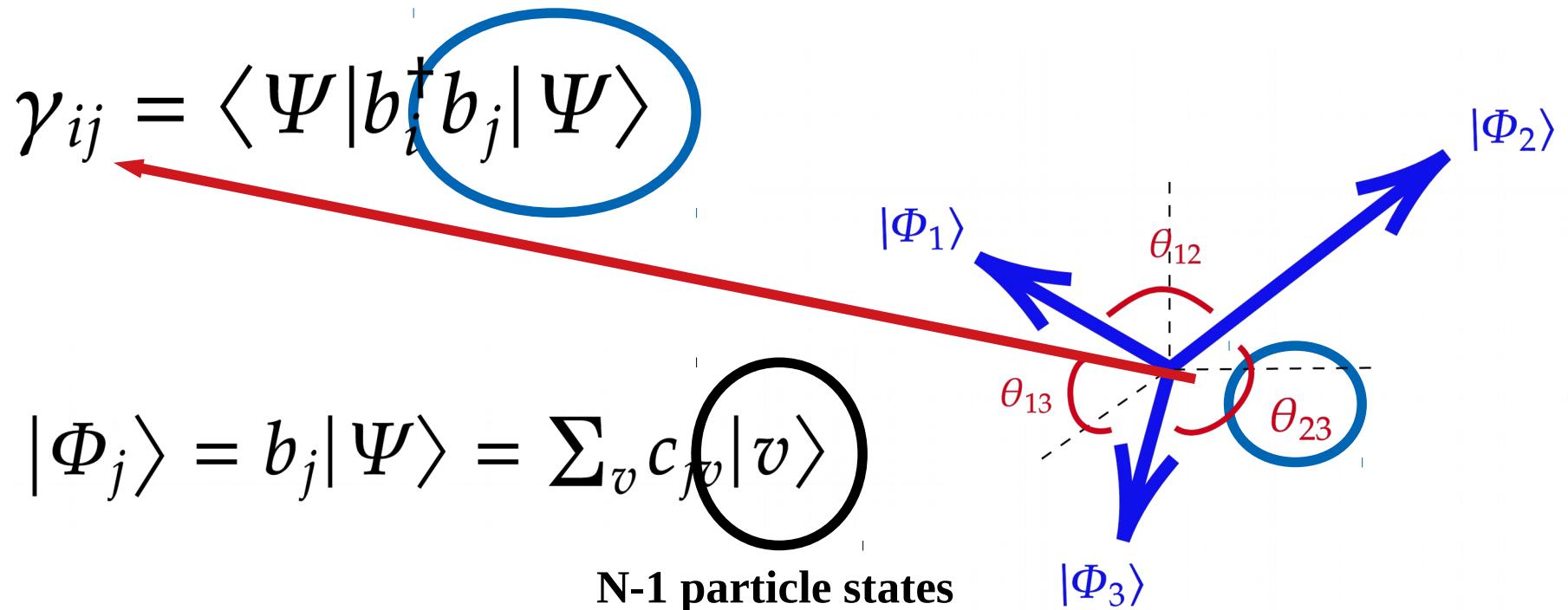
$$\gamma_{ij} = \langle \Psi | b_i^\dagger b_j | \Psi \rangle$$

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

N-1 particle states

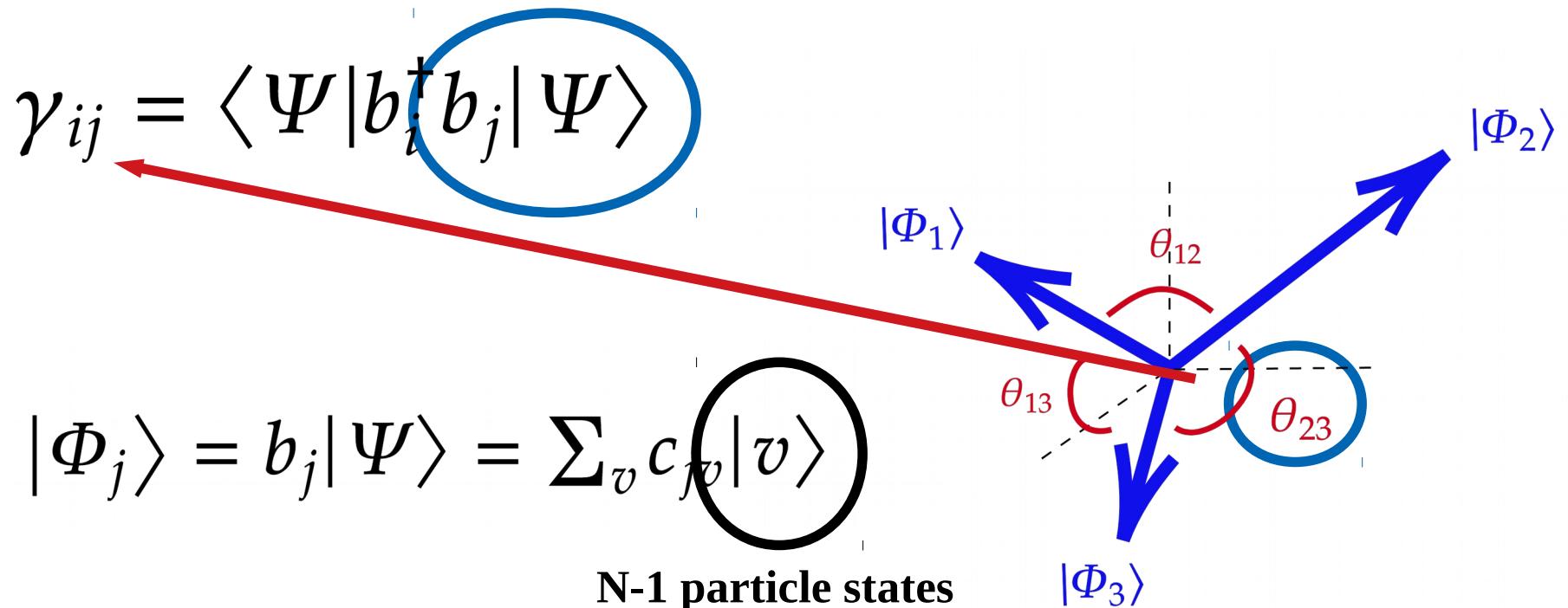
J Schmidt, M Fadel, and **CLBR**, PRR 2021

Universal bosonic functionals



J Schmidt, M Fadel, and CLBR, PRR 2021

Universal bosonic functionals

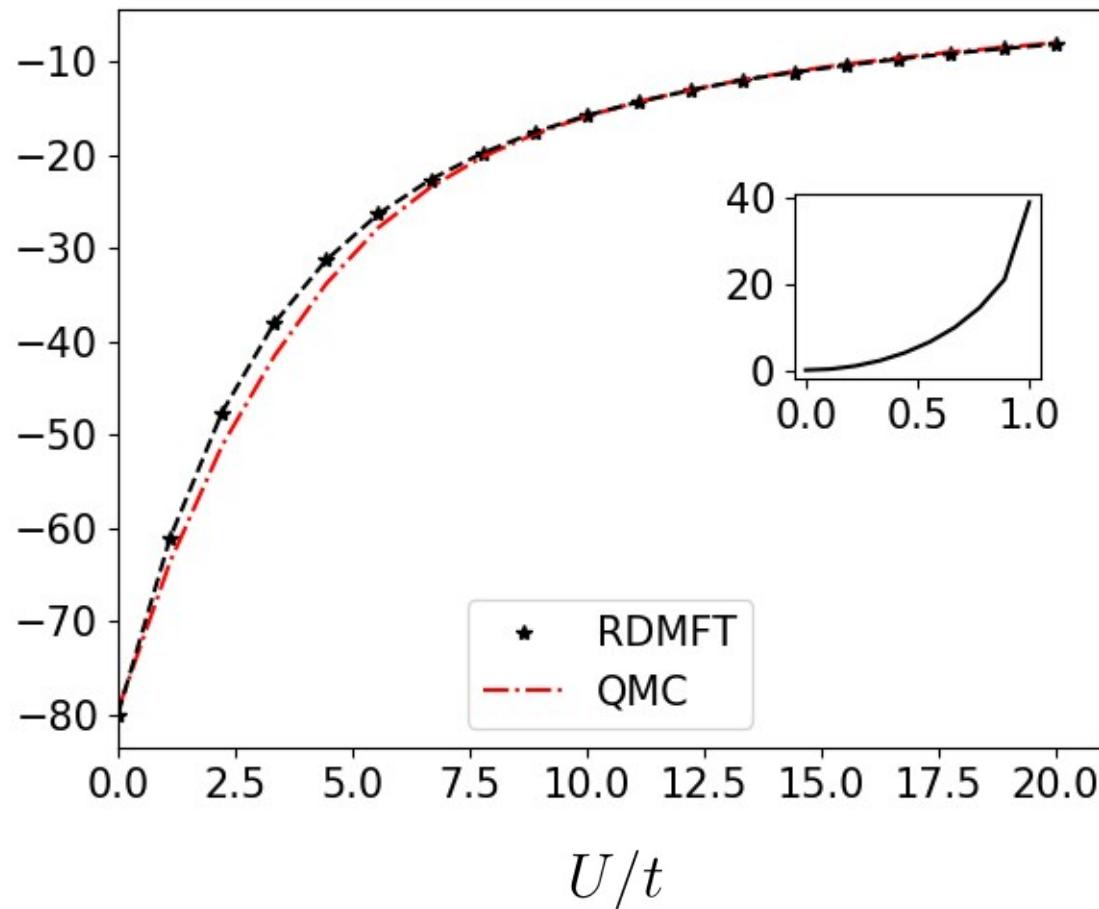


$$c = U\Sigma V$$

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

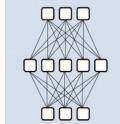
$$\mathcal{F}[\gamma] = \min_{V \in SO(M)} \sum_{\alpha\beta} \sqrt{n_\alpha n_\beta} \Delta_{\alpha\beta}(U_\gamma, V)$$

J Schmidt, M Fadel, and CLBR, PRR 2021



J Schmidt, M Fadel, and CLBR, PRR 2021

Outlook



machine learning universal 1-RDMFT functionals

$$\mathcal{F}_\theta(\gamma)$$

MAX PLANCK
GESELLSCHAFT

