Conditional generative adversarial networks for quatum many-body systems

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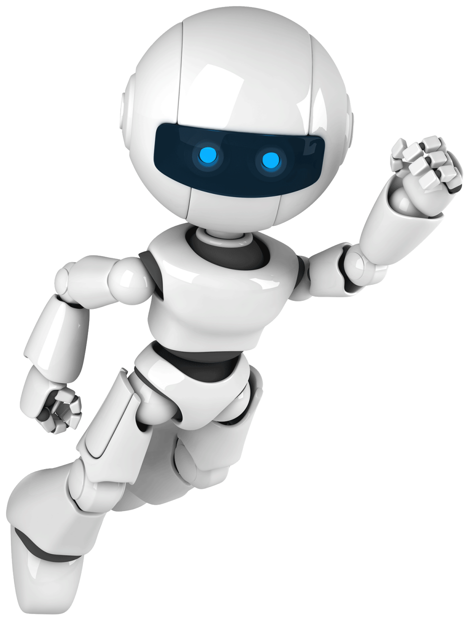
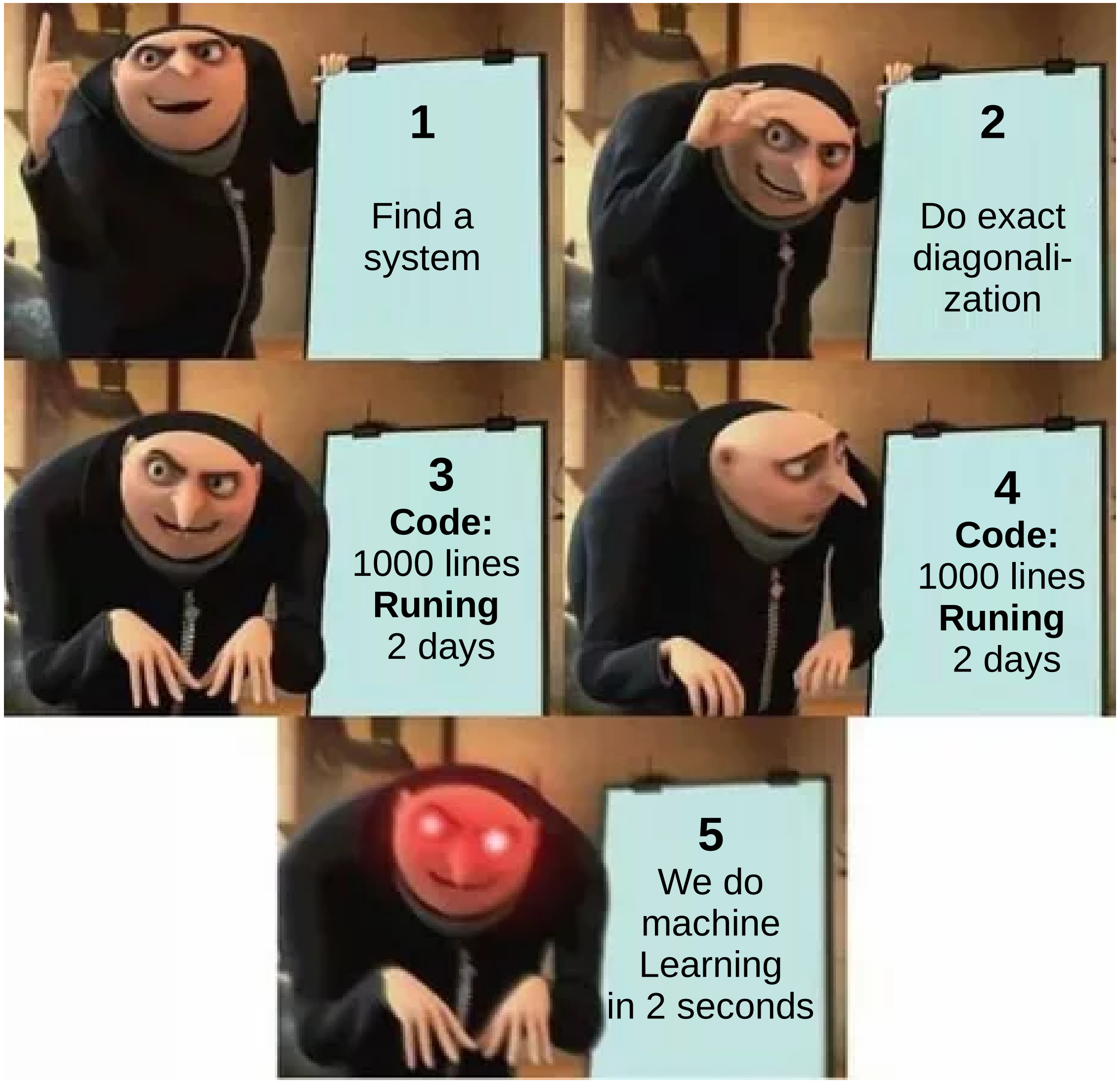
Summary

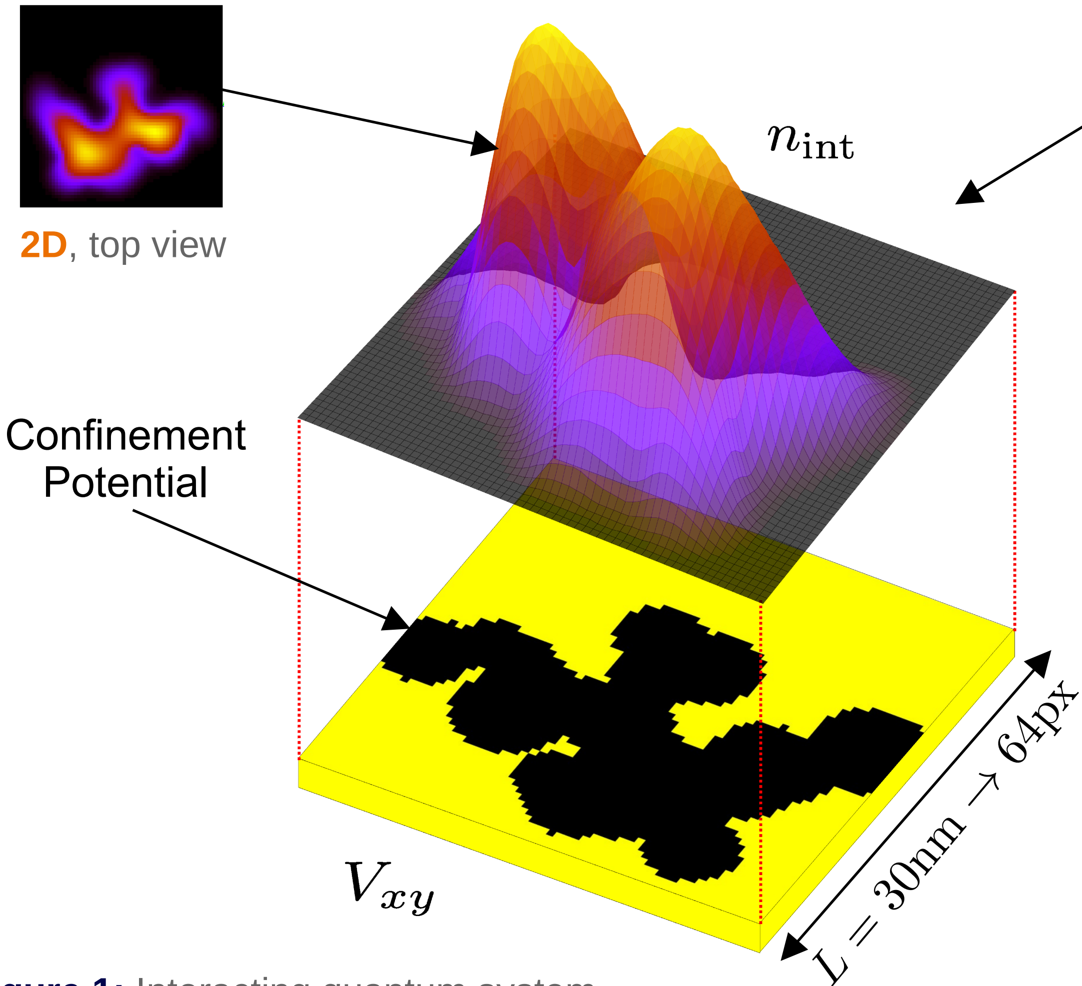
- Motivation
- Model system
- Many-body formalism
- Exact Diagonalization (**ED**)
- Machine Learning (**ML**)
- Results



Motivation


1
Find a system
2
Do exact diagonali-zation
3
Code:
1000 lines
Runing
2 days
4
Code:
1000 lines
Runing
2 days
5
We do machine Learning in 2 seconds

Model system



$V_s = 0.5eV$

$V_0 = 0eV$

$N = 2$

$N_{QW} = 25$

$\frac{L}{16} < R < \frac{L}{8}$

$A_{N_{\max}} = \frac{3}{4}$

$A_{\max} = 80\%$

Figure 1: Interacting quantum system

Ex: two-dimensional self-assembled functionalized graphene QDs

Many-body formalism

- **Hamiltonian in Second Quantization**

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\text{int}} = \sum_a \epsilon_a c_a^\dagger c_a + \frac{1}{2}\sum_{abcd} V_{abcd} c_a^\dagger c_b^\dagger c_d c_c$$

- **Single particle solution**

$$|\Phi_a\rangle = \sum_{\sigma_z} \phi_{a,\sigma_z}(\mathbf{r})|\sigma_z\rangle$$

- **Coulomb Potential**

$$V_C(\mathbf{r}-\mathbf{r}') = \frac{1}{4\pi\varepsilon_0\varepsilon_r}\frac{e^2}{|\mathbf{r}-\mathbf{r}'|}$$

- **Matrix Elements of Coulomb Potential**

$$V_{abcd} = \langle \phi_a(\mathbf{r})\phi_b(\mathbf{r}')|V_C(\mathbf{r}-\mathbf{r}')|\phi_c(\mathbf{r})\phi_d(\mathbf{r}')\rangle$$

$$= \int d\mathbf{r} \int d\mathbf{r}' \sum_{\sigma_z,\sigma_z'} \phi^*_{a,\sigma_z}(\mathbf{r})\phi^*_{b,\sigma_z'}(\mathbf{r}')\frac{1}{4\pi\varepsilon_0\varepsilon_r}\frac{e^2}{|\mathbf{r}-\mathbf{r}'|}\phi_{c,\sigma_z}(\mathbf{r})\phi_{d,\sigma_z'}(\mathbf{r}')$$

Exact Diagonalization ED

- **Single particle Hamiltonian**

$$\mathcal{H}_0\Phi_a(x,y) = \epsilon_a\Phi_a(x,y)$$

- **Occupation number representation**

$$|\psi_k\rangle = |n_1^{(k)}, n_2^{(k)}, ..., n_s^{(k)}, ...\rangle$$

- **Schrodinger equation**

$$\mathcal{H}\Psi_n = E_n\Psi_n$$

$$\Psi_n \equiv \Psi_n(\mathbf{r}_1\sigma_{z_1}, ..., \mathbf{r}_n\sigma_{z_n})$$

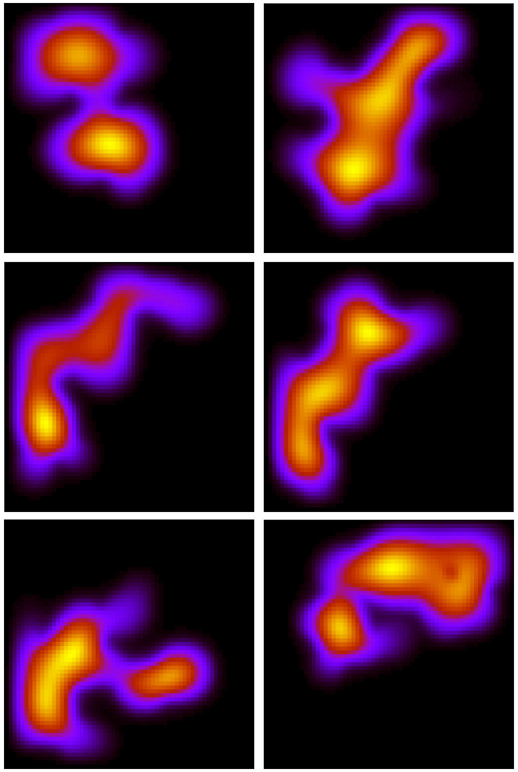


Figure 2: Computed interacting ground state charge densities

Exact Diagonalization **ED**

- **Charge density**

$$\bar{\rho}_n(\mathbf{r}) = \sum_k |C_{nk}|^2 \sum_{p=1}^{N} [|\phi_{i_p,\uparrow}|^2 + |\phi_{i_p,\downarrow}|^2]$$

- **Spin density**

$$\bar{\sigma}_{z,n}(\mathbf{r}) = \sum_k |C_{nk}|^2 \sum_{p=1}^{N} [|\phi_{i_p,\uparrow}|^2 - |\phi_{i_p,\downarrow}|^2]$$

- **Ground State**

$n = 0$

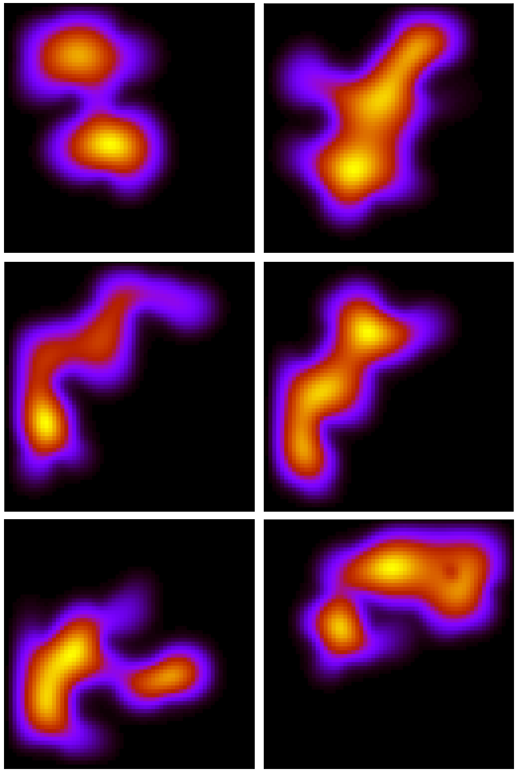
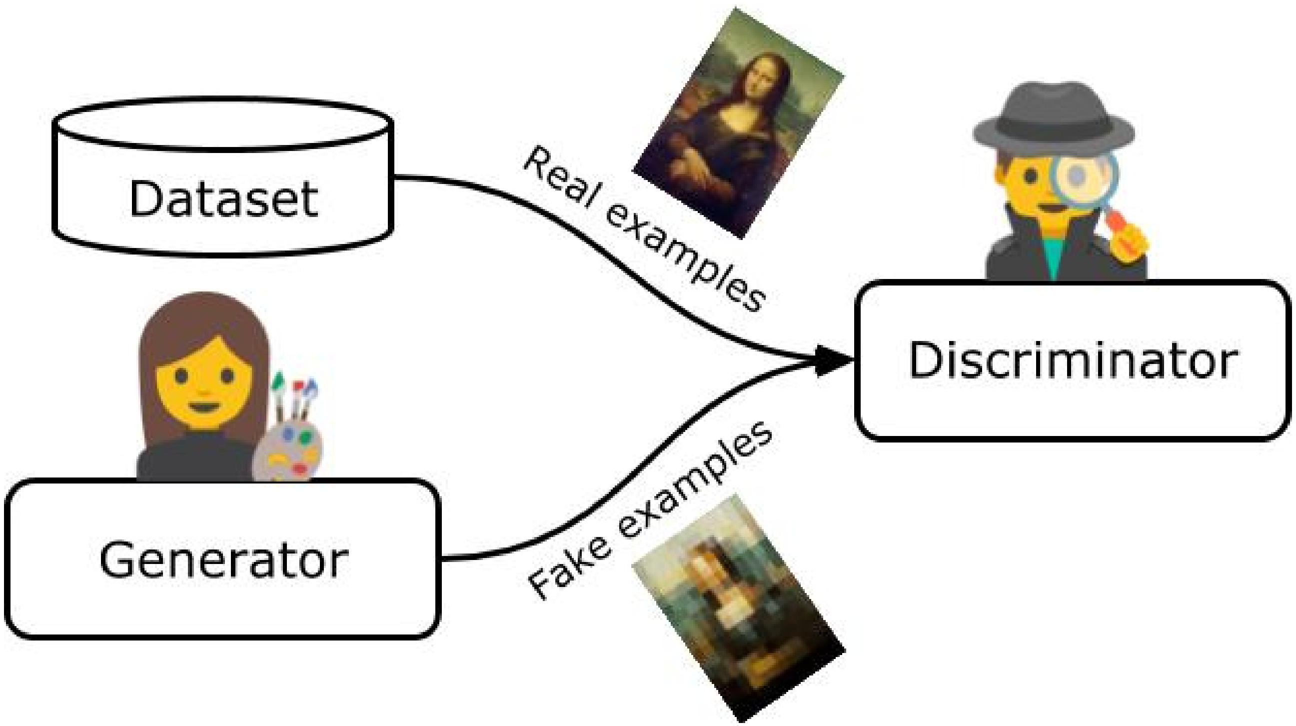


Figure 2: Computed interacting ground state charge densities

Machine Learning **ML**

Figure 3: Mapping confinement potential to interacting and non-interacting charge densities, investigating the inverse problem as well.

Generative Adversarial Neural Networks **GANs**



Main Results

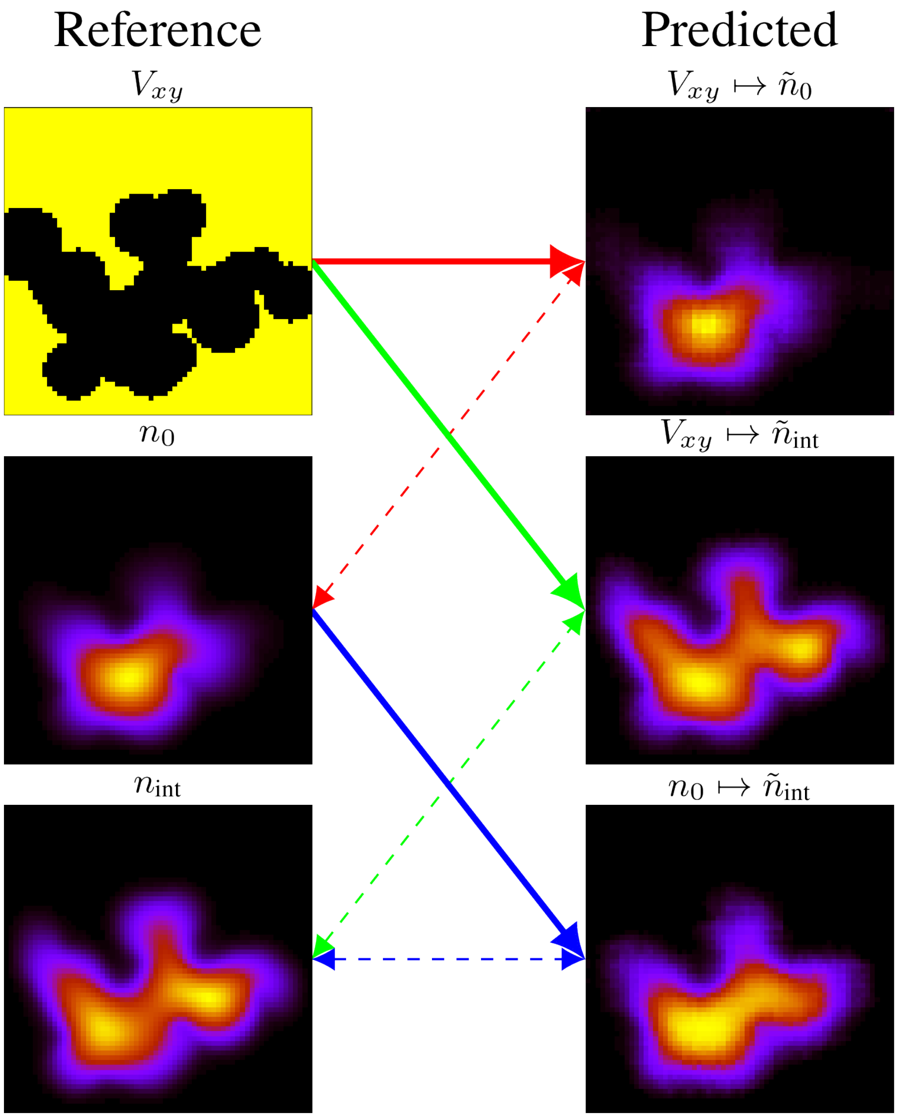


Figure 4: Mapping confinement potential to interacting and non-interacting charge densities. A mapping from non interacting to interacting is performed as well.

Main Results

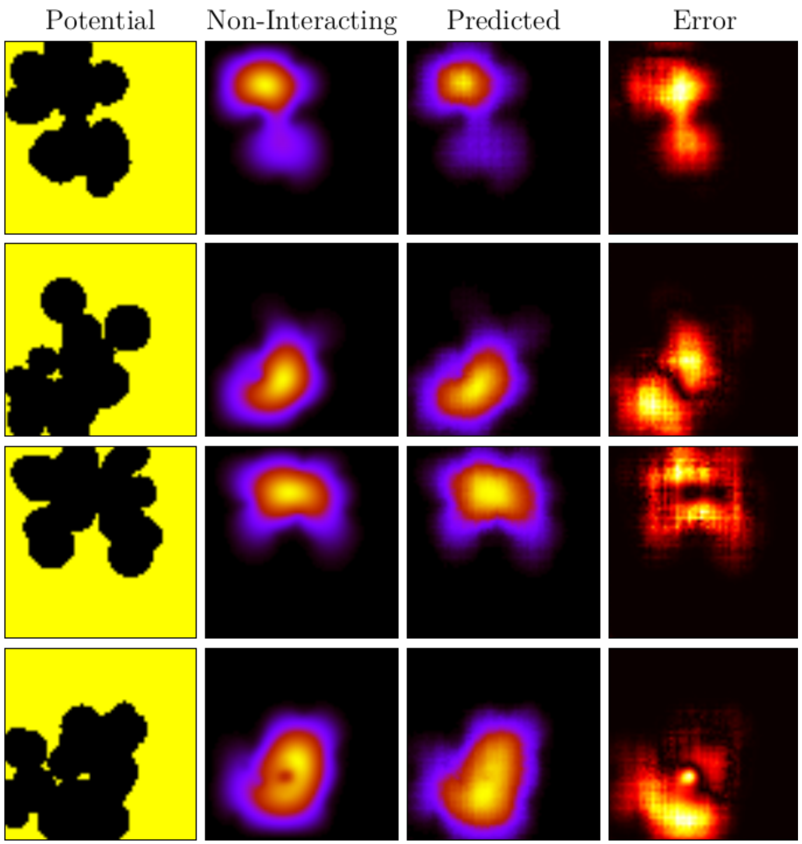


Figure 5: Mapping confinement potentials to **non-interacting** ground state charge densities

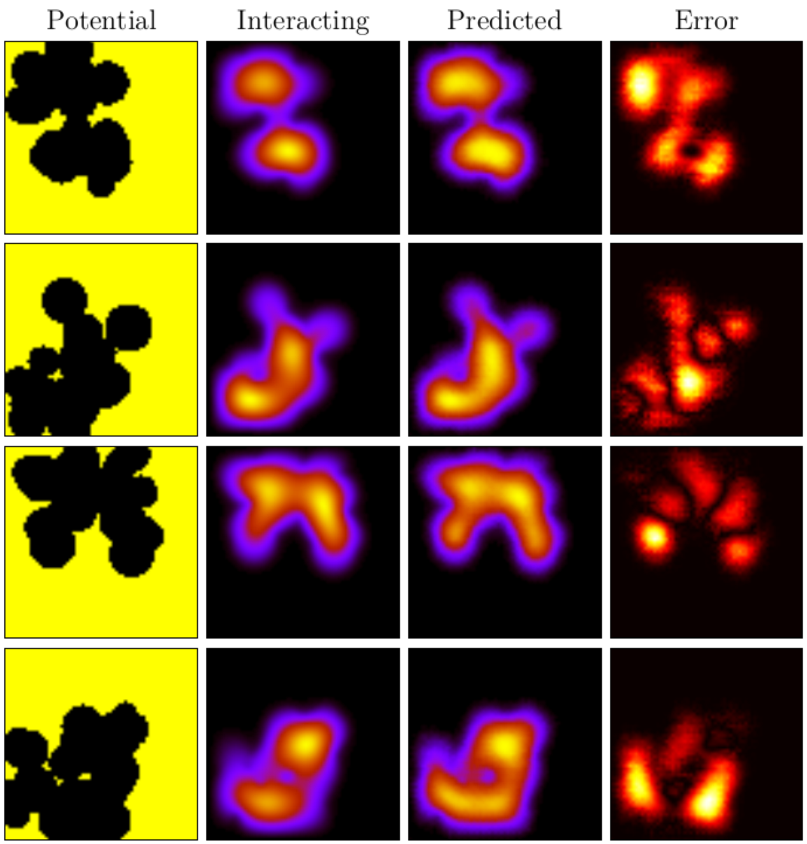


Figure 6: Mapping confinement potentials to **interacting** ground state charge densities

Outliers

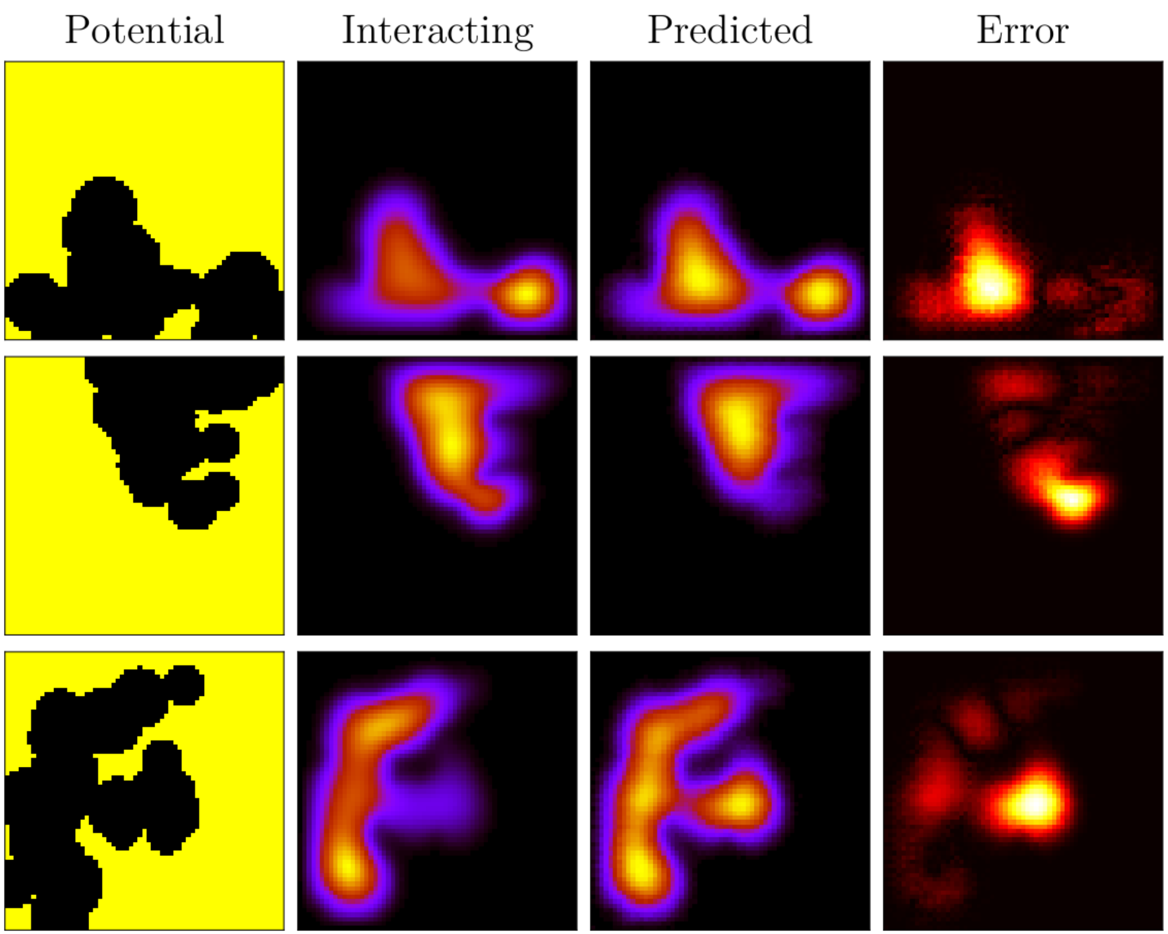


Figure 7: Three examples of outliers that exhibited the highest deviation from the real images.

Inverse Problem

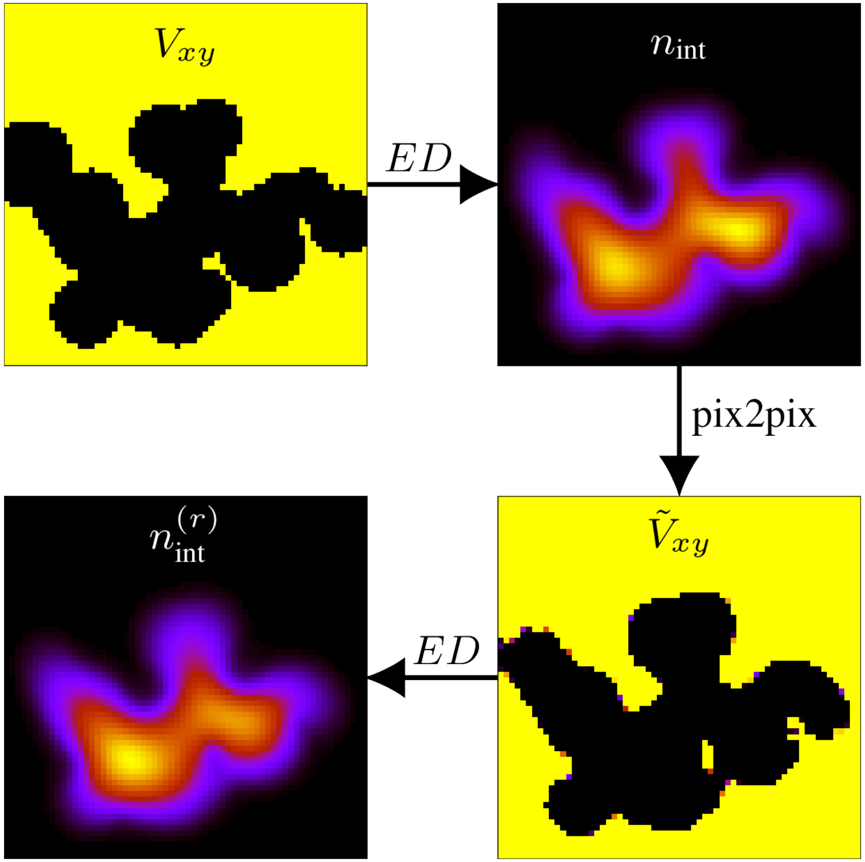


Figure 8: Mapping interacting charge densities to confinement potential.

ν-representability !!!

Not every proposed ground state charge density can be obtained from a potential.

Inverse Problem

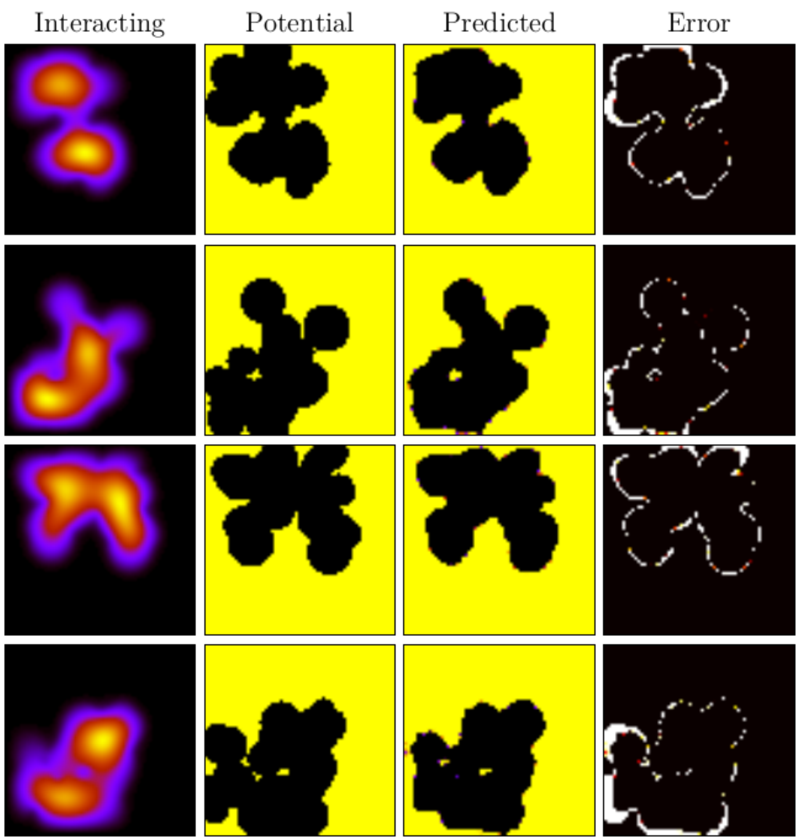


Figure 9: Mapping interacting ground state charge densities to **confinement potentials**.

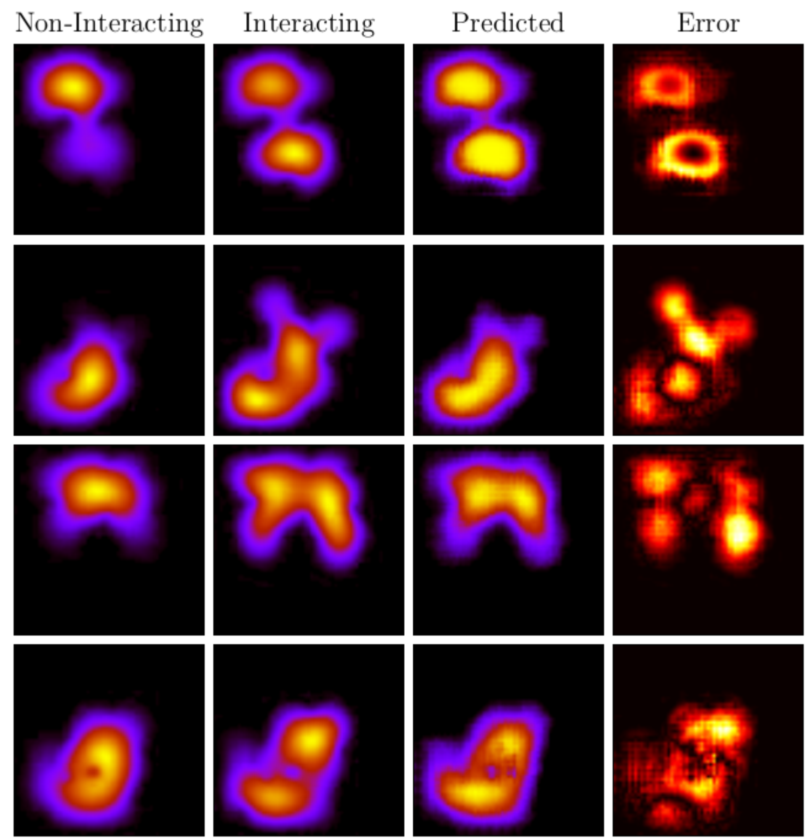


Figure 10: Mapping non-interacting to **interacting** ground state charge densities.

Multiple particles

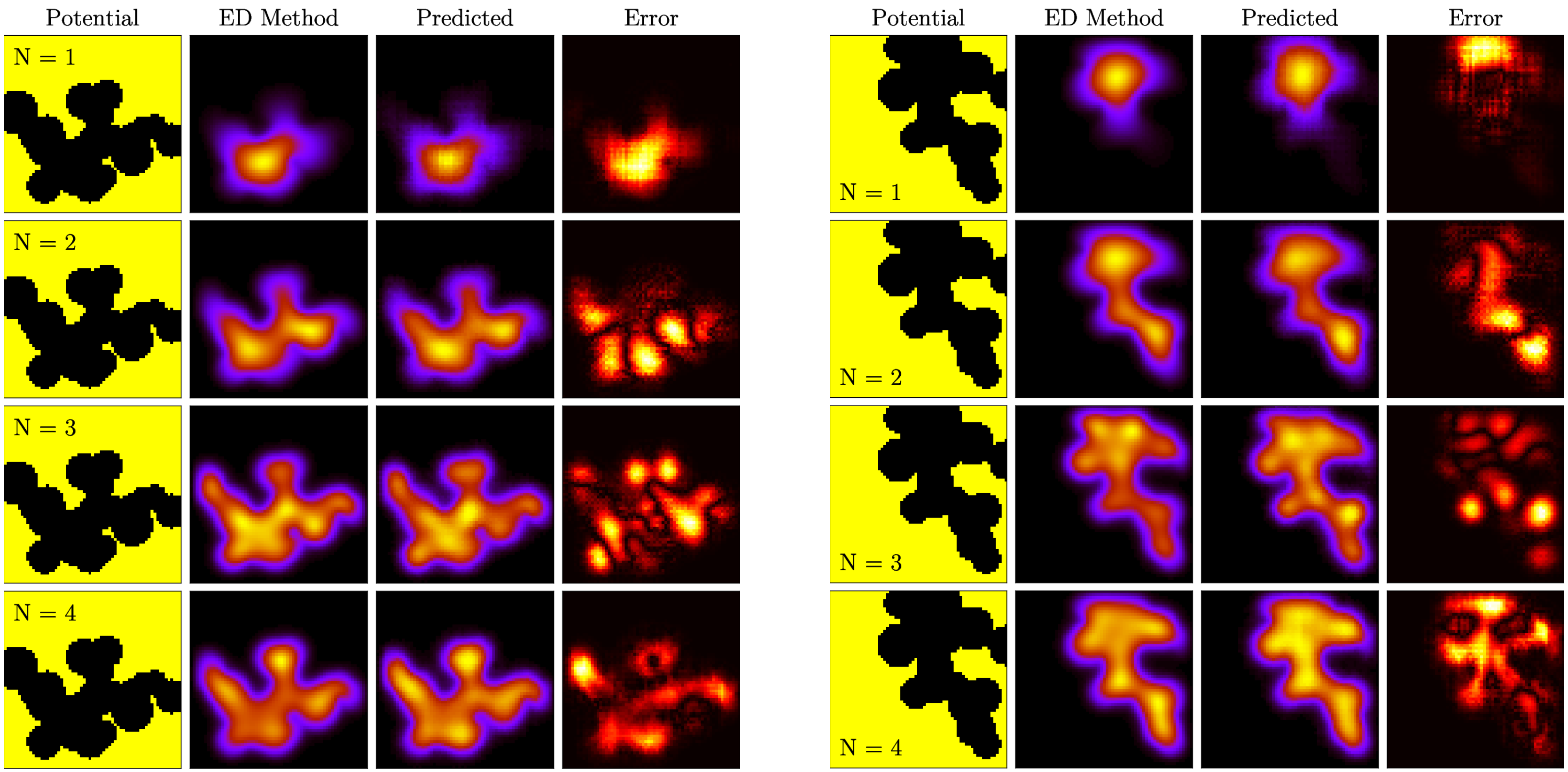


Figure 11 & 12: Pix2pix method has successfully mapped the interacting ground state charge density for systems consisting of **more than two electrons**.

Conclusions

- Successfully bypassed Exact Diagonalization
- Good accuracy of results have been obtained
- Training and predicting procedures are fast
- Ansatz free method
- Inverse problem can be approached