Title: Neural quantum states for simulating strongly interacting fermions in continuous space

Speakers:

Collection: Machine Learning for Quantum Many-Body Systems

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Abstract: ZOOM: https://pitp.zoom.us/j/94595394881?pwd=OUZSSXpzYlhFcGlIRm81Y3VaYVpCQT09

We introduce a novel neural quantum state architecture for the accurate simulation of extended, strongly interacting fermions in continuous space. The variational state is parameterized via permutation equivariant message passing neural networks to transform single-particle coordinates to highly correlated quasi-particle coordinates. We show the versatility and accuracy of this Ansatz by simulating the ground-state of the 3D homogeneous electron gas at different densities and system sizes. Our model respects basic symmetries of the Hamiltonian, such as continuous translation symmetries. We compare our ground-state energies to results obtained by different state-of-the-art NQS Ansaetze for continuous space, as well as to different quantum chemistry methods. We obtain better or comparable ground-state energies, while using orders of magnitudes less variational parameters and optimization steps. We investigate its capability of identifying and representing different phases of matter without imposing any structural bias toward a given phase. We scale up to system sizes of N=128 particles, opening the door for future work on finite-size extrapolations to the thermodynamic limit.

Neural quantum states for simulating fermions in continuous space

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Computational Quantum Science Lab.

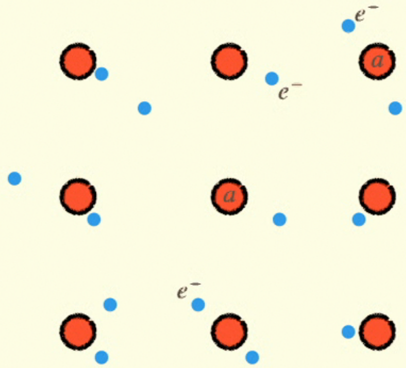
Microsoft

EPFL

Machine Learning for Quantum Many-Body Systems, June 2023

Hamiltonian

$$H = -\frac{1}{2m}\sum_i \nabla_i^2 + \sum_{i<j} V_{ee}(\|\mathbf{r}_i - \mathbf{r}_j\|) + \sum_i \sum_a V_{ea}(\|\mathbf{r}_i - \mathbf{R}_a\|)$$



$$\Psi(\mathbf{r}_1, ..., \mathbf{r}_N)$$

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Restriction: impose anti-symmetry

How to design fermionic Neural network Quantum States (NQS)?

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

Fermionic-NQS in 1st quantization

Mean field
(Hartree Fock)

$x = (\mathbf{r}_1, ..., \mathbf{r}_N)$

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

Fermionic-NQS in 1st quantization

Mean field (Hartree Fock)

Backflow $\tilde{\phi}_\mu(\mathbf{r}_1; x) = \phi_\mu(f(\mathbf{r}, x))$

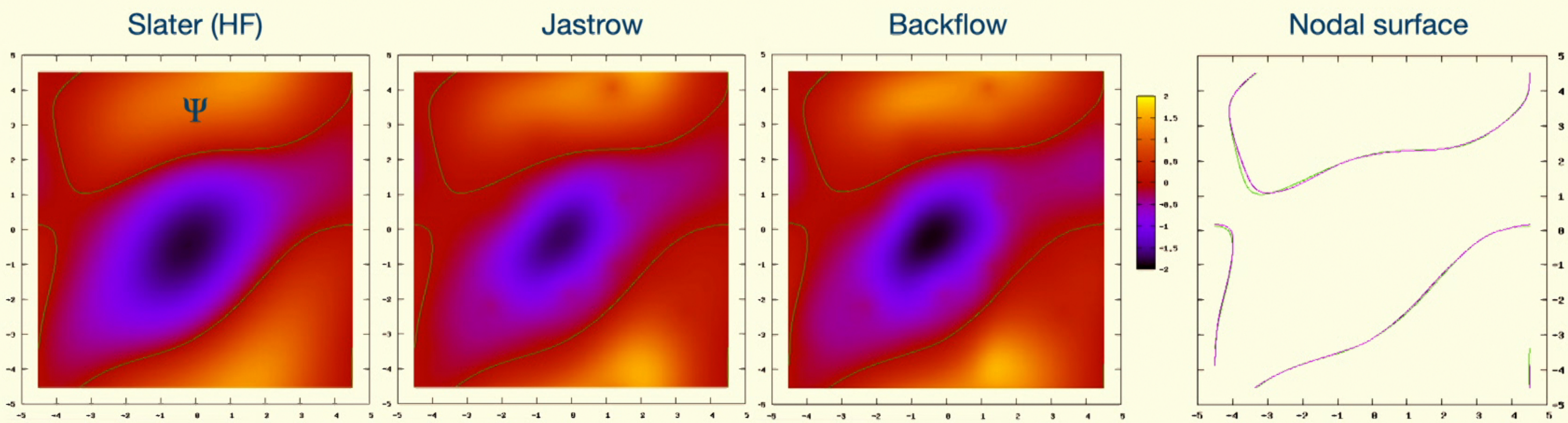
$x = (\mathbf{r}_1, ..., \mathbf{r}_N)$

$$\Psi(x) = \begin{vmatrix} \tilde{\phi}_1(\mathbf{r}_1; x) & \cdots & \tilde{\phi}_1(\mathbf{r}_N; x) \\ \vdots & \ddots & \vdots \\ \tilde{\phi}_N(\mathbf{r}_1; x) & \cdots & \tilde{\phi}_N(\mathbf{r}_N; x) \end{vmatrix} e^{J(x)}$$

Jastrow

D Luo, BK Clark, PRL (2019)

Nodal surface



Fix N-1 electron positions

Figures from Pablo López Ríos

Backflow as coordinate transformations

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

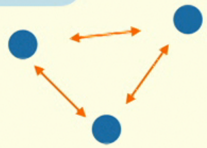
$$\Phi_\tau(\mathbf{X}) = \int_\Omega d\mathbf{X}' G_\tau(\mathbf{X}, \mathbf{X}') \Phi_0(\mathbf{X}') = \mathrm{Vol}(\Omega) \times G_\tau\left(\mathbf{X}, \mathbf{Y}(\mathbf{X})\right) \Phi_0(\mathbf{Y}(\mathbf{X}))$$

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

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

Message-Passing BackFlow (MPNN-BF)

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



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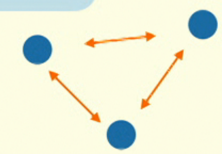

Skip Connection

$$\mathbf{x}_i^{(t)} = \left[\mathbf{x}_i^{(0)}, \mathbf{h}_i^{(t)}\right]$$
$$\mathbf{x}_{ij}^{(t)} = \left[\mathbf{x}_{ij}^{(0)}, \mathbf{h}_{ij}^{(t)}\right]$$

$$\mathbf{K}_{ij}^{(t)} = W_K^{(t)} \cdot \mathbf{x}_{ij}^{(t)}$$
$$\mathbf{Q}_{ij}^{(t)} = W_Q^{(t)} \cdot \mathbf{x}_{ij}^{(t)}$$

Particle Attention

$$\boldsymbol{\omega}_{ij}^{(t)} = \mathrm{GELU}\left(\sum_l \mathbf{Q}_{il}^{(t)} \mathbf{K}_{lj}^{(t)}\right)$$

$$\mathbf{m}_{ij}^{(t+1)} = \boldsymbol{\omega}_{ij}^{(t)}(\mathbf{x}_{ij}^{(t)}) \odot \boldsymbol{\phi}(\mathbf{x}_{ij}^{(t)})$$

Message-Passing BackFlow (MPNN-BF)

$$\mathbf{x}_i^{(0)} = \mathbf{e}$$

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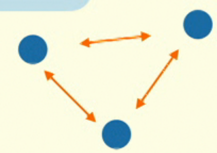

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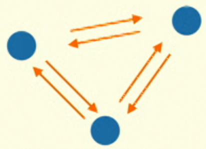
$$\mathbf{h}_{ij}^{(t+1)} = \boldsymbol{g}\left(\mathbf{x}_{ij}^{(t)}, \mathbf{m}_{ij}^{(t+1)}\right)$$

Message-Passing BackFlow (MPNN-BF)



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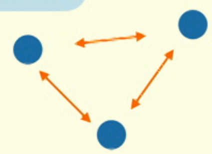

$$\mathbf{h}_i^{(t+1)} = \boldsymbol{f}\left(\mathbf{x}_i^{(t)}, \sum_{j \neq i} \mathbf{m}_{ij}^{(t+1)}\right)$$

$$\mathbf{K}_{ij}^{(t)} = W_K^{(t)} \cdot \mathbf{x}_{ij}^{(t)}$$
$$\mathbf{Q}_{ij}^{(t)} = W_Q^{(t)} \cdot \mathbf{x}_{ij}^{(t)}$$

Message Passing

Particle Attention

$$\boldsymbol{\omega}_{ij}^{(t)} = \mathrm{GELU}\left(\sum_l \mathbf{Q}_{il}^{(t)} \mathbf{K}_{lj}^{(t)}\right)$$

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Message-Passing BackFlow (MPNN-BF)

$$\mathbf{x}_i^{(0)} = \mathbf{e}$$

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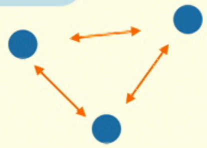

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$$\delta \mathbf{r}_i\,(\mathbf{X}) = W \cdot \mathbf{x}_i^{(T)}$$

Message Passing

Particle Attention

$$\boldsymbol{\omega}_{ij}^{(t)} = \mathrm{GELU}\left(\sum_l \mathbf{Q}_{il}^{(t)} \mathbf{K}_{lj}^{(t)}\right)$$

$$\mathbf{y}_i(\mathbf{X}) = \mathbf{r}_i + \delta \mathbf{r}_i(\mathbf{X})$$

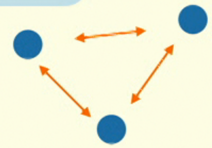
$$\mathbf{m}_{ij}^{(t+1)} = \boldsymbol{\omega}_{ij}^{(t)}(\mathbf{x}_{ij}^{(t)}) \odot \boldsymbol{\phi}(\mathbf{x}_{ij}^{(t)})$$

$$\mathbf{h}_{ij}^{(t+1)} = \boldsymbol{g}\left(\mathbf{x}_{ij}^{(t)}, \mathbf{m}_{ij}^{(t+1)}\right)$$

Message-Passing BackFlow (MPNN-BF)

$$\mathbf{x}_i^{(0)} = \mathbf{e}$$

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



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$$\delta\mathbf{r}_i(\mathbf{X}) = W \cdot \mathbf{x}_i^{(T)}$$

$$\mathbf{y}_i(\mathbf{X}) = \mathbf{r}_i + \delta\mathbf{r}_i(\mathbf{X})$$

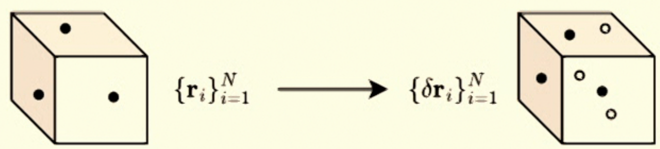
$$\Phi_0(\mathbf{Y}(\mathbf{X}))$$

Model summary

Mean field orbitals

$$\phi_\mu(\mathbf{r}) = e^{i\mathbf{k}_\mu \cdot \mathbf{r}}$$

Backflow transformations (quasi particles)



Generalised Slater determinants

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

Homogeneous Electron Gas

Experiments

Homogeneous Electron Gas (3D)

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

- Maintains symmetries
  - Translation invariant (**K** = 0): floating
  - Spin-inversion symmetric
- Unbiased: cubic simulation cell
- Orders of magnitude less parameters (~19k)
- Allows to use Stochastic Reconfiguration, aka (quantum) Natural Gradients
- Fast convergence (~500 steps vs 500k steps)

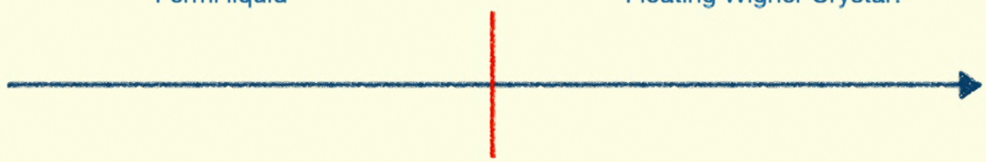
Experiments

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

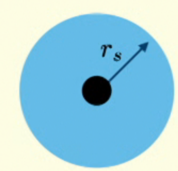
Low density:
Floating Wigner Crystal?



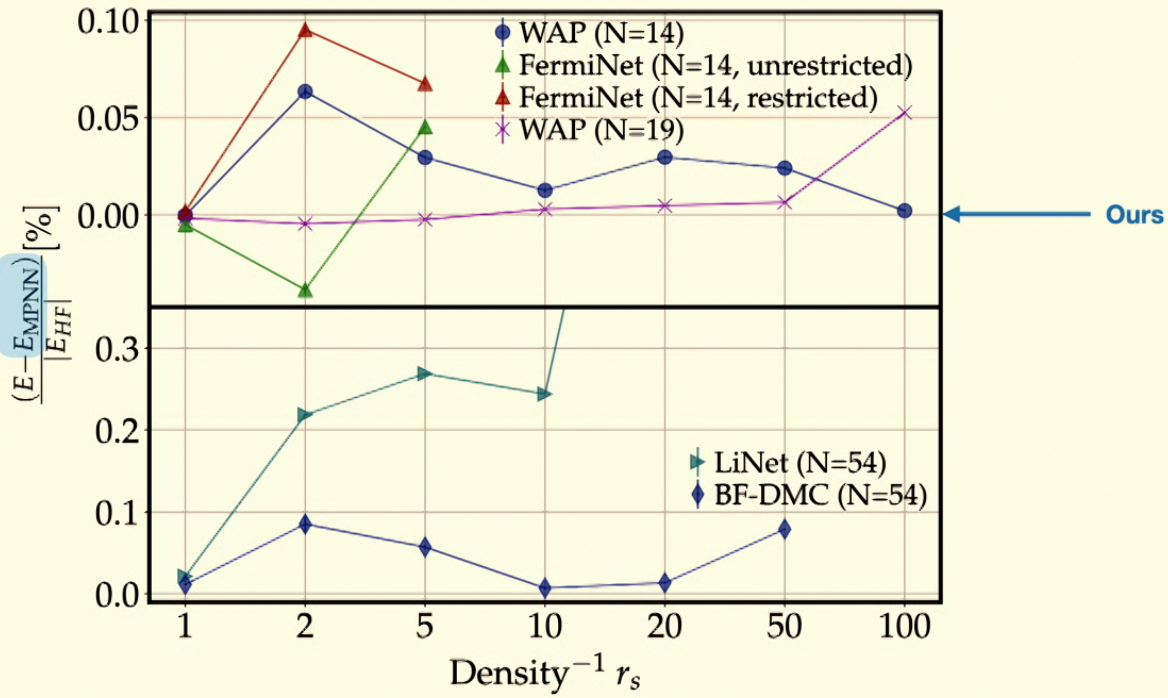
r_s

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

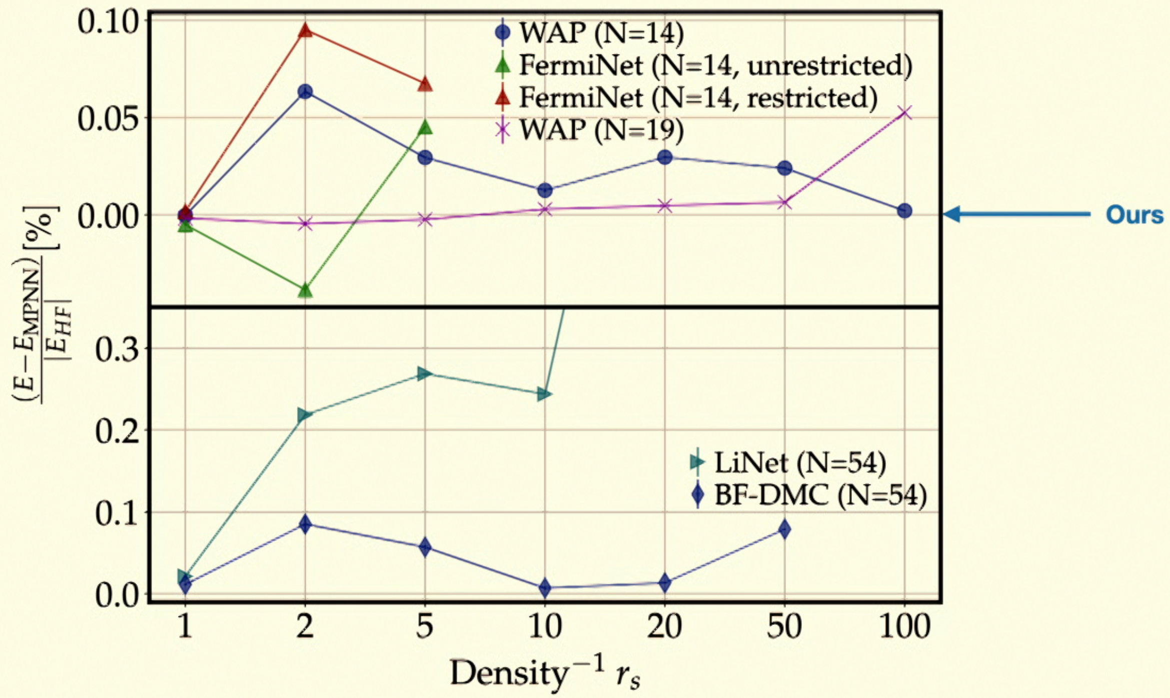
$$\frac{1}{r_s}\sum_{i<j}\frac{1}{\|\mathbf{r}_i - \mathbf{r}_j\|}$$



Benchmark: small systems



Benchmark: small systems



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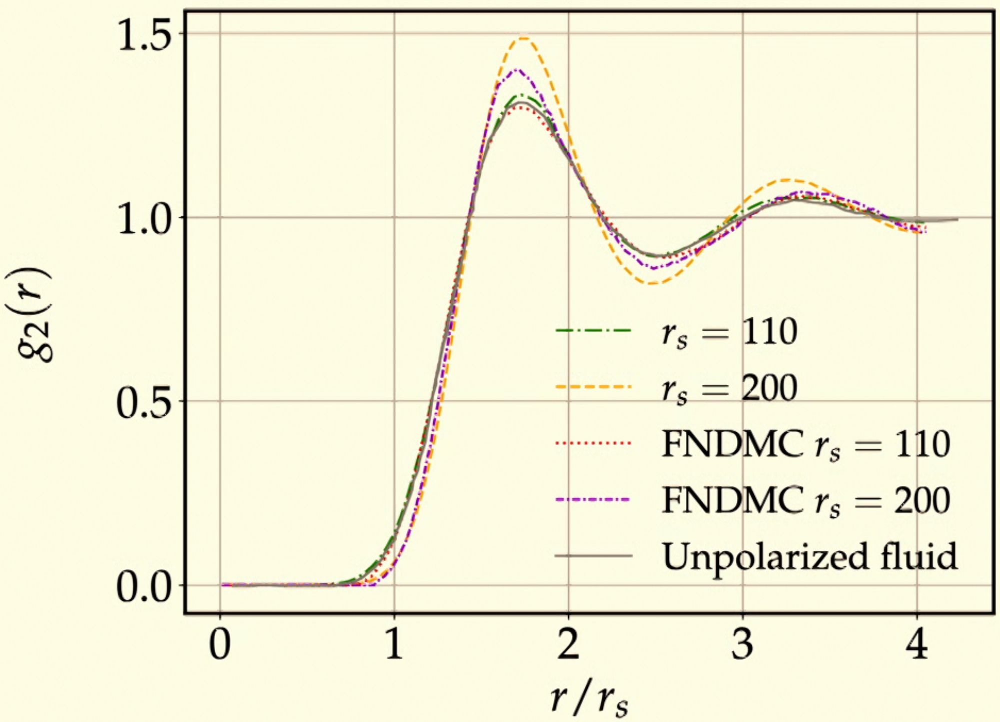
Results



- Uniform 1-body density: floating
- Exclude Wigner crystal to r_s=110
  - Recent work [Cassella et al, PRL (2023)]: 27 particles, crystal from r_s=2-5
- Largest electronic simulation: 128 electrons

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Ultra-cold Fermi gas

Restrictions: 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?

Pairing fermions with Pfaffians

Definitions

$$\phi(\mathbf{r}_i, \sigma_i; \mathbf{r}_j, \sigma_j) = \langle \sigma_i \sigma_j | \, \alpha(\mathbf{r}_i, \mathbf{r}_j) \left(\frac{|\uparrow\downarrow\rangle - |\uparrow\downarrow\rangle}{\sqrt{2}} \right)$$

$$+ \langle \sigma_i \sigma_j | \left[\beta^{\uparrow\downarrow}(\mathbf{r}_i, \mathbf{r}_j) \left(\frac{|\uparrow\downarrow\rangle + |\uparrow\downarrow\rangle}{\sqrt{2}} \right) + \beta^{\uparrow\uparrow}(\mathbf{r}_i, \mathbf{r}_j) \, |\uparrow\uparrow\rangle + \beta^{\downarrow\downarrow}(\mathbf{r}_i, \mathbf{r}_j) \, |\downarrow\downarrow\rangle \right]$$

(

Odd

Pairing fermions with Pfaffians

Definitions

Singlet pairing (BCS)

$$\mathrm{pf}\begin{bmatrix} 0 & \boldsymbol{\alpha} \\ -\boldsymbol{\alpha}^T & 0 \end{bmatrix} = \det|\boldsymbol{\alpha}|$$

Even

$$\phi(\mathbf{r}_i, \sigma_i; \mathbf{r}_j, \sigma_j) = \langle \sigma_i \sigma_j | \, \alpha(\mathbf{r}_i, \mathbf{r}_j) \left(\frac{|\uparrow\downarrow\rangle - |\uparrow\downarrow\rangle}{\sqrt{2}} \right)$$

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Odd

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Pairing fermions with Pfaffians

Definitions

Singlet pairing (BCS)

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$$\phi(\mathbf{r}_i, \sigma_i; \mathbf{r}_j, \sigma_j) = \langle \sigma_i \sigma_j | \, \alpha(\mathbf{r}_i, \mathbf{r}_j) \left(\frac{|\uparrow\downarrow\rangle - |\uparrow\downarrow\rangle}{\sqrt{2}} \right)$$

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Odd

Odd

Triplet pairing

$$\mathrm{pf}\begin{bmatrix} \boldsymbol{\beta}^{\uparrow\uparrow} & 0 \\ 0 & \boldsymbol{\beta}^{\downarrow\downarrow} \end{bmatrix} = \mathrm{pf}[\boldsymbol{\beta}^{\uparrow\uparrow}] \times \mathrm{pf}[\boldsymbol{\beta}^{\downarrow\downarrow}]$$

Neural backflow Pfaffian

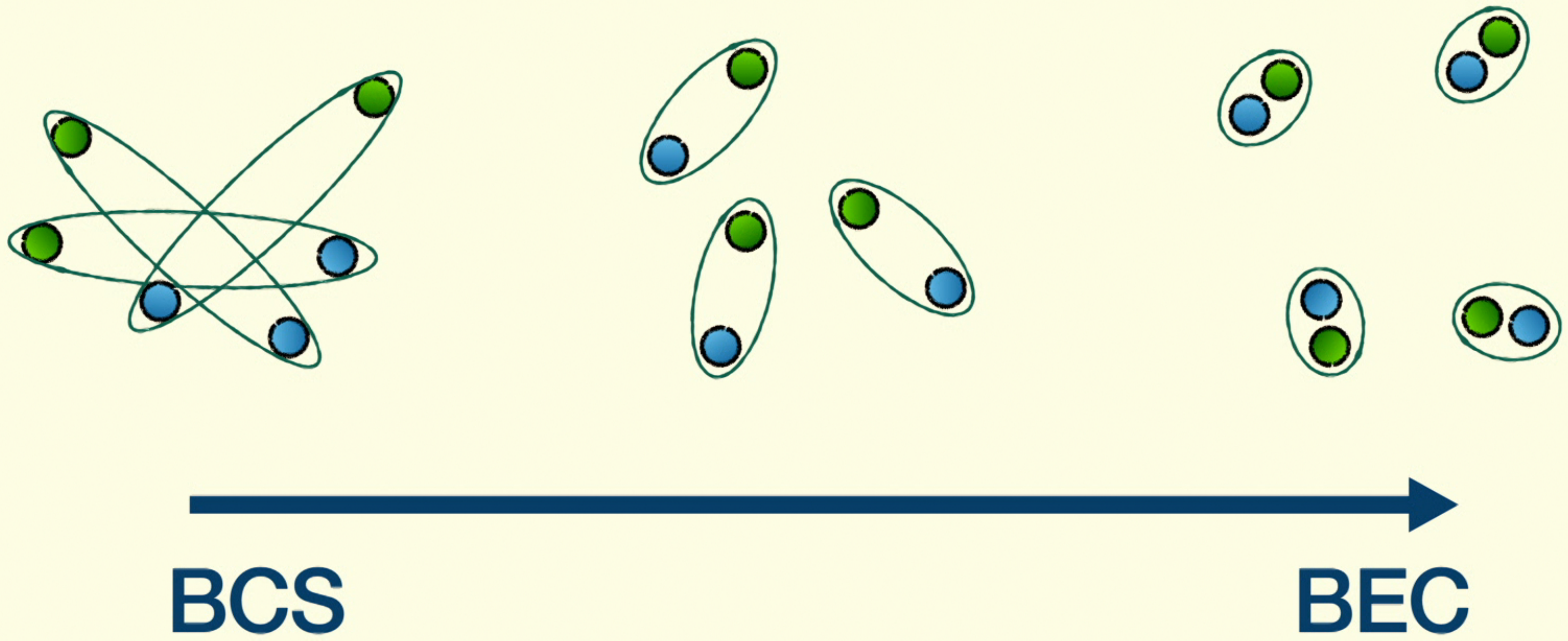
$\mathbf{x}_i = (\mathbf{r}_i, \sigma_i)$

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

Unpolarized, capture singlet and triplet

Ultra-cold Fermi gas

BCS-BEC Crossover

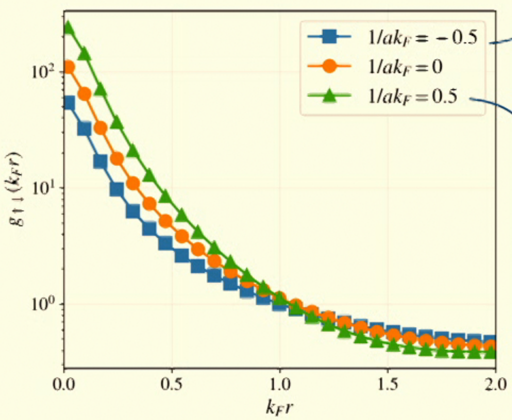


Results

- Poschl-Teller interaction

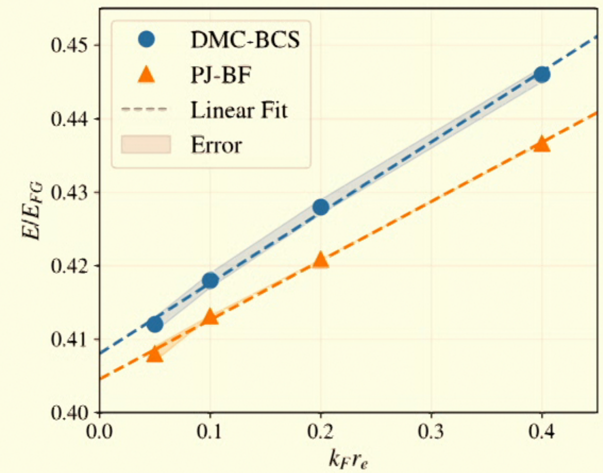
$$v_{ij} = (\delta_{s_i,s_j} - 1) v_0 \frac{2\hbar^2}{m} \frac{\mu^2}{\cosh^2(\mu r_{ij})}$$

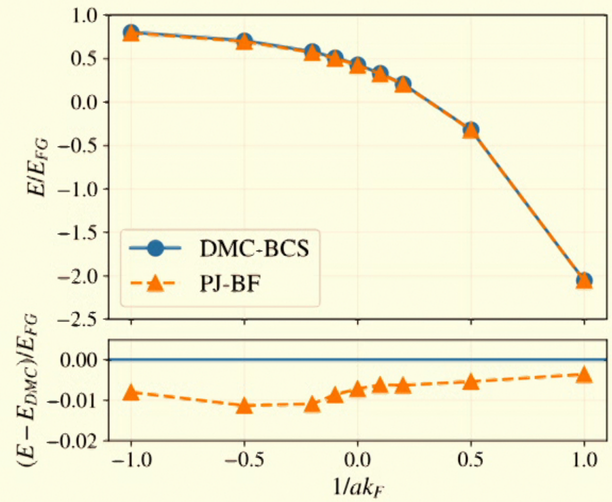
Only opposite spins: attractive



BCS (long range Cooper pairs)

BEC (tightly bound repulsive dimers)





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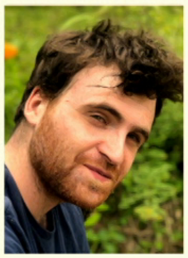
Team

Giuseppe Carleo   Gabriel Pescia

Jan Kim   Alessandro Lovato

Computational Quantum Science Lab.

EPFL

Michigan State University, Founded 1855

Argonne NATIONAL LABORATORY

NetKet

Net

The Machine-Learning toolbox for Quantum Physics

Contains: Fermions, NQS, (MC)MC, Automatic Diff, Hamiltonians, Stochastic Reconfiguration, Optimisers, ...

Vicentini, ..., **Nys**, ..., Carleo, SciPost Phys. Codebases 7 (2022)

References

- **First quantization:**
  - [MPNN+HEG] G Pescia, **J Nys**, J Kim, A Lovato, and G Carleo. "Message-Passing Neural Quantum States for the Homogeneous Electron Gas." arXiv:2305.07240 (2023).
  - [Pfaffian] J Kim, G Pescia, B Fore, **J Nys**, G Carleo, S Gandolfi, M Hjorth-Jensen, A Lovato. “Neural-network quantum states for ultra-cold Fermi gases.” arXiv:2305.08831 (2023)
- **Second quantization:**
  - [CC] *Variational solutions to fermion-to-qubit mappings in two spatial dimensions*, **J Nys** & G Carleo, Quantum 6, 833 (2022)
  - [QC] *Quantum circuits for solving local fermion-to-qubit mapping*, **J Nys** & G Carleo, Quantum 7, 930 (2023)