Neural Network Quantum States for Spinless Fermions

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Outline of this talk

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Outline - Condensed Matter

Studying NQS to many-body problem in Condensed Matter physics.

- Few-body system of up to 6 particles **harmonically trapped** interacting via a 2-body finite-range.
- Benchmarked against Direct **Diagonalization** and Hartree-Fock.
- **Finite-range** interaction: Leads to two distinct physical phenomena; Bosonization & Wigner crystallization


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The Many-Body Problem

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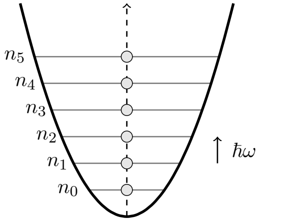
Hamiltonian: 1D Space

- Harmonic Oscillator (HO) + **finite-range** interaction:

$$\hat{H} = \underbrace{-\frac{1}{2}\sum_i \nabla_i^2 + \frac{1}{2}\sum_i x_i^2}_{\text{Harmonic Oscillator}} + \underbrace{\frac{V_0}{\sqrt{2\pi}\sigma_0}\sum_{i<j}\exp\left(-\frac{(x_i - x_j)^2}{2\sigma_0^2}\right)}_{\text{Finite-range interaction}}$$

- **Finite-range** interaction due to '**Spinless**' (fully-polarized) fermions due to Pauli exclusion principle.
- **Physical Phenomena**: Bosonization / Wigner Crystallization.

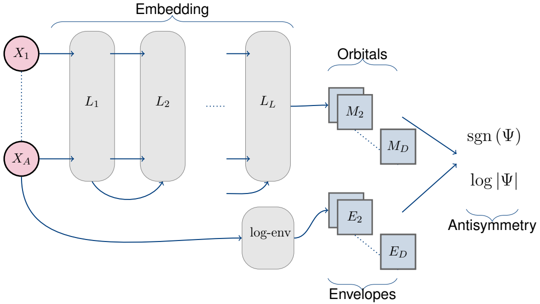


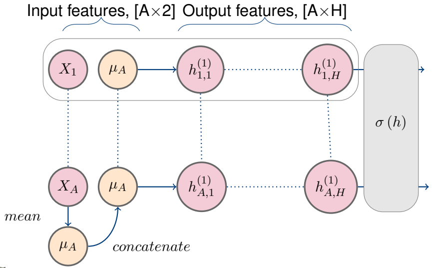
$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega$$

Methodology: NQS + VMC

- Construct **NQS** of given architecture to represent many-body wavefunction.
- Pre-train to set of 'target' orbitals (**Hermite Polynomials**).
- Follow **VMC** methodology (repeat until convergence):
  - Generate Samples via Markov Chain (**Metropolis-Hastings**).
  - Compute expectation of the energy via **Statistical Estimator**.
  - Update ansatz via **gradient-descent**: Adam [Kingma, Ba (2014)]
- **Access to wavefunction**: Compute **many-body observables** to benchmark accuracy.

Neural Quantum States: FermiNet





The Ansatz

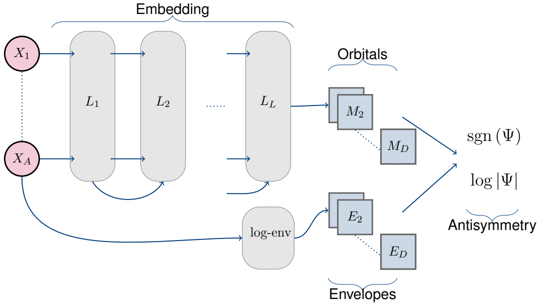
- Universal approximation under the 'width' of its hidden layers
- Includes a generic form of backflow leads to 'Generalised' Slater Determinants (GSD)

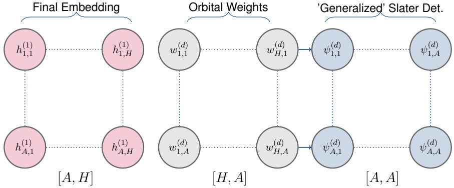
Equivariance

- Permutation equivariance is enforced via weight-sharing & permutation-invariant (mean position) information.

Pfau et al. (2020) Physical Review Research, 2(3), p.033429.
Sannai et. al. (2019) arXiv:1903.01939.

Neural Quantum States: FermiNet





The Ansatz

- Universal approximation under the 'width' of its hidden layers
- Includes a generic form of backflow leads to 'Generalized' Slater Determinants (GSD)

Antisymmetry

- Antisymmetry enforced by $D = 1$ determinant over all 'many'-body orbitals.
- NQS can have multiple determinants if needed.

Pfau, et al. (2020) Physical Review Research, 2(3), p.033429.

Markov Chain Monte Carlo

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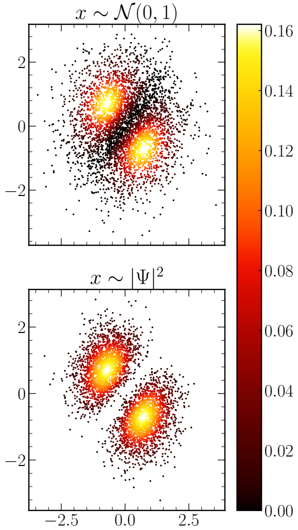
Evaluating the Energy in A-dim space

- Reformulate as statistical estimator:
  $\langle E(\theta)\rangle = \frac{\langle\Psi|\hat{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \mathbb{E}_{x\sim|\Psi|^2}\left[\Psi^{-1}\hat{H}\Psi\right]$
- $\langle E\rangle$ now **independent** of dim.
- How to generate $x \sim |\Psi|^2$?

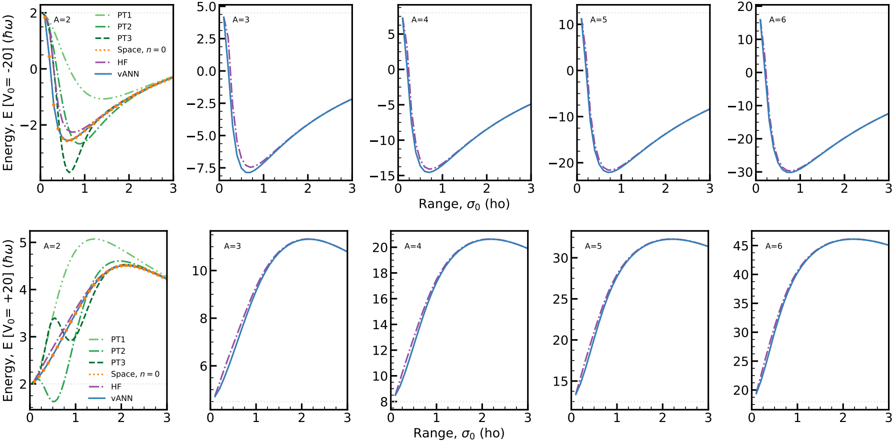
Generating data via MH-Sampler

- **Initialize**: $x_0 \sim \mathcal{N}(0,1)$.
- **Propose**: $x_{n+1} \sim \mathcal{N}(x_n, \sigma_n)$
- $\times$ 10
- **Accept**: $\min\left(1, \frac{|\Psi(x_{n+1})|^2}{|\Psi(x_n)|^2}\right)$
- **Distributed**: $x_n \sim |\Psi|^2$ (not *i.i.d*!)



Metropolis and Ulam. "The monte carlo method." J. Am. Stat. Assoc. 44.247 (1949): 335-341.

Ground-state energy - Range

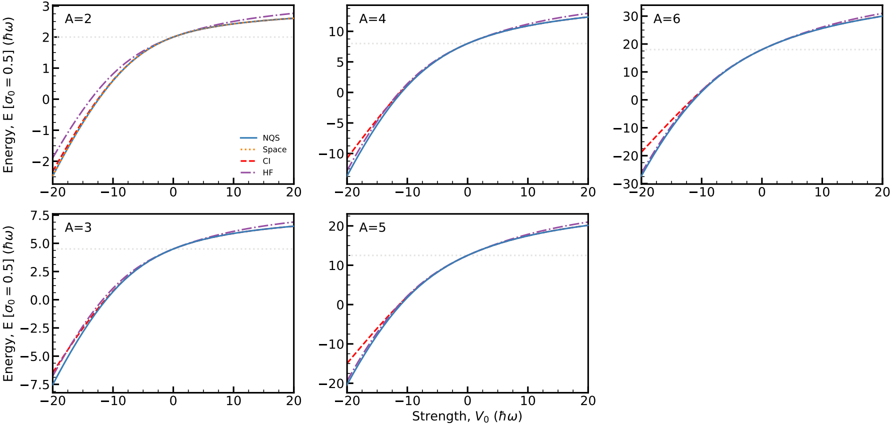


- Bosonisation ($V_0 \to -20\hbar\omega$) leads to fermions having a bosonic density profile.
- Wigner Crystallisation: ($V_0 \to +20\hbar\omega$) leads to crystalline density profile.
- Non-perturbative near $\sigma_0 = 0.5$, ideal to test NQS here.

$$\hat{H} = -\frac{1}{2}\sum_i \nabla_i^2 + \frac{1}{2}\sum_i x_i^2 + \frac{V_0}{\sqrt{2\pi}\sigma_0}\sum_{i<j}\exp\left(-\frac{(x_i - x_j)^2}{2\sigma_0^2}\right)$$

Keeble et. al. - arXiv:2304.04725.

Ground-state energy - Int. Strength



- Variational principle infers best methodology (Lower is better).
- CI restricted basis in $V_0 \ll 0$ limit, converged in $V_0 \gg 0$ limit.
- HF lacks correlation energy for $V_0 \neq 0$.

$$\hat{H} = -\frac{1}{2}\sum_i \nabla_i^2 + \frac{1}{2}\sum_i x_i^2 + \frac{V_0}{\sqrt{2\pi}\sigma_0}\sum_{i<j} \exp\left(-\frac{(x_i - x_j)^2}{2\sigma_0^2}\right)$$

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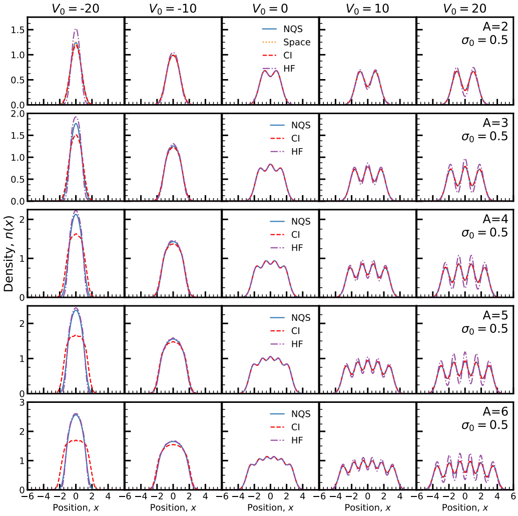
One-Body Density



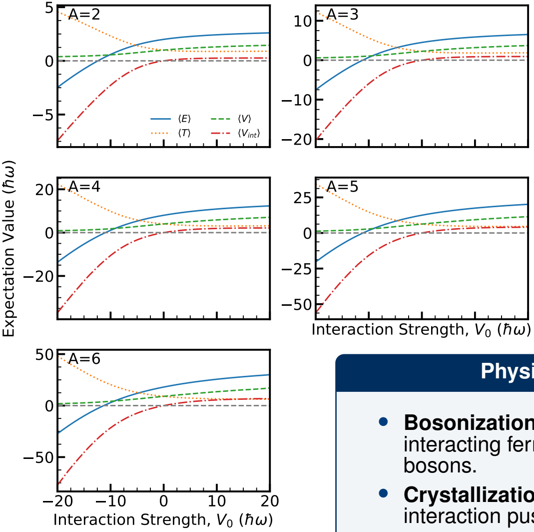
Different physical phenomena as V_0 varies,

- $V_0 \ll 0$ results in Bosonisation (Fermi-Bose duality).
- $V_0 \gg 0$ results in Wigner crystallisation.

NQS methodology performs well in all values of V_0 studied,

- $V_0 \ll 0$ CI fails due to model truncation
- $V_0 \gg 0$ HF fails due to lack of correlation energy

Rojo-Francàs et. al., 2020. Static and dynamic properties of a few spin 1/2 interacting fermions trapped in a harmonic potential. Mathematics, 8(7), p.1196.



Bosonization

- **Minimize** $\langle V \rangle \approx 0$.
- **Maximize** $\langle T \rangle$
- $\langle V_{\text{int}} \rangle$ **dominates** $\langle T \rangle$,

Wigner Crystallization

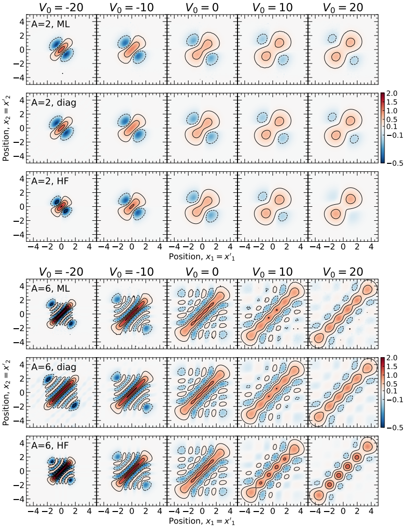
- **Maximize** $\langle V \rangle$.
- **Minimize** $\langle T \rangle \approx 0$
- $\langle V_{\text{int}} \rangle \approx \langle T \rangle$

Physical Interpratation

- **Bosonization**: Fermi-Bose duality, interacting fermions $\approx$ non-interacting bosons.
- **Crystallization**: Localization emerges from interaction pushing particles apart.

Keeble et. al. - arXiv:2304.04725.

One-Body Density Matrix



Benchmarks A = 2 & 6

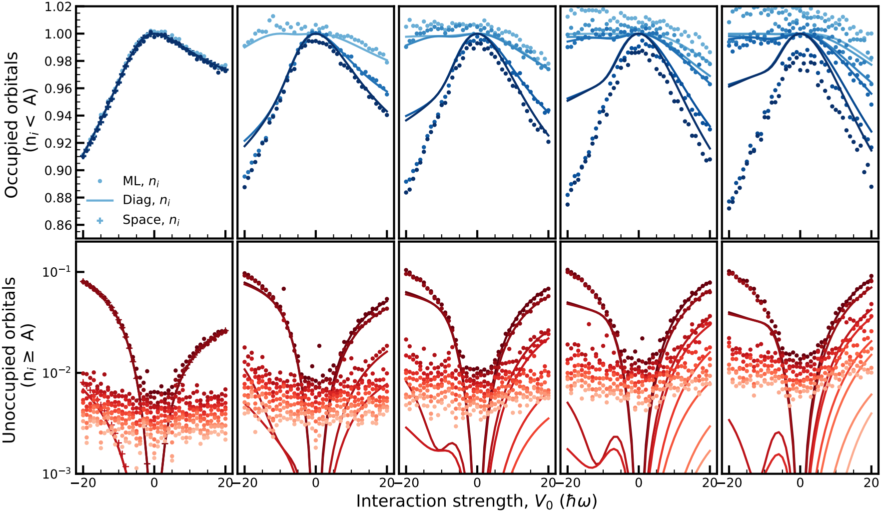
- Compared against HF & CI (diag)
- **HF**: Single-particle orbitals, distinct circular peaks in OBDM.
- **CI**: Converged in $V_0 \gg 0$ limit & truncated in $V_0 \ll 0$ limit. ML agrees with CI (some artifacts).
- Bosonization $V_0 \ll 0$ & Wigner Crystallization $V_0 \gg 0$.

Physical Interpretation - OBDM

- Fermionic structure shown along **off-diagonal** (mixing of natural orbitals).
- OBDM represents how arb. positions **relate** to one another.

McMillan, W.L., 1965. Ground state of liquid He 4. Physical Review, 138(2A), p.A442.

Occupation Numbers



- Noise emerges from sign problem along off-diagonal matrix elements of OBDM.

Keeble et. al. - arXiv:2304.04725.

Pairing Gap Energies

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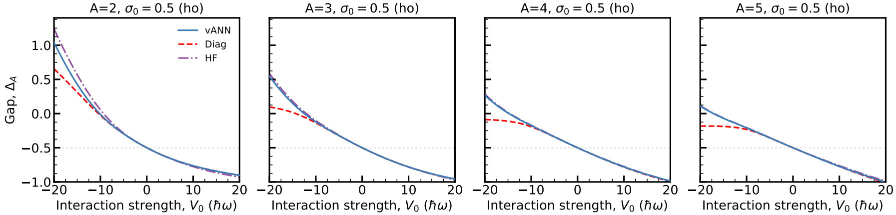


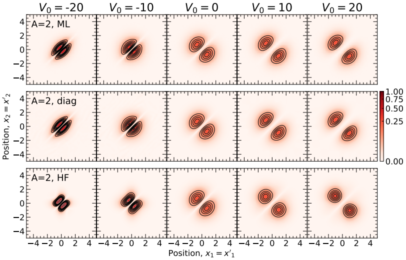
Pairing-gap Energies:

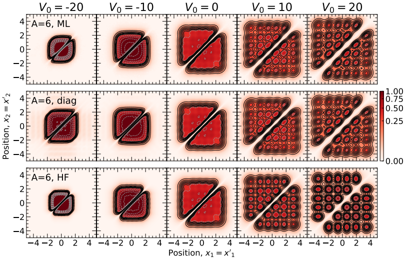
- Fermions of the same spin tend to 'pair' together (**lowers** ground-state energies, **increases** binding energy).

$$\Delta_A = \langle E_A \rangle - \frac{1}{2} \left(\langle E_{A+1} \rangle + \langle E_{A-1} \rangle \right).$$

- $+\Delta_A$ increases ground-state (reduces binding energy).
- $-\Delta_A$ decreases ground-state (increases binding energy).

Two-Body Density





Benchmarks A = 2 & 6

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- Bosonization $V_0 \ll 0$ & Wigner Crystallization $V_0 \gg 0$.

Physical Interpretation - TBD

- Zero probability along diagonal (Pauli-Exclusion Principle).
- Two-body density represents probability of arb. pairs of particles.

Löwdin, P.O., 1955. Quantum theory of many-particle systems. I. Physical Review, 97(6), p.1474.

To Conclude

Conclusions

- 'Spinless' fermions solved up to 6 fermions, **good** accuracy for all V_0 & σ_0 studied. **Code**: github.com/jwtkeeble/SpinlessFermions
- One/Two-body densities **accurately** represented with **same** NQS.
- Density matrix looks **great**, but has **poor** occupation numbers & natural orbitals.

Open Questions?

- Are the same advancements possible for real-time **dynamics**?
- What **modifications** of NQS for **nuclear** systems? Spin/Isospin?

Other talks to look out for!

- Anti-symmetrized neural quantum states - J. Rozalén (Barcelona)
- Transfer learning for many-body physics - A. Azzam (Barcelona)
- Optimising Fermionic Neural Networks with Decision Geometry - M. Drissi (TRIUMF)

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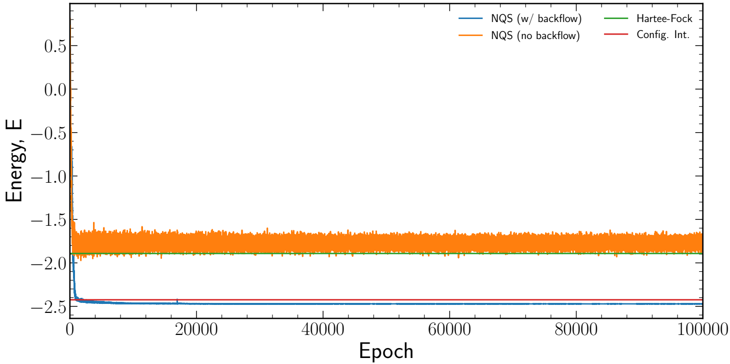
Backup slides...

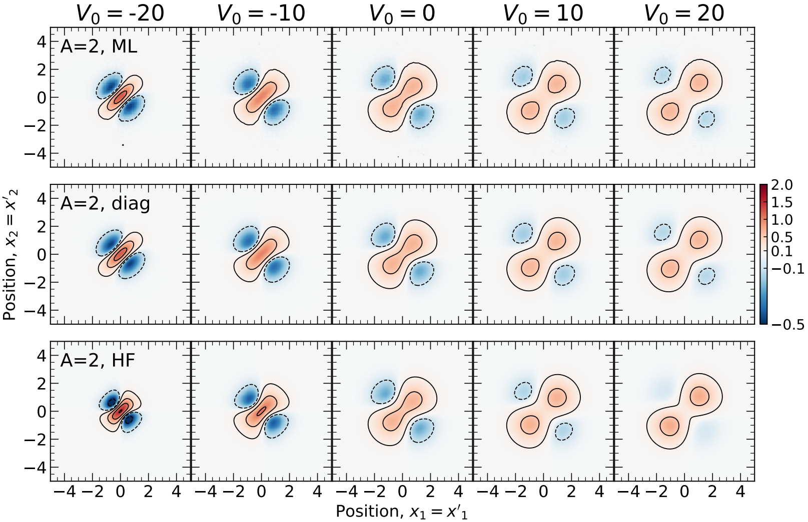
Comparing Backflow in the NQS



- Removed mean-body position (invariant information)
- **No backflow** → **No correlation** energy
- Best possible result is **Hartree-Fock**.

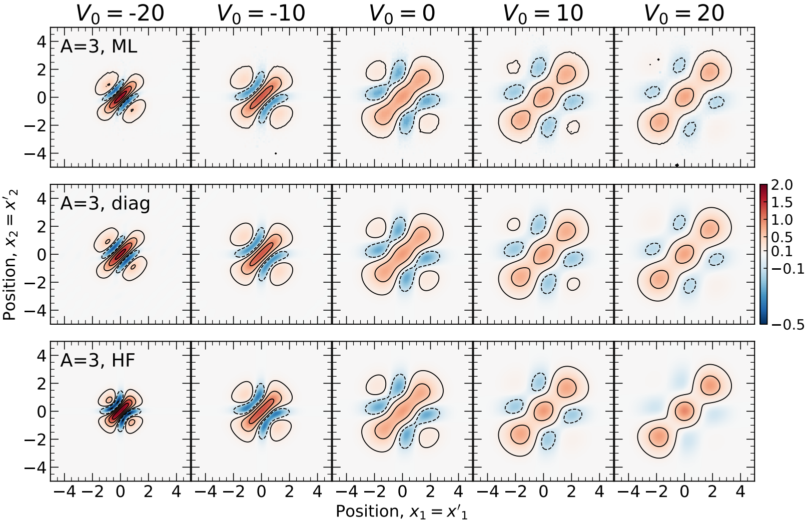
Keeble et. al. - arXiv:2304.04725.

One-Body Density Matrix: A=2



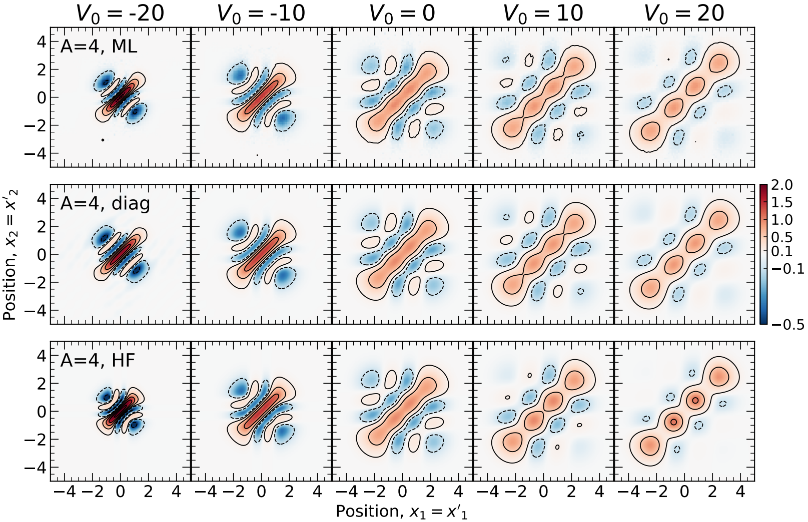
McMillan, W.L., 1965. Ground state of liquid He 4. Physical Review, 138(2A), p.A442.

One-Body Density Matrix: A=3



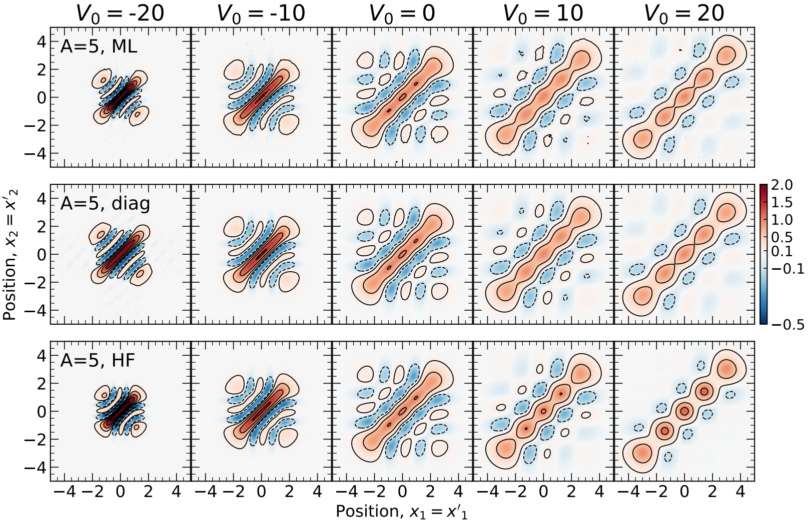
McMillan, W.L., 1965. Ground state of liquid He 4. Physical Review, 138(2A), p.A442.

One-Body Density Matrix: A=4



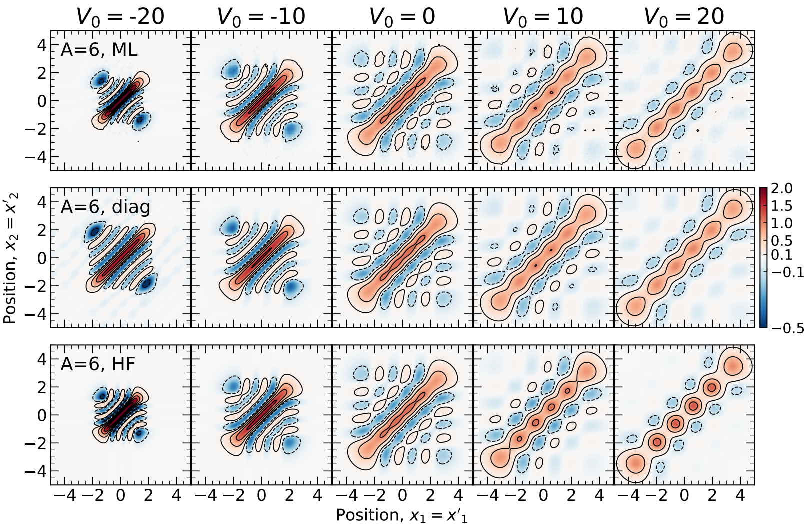
McMillan, W.L., 1965. Ground state of liquid He 4. Physical Review, 138(2A), p.A442.

One-Body Density Matrix: A=5



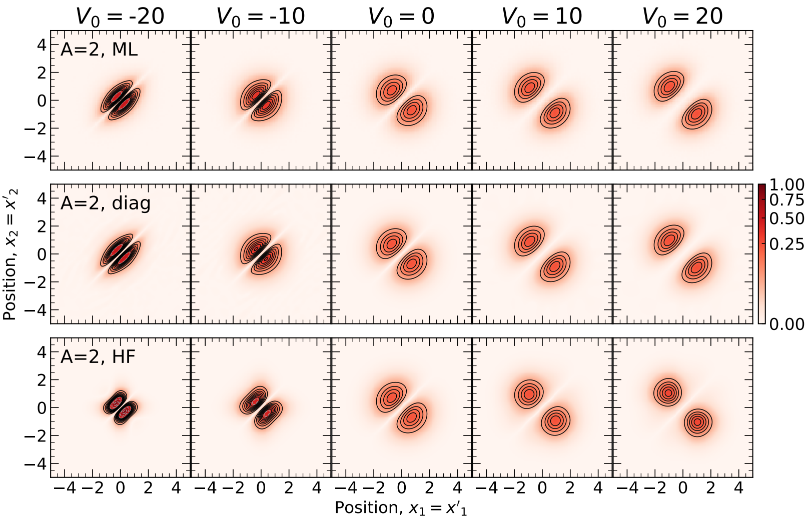
McMillan, W.L., 1965. Ground state of liquid He 4. Physical Review, 138(2A), p.A442.

One-Body Density Matrix: A=6



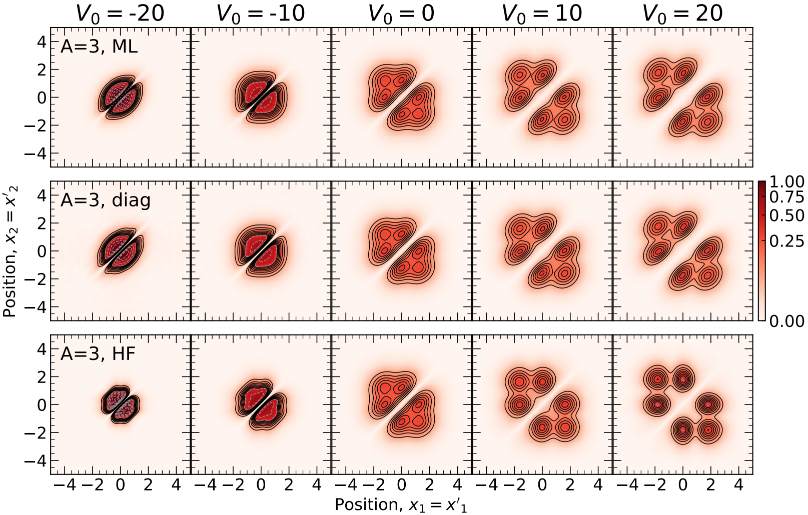
McMillan, W.L., 1965. Ground state of liquid He 4. Physical Review, 138(2A), p.A442.

Two-Body Density: A=2



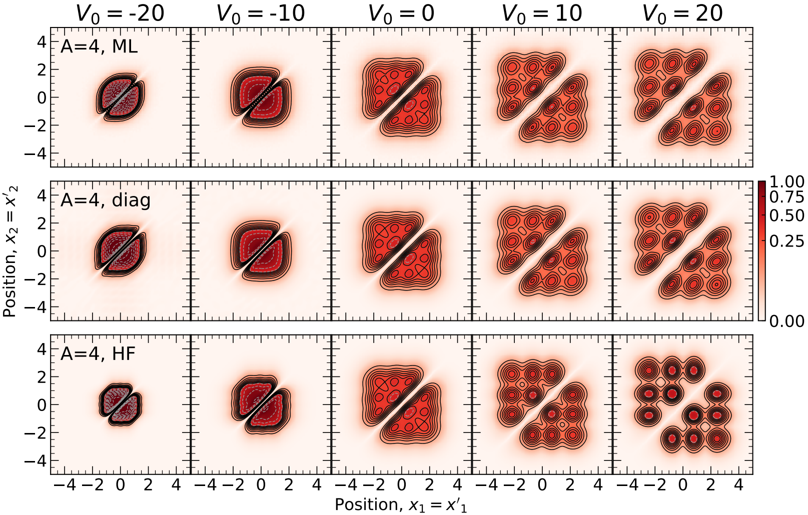
Löwdin, P.O., 1955. Quantum theory of many-particle systems. I. Physical Review, 97(6), p.1474.

Two-Body Density: A=3



Löwdin, P.O., 1955. Quantum theory of many-particle systems. I. Physical Review, 97(6), p.1474.

Two-Body Density: A=4



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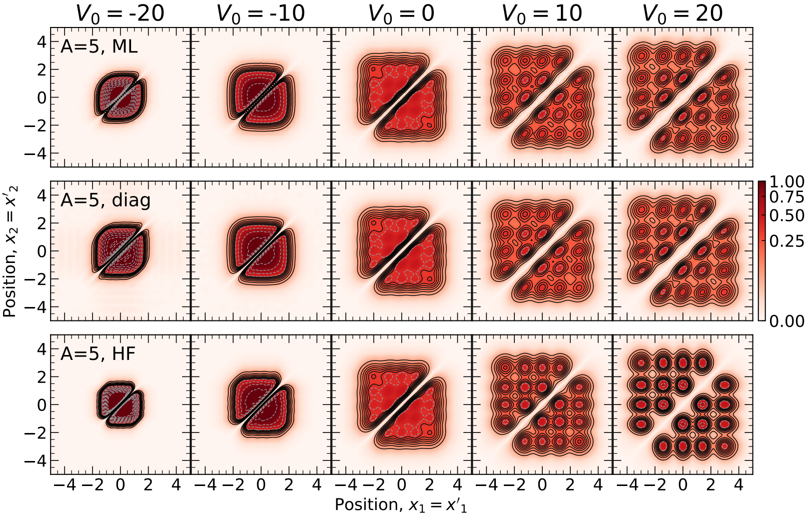
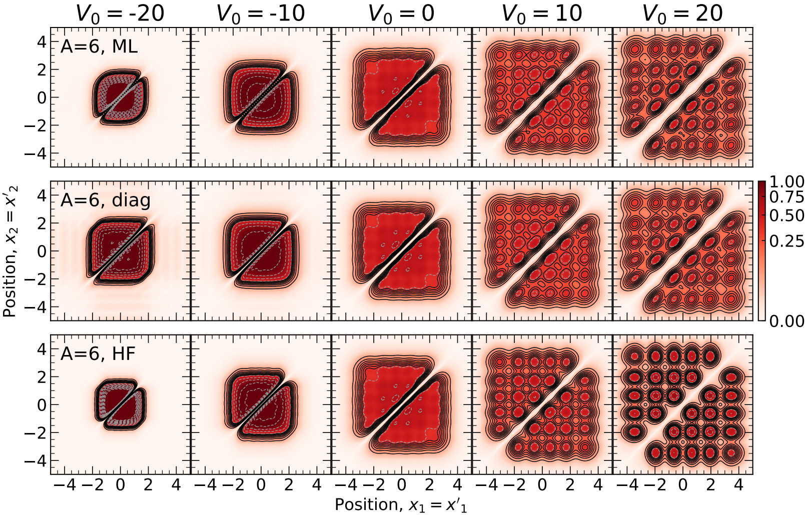
Two-Body Density: A=5



Löwdin, P.O., 1955. Quantum theory of many-particle systems. I. Physical Review, 97(6), p.1474.

Two-Body Density: A=6



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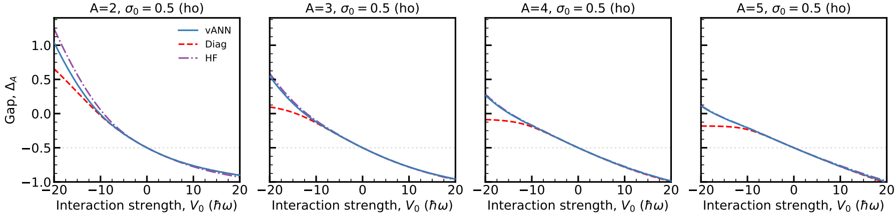
Pairing Gap Energies

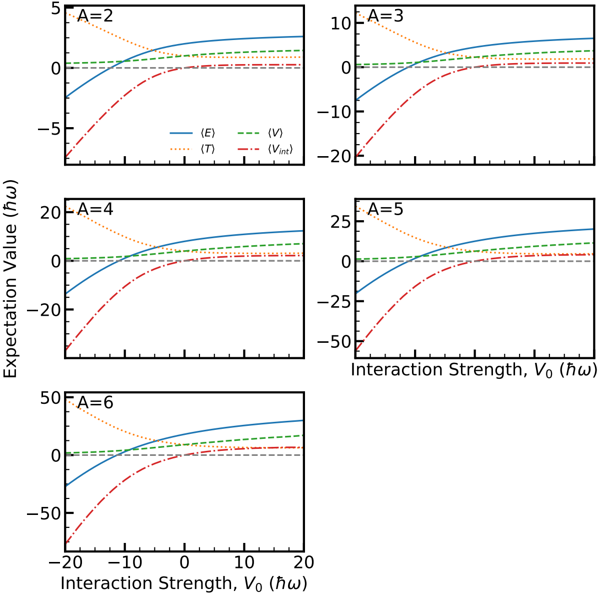


Pairing-gap Energies

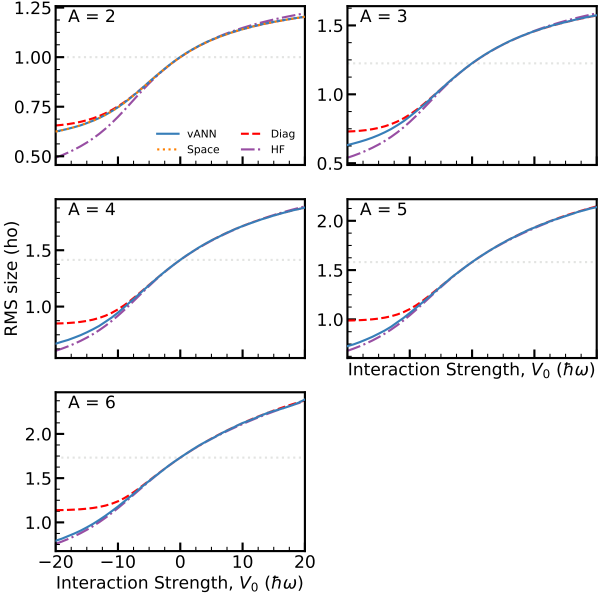
- Nucleons of same spin tend to 'pair' together (leads to lower ground-state energies).
- Pairing-gap energy, Δ_A, defined as,

$$\Delta_A = \langle E_A \rangle - \frac{1}{2} \left(\langle E_{A+1} \rangle + \langle E_{A-1} \rangle \right).$$

Individual Contributions to Energy



Root-Mean-Square Size



Occupation Numbers