Machine Learning as an Alternative Wavefunction Ansatz to Improve Variational Monte Carlo

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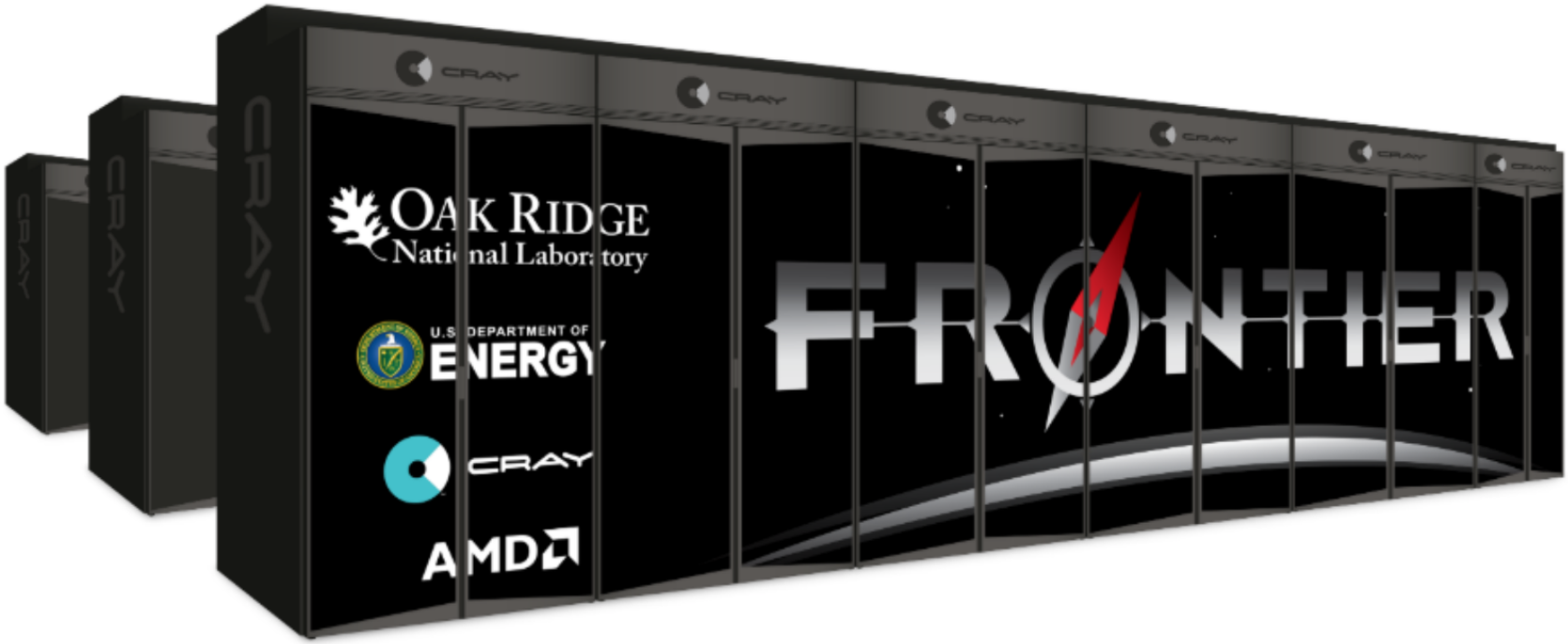
Intro

1. AMD and Quantum Monte Carlo
2. Variational Quantum Monte Carlo: Introduction
3. N electron systems
   - The need for antisymmetry
   - Comparison of Slater and Vandermonde determinants
4. Deep-learning-based ansatz: PauliNet
   - Description of PauliNet
   - Proposed improvement: Vandermonde with PauliNet
5. Conclusions and new directions

Outline for section 1

AMD and Frontier (exascale computing)



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- Radeon GPUs

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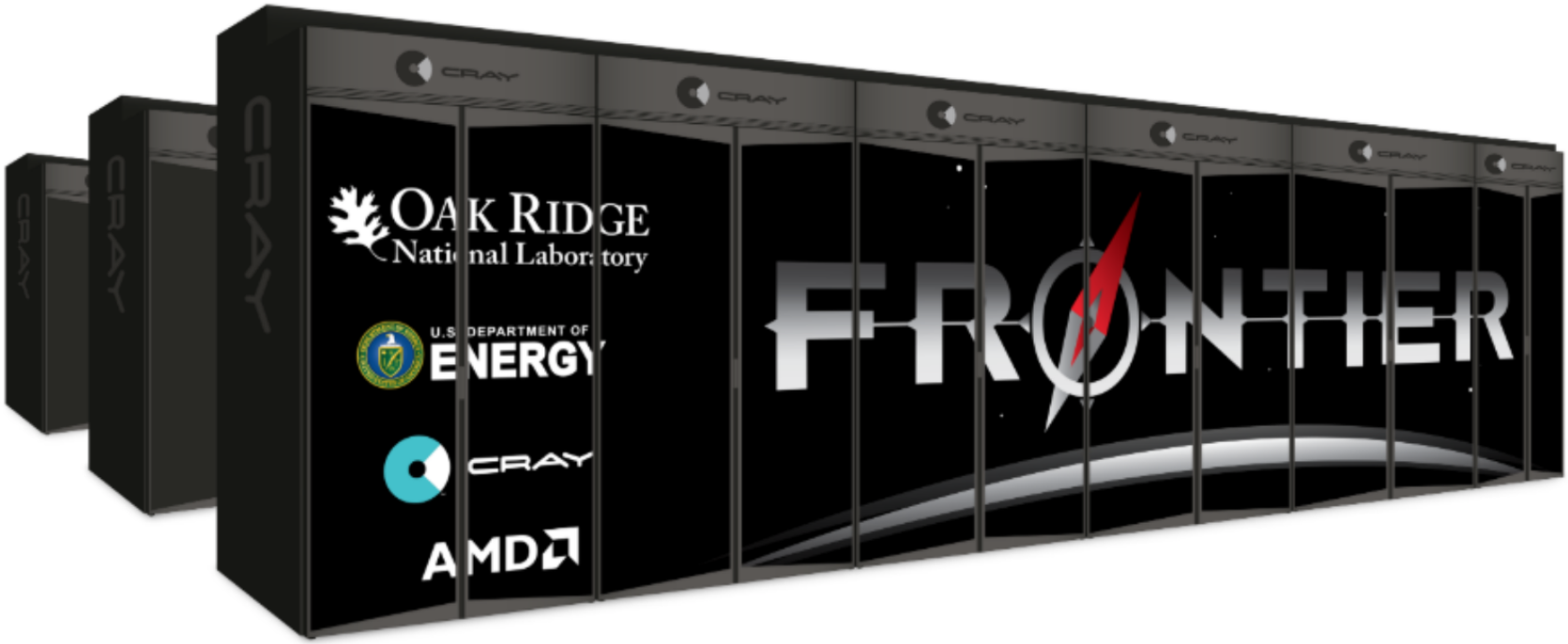
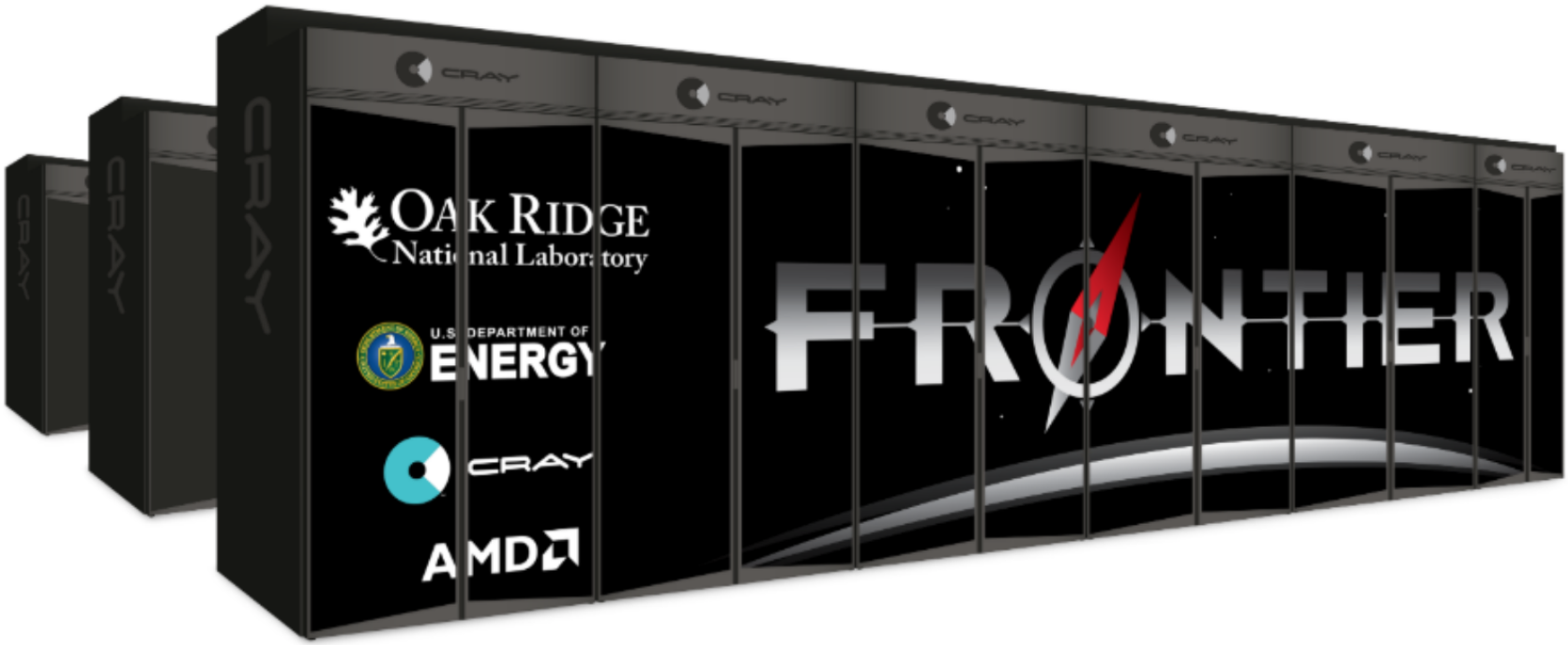
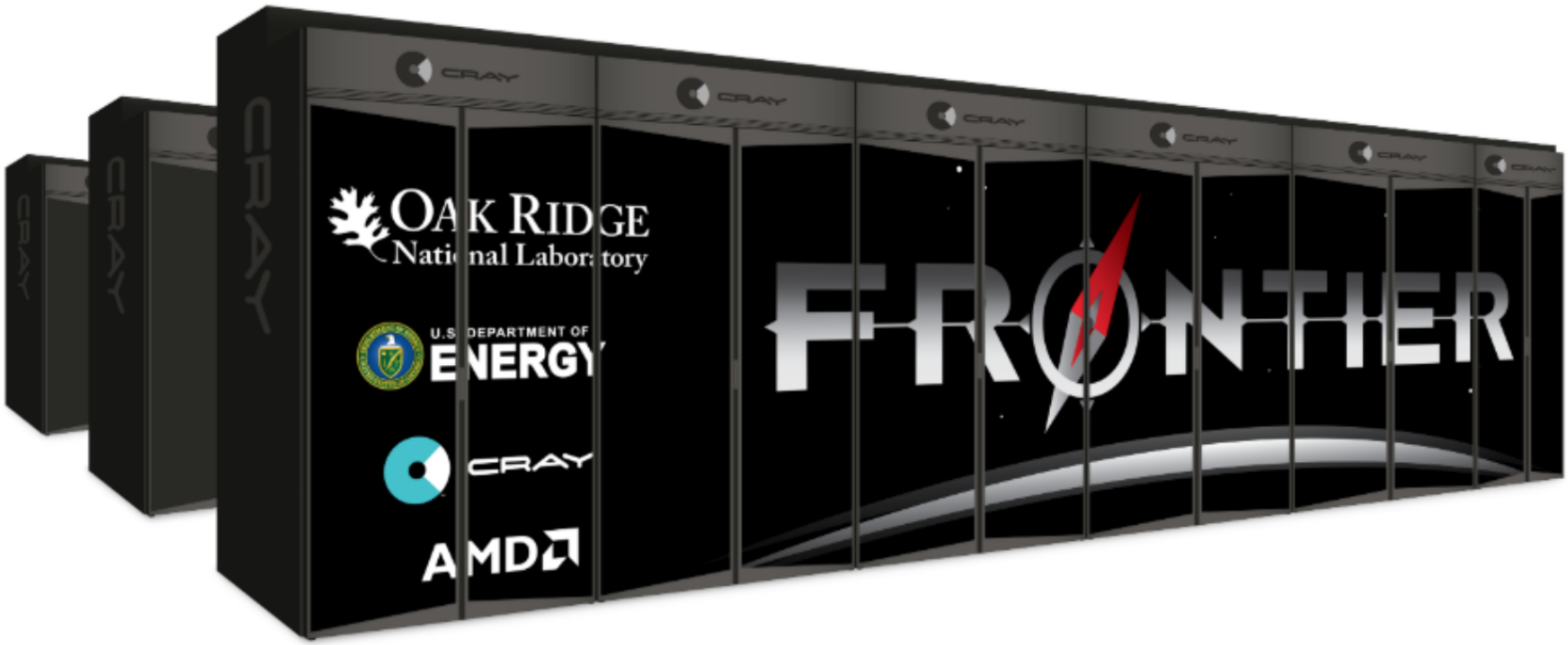


- Epyc CPUs
- Radeon GPUs
- In 2021: Frontier will become the largest supercomputer ever constructed.

QMCPACK


CRAY
OAK RIDGE
National Laboratory
U.S. DEPARTMENT OF
ENERGY
CRAY
AMD
FRONTIER

QMCPACK



- Uses **Quantum Monte Carlo** methods to solve the Schrödinger equation $\hat{H}\Psi = E\Psi$.

Significance of Quantum Monte Carlo

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- Knowing the configuration of electrons can help infer chemical properties of molecules and materials.

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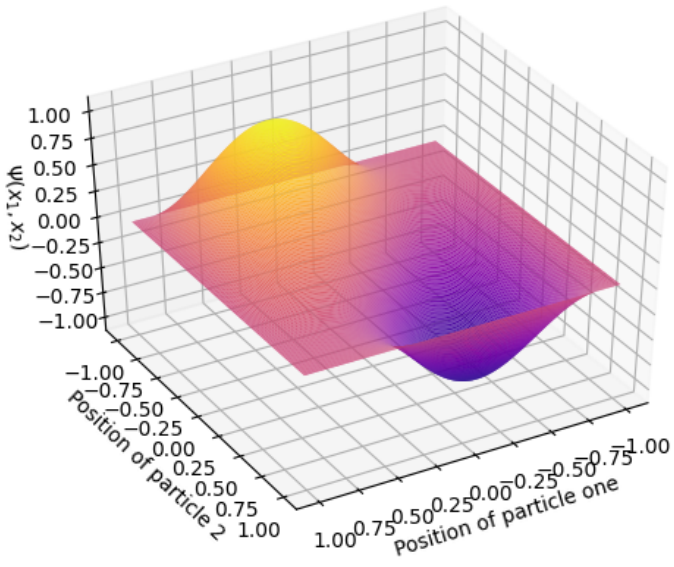
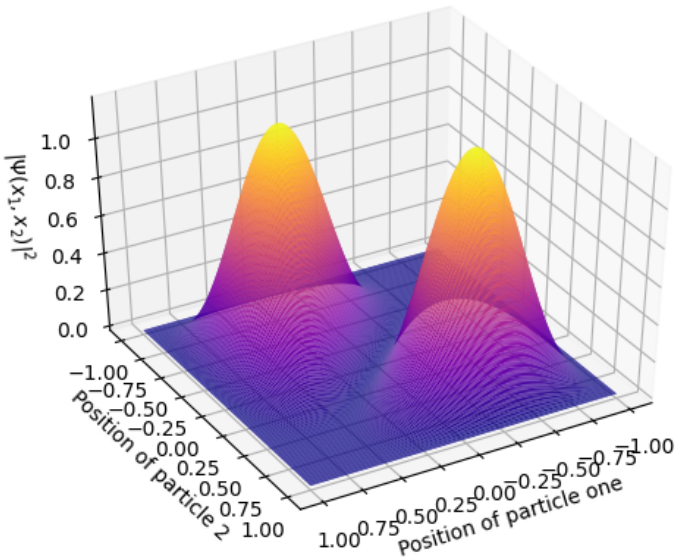
- In mathematical terms, the wavefunction must obey **antisymmetry**. This means that **exchanging two particles must flip only the sign of the wavefunction**:

$$\Psi(\cdots, r_i, \cdots, r_j, \cdots) = -\Psi(\cdots, r_j, \cdots, r_i, \cdots)$$

Example: two fermions in a 1-dimensional box





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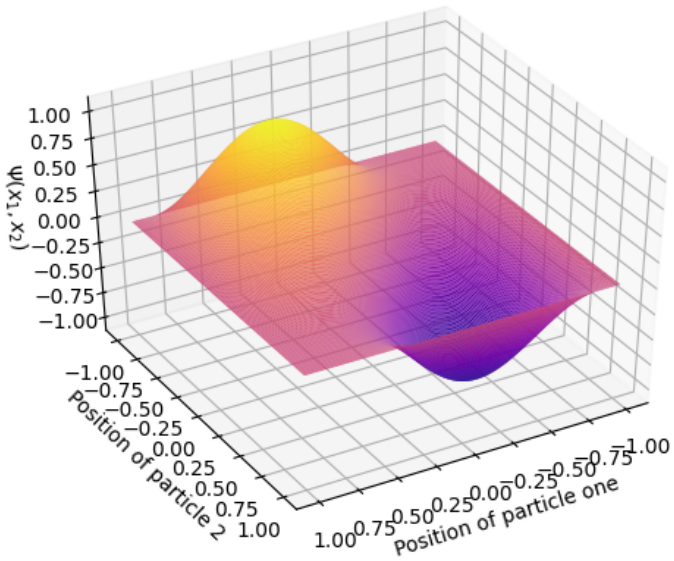

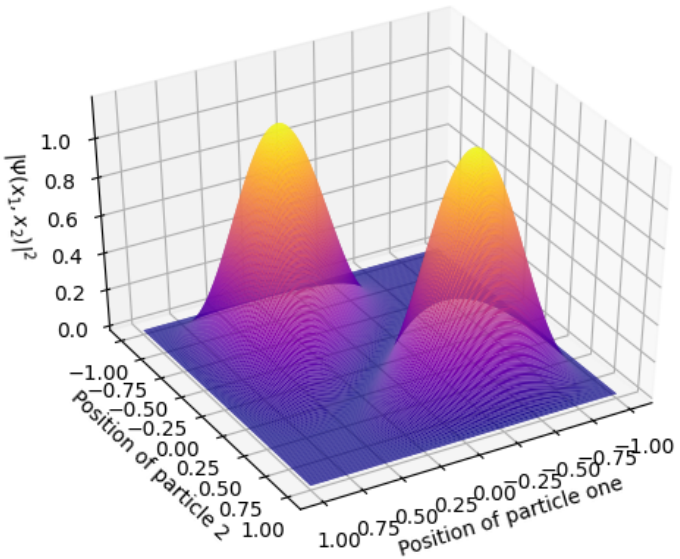

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- **Solution 2** Use neural networks as function approximators.

Many methods e.g. PauliNet do both.

Our focus

- We aim to investigate the feasibility of **deep learning** to produce new and powerful forms of **ansatz**.
- Need to enforce a property known **antisymmetry** due to the **Pauli exclusion principle**.
- The traditional method for enforcing antisymmetry uses a technique known as the **Slater determinant**, which is a major part of the computational cost of ansatz that use it.
- We focus on a different technique for enforcing antisymmetry known as the **Vandermonde determinant**.

Slater determinants

$$\Psi(r_1, \cdots, r_N) = \begin{vmatrix} \varphi_1(r_1) & \varphi_2(r_1) & \cdots & \varphi_N(r_1) \\ \varphi_1(r_2) & \varphi_2(r_2) & \cdots & \varphi_N(r_2) \\ \vdots & \vdots & \ddots & \vdots \\ \varphi_1(r_N) & \varphi_2(r_N) & \cdots & \varphi_N(r_N) \end{vmatrix}$$

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Computational cost: $O(N^3)$

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Computational cost: $O(N^2)$

Outline for section 2

The ground state energy of the system

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- Variational Monte Carlo is used to find the **ground state energy** of the system.
- All wavefunctions ϕ other than the true ground state Ψ_0 have higher energy: $\mathbb{E}_{\Psi_0}[E] \leq \mathbb{E}_{\phi}[E]$.
- The system's properties are defined by an operator H known as the Hamiltonian. Given H and the wavefunction Ψ, the expected energy of the system is:

$$\mathbb{E}[E] = \frac{\int \Psi_\alpha^*(\vec{r}) H \Psi_\alpha(\vec{r}) dV}{\int |\Psi_\alpha(\vec{r})|^2 dV}$$

We want to minimize this quantity.

In general, the expected energy cannot be computed analytically. An approximation is

$$\mathbb{E}[E] \approx \frac{1}{N} \sum_{i=1}^{N} E_L(x_i)$$

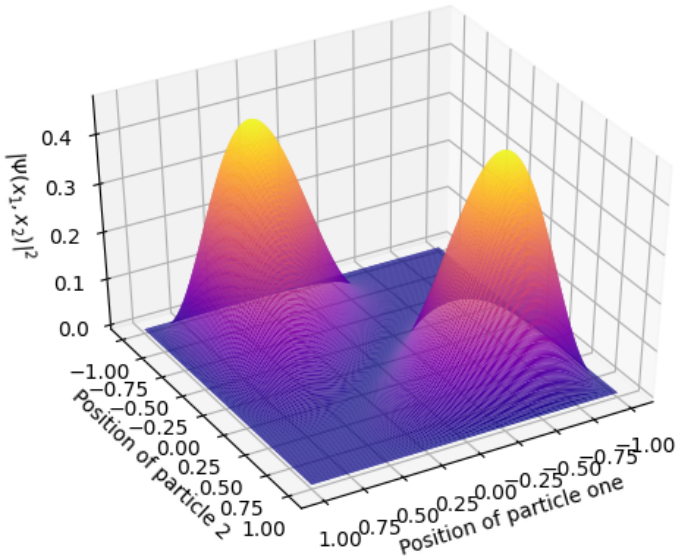
- E_L is the **local energy** associated with a particle in a single, specific configuration.
- $\{x_i\}$ is a set of random samples from $|\Psi_\alpha(\vec{r})|^2$. These are drawn using Markov-chain Monte Carlo (MCMC).

Sampling with Markov-Chain Monte Carlo

Using the two particles in a box ansatz as an example. We set $(\alpha_1, \alpha_2) = (1.95, 0.95)$.

$\Psi_{\alpha_1,\alpha_2}(x_1, x_2) = (1 - x_1^{2\alpha_1})(1 - x_2^{2\alpha_2})x_2 - (1 - x_2^{2\alpha_1})(1 - x_1^{2\alpha_2})x_1$

Sampling with MCMC 4500 times.



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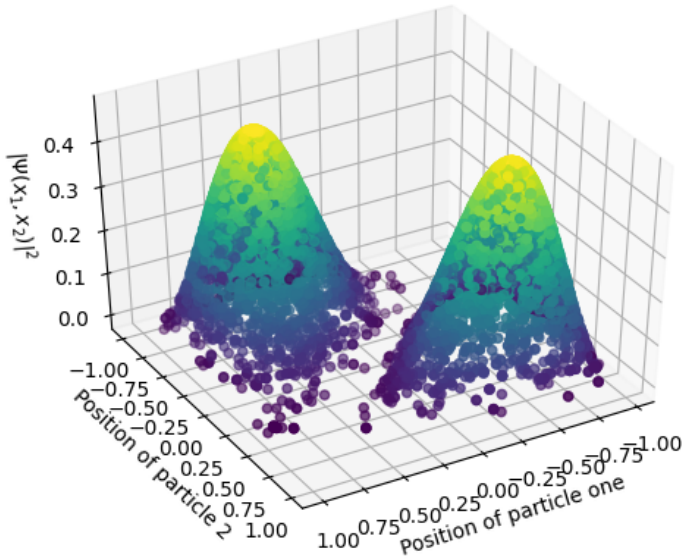
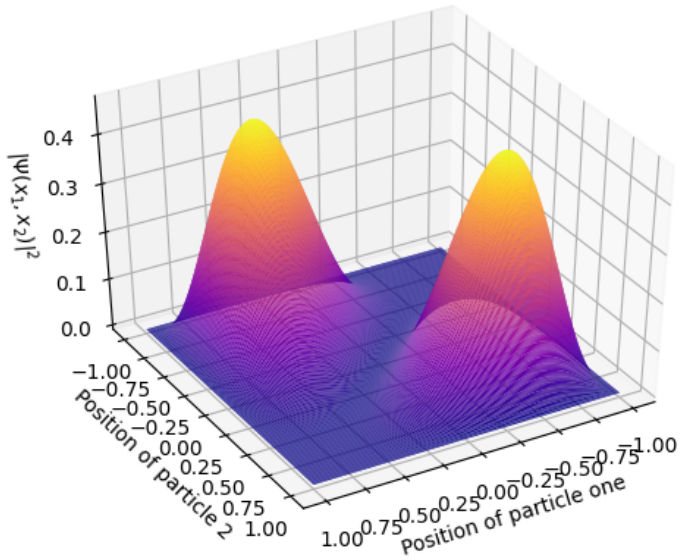


Sampling with MCMC 10000 times.



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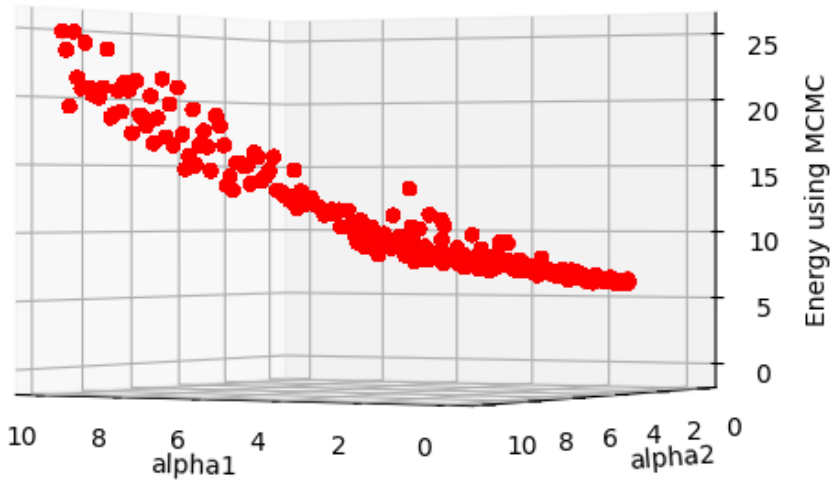
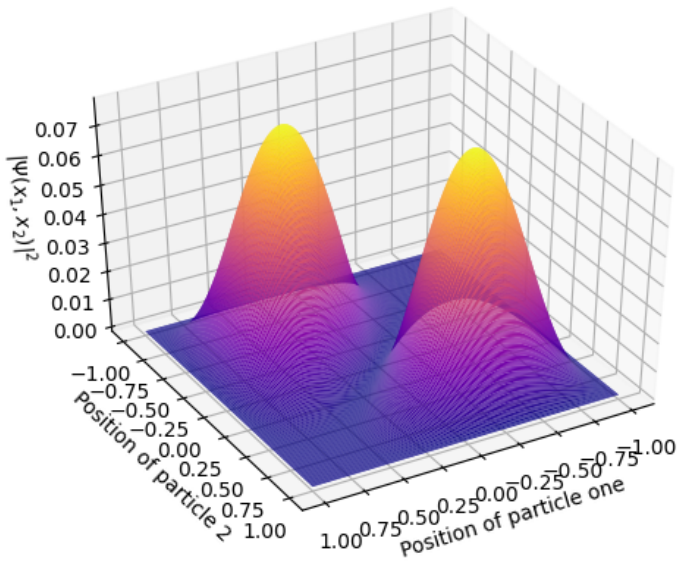
Gradient descent on the approximated energy

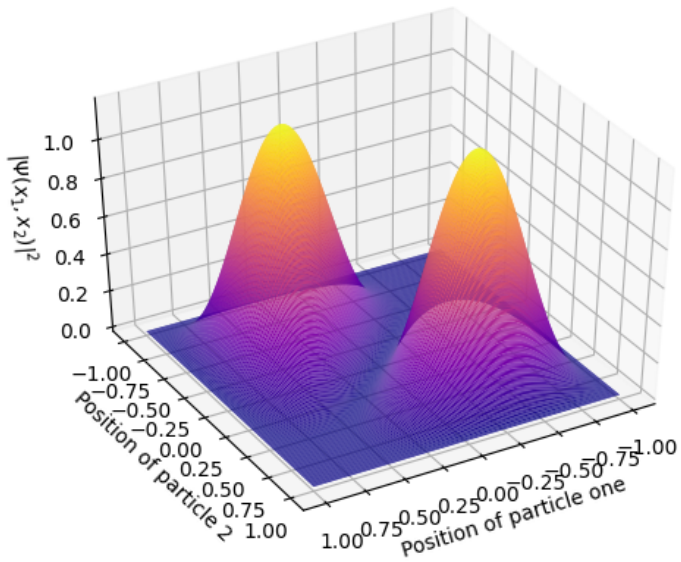


GD to approximate ground state energy of the two fermions in a box model. $E_0 = 6.168$ in our units. Converges to $\alpha_1 = 0.876$ and $\alpha_2 = 0.52$.

Ansatz with optimal alphas vs Exact solution



Using $\alpha_1 = 0.876$ and $\alpha_2 = 0.52$ with our ansatz.



Exact solution.

Outline for section 3

N-electron systems

We focus on the study of N-electron systems: that is, atoms and molecules with electrons surrounding the nucleus. The Hamiltonian (which defines the energy) of systems like is:

$$\sum_{i=1}^{N}(-\frac{\hbar^2}{2m}\nabla_i^2) + V_{e-n}(\vec{r_1},...,\vec{r_N}) + V_{e-e}(\vec{r_1},...,\vec{r_N})$$

- Kinetic energy of electrons: defined in terms of Laplacian of the wavefunction.
- Electron-nucleus energy
- Electron-electron energy

Pauli exclusion principle

Recall the: **Pauli exclusion principle:** Two identical fermions cannot occupy the same state.

- $|\Psi(\cdots, r_i, \cdots, r_j, \cdots)|^2 = |\Psi(\cdots, r_j, \cdots, r_i, \cdots)|^2$.
- $\Psi(\cdots, r_i, \cdots, r_j, \cdots) = -\Psi(\cdots, r_j, \cdots, r_i, \cdots)$

A first attempt at an ansatz

Suppose we have single-electron basis functions φ_j. A first attempt at an ansatz might be:

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This is known as the Hartree product ansatz, but it does not enforce antisymmetry when r_i, r_j switched.

One can extend the idea of the Hartree product ansatz as follows:

$$\Psi(r_1, \cdots, r_N) = \begin{vmatrix} \varphi_1(r_1) & \varphi_2(r_1) & \cdots & \varphi_N(r_1) \\ \varphi_1(r_2) & \varphi_2(r_2) & \cdots & \varphi_N(r_2) \\ \vdots & \vdots & \ddots & \vdots \\ \varphi_1(r_N) & \varphi_2(r_N) & \cdots & \varphi_N(r_N) \end{vmatrix}$$

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Because this is a determinant, permuting r_i, r_j swaps rows and therefore swaps sign – antisymmetry is enforced perfectly.

The Vandermonde determinant

Suppose we have some basis function φ applied to each electron configuration. The Vandermonde determinant is defined as:

$$\det_V = \begin{vmatrix} 1 & \varphi(r_1)^1 & \varphi(r_1)^2 & \cdots & \varphi(r_1)^{N-1} \\ 1 & \varphi(r_2)^1 & \varphi(r_2)^2 & \cdots & \varphi(r_2)^{N-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \varphi(r_N)^1 & \varphi(r_N)^2 & \cdots & \varphi(r_N)^{N-1} \end{vmatrix}$$

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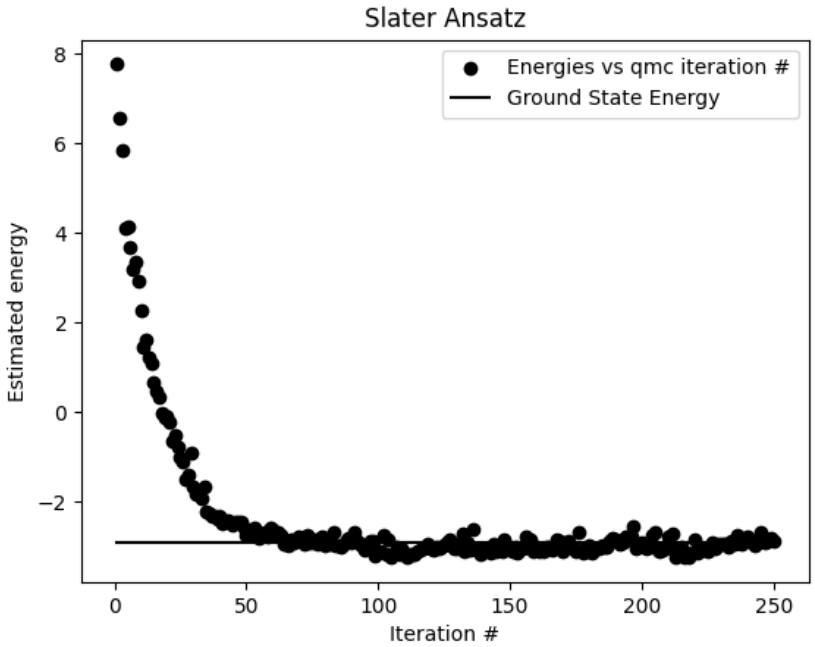
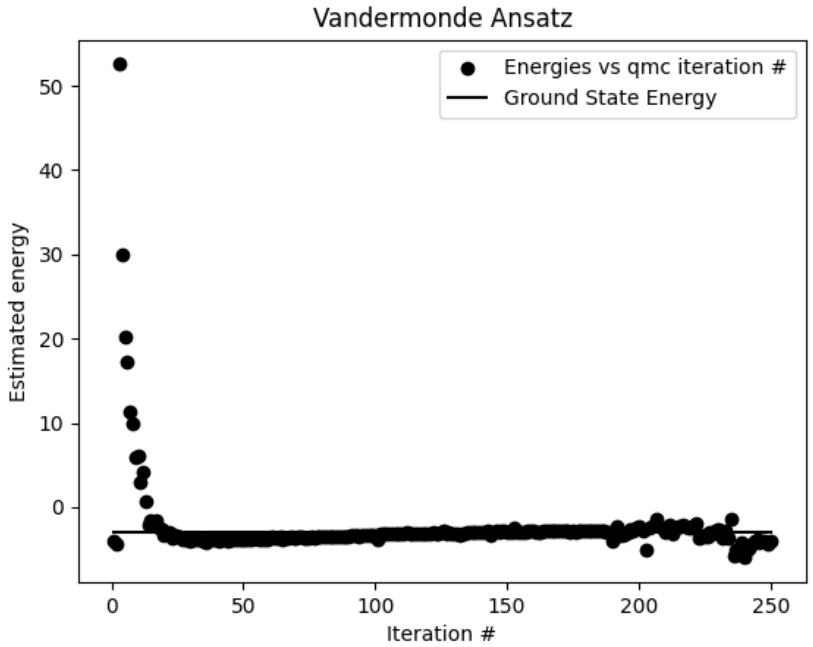
But it can be computed using a more efficient expression.

$$\det_V = \prod_{i<j} (\varphi(r_i) - \varphi(r_j))$$

Helium (2 electrons)
Slater vs Vandermonde

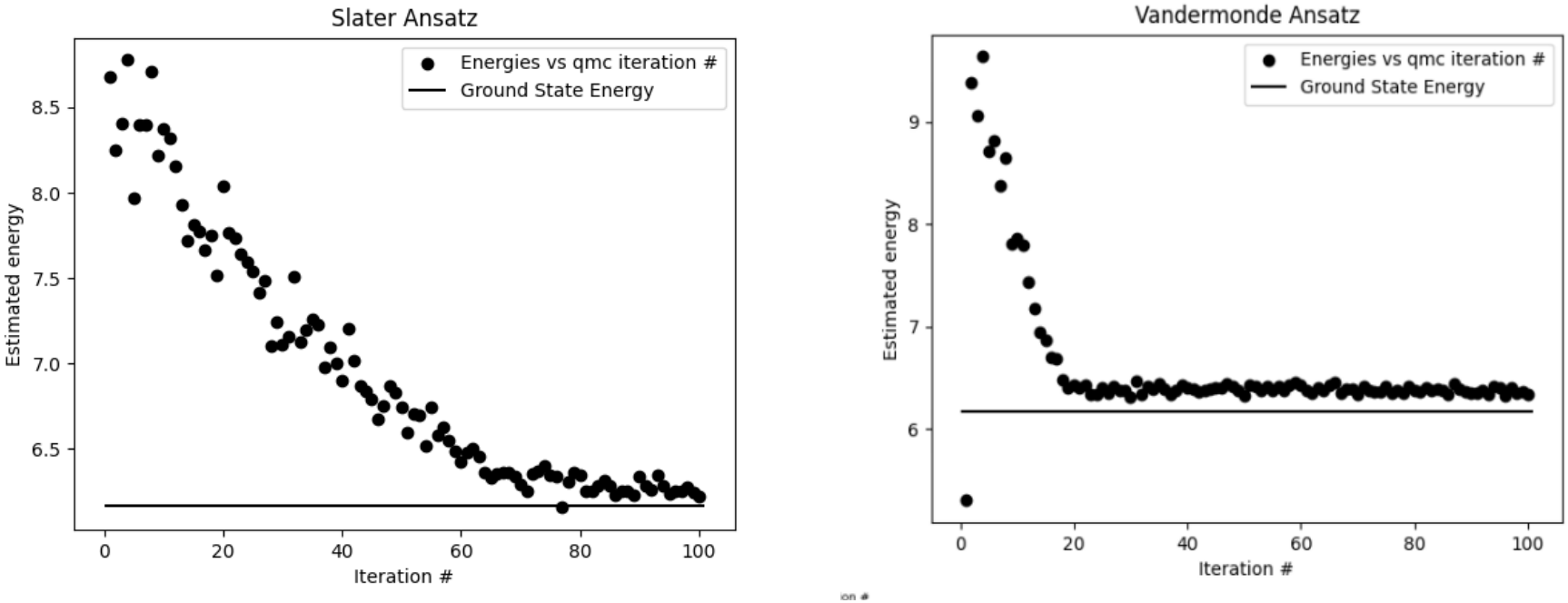




$$\Psi_{slat}(r_1, r_2) = e^{-\alpha_1 r_1} e^{-\alpha_2 r_2} - e^{-\alpha_1 r_2} e^{-\alpha_2 r_1}$$

$$\Psi_{Van}(r_1, r_2) = e^{-\alpha_1 (r_1 + r_2)} (e^{-\alpha_2 r_1} - e^{-\alpha_2 r_2})$$

Two particles in a box: Vandermonde and Slater



Convergence plot for the two-fermions-in-a-box system near the ground state energy

Outline for section 4

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- The structure of the ansatz has a widely-used design – what is known as a "Slater-Jastrow-Backflow" ansatz. (QMCPACK uses a similar form.)
- But parts of this are replaced with flexible neural networks. The weights of these networks are what varies to minimize the energy.

PauliNet: the ansatz itself

For electrons with coordinates r_i, the ansatz is as follows:

$$\Psi_\alpha(r) = e^{\gamma(r)+J_\alpha(r)} \sum_p c_p \det(\tilde{\varphi}^\uparrow_{\mu_p}(r)) \det(\tilde{\varphi}^\downarrow_{\mu_p}(r))$$

$$\tilde{\varphi}_\mu(r)_i = \varphi_\mu(r_i) f_{\mu,\alpha}(r)_i$$

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- $f_{\mu,\alpha}$ are the backflow factors which scale the Hartree-Fock functions: another neural network.

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- J_α is what is known as the Jastrow factor, represented as a neural network.
- $f_{\mu,\alpha}$ are the backflow factors which scale the Hartree-Fock functions: another neural network.
- $\gamma(r)$ enforces electron-electron cusp conditions.

PauliNet: the ansatz itself

For electrons with coordinates r_i, the ansatz is as follows:

$$\Psi_\alpha(r) = e^{\gamma(r)+J_\alpha(r)} \sum_p c_p \det(\tilde{\varphi}^\uparrow_{\mu_p}(r)) \det(\tilde{\varphi}^\downarrow_{\mu_p}(r))$$

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- $\gamma(r)$ enforces electron-electron cusp conditions.
- Slater determinants are used (split by spin up/down of particles).

Modification to PauliNet: Vandermonde Determinants

- We replace the Slater determinants in the PauliNet ansatz with Vandermonde determinants.
- We define $\tilde{\varphi}(r_j) = \prod_{i=1}^{N} \tilde{\varphi}_i(r_j)$ and then take a Vandermonde determinant of $(\tilde{\varphi}(r_1), \tilde{\varphi}(r_2), \cdots)$

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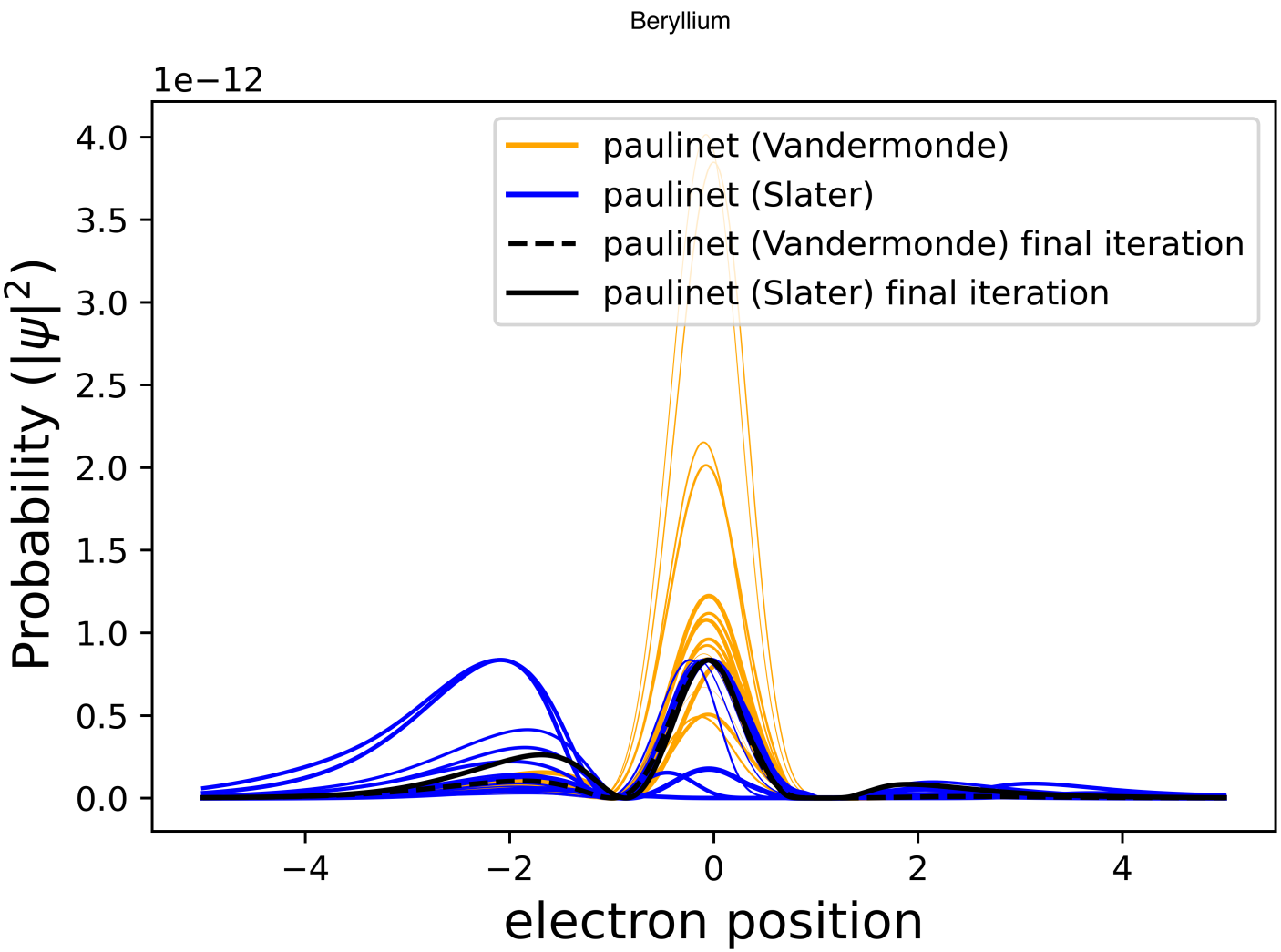
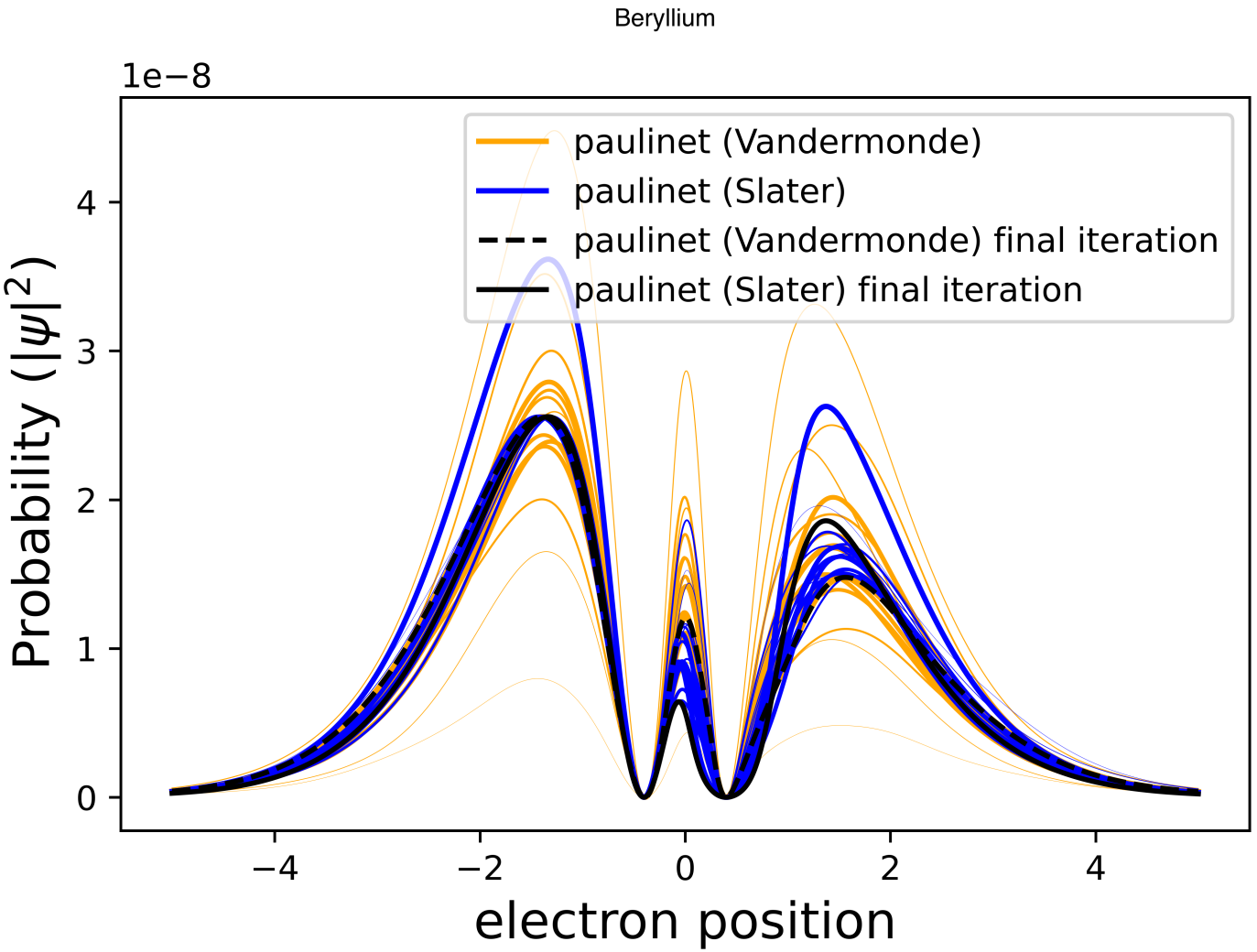
- Certain boundary conditions are preserved by Slater determinant but lost when moving to the Vandermonde determinant. We premultiply by a wavefunction applied to each electron $\varphi(r_1)\varphi(r_2)\cdots$ to preserve this property.

PauliNet: Slater v Vandermonde



PauliNet: Slater v Vandermonde



Outline for section 5

The Vandermonde determinant

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- While the use of neural networks in VMC can result in highly accurate solutions, further new approaches are needed to best balance computational cost with accuracy.

Conclusions and new directions

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Conclusions and new directions

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- In principle a neural network can learn any arbitrary function. But even with the most complex and flexible deep learning ansatz, enforcement of physical properties by construction seems to be quite valuable.
- We have focused only on the ground state and the time-independent Schrödinger equation. Considering whether VMC techniques could be used to solve for higher excited states, or a time-evolving version of the equation, would be interesting.

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Questions?