Exercise Sheet 4

Due: 21.05.24 14h00

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General Regulations.

- Please hand in your solutions in groups of up to two people.
- Your solutions to theoretical exercises can be either handwritten notes (scanned), or typeset using LaTeX. In case you hand in handwritten notes, please make sure that they are legible and not too blurred or low resolution.
- For the practical exercises, always provide the (commented) code as well as the output, and don't forget to explain/interpret the latter. Please hand in both the notebook (`.ipynb`), as well as an exported pdf.
- Submit all your files in the Übungsgruppenverwaltung, only once for your group.

1 Two electrons on a ring

Consider the following scenario, two electrons are in a one dimensional periodic potential, with the following Hamiltonian:

$$\hat{H} = -\frac{1}{2}\left(\nabla_1^2 + \nabla_2^2\right) + \frac{1}{2}V(x_1 - x_2), \quad x_1, x_2 \in [0, 2\pi), \tag{1}$$

where the potential is given parametrized by an interaction strength k

$$V(x_1 - x_2) = \frac{k}{\sqrt{2 - 2\cos(x_1 - x_2)}}. \tag{2}$$

The potential is the Coulomb force the electron feels, from the electron across the ring with radius 1 embedded in a 2D space.

(a) Think about their wave function $\Psi(x_1, x_2)$. List the complete set of conditions that the wave function must fulfill.

Hint: Remember antisymmetry requirement and that the domain is periodic. (2 pts)

(b) Consider two limiting cases, of the electrostatic interaction being small ($k \approx 1$) and large ($k \gg 1$) relative to the kinetic contribution. Reason about the appearance of the lowest energy state in both cases, keeping in mind your previous answer. (2 pts)

In the next step, we will approximate the ground state by using gradient descent to minimize the energy of the system. For this we will discretize the system, and solve it on a $M \times M$ grid.

(c) Write down the Hamiltonian in a discretized fashion, such that you can use it to calculate the total energy of a state given by a real matrix $\Psi \in \mathbb{R}^{M \times M}$, where the elements correspond to values of the wave function on the grid.

Hint: Look up how the second derivative is calculated on a grid. (3 pts)

(d) Calculate a random initial state, plot it and calculate the energy of this state.

Hint: What property does the initial state matrix need to have? (3 pts)

(e) Use the gradient descent algorithm and the derivative of the total energy to calculate updates, to your random initial state. Plot your resulting ground state for the interaction strengths $k = 1$ and $k = 100$. Do the experiments support your theoretical considerations from task **(b)**?

Hint: Normalize your state after each gradient step and if the energy increases rather than decreases, your step size is probably too large. You do not need to enforce symmetry conditions, when optimizing your state. (6 pts)

(f) In the limit of strong electrostatic interaction ($k \gg 1$): argue if a Slater determinant can represent the ground state faithfully. (2 pts)

(g) Estimate the memory footprint of finding the ground state for $N = 2, 10, 100$ electrons on a ring. (2 pts)

(h) Use an automatic differentiation framework such as pytorch and repeat your experiments from **(e)**. Compare the speed. (**Bonus:** 3 pts)

(i) Use the automatic differentiation framework to find the best Slater determinant in the strong correlation limit ($k = 100$). Compare to your insights from **(f)**. (**Bonus:** 2 pts)