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Neural Network Variational Monte Carlo for Positronic Chemistry

Friday 5 April 2024 12:00 (30 minutes)

In recent years, several authors have demonstrated that deep neural networks can produce excellent representations of the many-body wavefunction for use in variational Monte Carlo calculations of the ground-state properties of atoms, small molecules, and simple solids. In this talk, I will briefly introduce the principle of neural network variational Monte Carlo, and discuss how it is quite straightforward to extend the neural network wavefunction to the description of multi-component (positrons and electrons) wavefunctions. I will share our initial, quite promising, results for the positron binding energy and annihilation rate of several well-studied molecules, and discuss why NNVMC may be particularly well suited for this problem.

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