Semester Project: Variational Monte-Carlo for strongly correlated bosons in continuous space

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Introduction

Variational Monte-Carlo

Exploits the *variational principle*, which states that the ground-state $|\Psi_0\rangle$ minimizes the energy:

$$|\Psi_0\rangle = \underset{|\Psi\rangle}{\operatorname{argmin}} \left[\frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle} \right] \tag{1}$$

Given an ansatz $|\Psi(\boldsymbol{\theta})\rangle$, the parameters are optimized so as to reach the minimum in energy.

Observables: Almost every observable can be estimated as a stochastic expectation value over its *local* counterpart:

$$\langle \hat{O} \rangle = E_{\Pi(\boldsymbol{x})} \left[O_{\mathrm{loc}}(\boldsymbol{x}) \right] \text{ where } O_{\mathrm{loc}}(\boldsymbol{x}) = \int d\boldsymbol{x}' O_{\boldsymbol{x}\boldsymbol{x}'} \frac{\Psi(\boldsymbol{x}')}{\Psi(\boldsymbol{x})} \tag{2}$$

Simulation of Heisenberg model

$$H_{2-spin} = -J(\sigma_x^{(1)}\sigma_x^{(2)} + \sigma_y^{(1)}\sigma_y^{(2)} + \sigma_z^{(1)}\sigma_z^{(2)})$$

$$H_{3-spin} = -J(\sigma_x^{(1)}\sigma_x^{(2)} + \sigma_x^{(2)}\sigma_x^{(3)} + \sigma_y^{(1)}\sigma_y^{(2)} + \\ + \sigma_y^{(2)}\sigma_y^{(3)} + \sigma_z^{(1)}\sigma_z^{(2)} + \sigma_z^{(2)}\sigma_z^{(3)})$$

Conclusions

- A quantum computer would potentially allow to study many unexplored systems.
- NISQ still far away from having fully functional UQS at disposal.
- Accuracy of a simulation to be assessed by considering digital and hardware error.