Bosonic and Fermionic NN-VMC

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1 Bosonic Ansatz

Consider the system of N bosons, with Hamiltonian:

$$\hat{H} = \sum_{i=1}^{N} \left(-\frac{1}{2m} \frac{\partial^2}{\partial x_i^2} + \frac{1}{2} m\omega^2 x_i^2 \right) + \sum_{i<j}^{N} \left(g\delta \left(x_i - x_j \right) + \sigma |x_i - x_j| \right)$$

Where our interaction strength parameters are g and σ.

We define our bosonic ansatz ψ_B:

$$\psi_B \left(x_1, x_2, \ldots, x_N \right) = e^{-\mathcal{A}(x_1, x_2, \ldots, x_N)}$$

where

$$\mathcal{A} \left(x_1, x_2, \ldots, x_N \right) = \mathrm{NN} \left(\xi_1, \xi_2, \ldots, \xi_N \right) + \omega \sum_{i}^{N} x_i^2$$

Where NN is the neural network function, and ω is a constant.

1.1 Energy and Gradient

We can compute the energy expectation value:

$$\mathcal{E} = \left\langle \sum_i \frac{1}{2m} \left(\frac{\partial^2 \mathcal{A}}{\partial x_i^2} - \left(\frac{\partial \mathcal{A}}{\partial x_i} \right)^2 \right) + \frac{1}{2} m\omega^2 x_i^2 + \sum_{i<j} \left(\sigma |x_i - x_j| \right) + g \frac{N \left(N-1 \right)}{2} \frac{e^{-2\mathcal{A}(x_1, x_1, \ldots, x_N)}}{e^{-2\mathcal{A}(x_1, x_2, \ldots, x_N)}} \mathcal{D} \left(x_2 \right) \right\rangle_{\psi}$$

And the gradient in parameter space:

$$\begin{aligned}
\frac{\partial \mathcal{E}}{\partial \theta} = 2\mathcal{E} \cdot \left\langle \frac{\partial \mathcal{A} \left(x_1, \ldots, x_N \right)}{\partial \theta} \right\rangle_{\psi} \\
- 2 \left\langle \frac{\partial \mathcal{A} \left(x_1, \ldots, x_N \right)}{\partial \theta} \left[\sum_i \frac{1}{2m} \left(\frac{\partial^2 \mathcal{A}}{\partial x_i^2} - \left(\frac{\partial \mathcal{A}}{\partial x_i} \right)^2 \right) + \frac{1}{2} m\omega^2 x_i^2 + \sum_{i<j} \left(\sigma |x_i - x_j| \right) \right] \right\rangle_{\psi} \\
- 2g \frac{N \left(N-1 \right)}{2} \left\langle \frac{\partial \mathcal{A} \left(x_1, x_1, \ldots, x_N \right)}{\partial \theta} \frac{e^{-2\mathcal{A}(x_1, x_1, \ldots, x_N)}}{e^{-2\mathcal{A}(x_1, x_2, \ldots, x_N)}} \mathcal{D} \left(x_2 \right) \right\rangle_{\psi}
\end{aligned}$$

2 Fermionic Ansatz