Variational Monte-Carlo for strongly correlated bosons in continuous space

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Contents

Introduction

- Many-body quantum systems very difficult to study - *ab initio* simulations often unfeasible (e.g. N constituents with d d.o.f $\implies \text{dim}(\mathcal{H}) = d^N$).

- **Possible solution:**
  Machine Learning (ML) techniques + MC statistical methods.
  ANNs = Universal function approximators. Can also encode relevant physical symmetries in the architectures.

- Recent **state-of-the-art** has allowed to study systems with both discrete and continuous degrees of freedom [1–6].

In this study: 2D boson particles interacting through a gaussian core potential.

Variational Monte-Carlo (VMC)

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

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

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:

$$\langle\hat{O}\rangle = E_{\Pi(\boldsymbol{x})}\Big[O_{\mathsf{loc}}(\boldsymbol{x})\Big] \text{ where } O_{\mathsf{loc}}(\boldsymbol{x}) = \int d\boldsymbol{x}' O_{\boldsymbol{x}\boldsymbol{x}'} \frac{\Psi(\boldsymbol{x}')}{\Psi(\boldsymbol{x})}$$

over the distribution $\Pi(\boldsymbol{x}) = \frac{|\Psi_{\boldsymbol{\theta}}(\boldsymbol{x})|^2}{\int d\boldsymbol{y} |\Psi_{\boldsymbol{\theta}}(\boldsymbol{y})|^2}$.

Periodic Boundary Conditions (PBCs)

PBCs allow to access the bulk properties of a system. For a simulation box of size $\boldsymbol{L} = (L_1, ..., L_d)$ we map each vector $\boldsymbol{x}_i$ describing said system into a periodic representation:

$$\boldsymbol{x}_i \longmapsto \boldsymbol{r}_i = \left(\sin\left(\frac{2\pi}{\boldsymbol{L}}\boldsymbol{x}_i\right), \cos\left(\frac{2\pi}{\boldsymbol{L}}\boldsymbol{x}_i\right) \right)$$

To compute the euclidean distance between two particles, we adopt the *minimum image* convention:

$$d(i,j) = \left\| \boldsymbol{x}_i - \boldsymbol{x}_j - \boldsymbol{L} \left\lfloor \frac{\boldsymbol{x}_i - \boldsymbol{x}_j}{\boldsymbol{L}} \right\rceil \right\|$$

In the NQS architecture we will instead use the differentiable variant:

$$d_{\sin}(i,j) = \left\| \sin\left(\frac{\pi(\boldsymbol{x}_i - \boldsymbol{x}_j)}{\boldsymbol{L}} \right) \right\|$$

Gaussian cores

In this study, we investigate the physical properties of bosons with spin zero in PBCs interacting through a repulsive **gaussian core** potential in 2D. The entire Hamiltonian reads:

$$\hat{H} = \hat{T} + \hat{V} = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\vec{\nabla}_i^2 + \varepsilon\sum_{i<j}^{N}\exp\left(-\frac{d(i,j)}{2\sigma^2}\right) =$$

$$= -\frac{\Lambda}{2}\sum_{i=1}^{N}\vec{\nabla}_i^2 + \sum_{i<j}^{N}\exp\left(-\frac{d(i,j)}{2}\right)$$

where in the last equality we simplified the expression by renormalizing the coordinates by σ^2 and defining $\Lambda = \hbar^2/m\varepsilon\sigma^2$.

NQS architecture (1)

Message-passing neural networks (MPNNs) to represent data as graphs (nodes+edges). Able to encode symmetries [7].

We transform the data by feeding it into a composition of $\mathcal{N}$ graphs. We are interested in spatial structure of system $\implies$ nodes: 1-body coord's / edges: 2-body coord's. For the μ-th graph:

$$\boldsymbol{n}_i^{(\mu)} = \left(\boldsymbol{r}_i, \boldsymbol{h}_i^{(\mu)}\right)$$

$$\boldsymbol{e}_{ij}^{(\mu)} = \left(\boldsymbol{r}_{ij}, d_{\sin}(i,j), \boldsymbol{h}_{ij}^{(\mu)}\right)$$

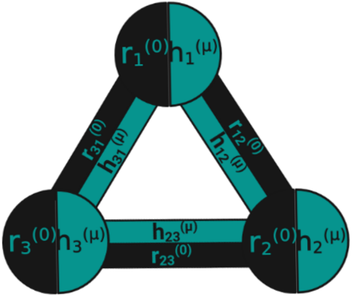

Figure: Schematic of three-particle MPNN, with nodes (circles) and edges (connections).

NQS architecture (2)

Hidden nodes and edges:

$$\boldsymbol{h}_i^{(\mu)} = \boldsymbol{f}\left(\boldsymbol{n}_i^{(\mu-1)}, \sum_{i\neq j} \boldsymbol{m}_{ij}^{(\mu)}\right), \quad \boldsymbol{h}_{ij}^{(\mu)} = \boldsymbol{g}\left(\boldsymbol{e}_{ij}^{(\mu-1)}, \boldsymbol{m}_{ij}^{(\mu)}\right)$$

where $\boldsymbol{m}_{ij}^{(\mu)} = \boldsymbol{\phi}\left(\boldsymbol{e}_{ij}^{(\mu-1)}\right)$. The functions $\boldsymbol{f}, \boldsymbol{g}, \boldsymbol{\phi}$ are simple feed-forward artificial neural networks.

Permutation equivariance: ensured by taking same initial hidden variables for all (i, j). In summary, we construct the ansatz by transforming the particle positions into backflow coordinates $\tilde{\boldsymbol{x}}_i = \mathsf{MPNN}(\boldsymbol{x})_i$ and feed them into a final MLP:

$$\log[\Psi_{\boldsymbol{\theta}}(\boldsymbol{x})] = \sum_i \boldsymbol{\rho}(\tilde{\boldsymbol{x}}_i) = \sum_i \boldsymbol{\rho}(\mathsf{MPNN}(\boldsymbol{x})_i)$$

Investigating the physical structure

Radial correlation function:

$$g_2(\boldsymbol{r}) = \frac{1}{N\rho} \langle \sum_{i \neq j}^{N} \delta(\boldsymbol{r} - \boldsymbol{r}_{ij}) \rangle$$

Pair correlation function:

$$g_2(r) = \frac{1}{N\rho} \frac{1}{4\pi r^2} \langle \sum_{i \neq j}^{N} \delta(r - r_{ij}) \rangle$$

Both give us insight on the probability to find a particle in position $\boldsymbol{r}$ (or r) given a particle at the origin.

The structure factor, useful in determining scattering properties, can be used to infer the structural arrangement. It is given by:

$$S(\boldsymbol{q}) = \frac{1}{N} \left| \langle \sum_{i=1}^{N} e^{-i\boldsymbol{q}\cdot\boldsymbol{r}_i} \rangle \right|^2$$

Results - MPNN performances

$N = 16$; $\Lambda = 1/30$; SGD + SR; samples $= 5 \cdot 10^3$. Firstly, we study the impact of number of graphs and number of hidden layers in the architecture.

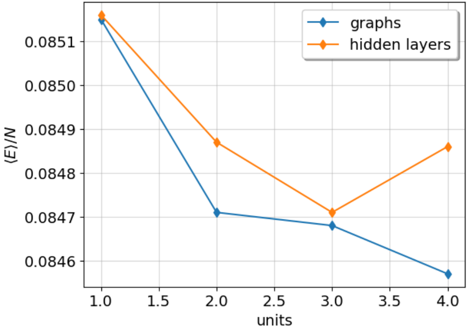

Figure: Ground-state energy at $\rho = 1/9$, for different number of graphs, hidden layers.

Table: Energy per particle for $\rho = 4/9, 1/9$ with and without applying LN after each activation layer in the MPNN architecture.

	No **LN**	**LN**
$\rho = 4/9$	1.00498	1.00403
$\rho = 1/9$	0.08534	0.08515

Results - phases of matter

Investigation of the average particle density's impact on the **phases of matter**

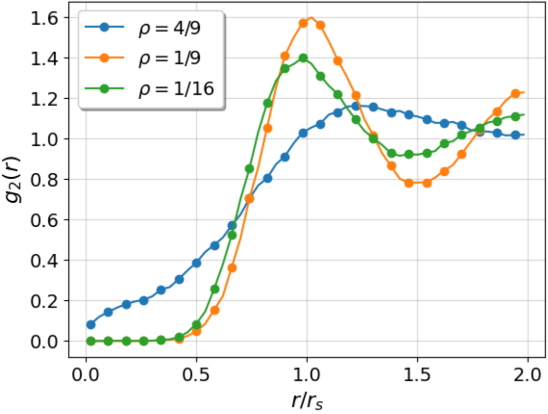

Figure: Pair correlation function at three different densities.

Results - geometry of the simulation box (1)

$\Lambda = 1/100$. Change of the aspect ratio of the simulation box
$\implies$ **relaxation** in energy up to $a = 2/\sqrt{3}$.

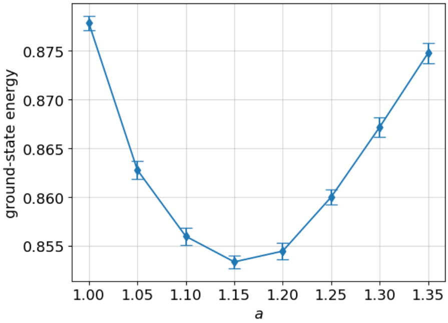

Figure: Ground-state energy against aspect ratio. Minimum in $a = 2/\sqrt{3}$.

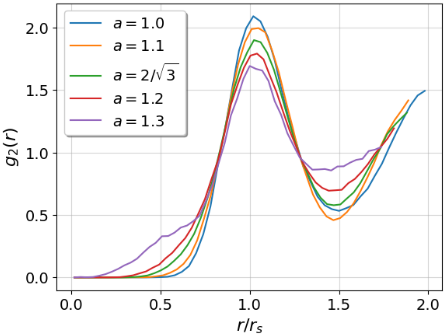

Figure: Pair correlation function at different values of the aspect ratio.

Results - geometry of the simulation box (2)

Radial correlation function localizes in well-defined **clusters** for higher a (two-particle unit cell becomes clearly visible). Structure factor also indicates a more rigid structure.

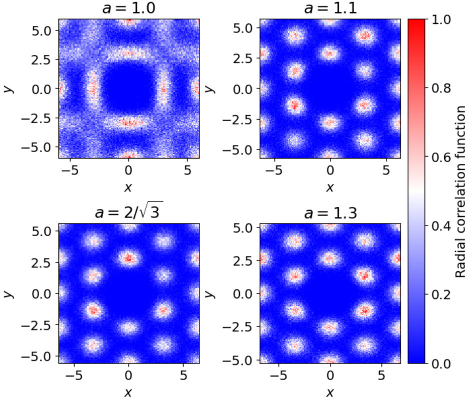

Figure: Radial correlation function for different aspect ratios.

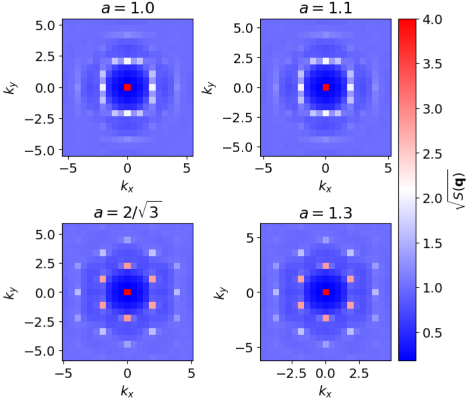

Figure: Square root of the structure factor for different aspect ratios.

Conclusions

- **MPNN** Neural Quantum States can **accurately** describe a continuous-variable system. Also largely **flexible**, no matter the physical parameters or the emergent structure of the system.
- Gaussian cores in **superfluid** phase at high and low densities. They instead self-assemble into a **crystalline** structure at intermediate densities ($\rho = 1/9$).
- Crystal is even more **rigid** when the environment conforms to the aspect ratio of the unit cell.

Thank you!

References

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