Analytic and Machine Learning Approaches to Composite Quantum Impurities

Awardee: Wojciech Rzadkowski

Supervisor: Prof. Dr. Mikhail Lemeshko

IST Austria (Institute of Science and Technology Austria)

Motivation

Many-body quantum physics – exponentially growing Hilbert space

In quantum mechanics, the size of the N- particle Hilbert space associated with grows exponentially with N, i.e. if a single body can be described with d-dimensional Hilbert space, the full N-body space is d^N-dimensional. In this project, we deal with this problem by harnessing the power of recently emerged techniques.

Recent developments in quasiparticle physics

The angulon quasiparticle was introduced in 2015 by Richard Schmidt and project supervisor Mikhail Lemeshko [1]. It describes a quantum rotor (such as a rotating molecule in a many-body bosonic bath (e.g. superfluid helium nanodroplets). The angulon has already been used for explaining the renormalization of molecular moments of inertia in superfluid helium, broadening of lines in spectra of symmetric-top molecules, rotation of cold molecular ions in a Bose-Einstein condensate, and microscopic modeling of the Einstein–de Hass effect, to name a few.

Recent successes of machine learning methods in quantum physics

Recent years have witnessed a tremendous success of machine learning applications in quantum many-body physics [2, 3]. These techniques have been so far applied mainly to lattice spin and bosonic systems. In this DOC project, we extend this to quasiparticles.

Machine learning approaches

The core ideas begind the approach that we develop are roughly based on from Ref. [4]. This method used variational principle. The goal is to introduce an Ansatz, $\psi(\vec{s})$ and minimize the energy:

$$E = \frac{\langle\psi|\,\hat{H}\,|\psi\rangle}{\langle\psi|\psi\rangle}. \tag{1}$$

In this approach, a Restricted Boltzmann Machine, which is a well-established concept in computer science, is used as a variational ansatz for spin-1/2 systems. On top of the visible spins v_i, $i \in 1 \dots N$, the authors introduce additional „hidden" layer of spins h_j, $j \in 1 \dots M$. The complex variational parameters are $\{a_i\}$, $\{b_j\}$ and $\{W_{ij}\}$. Then, the Ansatz is:

$$\psi(\vec{s}) = \langle\vec{s}|\psi\rangle = \sum_{\{h_j\}} \exp\left(\sum_i a_i s_i + \sum_j b_j h_j + \sum_{ij} W_{ij} s_i h_j\right), \tag{2}$$

where $|\vec{s}\rangle$ is a Hilbert space basis vector corresponding to the visible layer (i.e. physical spins) configuration $\vec{s} = s_1, s_2, \dots, s_N$. The sum goes over all possible hidden spin configurations. Hence, it can be computed exactly and the ansatz assumes the following form:

$$\psi(\vec{s}) = \langle\vec{s}|\psi\rangle = \sum_{\{h_j\}} \exp\left(\sum_i a_i s_i\right) \prod_j \left(b_j + \sum_i W_{ij} s_i\right) \tag{3}$$

One performs stochastic sampling of the system with Metropolis-Hastings algorithm, which is a Monte Carlo method commonly used to get stochastic estimates of energy and its gradients with respect to variational parameters.

References

[1] Richard Schmidt and Mikhail Lemeshko. Rotation of quantum impurities in the presence of a many-body environment. Physical review letters, 114(20):203001, 2015.

[2] Vedran Dunjko and Hans J Briegel. Machine learning & artificial intelligence in the quantum domain: a review of recent progress. Reports on Progress in Physics, 81(7):074001, 2018.

[3] Vedran Dunjko and Peter Wittek. A non-review of Quantum Machine Learning: trends and explorations. Quantum Views, 4:32, March 2020.

[4] Giuseppe Carleo and Matthias Troyer. Solving the quantum many-body problem with artificial neural networks. Science, 355(6325):602–606, 2017.

[5] Wojciech Rzadkowski, Mikhail Lemeshko, and Johan H Mentink. Artificial neural network states for non-additive systems. arXiv preprint arXiv:2105.15193, 2021.

For further information:
wojciech.rzadkowski@ist.ac.at
mikhail.lemeshko@ist.ac.at

Key interim result

We developed [5] a novel machine-learning-based approach to the polaron quasiparticle.

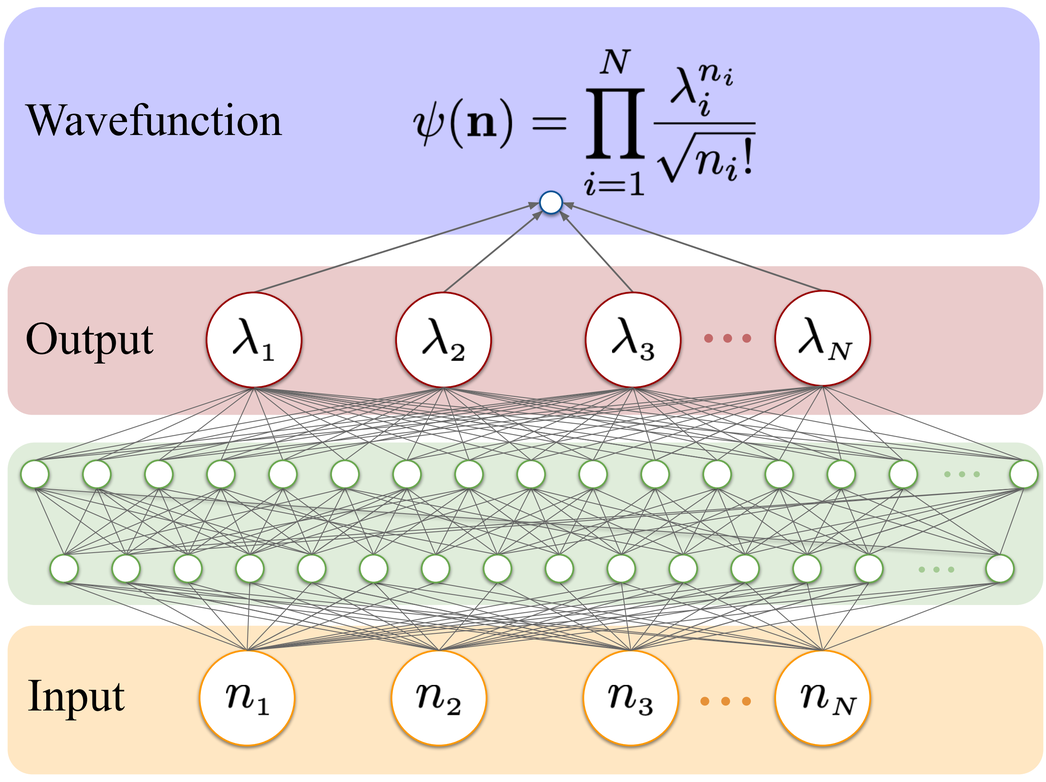

Figure 1: Visualization of the NCS approach. The input consists of Fock occupation numbers n_i for each of bosonic modes $i = 1, \dots, N$, corresponding to discrete k values k_i. The input is fed to a multilayer perceptron with arbitrary number and size of the hidden layers, see text for details. The number of neurons in the output layer is equal to the number of inputs (k-points). Each of the outputs λ_i, is transformed using the information from the input, $\lambda_i \to \lambda_i^{n_i}/\sqrt{n_i!}$. These numbers are multiplied to form the wavefunction ψ. All neurons in the hidden layers are densely connected to all neurons in the neighbouring layers; for clarity of the picture not all of them are visualized with grey lines. Figure adapted from Ref. [5].

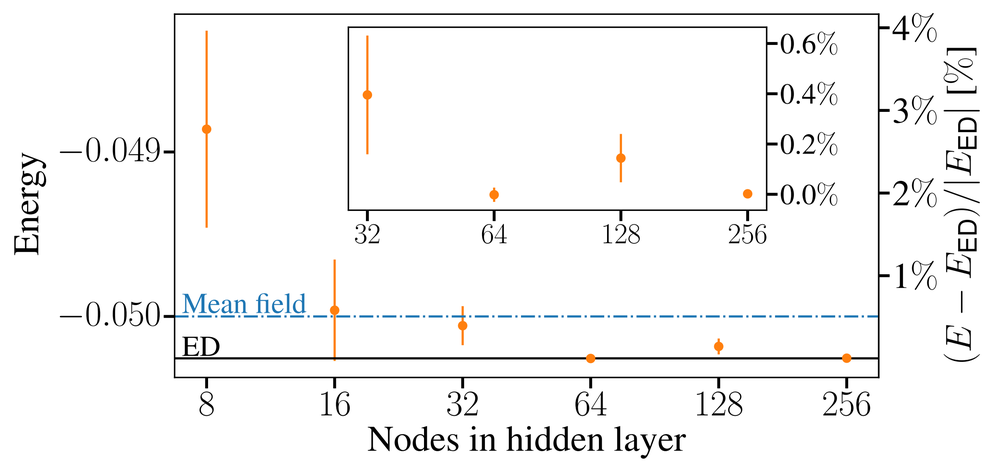

Figure 2: Representative power of the proposed approach. The optimized variational energy (orange dots, in units of $\hbar\omega_0$) is compared with exact diagonalization (ED), see right y-axis for percent scale relative to ED; and mean-field result for a system with 2 bosonic modes. The inset shows percent difference to ED for the four largest network sizes. Figure adapted from Ref. [5].

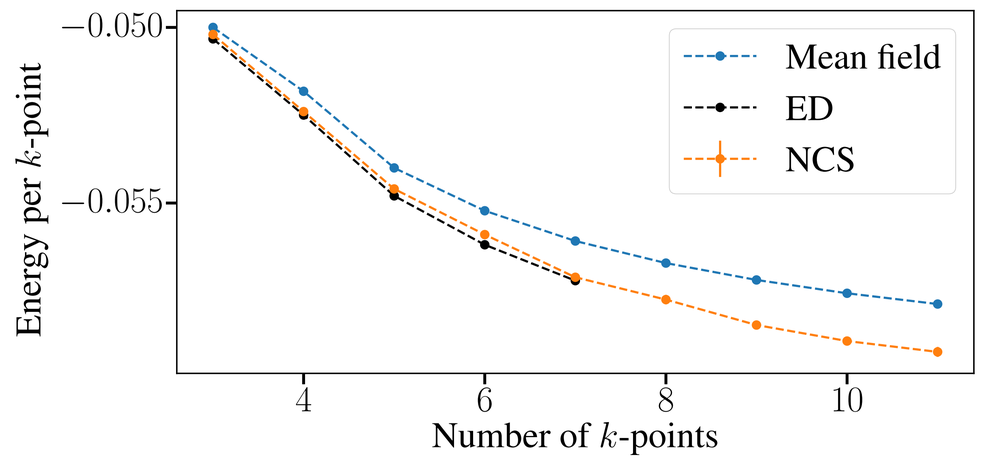

Figure 3: The energy divided by number of k-points calculated with the NCS approach as a function of the number of k-points on an equidistant grid between $k = -1$ and $k = 1$. Error bars for NCS approach are smaller than point size. Dashed lines guide the eye. Figure adapted from Ref. [5].