Contribution ID: **161** Type: **Oral**

Self-consistent evolution: new neural network approach to bound state calculations

Tuesday 2 July 2024 09:50 (20 minutes)

An application of neural networks for solving quantum mechanical problems has been suggested in [1,2]. Many improvements, including an adaptation of deep neural network techniques [3], have been proposed since. Development of a new computational technology which could lift the curse of dimensionality, however, has not yet been completed, although some steps in this direction have already been made [4,5].

We propose a new approach to training neural networks for approximation of quantum Hamiltonian invariant subspaces corresponding to bound states. The approach is based on training an artificial neural network to solve the Schrödinger equation in imaginary time with initial conditions that put the solution into an invariant subspace.

The advantage of the proposed approach is a simpler objective function which leads to better performance.

Theoretical results are illustrated with numerical examples.

[1] I.E. Lagaris, A. Likas, and D.I. Fotiadis, Artificial Neural Networks for Solving Ordinary and Partial Differential Equations // IEEE TRANSACTIONS ON NEURAL NETWORKS 1998, V. 9, N. 5, P.987
[2] I.E. Lagaris, A. Likas, and D.I. Fotiadis, Artificial neural networks in quantum mechanics // Comp. Phys. Comm. 1997, V.104, P.1-14
[3] Sirignano, J., Spiliopoulos, K., DGM: A deep learning algorithm for solving partial differential equations// arXiv preprint arXiv:1708.07469
[4] Hong Li, Qilong Zhai, Jeff Z. Y. Chen, Neural-network-based multistate solver for a static Schrödinger equation // Phys.Rev. A 2021,V. 103, P. 032405
[5] V.A. Roudnev, M.M. Stepanova, Deep learning approach to high dimensional problems of quantum mechanics // Proceedings of Science 2022, V.429, P. 13

Section

Nuclear structure: theory and experiment

Primary author: ROUDNEV, Vladimir (St-Petersburg State University)

Co-author: Mr KOZLOV, Alexander (St-Petersburg State University)

Presenter: ROUDNEV, Vladimir (St-Petersburg State University)

Session Classification: Nuclear structure: theory and experiment