Quantum Mechanical Many-body Problems with Machine Learning Algorithms

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I. INTRODUCTION AND MOTIVATION

Traditional many-body methods like full configuration interaction theory (FCI), coupled-cluster (CC) theory, many-body perturbation theory (MBPT), in-medium similarity renormalization group (IMSRG), various Monte Carlo methods and many other many-body approaches, have been rather successful in describing properties of interacting many-body systems. These methods have been widely used in condensed matter physics, nuclear physics, quantum chemistry and materials science, just to mention a few of the areas of applicability.

However, essentially all of these methods face what is normally called the curse of dimensionality. For wave function based method like FCI or CC theories where the original continuous problem is discretized in terms selected basis functions and/or many-body excitations, the dimensionality of the systems under study grows almost exponentially when larger basis sets and/or number of particles are included. As an example, nuclear physics systems close to the limits of stability pose in particular a tough problem to many-body practitioners in terms of a dramaticn increase of the number of relevant degrees of freedom. To describe say weakly bound nuclei within the framework of a wave function based approach, requires often a single-particle basis which includes bound, weakly bound and unbound states, increasing thereby considerably the number of many-body basis states. This renders often a standard FCI calculation infeasible. Within the above mentioned many-body methods there are however several interesting theoretical approachs which attempt at circumventing the dimensionality curse. Smarter basis sets is one of these approaches, as well as the resummation of specific correlations and the recently proposed stochastic sampling of many-body states in both FCI and CC calculations.

Recently, several authors have pointed to possibilities within the broad fields of Machine Learning and Quantum Computing as approaches that hold great promise in tackling the ever increasing dimensionalities. There are several groups worldwide which now focus on Machine Learning and/or Quantum Computing applied to many-body problems. Machine learning (ML) is an extremely rich field, in spite of its young age. The increases we have seen during the last three decades in computational capabilities have been followed by developments of methods and techniques for analyzing and handling large date sets, relying heavily on statistics, computer science and mathematics. The field is rather new and developing rapidly.

Machine Learning based methods offer several possibilities to circumvent the abovementioned dimensionality problems, as well as allowing us to model quantum mechanical systems with less a priori knowlegde. For complex many-body systems like those which arise in nuclear physics (in particular with the increase in the number of degrees of freedom for nuclei close to their limits of stability).

We have recently started to explore several approaches based on deep learning algorithms, with an emphasis on neural networks and so-called Boltzmann machines, with several promising results for interacting many-fermion systems, see some of the results below. Our applications so far have been to systems of electrons confined to move in two or three-dimensional regions (so-called quantum dots) and systems of bosons (weakly and strongly interacting) using a mix of neural network based algorithms and variational quantum Monte Carlo approaches. Furthermore, we have also explored the solution of the Similarity Renormalization Group set of equations using deep learning algorithms.

II. OPPORTUNITIES, CHALLENGES AND NEW ADVANCES

Neural-network quantum states (NQS) are a representation of the many-body wave-function in terms of artificial neural networks (ANNs). A commonly adopted choice is to parameterize wave-function amplitudes as a feed-forward neural network.

One of the specific challenges emerging in the quantum domain is imposing physical symmetries in the NQS representations. In the case of a periodic arrangement of matter (often used in the simulation of infinite systems like nuclear matter and the homogeneous electron gas), spatial symmetries can be imposed using convolutional architectures similar to what is used in image classification tasks. While spatial symmetries have analogous counterparts in other ML applications, satisfying more involved quantum symmetries often needs a deep rethinking of ANN architectures. The most notable case in this sense is the *exchange symmetry*. For bosons, this amounts to imposing the wave-function to be permutationally invariant with respect to exchange of particle indices. The Bose-Hubbard model has been adopted as a

benchmark for ANN bosonic architectures, with state-of-the-art results having been obtained. The most challenging symmetry is, however, certainly the fermionic one. In this case, the NQS representation needs to encode the antisymmetry of the wave-function (exchanging two particle positions, for example, leads to a minus sign). In this case, different approaches have been explored, mostly expanding on existing variational ansatz for fermions. We have for example explicitely included the fermion antisymmetry by multiplying the NQS with an explicit Slater determinant. The situation for fermions is certainly the most challenging for ML approaches at the moment, owing to the specific nature of the symmetry. On the applications side, NQS representations have been used so-far along three main different research lines. These are:

1. Representation of states: An active area of research concerns the general expressive power of NQS, as also compared to other families of variational states. Theoretical activity on the representation properties of NQS seeks to understand how large, and how deep should be neural networks describing interesting interacting quantum systems.

2. Learning from data: Parallel to the activity on understanding the theoretical properties of NQS, a family of studies in this field is concerned with the problem of understanding how hard it is, in practice, to learn a quantum state from numerical data. This can be realized using either synthetic data (for example coming from numerical simulations) or directly from experiments.

   This line of research has been explored in the supervised learning setting, to understand how well NQS can represent states that are not easily expressed (in closed analytic form) as ANN. The goal is then to train a NQS network to represent, as close as possible, a certain target state whose amplitudes can be efficiently computed.

3. Finally, one of the main applications for the NQS representations is in the context of variational approximations for many-body quantum problems. The goal of these approaches is, for example, to approximately solve the Schrödinger equation using a NQS representation for the wave-function. In this case, the problem of finding the ground state of a given quantum Hamiltonian H is formulated in variational terms as the problem of learning NQS weights W minimizing $E(W) = \langle\Psi(W)|H|\Psi(W)\rangle/\langle\Psi(W)|\Psi(W)\rangle$. This is achieved using a learning scheme based on variational Monte Carlo optimization. Within this family of applications, no external data representative of the quantum state is given, thus they typically demand a larger computational burden than supervised and unsupervised learning schemes for NQS.

We have worked on the latter approach in connection with studies of quantum dot systems (confined two-dimensional and three-dimensional electron systems). Using Quantum Monte Carlo samplings (QMC), a practical issue often resulting is that of providing efficient sampling schemes of high-dimensional spaces (path integrals, perturbation series, etc..). This requires a careful tuning which is often problem-dependent. Devising general-purpose samplers for these representations is therefore a particularly challenging problem. Unsupervised ML methods can, however, be adopted as a tool to speed-up Monte Carlo sampling for both classical and quantum applications. In the figure here, we show the speed-up obtained when using Restricted Boltzmann machines (RBM) for systems of two-dimensional quantum dots (with $N = 2, 6, 12, 20, 30, 42, 56, 72$ electrons) compared with a Variational Monte Carlo calculation (VMC). The results for the energies are similar. The main speed-up is due to a simpler mathematical form for the correlated part of the trial wave function. In the RBM calculation we used a simple Slater determinant for the electrons using Hermite polynomials only. However, the results for energies and other observables can be improved upon by multiplying the NQS with a Jastrow factor (RBM+PJ/SJ). This leads however to an increase in CPU time since the number of parameters to optmize increases. How to speed up the calculation of the Jastrow factor is also an important issue.

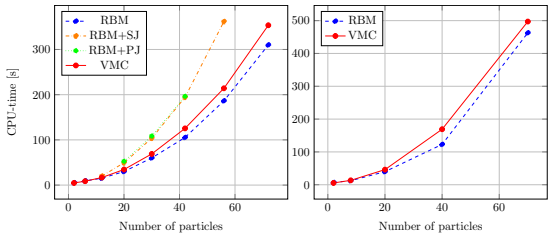

FIG. 1. Speed-up obtained when using Restricted Boltzmann machines (RBM) for systems of two-dimensional quantum dots (with $N = 2, 6, 12, 20, 30, 42, 56, 72$ electrons) compared with a Variational Monte Carlo calculation (VMC). The results for the energies are similar. The main speed-up is due to a simpler mathematical form for the correlated part of the trial wave function. In the RBM calculation we used a simple Slater determinant for the electrons using Hermite polynomials only. However, the results for energies and other observables can be improved upon by multiplying the NQS with a Jastrow factor (RBM+PJ/SJ).

While exact for a large family of bosonic and fermionic systems, QMC techniques typically incur in a severe sign problem when dealing with several interesting fermionic models, as well as frustrated spin Hamiltonians. In this case, it is tempting to use ML approaches to attempt a direct or indirect reduction of the sign problem. While only in its first stages, this family of applications has been used to infer information about fermionic phases through hidden information in the Green's function.

Similarly, ML techniques can help reduce the burden of more subtle manifestations of the sign problem in dy-

namical properties of quantum models. In particular, the problem of reconstructing spectral functions from imaginary-time correlations in imaginary time is also a field in which ML can be used as an alternative to traditional maximum-entropy techniques to perform analytical continuations of QMC data.

Applications of ML to quantum many-body problems have seen a fast-pace progress in the past few years, touching a diverse selection of topics ranging from numerical simulation to data analysis. The potential of ML techniques has already surfaced in this context, already showing improved performance with respect to existing techniques on selected problems. To a large extent, however, the real power of ML techniques in this domain has been only partially demonstrated, and several open problems remain to be addressed. In the context of variational studies with NQS, for example, the origin of the empirical success obtained so far with different kind of neural network quantum states is not equally well understood as for other families of variational states, like tensor networks. Key open challenges remain also with the representation and simulation of fermionic systems, for which efficient neural-network representation are still to be found.

Tensor-network representations for ML purposes, as well as complex-valued networks like those used for NQS, play an important role to bridge the field back to the arena of computer science. Challenges for the future of this research direction consist in effectively interfacing with the computer-science community, while retaining the interests and the generality of the physics tools.

We have been able recently to study both interacting bosonic systems and interacting fermions such as electrons confined to two- or three-dimensional regions. We are planning to study infinite systems like the homogeneous electron gas. We plan to address several of the above issues in the next few years (a three to five year perspective). The real challenge however is to extend these studies to nuclear systems. Applying ML methods to nuclear systems based on the above approaches is our central goal for the next five to ten years.