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Letter of Evaluation of the Dissertation of Anna Dawid-Łekowska on Quantum many-body physics with ultracold atoms and molecules: exact dynamics and machine learning

The doctoral thesis by Anna Dawid-Łekowska investigates complex quantum many-body problems, the challenges they impose on classical computations due to their exponentially growing state space, and applications to study and exploit their properties via quantum simulation and machine learning.

The thesis is, besides an introduction to the necessary concepts and motivation, separated into two large sections: Investigation of molecules for quantum simulations, and applications of machine learning for quantum phase detection.

Introduction:
The thesis starts with a very accessible chapter that explains the basis and motivation of the two main sections. First, the idea of quantum simulation is described, specifically with the motivation in mind of replacing atoms with molecules. Atoms are in many cases easier to handle experimentally (and theoretically/computationally), however, they have strict natural limitations on the complexity of their interactions. Molecules however have additional interaction possibilities, for example, via rotational and vibrational states. The broader goal of the first part of this thesis is to better understand the behaviour of molecular quantum simulators. The second part concerns machine learning algorithms for the detection of phases. The particularly interesting part here is the application of a mathematically closely related set of technologies to "interpret" what and how the machine is learning. This question stems from the problem that conventionally, machine learning algorithms – and in particular neural networks – are black boxes. We cannot understand/explain/interpret their behaviour except for trivially small examples. Of course, if we have computer algorithms that at some point outperform our capabilities to solve physics questions – we want to know why and how

they do it. The results presented in the subsequent chapters make an important step towards this ambitious goal.

Part I: Ultracold Molecules in a trap

The first main part of the thesis considers molecules for quantum simulation. In the beginning, the necessary quantum many-body concepts are explained, with a particular focus on the difference between atomic and molecular systems. The underlying Hamiltonian is explained, as well as a method for exact diagonalization by separating the center-of-mass Hamiltonian and the relative motion contribution. Very relevant for what follows is the explanation of experimental feasibility which ensures that the results of the subsequent studies could be used in laboratories.

In the next section, the interaction and dynamics of two polar molecules in a 1D trap are investigated. The molecules interact via a short-range anisotropy of intermolecular interactions. The dynamic of the system is investigated in detail, with a focus on the characteristic molecular properties. Interesting conclusions are drawn, such as the emergence of a molecular super-Tonks-Girardeau state, an analogue to the Einstein-de-Haas effect. Interestingly, quantum chaotic behaviour is excluded which has consequences for the integrability of the system.

Subsequently, the magnetization and quench dynamics of the system are studied. As a main result, it is found that magnetization can be controlled by external fields. Furthermore, it is found that most of the dynamics are guided by the impact of spin–rotation coupling and the anisotropy of the intermolecular interaction. Thereby, experimental implementations of these bi-molecular systems could be used to determine those physical properties.

Part II: Interpretable machine learning for phase detection

The goal of the second part of the thesis is to use machine learning for phase detection and go towards explaining/interpreting what impacted the training process particularly. At the beginning of this chapter, a very nice overview of artificial intelligence, machine learning and deep learning is presented, together with the types of training, explanations of neural networks and their different implements.

A very interesting section is 4.9, which introduces the *Hessian-based toolbox* for interpreting neural networks in the domain of quantum physics. The Hessian of the neural network parameters turns out to be a key concept in several techniques for interpreting the training behaviour of neural networks. For example, the impact of

removing one single training example from the training set can be approximated by the Hessian and gradients of the loss functions of the neural network.

Several related methods are discussed, starting from the Leave-one-out training, which is infeasible to compute. As an approximation, the Influence function (I) is built from the (inverse of the) Hessian and gradients of the Loss and has very interesting properties in terms of training example similarities. A normalized form of the influence function (relative influence function, relative-I), the resampling uncertainty estimations (RUE) and the local ensembles (LE) are also built from the Hessian and are used in the subsequent experiments. The combination of these techniques is called the "Hessian toolbox".

In the next section, it is demonstrated how the Hessian toolbox can be applied to the Fermi-Hubbard model for detecting quantum phases. The experiment indicates that the neural network has discovered a relevant order parameter describing a phase transition, and it is explained how the Influence function can be used to find the order parameter without prior knowledge. This is of course an exciting feature for a future project, where one wants to discover quantum phase transitions and order parameters of unknown systems, potentially directly from experimental data. The subsequent chapter 5.3 goes a significant step ahead and applies the full "Hessian toolbox" described above to the interpretation of the influence and the reliability of the training in the neural networks. It is observed that the influence function is very suitable in discovering anomalies in the training data which impacts the reliability of the training neural network, while the local ensembles function can identify the extrapolation quality of the neural network.

In the final section, it is described how an (unsupervised) ML method can detect quantum phases directly from experimental data. In this case, the system is a Haldane-like model of atoms. This task is of course significantly more difficult than detection in simulated data, because of experimental noise (potentially systematic one). Very interesting insights came from the 2d plot of a bottleneck latent space of a variational autoencoder – a key tool in AI-based scientific discovery. The culmination of the projects in this second part of the thesis indicates a realistic path towards the ML-based discovery of new phases of matter, potentially directly from experiments. The results from this thesis significantly contribute to that important goal of the physics community.

While it is not an explicit part of the thesis but is only mentioned in the List of Publications under "Other works", I want to highlight a book – first authored by Anna

Dawid-Łekowska – on “Modern applications of machine learning in quantum sciences”. This is a remarkable and highly educational text, and it shows Anna Dawid-Łekowska’s outstanding role in the ML for Quantum Science community, and as an exceptional organizer who made this project (consisting of nearly 30 co-authors) a reality.

In conclusion, I find the doctoral thesis to be of the highest quality, presenting new and innovative results in an exciting research field. Based on the written quality of the thesis and the results achieved therein, I recommend the best possible grade: 1.0 (Very Good)

Furthermore, I strongly recommend the PhD thesis be considered for a distinction.
While the entire thesis is of very high quality, I want to specifically highlight here that in my opinion the “Hessian toolbox” is an extremely powerful collection of computational methods with clear-cut interpretations. This thesis shows high potential for their application and interpretation in the field of quantum science that will inspire many future applications in quantum many-body physics and beyond. The Hessian toolbox seems to be highly applicable to diverse problems. Crucially, it does not require to modify the neural network architecture, therefore it can directly be applied to many other physics-based neural networks projects.

Sincerely,

Dr. Mario Krenn, 11. July 2022