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Report on the PhD Thesis "Quantum many-body physics with ultracold atoms and molecules: exact dynamics and machine learning" by Anna Dawid-Lekowska

The PhD thesis by Anna Dawid-Lekowska has two main parts. The first one focuses on the analysis of two interacting molecules on a one-dimensional trap. The motivation comes from the fact that while experiments with ultra-cold atoms have been proven very successful in the last years, with an emphasis on the quantum simulation of relevant quantum many-body systems out of reach for classical computers, the situation is much more challenging when considering molecules, due to their much more complex internal structure. Cooling techniques, for instance, are much more difficult in this context. To shed light into this problem, the student analysis a system composed of two molecules on a one-dimensional trap. The molecules are approximated with a rigid quantum rotor model. A Hamiltonian is introduced taking into account their rotation and spin degrees of freedom, the field and the interactions between molecules and the field. Then, the system is solved through exact diagonalization in a basis set defined by the field number states and the eigenvectors of the total rotational angular momentum operator. The quench dynamics of the system is also analysed.

The main results of the study were published in two articles in Phys. Rev. A and Phys. Chem. Chem. Phys., both with the student as first author. The analysis in the first article demonstrates that, in some regime of parameters: (i) the ground state can have total angular momentum larger than zero and be degenerate; (ii) a molecular equivalent of the atomic super-Tonks-Girardeau limit can emerge; (iii) energy spectra can be highly complex with a high density of states and also level crossings. Interestingly, no signatures of chaotic behaviour were found. The second article focuses on the magnetic properties and dynamics. It shows that the magnetization of the system can be controlled by external fields and study the dependence of the magnetization after an electric or magnetic quench.

The second part of the Thesis focuses on the use of (classical) machine learning techniques to analyse many-body systems, in particular in the context of phase detection. Machine learning techniques are having a tremendous impact in our daily lives and this impact also includes research. In fact, many of the scientific challenges we face today are caused by the need to understand and process huge amount of data. It is therefore no surprising that machine learning techniques find an application here. A paradigmatic example is the study of quantum many-body systems, where the number of parameters, or equivalently the dimension of the involved systems, grows exponentially with the number of constituents. In the last years, many different works have applied machine learning techniques in this context. However, two relevant scientific questions have hardly been explored: (1) how do we interpret the results obtained after the application of machine learning? And (2) how do these techniques apply to real experimental many-body setups? To my knowledge, the present Thesis represents one of the first efforts to address these questions.

Concerning the interpretability of machine learning results, the student first applies machine learning techniques to reconstruct the phase diagram of a Fermi-Hubbard model. Then, the student

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and co-workers apply the so-called influence functions to understand how the method reconstruct the phase transitions and how is able to detect unknown phases. The results were presented in an article published in New J. Phys. with the student as first author. In a second work, which appeared in Mach. Learn.: Sci. Technol. with, again, the student as first author, they add more tools to attain interpretable and reliable machine learning in the many-body context: the previously considered influence functions, but also relative influence functions, resampling uncertainty relations, which can be considered as a method to introduce an analogue of error bar, and local ensembles, that may detect if a machine learning model makes predictions with a high level of extrapolation. It is demonstrated how these tools can be used to improve the reliability of the machine learning predictions.

Concerning the application of machine learning to experimental data, this is a collaboration with the experimental group of Prof. Sengstock on the quantum simulation of a topological model. The analysis is performed on raw experimental data, such as time-of-flight images. The analysis reveals that the problem is difficult and that a proper post-processing of the raw data is required for the machine to "properly" learn. However, the successful identification of the phase diagram demonstrates that unsupervised machine learning can correctly identify phases even for noisy data and despite the finite temperature of the system, which is in my opinion a remarkable result.

After this quick overview, my assessment about the work in the thesis is highly positive. All the considered problems are relevant and the obtained results represent significant advances on the identified questions. They have appeared in very good international journal and in all of them but one the student appears as first author. The thesis is also very rich in methods, especially in the machine learning part where the student has considered many different methods to study the interpretability and reliability of the applied techniques. Perhaps because closer to my work, I find all the works on the application of machine learning to the study of quantum many-body systems highly original and innovative.

Based on all these points, my assessment on the thesis work is openly positive and it deserves a distinction. In my opinion, it clearly belongs to the top 5% of thesis in the field in Poland.

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