a place of mind
THE UNIVERSITY OF BRITISH COLUMBIA

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6 July 2022

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Review of the dissertation of Anna Dawid-Lekowsa

Dear Sir or Madam,

I am writing in response to your request to review the dissertation of Ms. Anna Dawid-Łękowska submitted to the University of Warsaw for the degree of doctor.

My letter will address in detail the following two questions explicitly.

1) The doctoral dissertation presents the candidate's general theoretical knowledge in a discipline or disciplines as well as the ability to independently conduct scientific work.
2) The subject of the doctoral dissertation is an original solution to a scientific problem or an original solution in the field of applying the results of own scientific research in the economic or social sphere.

On question 1), my recommendation is: positive
On question 2), my recommendation is: positive

I will now provide justification for my recommendations.

On question 1):

The thesis considers two major research problems. One is understanding the interactions of ultracold molecules in a trap. This problem is relevant for a large number of ongoing experiments with ultracold molecules. In order to cool molecules to ultracold temperatures, one must trap them. The cooling process itself relies on energy equilibration in molecular collisions in traps. In order to use molecules for pretty much any goals that have been proposed and explored in the literature, one must trap molecules. Often the effects of trapping fields are ignored. However, they are not inconsequential. Part I of this dissertation (Chapters 3 and 4) presents rigorous calculations to elucidate the effects of trapping fields on interactions of ultracold molecules and the effect of interactions (and fields) on dynamics of trapped molecules.

Part II of this thesis addresses a different problem. Quantum calculations, including the calculations carried out in Part I of this dissertation, are exceedingly difficult. A major thrust of recent work has been to explore applications of machine learning algorithms for accelerating quantum calculations or enhancing the accuracy of approximate quantum calculations. However, machine learning models are generally complex and it is, therefore, often difficult, if not impossible to understand why machine learning works the way it does. Part II of this thesis aims to develop approaches that explain why and how machine learning algorithms, when applied to physics problems, work. This is a lofty goal, but this dissertation makes substantial progress towards it.

The doctoral candidate clearly demonstrates extensive knowledge of both of these fields in the present dissertation.

Thus, Part I opens with a detailed description of molecular structure relevant for ultracold molecules and rigorous quantum calculation techniques used later in the thesis. Notably, Section 2 includes a discussion of experimental feasibility, which demonstrates the author's understanding of the experimentally relevant systems and problems. The quantum calculations are rigorous and well explained and discussed. Again, the level of detail presented demonstrates that the author is in command of rigorous computation techniques for quantum problems.

Similarly, Part II begins with a general introduction of machine learning, including a description of supervised and unsupervised learning techniques as well as the key machine learning concepts such as regularization and generalization error. The discussion progresses to introduce various kinds of neural networks, and some of their applications. This is necessary to introduce the Hessian-based technique for interpretable machine learning, of central importance to this work.

The above arguments clearly support my positive recommendation on question 1).

On question 2):

This dissertation considers new dynamics regimes for interacting molecules in harmonic traps. The results will be useful both for the interpretation of ongoing experiments with molecules trapped in optical lattices as well as for new applications of ultracold molecules, such as quantum simulators. While the effect of external confinement on s-wave and p-wave scattering of ultracold systems had been studied before (with work dating back to Petrov and Shlyapnikov, Olshannii and even my own group – we investigated the effect of confinement on inelastic and reactive scattering of ultracold molecules in quasi-2D geometries), the interplay of confinement and interactions due to intra-molecular open-shell structure (such as spin-rotation interactions) has, to the best of my knowledge, not been previously explored. Therefore, the study published in this dissertation is novel. As open-shell molecules (such as molecules in a 2Sigma electronic state) can be laser cooled to ultracold temperatures or even (in the case of 3Sigma molecules) created from ultracold atoms, this study is directly relevant to ongoing experiments and the results presented in this dissertation can be tested in current experiments.

In Part II, this dissertation proposes novel algorithms for unsupervised learning to identify topological phase transitions in experimental data based on ultracold atoms. While the machine learning techniques utilized in this work were developed previously, the way these methods have been applied is novel. In particular, I like the author's use of variational autoencoder for standardizing the micromotion phase, which makes the analysis of seemingly different images containing similar physics feasible. The focus on interpretable machine learning for physics problems is particularly important, as this represents a significant advance compared to other efforts aiming to apply machine learning to physics research. All in all, this dissertation demonstrates a creative use of machine learning techniques for physics applications, paving the way for many applications of machine learning for solving physics problems.

Overall recommendation: Based on the arguments presented above, I believe that this is an excellent dissertation. I recommend that this dissertation be recognized by a distinction. The primary justification for the distinction is the work in Part II of the dissertation that paves the way for new approaches to solve physics problems, both within the research fields (AMO and condensed-matter physics) considered here but also in other fields, by creatively combining machine learning and rigorous quantum calculations.

Sincerely,

Roman Krems

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