Posudek práce

předložené na Matematicko-fyzikální fakultě
Univerzity Karlovy

☑ posudek vedoucího ❑ posudek oponenta
☑ bakalářské práce ❑ diplomové práce

Autor/ka: **Lukáš Frk**
Název práce: **Study of phase transitions in models with itinerant and localized particles via machine learning**
Studijní program a obor: Physics
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Jméno a tituly vedoucího/~~oponenta~~: RNDr. Martin Žonda, Ph.D.
Pracoviště: Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University
Kontaktní e-mail: martin.zonda@matfyz.cuni.cz

Odborná úroveň práce:
☑ vynikající ❑ velmi dobrá ❑ průměrná ❑ podprůměrná ❑ nevyhovující

Věcné chyby:
☑ téměř žádné ❑ vzhledem k rozsahu přiměřený počet ❑ méně podstatné četné ❑ závažné

Výsledky:
☑ originální ❑ původní i převzaté ❑ netriviální kompilace ❑ citované z literatury ❑ opsané

Rozsah práce:
❑ veliký ☑ standardní ❑ dostatečný ❑ nedostatečný

Grafická, jazyková a formální úroveň:
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Tiskové chyby:
☑ téměř žádné ❑ vzhledem k rozsahu a tématu přiměřený počet ❑ četné

Celková úroveň práce:
☑ vynikající ❑ velmi dobrá ❑ průměrná ❑ podprůměrná ❑ nevyhovující

Slovní vyjádření, komentáře a připomínky vedoucího/~~oponenta~~:

In his bachelor thesis, Lukáš Frk explored the possibility of automatically constructing the phase diagram of the Falicov-Kimball model (FKM) using a set of unsupervised machine learning (ML) techniques. The primary motivation was to develop and test methods capable of identifying novel phases or automatically constructing complex phase diagrams typical of strongly correlated electron systems, preferably using data that is experimentally accessible.

The FKM was selected for several reasons. First, this model is accesible to exact methods, including semi-classical Monte Carlo simulations. Second, even at half-filling, it possesses a complicated phase diagram with phases that are still under debate. Finally, the FKM has recently gained interest in the development of novel ML methods for unsupervised phase classification.

Monika Richter-Laskowska et al. [Phys. Rev. E 108, 024113 (2023)] demonstrated that the "learning by confusion" method can identify the transition from the ordered to disordered phase. However, there are challenges: the method is effective only for continuous transitions, whereas for weak interactions, the order-disorder transition in FKM is discontinuous. Additionally, the phase diagram of the FKM is much richer than just the ordered and disordered phases.

Lukáš's goal was to identify methods that are reliable for the order-disorder transition across all interaction strengths and potentially capable of identifying other phases as well. An important restriction was that the only information available to the ML techniques were Monte Carlo snapshots of the particle occupations and the parameters at which they were calculated.

The first goal was met to a great extent as Lukáš identified several methods that outperform learning by confusion, including a novel variant of PCA classification that is much simpler and faster. Lukáš managed to partially fulfill the second goal. What has not worked was the identification of the phase boundary between the Mott insulator and Anderson insulator phases or the location of the ordered phase with and without a finite density of states at the Fermi level. The reason for this seems to be that the necessary information to distinguish these phases is not available within the snapshots.

However, Lukáš succeeded in automatically identifying the phase boundary between the weakly localized and Anderson localized phases. This achievement is remarkable, considering that the boundary was only identified in 2016 after an extensive investigation of the Inverse Participation Ratio (IPR), which measures the localization of otherwise itinerant electrons. The PCA-based algorithm can identify this boundary automatically just from the snapshots of particle occupations. Although it was not clear why this worked during the writing of the thesis, Lukáš continued working on the problem and we have since developed a working theory explaining the physical effect that allows this automatic identification.

Lukáš worked independently, generating his own ideas, and testing them. He mastered the use of standard ML packages in physics, understood, and implemented novel methods for automatic phase classification. Additionally, he learned various methods of theoretical physics to deepen his understanding of the FKM model. A notable example is his usage of small-cluster exact diagonalization to produce data for crucial tests.

Lukáš has already presented his research at the Student Scientific Conference in Košice, where he won second place in his category. Even more importantly, his results are worthy of publication. We are therefore continuing to work on the problem and should soon have a first complete draft of a paper aimed at publication in Physical Review E (PRE) or Physical Review B (PRB).

Případné otázky při obhajobě a náměty do diskuze:

I have no questions.

Práci
☑ doporučuji
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Navrhuji hodnocení stupněm:
☑ výborně ❑ velmi dobře ❑ dobře ❑ neprospěl/a

Místo, datum a podpis vedoucího/~~oponenta~~: 12. 6. 2025 v Praze