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Review of the doctoral dissertation entitled

„Unconventional superconductivity, topology and strong electronic correlations in two dimensional transition-metal dichalcogenide moiré bilayers"

by Waseem Akbar

The reviewed doctoral dissertation was carried out by Waseem Akbar at the Academic Centre for Materials and Nanotechnology, AGH University of Kraków, under the supervision of dr. hab. inż. Michał Zegrodnik (prof. AGH) and auxiliary supervision of dr. hab. Andrzej Biborski (prof. AGH). The dissertation consists of a collection of four scientific publications, with reprints supplemented by a concise summary. The thesis is preceded by three introductory chapters covering unconventional superconductivity in moiré superlattices, motivational experimental data, and the theoretical framework, including models for strongly correlated electron systems and the methodology used to approach them (specifically, the Gutzwiller approximation). The dissertation is written in English, as are all included publications.

The dissertation addresses a fundamental understanding of superconductivity observed or proposed in widely studied moiré superlattices. These systems are formed in bilayer configurations where either a relative twist angle or a lattice mismatch creates periodic superstructures spanning multiples of the primitive unit cell. Moiré systems are particularly interesting due to the non-trivial interplay between strong electronic correlations and geometric features, as well as their high tunability via external parameters, such as electric field induced carrier doping.

The doctoral candidate, in collaboration with his supervisors, analyzed single orbital models incorporating strong correlations via different many-body terms to effectively describe the physics of a WSe_2 homobilayer and a WS_2/WSe_2 heterobilayer. The ultimate motivation for this research is to understand where superconductivity emerges on the doping phase diagram for these material systems, identify the symmetry of the order parameter, and evaluate how well experimental observations are captured under the assumption that strong correlations drive the superconductivity.

Key results of the dissertation concern the realization of various superconducting order parameter symmetries, including topologically non-trivial ones, depending on the strength and type of correlations assumed for the system, as well as features in the density of states such as Van Hove singularities. Where possible, a comparison and rationalization of experimental observations are discussed based on the obtained results. To determine these results, the candidate solved a version of the single orbital extended t-J model accounting for possible superconducting order parameter with the Gutzwiller approximation method.

More precisely, the original scientific contributions of the dissertation include:

- providing a theoretical argument for the realization of topologically non-trivial superconducting phases in a t-J model adjusted to mimic low-energy properties of a twisted WSe_2 bilayer,
- rationalizing experimental observations for a twisted WSe_2 bilayer regarding superconductivity bounded to single dome near half-filling using a single orbital t-J-U-V model,
- comparing superconducting modeling obtained via the t-J-U-V model against the negative U Hubbard model in light of the phase diagram of a twisted WSe_2 bilayer, and
- extending the analysis of correlation driven unconventional superconductivity in the t-J-U-V model to a heterobilayer setup capturing the low-energy physics of a WS_2/WSe_2 heterobilayer.

The numerical results and their interpretations form a coherent body of research aimed at understanding superconductivity driven by strong electronic correlations in model systems effectively tuned to capture the low-energy physics of experimentally studied twisted homobilayers and heterobilayers.

The doctoral dissertation comprises an introductory chapter on unconventional superconductivity and moiré superlattices, a chapter on research motivations deeply rooted in experimental observations, a chapter describing models and modeling techniques, a chapter summarizing the articles included in the thesis, four attached reprints of published scientific papers, a summary chapter, and a bibliography. The quality of writing in this dissertation is generally high, and I did not spot any major issues regarding formatting or typos. The only notable omissions I noted are the absence of an explicit text reference to Fig. 1.4 in the introductory chapter, and a missing information regarding the exact material for which a particular phase diagram in this figure was obtained.

In the first chapter, the candidate opens with a historical overview of developments in unconventional superconductivity, placing special focus on strongly correlated systems, before introducing moiré superlattices from the perspective of early experimental observations and rapid advancements in condensed matter physics. In the second chapter, the candidate focuses specifically on experimental observations concerning superconductivity in transition metal dichalcogenide bilayers, including reproduced phase diagrams with control parameters such as carrier density, displacement field, and temperature, concluding with a concise motivation aimed at developing a unified theoretical understanding of emergent superconducting phases. The third chapter introduces effective correlated electron models in the extended t-J family, providing rationale for the included many-body terms and the specific single particle sectors tuned to model band structures. Additionally many-body theoretical tool Gutzwiller Approximation is well introduced within third chapter.

In this place the general comments regarding described parts of the thesis is in place. Given the complexity of the considered materials and the heuristic arguments used to introduce various many-body terms, these models should be regarded as phenomenological models for correlation driven superconductivity rather than a fully microscopic treatment. Additionally, the doctoral candidate is leveraging the Gutzwiller approximation for solving the models. While well suited as a qualitative approach to the correlated electron problems defined in the thesis, I hesitate to label it as an advanced many-body tool, that doctoral candidate mastered as a part of the doctoral training. This however does not diminish quality of demonstrated physical insights.

In the initial three chapters, I missed a dedicated discussion on the geometric and topological properties introduced by spin orbit coupling, which is one of the reasons the condensed matter community pays close attention to superconductivity in considered materials. Given that articles include calculations of Chern numbers, **I would be happy to discuss topological properties and their consequences in moiré**

superlattices, during the public defense. Furthermore, during the public defense, I would like the candidate to elaborate on the nature and presence of Mott insulating phases in the addressed materials and models. In particular, why the insulating region in Fig. 2.1 spans a large range of carrier concentration, whereas in the modeling it exists precisely at half-filling. Additionally, why no Mott insulating phase appears in Fig. 3.1 despite stating on page 16 that one is formed, and clarify why the Gutzwiller wave function under the Gutzwiller approximation realizes a Mott state in the Hubbard model while a diagrammatic expansion does not.

The fourth chapter provides a summary of the key results achieved in each publication, providing clear and substantive summaries that trace the progression of the research, followed by reprints of the respective articles. The summary chapter ties the research together into a coherent narrative connecting back to the core motivation of understanding fundamental properties of the superconducting state in transition metal dichalcogenide superlattices, while also outlining potential future directions. **During the public defense, I would like the doctoral candidate to elaborate on his intuition regarding the proposed inclusion of multiorbital effects and what consequences starting from a multiorbital model would potentially have on effective models, many-body terms, topological properties, and superconducting order parameters.** The bibliography is appropriate in both scope and length, proving that the PhD candidate has conducted proper literature research.

The research problem described in the dissertation is reflected in four original scientific papers published by Mr. Waseem Akbar. In three of these, the candidate is the first author, while in one he is the second author among four. For the papers where the candidate is the primary author, I have no reservations about including them as core publications forming the dissertation. For the article where the candidate is second author, the absence of an explicitly labeled Authors' Contribution section makes his exact contribution harder to assess directly. However, the publication is clearly a follow-up work deeply rooted in the candidate's primary publications, so I am convinced that his contribution was significant enough to warrant inclusion.

In "Topological superconductivity with mixed singlet-triplet pairing in moiré transition metal dichalcogenide bilayers" published in Physical Review B in 2024, the authors explore the stability of superconducting phases with various order parameters and spin states in a single orbital t-J model on a triangular lattice. The model is solved using the Gutzwiller approximation and a superconducting phase diagram is mapped out that qualitatively captures experimental observations and reveals a mixed chiral triplet p and singlet d paired state with Chern numbers equal to ± 2 or ± 4.

In "Optimal superconductivity in twisted bilayer WSe_2 where the Van Hove singularity crosses half-filling" published in Physical Review Research in 2026, the authors extend their analysis using an extended t-J-U-V model, showing that in a moderate correlation regime an interplay between the Van Hove singularity and correlation effects near half-filling rationalizes the behavior of superconductivity as a function of displacement field observed in experiment for WSe_2.

In "Superconductivity in moiré transition metal dichalcogenide bilayer: comparison of two distinct theoretical approaches" published in Acta Physica Polonica B in 2026, the authors conclude their studies on twisted WSe_2 homobilayers by solving a negative U Hubbard model with the Hartree-Fock approximation and demonstrating an unfavorable comparison of this mechanism to t-J type models when benchmarked against experimental observations.

Finally, in "Unconventional superconductivity in the presence of long-range interactions in transition metal dichalcogenide moire heterobilayers", published in Scientific Reports in 2026, the authors address superconductivity in a WS_2/WSe_2 heterobilayer using a single orbital t-J-U-V model reflecting low-energy physics of this material, constructing a phase diagram in the strong correlation regime where again a mixed p triplet and d singlet superconducting state is realized with the p triplet amplitude prevailing.

Proceeding to the final evaluation of the candidate, I state that Waseem Akbar meets all the criteria set out for PhD candidates in the Polish Law: Ustawa Prawo o Szkolnictwie Wyższym i Nauce z 20 lipca 201 r. (Dz. U. 201 poz. 166 z późn. zm). The candidate has proven fluency in numerical simulations of superconducting states in correlated models, and the doctoral dissertation proves a solid understanding of the physics of the addressed phenomena. Dissertation addresses original research problem solved by Mr. Waseem Akbar (in reference to art. 187.2) and demonstrates his broad theoretical knowledge in physical sciences discipline (in reference to art. 187.1). It should be also emphasized that the results achieved have been published in reputable scientific journals: in Physical Review B (IF: 3.9), Physical Review Research (IF: 4.0), Scientific Reports (IF: 4.9), and Acta Physica Polonica B (IF: 1.0). Taking all this into account, I strongly recommend that Mr. Waseem Akbar be admitted to the public defense.

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