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Recenzja rozprawy doktorskiej mgr. Waseema Akbar, zatytułowanej *"Unconventional Superconductivity, Topology and Strong Electronic Correlations in Two Dimensional Transition-Metal Dichalcogenide Moiré Bilayers"*

This doctoral work of Waseem Akbar was performed in the *Academic Centre for Materials and Nanotechnology* at *AGH University of Kraków* under the supervision of dr hab. inż. Michał Zegrodnik, along with auxiliary supervisor dr hab. Andrzej Biborski. In his thesis Waseem Akbar investigates WSe_2 and WS_2 Moiré bilayers, with a particular focus on their topological and superconducting properties due to correlation effects. The thesis comprises of three introductory chapters followed by four collected papers, a total of 116 pages in length. The introductory chapters are clear and well written in good scientific English. Chapter one covers some background material on the history of superconductivity, through to the discovery of unconventional superconductivity - particularly in the cuprates. This is followed by a brief section on twisted bilayer systems. Chapter two gives an overview of the experimental evidence for superconductivity on twisted bilayer WSe_2, which is the main motivation of the theoretical work in the thesis. Chapter three introduces the theoretical model which will be used, as well as the main calculations technique used to solve the model. There then follows four papers of which the PhD candidate is a coauthor, each with a brief introduction.

Of the four papers Waseem Akbar is the first author of three of them, and the second author of one. All are now published. The papers are all coauthored with the PhD supervisor, and three have additionally the auxiliary supervisor and an external researcher as coauthors. All supplemental material is also included. I must note that the short introductions to the papers do not add much more to the abstract and conclusions of the papers themselves. Much more useful to my mind would have been an explanation of which parts of each paper were the PhD candidates own work, and which parts were the work of his coauthors. This is perhaps especially true in this case as the techniques used appear to be standard in the group, and parts of the introductory chapters are almost word for word reproduced from text of the papers, a fact which I will return to below. Considering the very close thematic range of the papers included in the thesis I feel it is a shame the candidate did not choose to

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write a standard thesis, though of course he is well within his rights to present the thesis as it is. In the absence of clear information on who contributed what to the papers, I will proceed under the assumption that the calculations are performed by the candidate, and the papers are cowritten by all authors. I hope that this can be clarified during the defence.

The papers are:

1. *Topological superconductivity with mixed singlet-triplet pairing in moiré transition metal dichalcogenide bilayers* by W Akbar, A Biborski, L Rademaker, M Zegrodnik, published in Physical Review B 110 (6), 064516;
2. *Optimal superconductivity in twisted bilayer WSe_2 where the Van Hove singularity crosses half-filling* by M Zegrodnik, W Akbar, A Biborski, L Rademaker published in Physical Review Research 8 (1), L012070;
3. *Superconductivity in moiré transition metal dichalcogenide bilayers: comparison of two distinct theoretical approaches* by W Akbar, M Zegrodnik (arXiv preprint arXiv:2605.04693), now published in Acta Phys. Pol. B 57, 5-A12 (2026); and
4. *Unconventional superconductivity in the presence of long-range interactions in transition metal dichalcogenide moiré heterobilayers* by W Akbar, A Biborski, L Rademaker, and M Zegrodnik, published in Scientific Reports.

The scientific quality of the work in the papers collected in the thesis is uniformly high, and contains important contributions to our understanding of transition-metal dichalcogenide Moiré bilayers, as well as interesting predictions for what could be seen in cases which have not yet been experimentally confirmed. Naturally all work presented in this thesis has already undergone rounds of peer review prior to being published, and I find that with regard to scientific validity I have no doubts. In the following I will therefore raise mostly various questions to clarify the background or to further explain the candidate's results. On this topic it would have been nice to have seen a chapter which gave an overview of the results here and tied them together, but the PhD candidate will in any case have the opportunity do this during the defence.

Chapter one contains an introduction to unconventional superconductivity and Moiré lattices. As motivation for why these lattices are interesting to look at the ease of tuning different model parameters is mentioned, for example electron density and electron interaction strengths, which is in stark contrast to unconventional superconductors such as the cuprates mentioned later. In general the cuprates make an interesting comparison due to the similarities in the phase diagrams when compared to those of the bilayer Moiré lattices which will be covered later in the thesis. I note that Mr Akbar mentions also the unconventional superconductor strontium ruthenate as possible having triplet pairing, citing the classic 2003 work which purported to establish this. In fact more recent work demonstrates that this is not actually the case (see A. Chronister et al., Proc. Natl. Acad. Sci. USA 118, e2025313118 (2021)). A more careful reading of the literature may have revealed this. I would also have appreciated including citations of statements such as "*proposed mechanisms ranging from Coulomb driven pairing ... to more conventional phonon mediated scenarios*". The introduction to the thesis should ideally include a literature review, which this thesis does not fully do. Although an exhaustive review of unconventional superconductivity would not at this stage be desirable, a bit more detail would have been appreciated. This criticism applies much less to the more recent work on superconductivity in the Moiré lattices, which is well covered. There are also multiple concepts introduced here which it would be better to explain the meaning of: such

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as a pseudogap and strange metal. Finally I note that referencing in this chapter and the next are inconsistent, but I leave all such further minor remarks to the end of this report.

Chapter two covers the experiments which were the motivation for the theoretical studies inside this thesis. The main focus is therefore on superconductivity in WSe_2 bilayers. Overall this is a clear introduction to the relevant experiments, though I do have several questions. In addition to vanishing resistivity, an important marker of the superconducting state is the Meissner effect, has this been measured, or could it be measured, in these bilayer lattices? I have the same question to the candidate about the Cuprates which are used as a comparison, has the Meissner effect been measured? When discussing charge ordering and Wigner crystallisation it is written that this implies that longer range coulomb interaction terms are important. What is the physical reason for this? The argument should be sketched out here. I note in this chapter both the electric field E and displacement field D are used, what is the relation for these particular materials?

Chapter three introduces the models and the method which the results of this thesis will be based upon. Starting from the Hubbard model, the t-J model is introduced (though not derived), and then extended. Indeed I think the thesis would benefit from more detail in these derivations, though I am happy to say the important physical concepts are touched upon here. Following this the way in which the Moiré bilayers will be modelled by low energy effective tight binding models is described, but not derived. This chapter ends with a description of the Gutzwiller variational method, which is then used to solve the models. I think it is a problem that this section appears to be largely copied, almost word for word in some parts, from the first of the included papers. As such the section does not seem to add anything to the thesis overall, as no opportunity was taken to flesh out this description. More importantly the paper from which it is taken is a multi-author paper, with presumably multiple authors contributing to the writing, as such within the body of the thesis it really needs to be rewritten and extended. This is compounded by the fact that no information is given about the role of each author in the papers themselves.

In chapter three the phrases "*BCS-like*"and "*non-BCS -like*" are used. Normally I would take "*BCS-like*" to refer to one of several things, such as superconductivity being phonon mediated, or describable by a mean-field theory. Here it refers to positive and negative kinetic energy gain. Why this means "*BCS-like*" and "*non-BCS -like*" is not explained. Here I also want to add that I do not think the phrase "*for details see...*" belongs in a thesis, though "*for* further *details see...*" would be permissible. Along these lines the Schrieffer-Wolf transformation could also be described in more detail, after all it is important for the foundational model used throughout the thesis. Towards the end of section 3.1 it is written that the model "*reproduce[s] selected fundamental properties of [the] cuprates*", the obvious question being which ones and why those?

In the section on the Moiré modelling a complex hopping term is introduced to describe spin-orbit like terms. Often spin-orbit terms are also written following a gauge transformation to the basis where hopping terms are real. In such a case they are often easier to interpret and I would like to have seen the same done here. the rest of this section is a good overview of the Moiré modelling. I have one question about the limits for the lattice constants given by Eq. 3.9. If I want to take the simple limit of no twist and identical lattice constants $a_1 = a_2$ for each layer, should one not find the bilayer lattice constant to be the same? Why does this not follow here?

Section 3.2 then focuses on the Gutzwiller approximation. As noted above this

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follows very closely to the descriptions in the papers, which is perhaps why some aspects are not explained in as much detail as a thesis requires. I would like to know the following about this methodology. What does the additional condition imposed on the correlation operator in (3.14) mean physically? Is it purely a matter of convenience or does it restrict the solution space? What is the diagrammatic expansion of the Gutzwiller wave function an expansion in? What are some examples of the diagrams included? What is the effective Hamiltonian scheme in this context? $\mathcal{F}$ is presumably the grand canonical potential at zero temperature, is that correct? Where do the relations 3.22 come from?

Following these three introductory chapters there are four articles of the PhD candidate included. As I have already mentioned these papers are generally of a high quality and other than the question of what contributions each coauthor made, I have the following general and interpretative questions.

In 4.1 why are only even Chern numbers observed. What would need to be added to the model to allow for odd Chern numbers to also be found? Could one measure experimentally the edge states which result from these topological phases? If so, how? I am slightly confused by the description of the topology. It is written there that each nodal point contributes a topological charge, however the Chern number is only defined if there is no degeneracy. Is the gap opened by another term in the Hamiltonian? Finally in the conclusions of the paper it is suggested that Majorana fermions could be found in these systems. However Majorana fermions only appear for crossings at high symmetry points of the band structure, which is not guaranteed for even Chern numbers. Could the band structure for an open system be calculated here to check this?

In 4.3 why is no direct comparison between the two models given, for example the equivalent of Fig. 2? Would this be possible? Could one generalise the attractive Hubbard model to better fit to the results of the t-J-U model?

Finally, I would remark that missing for me from the conclusion is a comparison of the work done throughout the series of papers, rather than simply a re-summarising of each. My final questions are what may be expected at non-zero temperature, would phases show up which are not present at zero temperature? To what extent are the phases seen restricted by the Gutzwiller method used?

PODSUMOWANIE

The original work contained in this thesis includes an important contribution to the study of unconventional superconductivity in bilayer Moiré lattices and is of a high scientific standard. There are some clarifications I hope to see in the defence, but these questions should not distract from the very nice work contained here. I also note that, although in some places lacking the detail I would have liked to see, the thesis was always very clear in what was presented. In summary this thesis fulfils the conditions for a doctoral thesis as set out in the Polish law on higher education, article 187. I recommend that Waseem Akbar passes on to the next stage of the procedure for awarding a doctoral degree.

Podsumowując, uważam, że przedstawiona rozprawa spełnia wymogi określone w art. 187 Ustawy Prawo o Szkolnictwie Wyższym i Nauce. W związku z tym oceniam ją pozytywnie i opowiadam się za dopuszczeniem pana mgr. Waseema Akbar do dalszych etapów postępowania w sprawie nadania stopnia doktora.

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FURTHER COMMENTS

1. In Fig. 1.1 the references for the sources of the figures are given directly rather than included in the bibliography.
2. In chapter two the reference to "Wang *et al.* is not properly referenced.
3. On p11 "see magnified phase diagram" could be less ambiguously referred to.
4. On p11 "(cf. Fig. 2.4)" - which panel?
5. In chapter two E is not defined until a caption later. Several other quantities are not defined fully in this chapter, even if they are normally clear from context.
6. In the caption to Fig. 2.4 the explanation of panel (b) appears to be mistaken.
7. In figure 3.2 it would be helpful to have the interaction strength marked on.
8. In figure 3.4 the reference should also be to the bibliography.

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