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Recenzja rozprawy doktorskiej mgr inż. Weroniki Pasek, zatytułowanej *"Quantum Simulation of Strongly Correlated Phases in Low-Dimensional Solid-State Systems"*

This doctoral thesis of Weronika Pasek was performed in the *Faculty of Physics, Astronomy, and Informatics* at *Nicolaus Copernicus University in Toruń* under the supervision of Dr hab. Paweł Potasz, along with auxiliary supervisor Dr Michal Zieliński. In her thesis Weronika Pasek investigates several strongly correlated systems. The first is a study of small "nano-flake" Moiré bilayers and their magnetic properties. The same Moiré systems are then shown to have possible valence-bond solid and quantum spin liquid ground states. The last topic is based on chains of graphene quantum dots which can possess interesting topological properties. These results are collected in chapters four, five, and six respectively. Chapters one and two give introductory background material and an overview of the field, while chapter three focuses on the methodology used. Overall the thesis itself, as well as the work represented inside it, are of a high quality. As such I have mostly minor questions and points that I will raise in the following report.

No full and explicit bibliographic information about the publications of the doctoral candidate is given but a search suggests that the candidate has two preprints in addition to the two published papers referenced in the thesis. One of each is a first author paper. The published works are *Superexchange mechanism in coupled triangulenes forming spin-1 chains*, Y. Saleem, T. Steenbock, ERJ. Alhadi, W. Pasek, G. Bester, and P. Potasz, Nano Letters **24**, 7417 (2024); and *Magnetic properties of moiré quantum dot arrays*, W. Pasek, M. Kupczynski, and P. Potasz, Physical Review B **108**, 165152 (2023). Both are good quality journals, with a reasonable number of citations already building up after a relatively short time. Additionally there are two preprints: *Engineering Biquadratic Interactions in Spin-1 Chains by Spin-1/2 Spacers*, Y. Saleem, W. Pasek, M. Korkusinski, M. Cygorek, and P. Potasz, arXiv:2510.26956; and *Arise of the gapless quantum spin liquid in moiré transition metal dichalcogenide due to ring exchange interaction*, W. Pasek, and Michał Kupczyński, https://doi.org/10.21203/rs.3.rs-6869593/v1. There are additionally contributions to several conference proceedings, all of which demonstrates an active participation in the research community.

The thesis is 125 pages in length, plus 321 references. It is clear and well written in good scientific English. My only comment to this end would be a plea for fewer acronyms which are on occasion hard to follow. The helpful list of acronyms at the beginning alleviates this issue slightly, but as there is no restriction for the length of the thesis perhaps it would be preferable, and certainly easier to read, if the acronyms were restricted only to those that are very common.

Chapter one contains an introduction to strongly correlated systems and topology in condensed matter physics. Focusing largely on spin chains, it covers relevant aspects of topology (such as long range entanglement and symmetry protected topology), the physics of the Kondo effect, and fractional Chern insulators. Some minor points: On page 2, although indeed a partial filling of a band would normally indicate metallic conductivity, it is less clear to me what the candidate means when they ascribe this outcome as "according to the Bloch theorem". In figure 1.2(a) the phase diagram is not fully explained. The parameter being changed, and possibly a link to the relevant equation, should be included in the caption. Occasionally references are made to ‘’ideas such as ‘Haldane's conjecture" or to "Coleman's theorem" which are not fully explained or referenced in the text and are not as well-known as for example Bloch's theorem. Similarly entanglement energy, on page 8, is a term I have not encountered before, entanglement eigenvalue is surely the more common term for eigenvalues of a reduced density matrix.

In chapter two we turn to some motivation of the thesis in terms of quantum simulators. The necessity of quantum simulators is reasoned for on the basis of the difficulty of numerically solving many models of interest, which is hard to argue with. The likely accuracy and applicability of any particular simulator to a particular problem of interest is not discussed in such detail. Several such quantum simulators are introduced, which will be further studied later in the thesis in the original work. Principally these include Moirè heterostructures and graphene nano-structures. This may be largely a matter of taste, but I find this justification rather unnecessary. Although the analogy of the effective models of, for example, a Moirè crystal to another physical system is interesting, the physics of the Moirè system itself is more than reason enough to study them. Additionally, using one of these systems as a test-bed for quantum criticality or another question of interest does not make them necessarily a "simulator". Finally, I would question how easy it is to measure "entanglement, topological order" in the ‘simulator’. Though it may sometimes be possible, this itself is a difficult experimental task.

Chapter three introduces the methods that will be used later, including a clear introduction to, and explanation of the following: exact diagonalisation, the density matrix renormalisation group, matrix product states, and the Lanczos algorithm. (I note Lanczos is unfortunately misspelt in one section heading.) In the description of variational techniques on page 36 it is not clear how the existence of a global minimum stops one from converging to a local minimum during the procedure? Otherwise this chapter is very clear, with all procedures well explained.

Chapter four contains some of the original results of the thesis. An effective model is developed for the Moiré lattice including several possible interaction terms and applied to different possible small configurations of the Moiré lattices. By tuning the twist angle and filling factor different parameters of the effective model are reached and the ground states of these are investigated. The results are nicely explained by physical reasoning and dependencies on geometry and possible finite size effects are discussed.

Following the magnetic behaviour of the ground state, chapter four turns to Wigner crystals. Here I found the justification for calling them Wigner crystals rather hard to follow. As the charge density is plotted only on the Moiré lattice sites, of which there are a small number, there is always going to be some arrangement of the charge density. If, as in one example, the charge density is higher in the three corners than the other 7 sites it is not clear that a Wigner crystal is forming that would still hold in larger samples. The difference in the charge density between figure 4.7(a) and (c) for different shapes may suggest it is not so straightforward. I do note that it is carefully written that these results show "Wigner molecules" rather than crystals, but I would have appreciated a little more detail on how they do or do not relate to the generalised Wigner crystals when the sample size is increased. In any case overall I find that chapter four contains several interesting new results.

In chapter five the same Moiré systems are found to also contain physics of quantum spin liquids. Appropriate order parameters and entanglement are calculated from an effective spin Hamiltonian. In figure 5.3 it is a little hard to see some of the differences in bond strength which result in the valence-bond solid. Perhaps the contrast of the thickness could have been increased to make this clearer. There is also the question of how large finite size effect are in the small systems available, and how reliable the resulting phase diagram, figure 5.4(b), will be. For the dimer structure factor I alse had some trouble to follow the definitions in equations 5.5 and 5.9 to be sure of what was plotted. In 5.9 there is a vector $\mathbf{D}$ which I assume is actually the scalar in (5.5). Probably a simple typo, but as D is used for two closely related quantities with the real space dependence only sometimes explicit this could have been clearer. Another very minor issue: there is a figure reference missing below equation (5.10).

For the quantum spin liquid phase the entanglement entropy is calculated, and compared to standard results from conformal field theory. The arguments given for using the results for one dimensional systems seems reasonable enough, but I wonder what is the cause of the discrepancy in the centre of the cylinder in Figure 5.6(a) between the theory and the numerical results? Is this really a finite size effect as suggested in the text? For larger dielectric constant the fit is already much better, although there is clearly a correction necessary to equation 5.12 giving the oscillations.

Chapter five also contains several very interesting new results on Moiré systems and the physics that can be seen in them, in this case valence-bond solids and quantum spin liquids.

Finally in chapter six is an investigation of nano-graphene quantum dots coupled together into chains. The quantum dots, of various sizes and shapes, are first modelled and effective Hamiltonians for the quantum dots and chains are developed. A model is obtained for the structures which is a Hubbard-like model for with onsite interactions and some longer range hopping terms, equation (6.7). There appear to be several typographical errors here in equations (6.7) to (6.10) as the hopping is purely on-site, so the model is unfortunately not exactly clear. Finally an effective model for the chain is obtained, and from this an effective spin model for the nano-graphene quantum dot chain is obtained. Obtaining this model is already an achievement and it is now used to investigate the topological properties of the chains which are shown to be tuneable to various phases. Appropriate string order parameters as well as entanglement spectra are calculated to back up the claims for the topological phase of the chains.

Chapters four, five, and six, which contain the original work of the thesis, contain many new results easily fulfilling criteria for an original contribution to the scientific field. Chapter seven concludes with an overview of the thesis. There follow two appendices containing some technical details and the references.

PODSUMOWANIE

In summary this thesis easily fulfils the conditions for a doctoral thesis as set out in the Polish law on higher education. I recommend that Weronika Pasek passes on to the next stage of the procedure for awarding a doctoral degree. I would like to stress at the end that most comments or questions I have had in the above are relatively minor, and that this is a very good thesis written to a high standard. Focusing on the minutiae is a testament to the lack of any more serious issues. I would also add finally that this thesis was a pleasure to read.

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 pani mgr inż. Weroniki Pasek do dalszych etapów postępowania w sprawie nadania stopnia doktora.

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