Review report on the doctoral thesis "Topological band theory of relativistic spintronics in antiferromagnets" by Libor Šmejkal

Dear Prof. Kratochvíl,

I was asked to review the doctoral thesis of Mr. Libor Šmejkal. Here is my assessment.

The thesis of Mr. Šmejkal summarizes results of his theoretical work in the field of antiferromagnetic spintronics and topological band theory in general. Most of the results presented in this thesis were published in peer reviewed journals, the rest, presumably under review, is available as arXiv preprints.

First, I shall state that I find the work of Mr. Šmejkal truly impressive. This is reflected in several ways in his publication list. He is a co-author of several articles in high profile journals such as Nature Physics or Physical Review Letters, in some cases being the first author. His papers are highly cited. The reputation of Mr. Šmejkal is also reflected in being the first author of a Nature Physics review article, without any of his supervisors being co-authors. The breadth of his thinking and scientific independence is documented also by a recent proposal to use topological antiferromagnets to detect the dark matter, Phys. Rev. Lett. **123,** 121601 (2019), again without co-authorship of his supervisors.

The thesis links two hot topic in condensed matter and applied physics – the antiferromagnetic spintronics and the topological bandstructure theory. Working in one of the leading groups in the field, Mr. Šmejkal addressed not only a theoretically interesting questions, but also questions with direct experimental relevance. There are number of valuable contributions to the studied topics in thesis, out of which I would like to point out three, that I find truly important: i) the systematic group theoretical approach to the studied phenomena and identification of candidate materials using this approach, ii) prediction and analysis 'relativistic metal-insulator transition' in CuMnAs – switching between Dirac and massive quasiparticle excitations by rotating the Neel vector, iii) the theory of spontaneous Hall effect in collinear antiferromagnet RuO_2.

The thesis is focused on fundamentally new physics rather than method development. The used numerical methods are standard in the field. The analysis of topological invariants is a modern chapter in bandstructure theory, while it does not require extensive method development, its mastering is mathematically rather involved and requires deep understanding of the basic concepts. During the work on his thesis Mr. Šmejkal used several different band structure codes (VASP, ELK) and tools for bandstructure analysis (wannier90) and demonstrated ability to use them efficiently.

The actual presentation of the subject in the thesis is somewhat disappointing to me, given the high scientific quality of the presented results. Personally, I know a number of PhD theses that I consider an excellent introduction to their respective topics including many details, e.g., analytic derivations normally missing the papers or books. The present thesis can hardly serve this role. It introduces number of concepts and methods, e.g., Berry phase and Berry curvature in the bandstructure context, magnetic symmetry groups, linear response theory, density functional theory, relativistic bandstructrue, coherent potential approximation. However, the level of presentation requires rather hight previous knowledge for it to be understandable. This is particularly a pity for the less standard modern topics such as the Berry curvature and the Chern numbers, while ts is less important for the description of numerical methods, which can be found in number of other sources.

Let me make a few specific remarks in this context.

- An explicit definition of 'gauge-covariance' in eq. 1.28 would be useful, as well as index forms of eqs. 1.30 and 1.31.
- Berry phase is multi-band case (calculated according to eq. 1.35) is not introduced.
- The mathematical notation is sometimes a bit erratic, for example the curly bracket {} is used to denote symmetry operations (e.g., in 1.41), general sets (1.42) and commutator (page 25)
- The discussion of the linear response on pages 20-21 is rather incomplete and inaccurate. Eq. 1.53 gives the static response not a response. The t-dependence of B, I believe, should refer to the corresponding operator in the Heisenberg picture rather than time dependent perturbation. The inverse temperature 'beta' in 1.53 is not introduced as well as the meaning of A and B (operators?). I think it would be better to drop 1.53 and simply refer to the cited literature for the complete discussion.
- Page 29, I do not agree that 'non-equilibrium steady-state properties can be expressed in terms of solely equilibrium ground state wavefunctions and operators'. This is in general only true if the deviation from equilibrium is infinitesimal.
- Discussing eq. 1.66, it is the Bloch gauge not the periodic gauge which fulfills 1.66.
- Page 33, 'Berry phase pi of the massless Dirac point'. So far Berry phase was introduced as a property of a path. How does one define a Berry phase of a point?
- In Eq. 1.74, Delta behaves like a chemical potential. I believe the author has in mind a staggered potential changing sign between the sublattices, (-1)^i\Delta ?
- On page 45, the author refers to 'density matrix' (non-local object \rho(r,r')), while he means spin density \rho_{ab}(r).
- It is not clear to me why to introduce normal ordering (pages 46-47) to explicitly normal ordered expressions (2.4, 2.7).

On other hand I appreciate the details on how to perform the calculations described in the thesis, e.g., names of the relevant routines of the used codes or necessary input files, which allows the calculations to be easily reproduced. The thesis also contains an extensive list of relevant literature, which can make it a useful reference on the subject.

Before concluding I would like to mention several scientific questions I would like to raise during the defense.

In Fig. 1.8 as well as later in text the authors use a symmetry operation consisting of a mirror plane and a sublattice translation perpendicular to it – the 'off-center mirror plane/line'. In my opinion, this is equivalent to an ordinary mirror plane (i.e., without any translation) at a shifted position. Am I wrong or what is the rational for introducing this symmetry operation?

Discussing the Dirac points (DPs) in section 1.6 the author uses the term 'DPs protected by symmetry'. However, I find this a bit an abuse of a language. In my opinion protected by symmetry refers to the situation found, e.g., in RuO_2 where in certain directions in the Brillouin zone only two- (or higher) dimensional irreducible representations exist and therefore the eigenstate must be at least two-fold degenerate. In the present case, on the other hand the bands cross because they belong to the different irreducible representations of the little group (at shown in the thesis). This is a typical situation that can be found in any material with higher symmetry and the band crossing can be removed by 'pulling the band apart'. Can you address this issue?

The gaps at Dirac points in CuMnAs opened by rotating the Neel vector are rather small. The calculations use static mean-field approximation, in which the conduction electrons are treated a non-interacting. Do you have a qualitative guess what would happen in a more complete treatment that would include thermal and/or quantum fluctuations of the Mn moments?

To conclude, I find the results contained in this thesis to be an important contribution to our understanding of metallic antiferromagnets, the topology of their bandstructure and related transport properties. Moreover, the work has direct connection to experiments and falls into a field that has been astonishingly fast in the transferring fundamental results to technological applications. Mr. Šmejkal has demonstrated, in my opinion beyond any doubt, the ability to conduct independent research and to come up with new and creative ideas.

Wien, February 21, 2020

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