NEW TECHNOLOGIES
RESEARCH CENTRE
UNIVERSITY
OF WEST BOHEMIA

Reviewer's report on the doctoral thesis of
RNDr. David Wagenknecht (Univerzita Karlova):

„Theory of spin-dependent transport in magnetic solids“

Research in the field of magnetic materials and spintronics has lead in the past two decades to the development of new technologies in context with the electron spin. In particular, significant impact has been achieved by considering new physical effects which are based on spin-orbit coupling concerning transport properties. An important role in these developments plays the calculational design by means of first principle approaches such as density functional theory. The main aim of Mr. Wagenknechts thesis is to investigate longitudinal and transverse transport properties in disordered alloy systems. In order to do so, D. Wagenknecht has been involved in the numerical implementations of the Kubo-Bastin formalism. The main focus of the thesis is devoted to the impact of finite temperatures on transport properties by means of the so called alloy analogy model.

In the first Introductory chapter, D. Wagenknecht introduces the topic of his thesis and he discusses it in a wider context. The following chapter is devoted to density functional theory and to the LMTO formalism which serves as a formal basis for the investigations presented here. The next chapter 2 reviews the so called alloy analogy model which allows to include spin and lattice fluctuations into the linear response formalism and its implementation in the LMTO Green function method is discussed in detail in chapters 3. All these chapters are very well and clear written. From these chapters it is clear that D. Wagenknecht internalized the complete theoretical methodology on a very high level.

The main results of this thesis are summarized in form of chapters 4 and 5. Most of the results are published in high ranking journals and furthermore in seven of them D. Wagenknecht is the first author. These are very interesting publications in the field of ab-initio description of transport properties at finite temperatures. Eventhought it is necessary to note that AAM was in the past implemented in other Green function techniques and D. Wagenknecht cites properly all relevant publications in the field.

University of West Bohemia
New Technologies – Research Centre
Univerzitní 8, 306 14 Plzeň, Czech Republic

Phone: (+420) 377 63 4771

E-mail: jminar@ntc.zcu.cz

To conclude, the submitted work of D. Wagenknecht is very well written and discusses many important aspects of electronic transport in solid state systems. However, there are some misprints and missing references to the figures. All together, D. Wagenknecht published remarkable number of publications. The submitted content-rich thesis undoubtedly reflects his competence and also proves his achieved scientific independence. Accordingly, I suggest this thesis to be defended.

In addition I have following questions:

– Section 2.1.2: Displacement matrix as shown in Eq. 2.6 implies that internal sums over angular momenta has to be converged. At least one additional angular momentum lmax+1 channel should be taken into account. Did author consider it, and did author some tests with this this respect?

– Author describe in his work that number of directions for the atomic displacements led to only minor changes of the results. Could you please discuss this point more in a detail? In particular, for crystals with lower symmetry then cubic one, it is known from X-ray diffraction studies, that displacements follow elliptical shape. Did author consider these issues.

– Author used experimental magnetization curves to model spin fluctuations (directions of local magnetic moment). Is there a way how to calculate it in ab-inition way?

– Spin fluctuations are included e.g. in dynamical mean field theory. Please comment how presented method is comparable, or if it can be generalized to other cases which are not possible to describe by local DMFT.

Plzen, 11.06.2019, Doc. Dr. Jan Minar

University of West Bohemia
New Technologies – Research Centre
Univerzitní 8, 306 14 Plzeň, Czech Republic

Phone: (+420) 377 63 4771

E-mail: jminar@ntc.zcu.cz