Physics of Functional Materials

Univ.-Prof. Dr. Wilfried Schranz
Boltzmanngasse 5
A-1090 Wien

T +43-1-4277-72771
F +43-1-4277-9727
wilfried.schranz@univie.ac.at

Prof. Jan Kratochvil

Studijní oddělení
Ke Karlovu 2027/3
121 16 Praha 2
Czech Republic

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Review on the PhD-thesis

"**Algebraic Approaches to Elementary Excitations in Media with Broken Spatial or Time-reversal Symmetry**"

by **Kay Condie Erb**

The doctoral thesis of Mr. Kay Condie Erb deals with structural phase transitions that exhibit macroscopic symmetry breaking. Group – subgroup transitions (Landau-type) are considered. These are transitions, where the low symmetry phase with space group G_1 is a subgroup of G_0, the space group of the high symmetry phase. Since the author is interested in macroscopic quantities, he can restrict himself to point group symmetry elements, where $P_1 < P_0$.
It was shown already some time ago, that there exist 212 distinct non-magnetic (Aizu-) species of macroscopic symmetry breaking phase transitions. If the corresponding quantity (order parameter), which appears spontaneously below T_c as a result of such symmetry breaking is polarization, magnetization or strain, the phase transition is called ferroelectric, ferromagnetic or ferroelastic. There exist extensive tables, which list possible spontaneous polarization, magnetization and strain components for all of the ferroic species.

In the present work the author makes use of a rather new group theoretically based concept to study the discriminability of macroscopic domain states - not only by polarization, magnetization or strain - but by all order parameters, which transform as vectors or vector-like quantities.
In fact, it was shown in 2014, by the supervisor of the thesis J. Hlinka, that group theory can be conveniently used to define 8 different "vector like" quantities (if one takes into account also time reversal operation in addition to spatial symmetries), which correspond to the basis functions of the irreducible representation of the group $D_{\infty h} \times \{1,1'\}$. It means, that all physical quantities defined by a sign, a magnitude, and an axis can be classified in eight symmetrically different categories.

The novelty of the present thesis is, that for the first time there exists now a full list of possible ferroic transitions between non-magnetic (212 species) and between magnetic point groups, classified with respect to the eight vector-like quantities. I.e. for all the possible ferroic phase transitions it is specified

which of the eight vector-like quantities appears spontaneously below the symmetry breaking transition. This task, which is virtually impossible to do manually, was achieved by Mr. Erb using extensive computer calculations.
One of the eight different vector-like quantities, that is worth mentioning here, is the chiroaxial vector. Its appearance is related to the existence of Bloch-skyrmion textures. Switchable skyrmion textures are of high interest in modern-day research, because of their potential to increase storage density substantially. The author found, that among the 212 species, there exist 105 chiroaxial species.

The tables (Attachments A - E), which are presented in the thesis of Mr. Erb are of invaluable value for people who are doing material science, materials design, either experimentally or theoretically by computational methods. They can be used in various ways. One possible application is, that for any required macroscopic property one gets a quick educated guess, for which material class it is worth to search.

Finally, I would like to make few remarks concerning some (mainly technical) details of the present work.

- The present thesis is divided into two parts. Chapters 1 - 5, introduce the basic theory, necessary to understand the results of the thesis. There are only very few misprints (e.g. “force matrix” on page 11, should better read “force constant matrix”, or $422 < 2_{\backslash} \rightarrow 422 > 2_{\backslash}$, etc.), but overall these chapters are well written and organized. On some places (e.g. page 23 on selection rules), I would have liked that the author dives a little deeper into the matter.
- Chapters 6 – 9 represent the core of Mr Erb´s PhD-thesis. The main results are summarized in the tables of Attachments A – E. These tables, which are made with great care and meticulosity are of their own beauty. But at the same time, they are of great value for many areas of solid state physics and materials research.
  Some of the results are already published and some others are intended to be published soon. Of particular note is chapter 6, on the chiroaxial transitions.
  Here I would also like to mention, that although chapters 6 – 9 are very well written from a general point of view, it would have been nice if the author had given few real examples from literature, which are showing some of the theoretically calculated properties.

In conclusion, the doctoral thesis of Mr Kay Condie Erb fulfils all the requirements of a high standard scientific work and offers a very important novel contribution in the field of symmetry breaking phase transitions. I am confident that the results will stimulate further research in materials science, e.g. by exploring the richness of functional properties which result from macroscopic symmetry breaking.
The doctoral thesis demonstrates undoubtedly that the candidate K.C. Erb is highly capable of conducting independent scientific high level research and I am looking forward to the defence.

In terms of grades, the dissertation of Mr Erb deserves the highest score.

Wilfried Schranz

Univ.-Prof. Dr.
Boltzmanngasse 5
A-1090 Wien, Austria