Report on Doctoral Thesis

“Microscopic Origin of Linear Magneto-Optical Effect in bcc Fe”
by Ondřej Stejskal

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When I was a PhD student, on the wall at the entrance to the department of computational physics of my home institute was written: “The aim of calculations is not a number but understanding”. The thesis submitted by Ondřej Stejskal follows exactly this motto.

Photon energy dependence of magneto-optical spectra of bcc Fe which are determined by the off-diagonal part of the permittivity tensor were calculated by many groups. This is actually a benchmark for any new \textit{ab initio} code for studying magneto-optical effects. However, to my knowledge nobody did such a detailed analysis of those features of the bcc Fe band structure which are responsible for peaks of the off-diagonal part of the permittivity tensor. To my opinion, finding interband transitions responsible for the peaks and, especially, \textit{k}-space regions giving dominant contributions are among most important achievements of the Thesis. This allowed to analyze how avoided band crossings appear when spin-orbit coupling (SOC) is taken into account and to show why interband transitions from \textit{k} volumes in the vicinity of the crossings contribute to the off-diagonal part of the permittivity tensor. I am particularly impressed by graphical representation of the analysis, e.g., BZ plots of constant energy difference surfaces for interband transitions decorated by the imaginary part of the $\langle |p_x| \langle |p_y| \rangle$ product of corresponding dipole matrix elements.

Another important achievement of the work is the development of the code for calculating the Berry curvature from band structure and momentum matrix elements. This allowed to study and to visualize topological properties of the bcc Fe band structure, in particular, Berry curvature monopoles at Weyl points, i.e., crossings of nondegenerate bands. Also very impressive is the visual analysis of the Berry curvature close to band crossing which become avoided because of SOC.

I have some comments and questions to the Thesis which are listed below.

1. p. 37: Strictly speaking Eq. (4.4)–(4.6) are incorrect since $V_{xc}[\rho]$ should be replaced by $E_{xc}[\rho]$ which is unknown exchange-correlation \textit{energy} functional. Then, Eq. (4.7)
should become $V_{xc} = \frac{\delta F_{xc}(\rho)}{\delta \rho}$, where $V_{xc}(r)$ is indeed exchange-correlation potential.

2. p. 38: It should be emphasized that $\varepsilon_{xc}(\rho)$ is not simply an unknown function of $\rho$ but by definition of LDA is the exchange-correlation energy of a homogeneous electron gas of the same density $\rho$.

The LDA exchange-correlation functional is not unique. There are, e.g., Barth–Hedin, Perdew–Zunger, Perdew–Wang parameterizations of $\varepsilon_{xc}(\rho)$.

As the whole work is devoted to ferromagnetic bcc Fe it would be appropriate to introduce here not only LDA but also Local Spin-Density Approximation (LSDA).

3. p. 38: Since one of main goals of the work is calculation of optical and MO spectra it would be appropriate to discuss in this section the Koopmans' theorem, i.e., the relation between LSDA one electron energies and excitation energies.

4. p. 38: The description of the LAPW basis set:

"WIEN2k uses the combination of the linearized augmented plane wave (LAPW) method, the augmented plane wave (APW) with local orbitals (+lo) method and local orbitals (LO). The basis sets for lo and LO differ despite being named identically." is too vague to my taste. Especially, taking into account that lo are important for proper accounting for SOC in compounds with heavy $p$ elements.

Also the sentence where "a linear combination of radial and spherical function" is mentioned sounds strange. Probably, a linear combination of a radial function and its energy derivative multiplied by spherical harmonics is meant here.

5. p. 40: The energy difference between a singlet and a triplet may be negative but not in an isolated atom. According to the first Hund's rule the direct exchange defined by Eq. (4.21) is always positive meaning that the exchange interaction favors the state with the highest possible spin $S$.

6. p. 41: The SO interaction is much weaker than the exchange one only for light elements. For instance, in Ir or U they are of the same order of magnitude.

7. p. 47: Eq. (4.60)–(4.62) would be more clear if it were shown which quantities explicitly depend on $k$. 

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8. p. 57: Momentum matrix elements in Eq. (5.42) are calculated with some precision. Also the number of bands in the sum over $n'$ may vary. How important is this numerical uncertainty for calculation of topological invariants. Is it possible to test the suggested approach to calculate the Berry curvature by comparing its results to those obtained from Wannier functions?

9. p. 57: Usually, band degeneracy is present along some high symmetry line in BZ and lifted in neighboring $k$ points. Can such a situation be treated by the algorithm? Can accidental degeneracy at a Weyl point cause any problems?

10. p. 62: Why $\text{Im} \epsilon_{zz}$ and $\text{Re} \epsilon_{xy}$ calculated from the same set of band energies and matrix elements differ (Fig. 6.1)?

11. p. 62: $\text{Im} \epsilon_{zz} \cdot E$ in Fig. 6.2 is proportional to $\sigma_{zz}(\hbar \omega)$ and should be an even function of $\hbar \omega$. Why the broadened curve goes to 0 with a nonzero derivative?

12. p. 65: “When the magnetization along the z-axis is introduced, the number of symmetries is reduced to 8.”

The Hamiltonian is invariant w.r.t. to another 8 symmetry operations which change the magnetization direction to the opposite if the latter are followed by the time reversal operation. Is it possible to use also these “combined” symmetry operations?

13. p. 95: I am confused by the definition of spin-up and spin-down states: usually, one calls majority- or spin-up states those spin states with $s_z = -1/2$ which lower their energy in the magnetic field, i.e., the WIEN2k definition is the commonly used one. The sign should be checked.

In spite of the large number of comments, I find the work presented in the Thesis to be very interesting and carefully done. The Thesis is clearly written and its author Ondřej Stejskal without any doubts qualifies for the Ph.D. degree.

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