Prediction and assignment of spectra from strongly magnetized White Dwarf stars using high-accuracy quantum chemistry

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Observational spectra from stellar objects allow insight about the composition of their atmospheres. In many cases the recorded spectra can be assigned using accurate experimental data for the species in question. Such assignments, however, become significantly more complicated – or even impossible - when strong magnetic fields are involved. For example, on magnetic White Dwarf (WD) stars magnetic fields of up to about 100 000 Tesla are encountered. On the other hand, on Earth, only up to 100 Tesla can be generated in specialized high-field labs. Hence, predictions can often not be made by experimental means. In such cases, high-level quantum-chemical predictions are essential for the assignment of respective magnetic WD spectra. Because the magnetic and Coulomb forces are equally important, they need to be treated on an equal footing. This is possible when *finite-field* quantum-chemical methods are employed. The development of finite-field Coupled-Cluster[1] (CC) and Equation-of-Motion CC methods[2-5] has enabled such predictions for systems with more than just a couple of electrons. In this contribution we will discuss how respective accurate and reliable predictions are made and present a recent successful assignment of an observational spectrum from a strongly magnetized WD star, through a fruitful interplay between astrophysics and quantum chemistry. The assignment involves the identification of metals in the atmosphere and an estimate of the strength of its magnetic field.[6]

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