Temperature-Dependence of the Ratio between Orbital and Spin Magnetic Moments and of the Magnetic Hyperfine Field by ab-initio Calculations

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Abstract: Elements-specific spin and orbital magnetic moments and especially their ratio are important material parameters in spintronics. For practical reasons, dependence of these characteristics on the temperature is very important. We apply ab initio calculations to predict that the ratio between the orbital and spin moments increases with increasing temperature for a range of systems. We interpret this as a consequence of unquenching of the orbital moment due to the decrease of symmetry if the temperature increases. The predicted increase of the ratio between the orbital and spin magnetic moments is large enough to be seen by XMCD experiments. Another family of spectroscopic techniques important for studying element-specific magnetism are those which measure the magnetic hyperfine field □ - such as nuclear magnetic resonance or Mössbauer spectroscopy. We apply ab initio calculations to investigate how □ and its relation to the magnetic moment depend on the temperature. We find that there are visible differences between calculated temperature dependence of the magnetization *M* and of the magnetic hyperfine field *B*. We conjecture that possibly the temperature-dependence of hyperfine field related spectra may involve some aspects not covered by direct comparison with *B*.