MAGNETIC ANISOTROPY OF 3d- AND 4f-METALS IN THE MODEL OF CRYSTAL FIELD WITH CALCULATION OF COVALENT BONDS AND THEIR FLUCTUATIONS 1. FERMION SPECTRA AND MAGNETIC ORDER

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Anomalous (in the existing theories of ferromagnetism) temperature dependences of magnetic anisotropy (MA) constants are explained on the basis of calculation of covalent bonds and their fluctuations (CBF). Soft CBF modes cause the strong temperature dependence of exchange parameters of unstable intermetallic compounds such as MnBi up to exchange inversion in MnAs. The varying of a sum of inter- and intraionic interactions in the operator form with respect to polarization of covalent electrons of different types allows us to obtain the Hamiltonian of crystal field (CF) in the form of MA energies. The parameters of the MA Hamiltonian are the functions of CBF correlators. The presence of CBF soft modes in ferrometals and compounds with polymorphism (Co, MnBi, Gd, etc.) defines the strong dependence of MA constants on temperature T, pressure P, etc. The soft modes are caused by the crossing of CBF branches with Fermi surfaces. The small CBF energies in extremal points (minimum) and the strong CBF dispersion in their vicinity lead to a strong (linear) T-dependence of MA constants, magnetization $M_S(T)$, and exchange parameters. The theory explains satisfactorily the MA constants $K_1(T)$ in Co, MnBi, and rare-earth metals (REM), in particular, the change of the $K_1(0)$ sign in the series of heavy REM.