Abstract Submitted
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Super-exchange in transition-metal oxides WALTER HARRISON, Stanford University — Using contemporary tight-binding theory and parameters[1]. Anderson's perturbation approach [2] gives a qualitatively correct energy difference (a factor 2.3 too high) between ferromagnetic and antiferromagnetic configurations for MnO, It corresponds to a Heisenberg model with $J_2/J_1 = 11/7$. Perturbation theory fails as the energy denominator gets smaller for FeO and CoO, and changes sign for NiO. Use of the special- points method to treat exchange-split bands gives smaller values not well characterized by a J_1 and J_2. Carrying it out self-consistently reorders the NiO levels and leads to still smaller energy differences near experiment for all four oxides, as estimated from the experimental Néel temperature TN , The theory predicts a variation with pressure corresponding to $(d/TN)\partial TN/\partial d = -12.2$ for MnO , near experiment, dropping to -9.1 for NiO. The theory is applicable also to the paramagnetic susceptibility.

[1] Walter A. Harrison, Elementary Electronic Structure, World Scientific (Singapore, 1999), revised edition (2004).
[2] P. W. Anderson, Phys. Rev. 115, 2 (1959).

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