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.