V. I. Anisimov, V. P. Antropov, V. A. Gubanov, M. I. Katsnel'son, and A. I. Likhtenshtein. *Band theory of magnetism in metals and alloys.* The problem of ferromagnetism and antiferromagnetism remains one of the most challenging problems in theoretical solid state physics, especially since it combines features of localized and collective behavior of magnetic electrons. Although this problem was clearly formulated as early as the 1930s in papers by F. Bloch, J. Slater, S. P. Shubin, and S. V. Vonsovskiĭ, E. Stoner, and others,[1] significant progress was achieved only in the late 1970s with the development of spin-fluctuation theories of magnetism.[2] However, these approaches are based on a number of model assumptions and employ fitting parameters, and this markedly reduces their utility in explaining and predicting the magnetic properties of real materials, especially alloys and complex intermetallic compounds. Fully nonempirical methods in the band theory of magnetism have appeared only recently. These do permit us to compute the characteristics of magnetic interactions and the related properties of specific materials.[3-6] Numerous band calculations of the ground state of ferromagnetic metals and dilute alloys in the local spin-density functional approximation have demonstrated agreement of calculated and experimental values of the magnetic moment (M_0) within a few percent.[7] By applying Andersen's "local force" theorem to magnetic excitations,[5,6] it becomes possible, in principle, to compute with the same accuracy other properties, such as the spin-wave stiffness (D) and the parameters of effective interatomic exchange interaction (J_{ij}). Although in metallic systems exchange is very much a non-Heisenberg interaction, the parameters J_{ij} can be rigorously defined in order to describe the energy of weakly inhomogenous distributions of spin density. Another important characteristic is the molecular field parameter

$$J_i = \sum_{j \neq i} J_{ij},$$

which describes the interaction of a magnetic moment at site i with the rest of the crystal.

Modern computational methods make it possible to study not only the energy spectra of solids, but also the parameters of the exchange interaction. The most convenient technique of computing magnetic interactions involves the multiple scattering formalism—the KKR or the LMTO Green's function methods. In these methods complete information on the electronic structure of the crystal is contained in the full scattering matrix T_{ij}, which is a function of both spin ($\sigma = \uparrow, \downarrow$) and orbital ($L = l, m$) variables, as well as the energy E. According to Refs. 5, 6 all properties of magnetic excitations at zero temperature can be expressed in terms of T_{ij} in the ground state, for example:

$$J_{ij} = \frac{1}{4\pi} \int^{E_F} \mathrm{Im}\, \mathrm{Sp}_L \left(\Delta_i T_{ij}^{\uparrow} \Delta_j T_{ji}^{\downarrow}\right) \mathrm{d}E,$$

$$J_0 = -\frac{1}{4\pi} \int^{E_F} \mathrm{Im}\ \mathrm{Sp}_L \left[\Delta_0 \left(T_{00}^{\uparrow} - T_{00}^{\downarrow}\right) + \Delta_0 T_{00}^{\uparrow} \Delta_0 T_{00}^{\downarrow}\right] \mathrm{d}E,$$

where $\Delta_i = (t_{i\uparrow}^{-1} - t_{i\downarrow}^{-1})$, t_i being the single-site scattering matrix. When this method[5,6] is generalized to the relativistic case one obtains expressions for the magnetic anisotropy constant and for the parameters of the antisymmetric Dzyaloshinskiĭ-Moriya interaction. In the mean-field approximation J_0 determines the Curie temperature T_c.[5] A computation of J_0 for an impurity in a magnetic matrix makes it possible to estimate the stability of the parallel and antiparallel orientations of the impurity spin. An analogous method can be extended to the paramagnetic state within the framework of the KKR coherent potential approximation, which makes it possible to calculate the magnetic susceptibility,[4] as well as the dependence of T_c on concentration in alloys.[6]

The promise of the nonempirical method in the theory of band magnetism was demonstrated by the computation of the magnetic properties of a large number of transition metals, their alloys and compounds. The obtained values of spin stiffness D for Fe and Ni (294 and 386 meV·Å^2) are in good agreement with experimental results (314 and 395 meV·Å^2). In all systems investigated thus far, the parameter J_0 explains the observed type of magnetic ordering (for example, ferromagnetic in $FePd_3$, $MnPt_3$ and antiferromagnetic in $FePt_3$, $MnPd_3$). By studying the dependence $J_0(E_F)$ for ideal crystals and impurities, we can analyze the mechanisms by which magnetic properties appear in a number of transition metals, in particular the tendency towards antiferromagnetism when the band is nearly half-filled and towards ferromagnetism at higher band filling (Fig. 1). The non-Heisenberg character of the exchange interaction in metals is most clearly manifested by the existence of two magnetic states ($M_0 > 0$ and $M_0 < 0$) stable with respect to moment rotation ($J_0 > 0$ in both states). This situation occurs for the Mn impurity in Fe and explains the experimental data on dilute FeMn alloys,[8] as well as on the Fe impurity in antiferromagnetic Cr (Fig. 2). Also note the presence of sharp impurity peaks in density of electron states near E_F for both magnetic states of the Fe impurity in the antiferromagnetic "pseudogap" of Cr. These peaks could explain the anomalous properties of dilute CrFe alloys.[9]

In order to focus on the extent of magnetic moment localization and the dependence of the exchange interaction

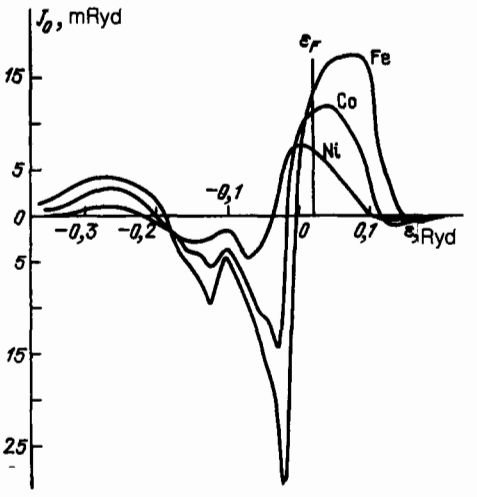

FIG. 1. Exchange parameter J_0 as a function of the Fermi energy for impurities in the hcp phase of ferromagnetic Co.

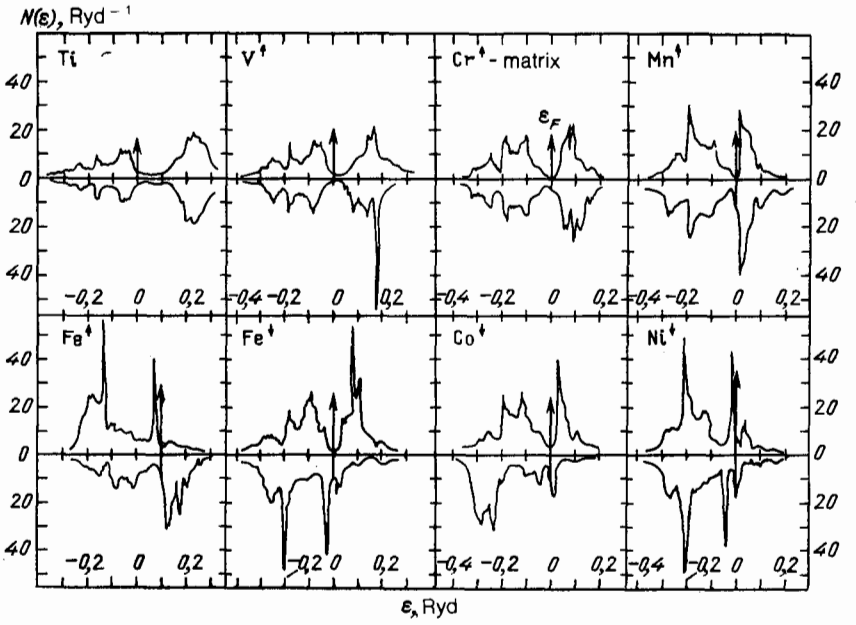

FIG. 2. Local densities of electronic states for transition metal impurities in antiferromagnetic Cr.

"constant" J_0 on magnetic configuration, we calculated the excited states of an "impurity" with a moment M_0 rotated by an angle θ. If the moment is fully localized M_0 is independent of θ, and the rotation energy $\delta E \sim 1 - \cos\theta$. With Fe we found that this picture is valid for $\theta < 45°$; at larger θM_0 (θ) becomes smaller, and at angles $\theta > 135°$ the self-consistent solution ceases to exist. In the case of an Mn impurity in Fe, M_0 depends weakly on θ throughout the $0 \leqslant \theta \leqslant 180°$ range, which points to stronger localization of the magnetic moment. Hence δE exhibits strongly non-Heisenberg behavior. The opposite situation of a weakly defined local moment occurs in pure Ni, where $M_0(\theta)$ falls sharply even at small θ.

In this manner, we can successfully determine the magnetic characteristics of crystals by focusing on the particular features of the electronic band structure. This particular approach should permit us to proceed with microscopic modeling of the properties of new magnetic alloys with varying degrees of electronic state localization.

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