CC/NUMBER 46
NOVEMBER 14, 1983

This Week's Citation Classic

Hodges L, Ehrenreich H & Lang N D. Interpolation scheme for band structure of noble and transition metals: ferromagnetism and neutron diffraction in Ni. *Phys. Rev.* 152:505-26, 1966.
[Div. Engineering and Applied Physics, Harvard Univ., Cambridge, MA]

This paper describes a simple interpolation scheme for face-centered-cubic (fcc) noble and transition metals in which d bands are represented by linear combinations of atomic orbitals and conduction bands by orthogonalized plane waves. It is used to calculate the ferromagnetic band structure of nickel. [The *SCI*® indicates that this paper has been cited in over 440 publications since 1966.]

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September 23, 1983

"This paper contains the work done for my PhD degree at Harvard University under Henry Ehrenreich, and bears the same title as my dissertation. Ehrenreich came to Harvard from General Electric in 1963. I was his first student, and he allowed me to choose a topic from among a list of several that he suggested. The success of this project was due more to his excellent list than to a wise choice on my part.

"This paper actually preceded the dissertation upon which it was based. After I had carried out my research, we wrote the paper and submitted it, so writing the dissertation was merely a matter of adding further details.

"Norton Lang, a later student of Ehrenreich who has gone on to a distinguished career at the IBM Yorktown Research Center, made many valuable contributions to the effort and was a coauthor.

"Our work built on other work from the early 1960s. Experimental evidence had begun to favor an itinerant description of the 3d electrons in noble and transition metals. Sophisticated band structure calculations were available that provided good electronic band structures for the paramagnetic state of nickel. Gutzwiller,[1] Hubbard,[2,3] and Kanamori[4] had showed how correlation effects giving rise to ferromagnetism in nickel could be described by an intra-atomic Coulomb interaction.

"We devised an interpolation scheme which fit the paramagnetic band structure, and then added an intra-atomic Coulomb interaction to give a ferromagnetic band structure that was in excellent agreement with many experimental features.

"This work has been extensively cited for two reasons. First, it gave a band structure for Ni which has been referred to in many later experimental and theoretical studies. Second, the interpolation scheme has proved an extremely useful tool for many other band structure calculations of 3d and 4d face-centered-cubic noble and transition metals.

"Since this paper was written, there has been a great deal of further development of the topics of transition-metal electronic band structures[5] and itinerant electron ferromagnetism."[6]

1. **Gutzwiller M C.** Effect of correlation on the ferromagnetism of transition metals. *Phys. Rev. Lett.* 10:159-62, 1963.
2. **Hubbard J.** Electron correlations in narrow energy bands. *Proc. Roy. Soc. London Ser. A* 276:238-57, 1963.
3. ----------. Citation Classic. Commentary on *Proc. Roy. Soc. London Ser. A* 276:238-57, 1963. *Current Contents/Physical, Chemical & Earth Sciences* 20(22):16, 2 June 1980.
4. **Kanamori J.** Electron correlation and ferromagnetism of transition metals. *Progr. Theor. Phys. Kyoto* 30:275-89, 1963.
5. **Mackintosh A R & Andersen O K.** The electronic structure of transition metals. (Springford M, ed.) *Electrons at the Fermi surface*. Cambridge: Cambridge University Press, 1980. p. 149-224.
6. **Lonzarich G G.** Fermi surface studies of ground-state and magnetic excitations in itinerant electron ferromagnets. (Springford M, ed.) *Electrons at the Fermi surface*. Cambridge: Cambridge University Press, 1980. p. 225-77.