

Finite-temperature ferromagnetism of nickel

W. Nolting, W. Borgiel,* V. Dose, and Th. Fauster

*Max-Planck-Institut für Plasmaphysik—EURATOM Association, D-8046 Garching bei München,
Boltzmannstrasse 2, Federal Republic of Germany*

(Received 24 February 1989)

By use of a generalized Hubbard model, we investigate the influence of electron correlations on the temperature dependence of the quasiparticle properties of ferromagnetic Ni. The one-particle energies of the model Hamiltonian are taken from a realistic band-structure calculation. The model contains only two parameters, Hubbard U and the interband exchange J . It is approximately solved by use of a self-consistent moment method. We find a ferromagnetic ground state, mainly caused by the uppermost d subband, a magnetic moment at $T=0$ of $0.56\mu_B$, a Curie temperature of $T_C=635$ K, a Brillouin-type magnetization curve, a strict Curie-Weiss behavior of the paramagnetic susceptibility, a satellite peak some 6 eV below the chemical potential μ as a consequence of strong electron correlations in the uppermost d subband, a temperature-dependent spin polarization of the satellite ($\cong 75\%$ at $T=0$), temperature-dependent exchange splittings at the top of the d band (0.23 – 0.36 eV at $T=0$), and an enhancement factor of the electronic specific heat $q(T=0) \cong -0.56$. All these results are in excellent agreement with the experiment. For the first time the full temperature dependence of the quasiparticle band structure and the quasiparticle density of states of ferromagnetic Ni are presented.

I. INTRODUCTION

The so-called “localized” magnetism, as represented by $4f$ materials such as EuO, EuS, and Gd, can be considered as rather well understood within the Heisenberg model. The itinerant magnetism, however, a prototype of which is the $3d$ transition metal Ni, persists to be a matter of intense study and controversial discussion.¹ The most important question therefore aims directly at the origin of the phenomenon. What is the physical reason for a spontaneous magnetic order of itinerant electrons? Many of the existing theories, very often based on Stoner-type approximations, predict unrealistic, high Curie temperatures. It is therefore not yet clear which theoretical model may be appropriate for the description of metallic magnetism leading, e.g., to reasonable T_C values. Furthermore, a modern theory of band magnetism encounters the fundamental problem of the incorporation of localized as well as itinerant features of the conduction electrons. We have to develop a model, which simultaneously describes localized aspects (Brillouin-function-type magnetization, Curie-Weiss behavior of the static susceptibility, etc.) as well as itinerant aspects (noninteger magneton numbers in the ground state, large cohesive energy,^{2,3} enhanced specific-heat coefficient,^{4,5} etc.).

Self-consistent one-electron band-structure calculations^{6,7} for Ni yield, at a first glance, rather convincing $T=0$ spectra. In detail, however, there are striking discrepancies with valence-band photoemission data, which have attracted the interest of numerous research groups in the recent past.⁸ The exchange splitting near the top of the fifth d subband [0.25 – 0.35 eV (Refs. 9–13)] is only half as large as predicted from band theory

[0.65 eV (Ref. 6)]. There appears a resonant satellite structure some 6 eV below the Fermi edge^{14–16} with a high spin polarization,¹⁷ which cannot be reproduced by one-electron band-structure calculations. The measured d -band widths¹¹ are smaller by about 20–30% than the calculated ones.⁶ It is the widely accepted opinion that these discrepancies are caused by strong electron correlations in the partially filled d band, which are obviously not taken into account by normal band theory. In this paper we want to present a new approach which is able to explain nearly quantitatively all the above-mentioned problems and questions.

The modern theory of magnetism in narrow-band systems normally starts from the Hubbard model,^{18–20} which can be used for discussing very general problems of band magnetism as well as for detailed statements about the electronic structure of certain magnetic materials. Investigations, which aim at the qualitative understanding of band magnetism, are based on the simple s -band Hubbard model. Since its exact solution is not available, the question, whether or not this model is able to describe collective magnetism, is not completely clarified. In the recent past a great number of approximate theories have been proposed, based on mean-field approximations,^{21,22} Green-function techniques,^{18,23} moment methods,^{24–26} functional integral procedures,^{27–34} variational approaches,^{35,36} and perturbation expansions.^{37,38} Interesting information can be drawn from numerical investigations of finite systems,^{39–43} where, however, the generalization of such results to the thermodynamic limit appears to be rather problematic. Most of the above-mentioned work confirms the possibility of collective magnetism within the framework of the Hubbard model, but under certain conditions on model parameters

like the Bloch density of states, the effective coupling constant, and the band occupation.²⁶

The simple s -band Hubbard model is, of course, completely overcharged if detailed statements about the electronic structure of classical band ferromagnets like Fe, Co, and Ni are required. The d -band degeneracy can no longer be neglected, the actual lattice potential must be incorporated into the one-particle part of the Hamiltonian, and the influence of the other charge carriers, which do not enter explicitly into the model, must be taken into account by a proper renormalization of the Bloch energies $\varepsilon_m(\mathbf{k})$. An appropriate procedure has recently been proposed for the $4f$ ferromagnet EuO (Refs. 44–46) to derive the full temperature dependence of the quasiparticle band structure. For this purpose a spin-polarized, self-consistent one-electron band calculation, performed on the basis of density functional theory, has been implemented into a many-body scheme for the d - f exchange model. An analogous concept should work for Ni, too, when we use a generalized Hubbard model as starting point.

Similar ideas have been applied already by some other authors. Treglia *et al.*⁴⁷ start from a model, which considers intra-atomic direct Coulomb interactions only and neglects all exchange terms. The “Stoner part” of the interaction is incorporated into the one-particle energies, which are then identified with the results of a band structure calculation.⁴⁸ The authors justify this identification by referring to Gunnarson,⁴⁹ who has shown that such band calculations for magnetic materials are quite consistent with a Stoner ansatz in which the exchange splitting is only slightly energy dependent. A perturbation theory for the electronic self-energy is then performed up to quadratic terms in U/W (U is the intra-atomic Coulomb matrix element, and W is the Bloch bandwidth). Although the basic idea and some final results are quite convincing, it is surely not unfair to say that the applied simplifications are too serious and sometimes even misleading. So it has recently been shown⁵⁰ that the satellite structure derived in Ref. 47 is nothing more than a consequence of the non-self-consistency of the applied theory, disappearing when the procedure is improved in this respect.

An interesting ansatz has been chosen by Davis and Feldkamp⁵¹ in order to explain why the measured d -band widths are up to 25–40% narrower than the calculated ones. The theory being restricted to $T=0$, uses as input a linear-combination of atomic-orbitals fit⁵² for the Ni d bands calculated by Wang and Callaway.⁶ The many-body part resembles an interpolation scheme,^{53,54} which is equivalent to the so-called Hubbard I approach.¹⁸ The results indeed remove a substantial portion of the discrepancy between experiment and previous $T=0$ band calculations.

Liebsch^{55,56} has applied a T -matrix approach^{57,58} to the extended Hubbard model¹⁹ for an approximate determination of the one-hole spectral density. Because of the small hole density in the Ni d bands the T -matrix procedure should work reasonably well. A well-known disadvantage of this method, however, is its non-self-consistency. Bandnarrowing, large quasiparticle damp-

ing, relatively small exchange splitting, and the existence of the satellite peak come out qualitatively correct, but cannot be fitted quantitatively with the same U . Furthermore, no statements about finite temperature properties are made.

In this paper we present a model calculation which provides us with the full temperature dependence of all important quasiparticle quantities of the transition metal Ni. A ferromagnetic ground state and a strikingly exact Curie temperature are found as results of a self-consistent treatment of a generalized Hubbard model, which are not at all predetermined by the input from the one-electron band calculation. The paper is organized as follows. In Sec. II we introduce the model and explain how the results of a realistic band calculation enter into our procedure. In Secs. III and IV we develop the many-body approach, the results of which are presented and compared to experimental Ni data in Sec. V.

II. MODEL HAMILTONIAN

Our model shall incorporate all interactions between electrons in the same Wigner-Seitz cell being, however, restricted to the d -band complex only. The most general Hamiltonian then, is the following: "

$$H = H_0 + H_1, \quad (2.1)$$

$$H_0 = \sum_{i,j,\sigma,m} T_{ij}^{(m)} a_{im\sigma}^\dagger a_{jm\sigma}, \quad (2.2)$$

$$H_1 = \frac{1}{2} \sum_{i,\sigma,\sigma',m_1,m_2,m_3,m_4} U(m_1, m_2; m_4, m_3) \times a_{im_1\sigma}^\dagger a_{im_2\sigma'}^\dagger a_{im_3\sigma} a_{im_4\sigma}. \quad (2.3)$$

$a_{im\sigma}$ ($a_{im\sigma}^\dagger$) is the annihilation (creation) operator of a Wannier electron with spin σ at site \mathbf{R}_i in an energy band with index m . $T_{ij}^{(m)}$ are the hopping integrals being connected with the one-electron Bloch energies by

$$T_{ij}^{(m)} = (1/N) \sum_{\mathbf{k}} \varepsilon_m(\mathbf{k}) e^{-i\mathbf{k} \cdot (\mathbf{R}_i - \mathbf{R}_j)}. \quad (2.4)$$

The sum extends over all \mathbf{k} vectors of the first Brillouin zone.

U is the Coulomb matrix element. To simplify the model as far as possible, but so that still enough structure is left to express the essentials of itinerant magnetism,⁵⁹ we restrict the Coulomb matrix elements to the “direct terms” ($m_1 = m_4 = m; m_2 = m_3 = m'$),

$$U_{mm'} = U(m, m'; m, m'), \quad (2.5)$$

and to the “exchange terms” ($m_1 = m_3 = m; m_2 = m_4 = m'$),

$$J_{mm'} = U(mm'; m'm). \quad (2.6)$$

Then, the interaction operator H_1 reads,

$$H_1 = \frac{1}{2} \sum_{i,\sigma,\sigma',m,m'} (U_{mm'} a_{im\sigma}^\dagger a_{im'\sigma'}^\dagger a_{im'\sigma} a_{im\sigma} + J_{mm'} a_{im\sigma}^\dagger a_{im'\sigma'}^\dagger a_{im\sigma} a_{im'\sigma}). \quad (2.7)$$

This Hamiltonian is very similar to the one used by Oles

and Stollhoff.⁶⁰ As they have shown, in the form of (2.7) H_1 represents the very general intra-atomic interaction part if the atomic symmetry is fully taken into account. We now introduce spin operators

$$\sigma_{im}^z = \frac{1}{2} \sum_{\sigma} z_{\sigma} n_{im\sigma}, \quad (2.8)$$

$$\sigma_{im}^{\sigma} = \sigma_{im}^x + iz_{\sigma} \sigma_{im}^y = a_{im\sigma}^{\dagger} a_{im-\sigma}, \quad (2.9)$$

where $n_{im\sigma} = a_{im\sigma}^{\dagger} a_{im\sigma}$ is the occupation number operator, and z_{σ} a sign factor ($z_{\uparrow} = +1, z_{\downarrow} = -1$). Using

$$\sigma_m^z \sigma_{m'}^z + \frac{1}{2} \sum_{\sigma} \sigma_m^{\sigma} \sigma_{m'}^{-\sigma} = \sigma_m \cdot \sigma_{m'}, \quad (2.10)$$

we get after simple manipulations

$$\begin{aligned} H_1 = & \frac{1}{2} \sum_{i,m,\sigma} (J_{mm} + U_{mm}) n_{im\sigma} n_{im-\sigma} \\ & - \sum_{\substack{i,m,m' \\ (m \neq m')}} J_{mm'} \sigma_{im} \cdot \sigma_{im'} \\ & + \frac{1}{2} \sum_{\substack{i,m,m' \\ (m \neq m')}} (U_{mm'} - \frac{1}{2} J_{mm'}) \hat{n}_{im} \hat{n}_{im'}. \end{aligned} \quad (2.11)$$

The last term is spin independent:

$$\hat{n}_{im} = \sum_{\sigma} n_{im\sigma}, \quad (2.12)$$

and is therefore irrelevant for magnetic phenomena. With sufficient accuracy and according to the basic ‘‘philosophy’’ of our procedure this term will be accounted for by a respective renormalization of the one-particle energies, as will be described below. Finally, we neglect the m dependence of the coupling constants,⁵⁹

$$J \equiv J_{mm'} \quad (m \neq m'); \quad U \equiv J_{mm} + U_{mm} \quad (2.13)$$

so that our model contains, henceforth, only two parameters. If we introduce the ‘‘local’’ spin operator

$$\mathbf{S}_{im} \equiv \sum_{\substack{m' \\ (m' \neq m)}} \sigma_{im'} \quad (2.14)$$

the model Hamiltonian can be reformulated as follows:

$$H = H_0 + H_C + H_{e-m}, \quad (2.15)$$

$$H_C = \frac{1}{2} U \sum_{i,\sigma,m} n_{im\sigma} n_{im-\sigma}, \quad (2.16)$$

$$H_{e-m} = -\frac{1}{2} J \sum_{i,\sigma,m} (z_{\sigma} n_{im\sigma} S_{im}^z + a_{im\sigma}^{\dagger} a_{im-\sigma} S_{im}^{-\sigma}). \quad (2.17)$$

The first term H_0 , defined in (2.2), contains via (2.4) the Bloch energies $\varepsilon_m(\mathbf{k})$, which should incorporate, as realistically as possible, all those interactions which are not explicitly taken into account by our model Hamiltonian (2.15). The second term H_C is the Hubbard-Coulomb interaction between electrons of the same d subband, which turns out to be decisive with respect to the appearance of spontaneous band ferromagnetism in Ni. The third term H_{e-m} can be interpreted as electron-magnon interaction. It consists of two parts, a diagonal Ising-type part be-

tween the z components of the electron spin and the ‘‘local’’ spin (2.14), and a nondiagonal part, which expresses spin-exchange processes between the two spin operators.

As mentioned above, we have to determine the one-electron energies $\varepsilon_m(\mathbf{k})$ in such a way that all the interactions, which are not directly covered by our model Hamiltonian (2.15), are accounted for by a proper renormalization of the $\varepsilon_m(\mathbf{k})$. For this purpose we performed a band-structure calculation for nickel with a parametrized Slater-Koster tight-binding scheme along the line proposed by Papaconstantopoulos.⁷ The root-mean-square error to a first-principles augmented-plane-wave (APW) calculation in the local-density approximation is 10 meV for the six energy bands which are of interest here. The ‘‘ d bands’’ were composed from the five states with the highest total d character at each \mathbf{k} point. They are arranged into five subbands, numbered by $m = 1, \dots, 5$, with increasing energy at each \mathbf{k} point. The main problem in this context is, not to count any interaction twice, once in the one-electron band calculation and then once more in the following many-body treatment of our model. In Ref. 44 such a double counting has been elegantly circumvented for the ferromagnetic $4f$ insulator EuO by exploiting an exactly solvable special case of the underlying d - f exchange model. This led to an exact one-to-one relationship between Bloch and quasiparticle energies, by which a double counting could be excluded. Such an exactly solvable limiting case is not available for the rather sophisticated model (2.15). Instead of this we use here the same arguments as given in Ref. 47, which are based on Gunnarsson’s observation⁴⁸ that standard band calculations on ferromagnetic materials are quite consistent with the Stoner model. In the paramagnetic phase, however, the Stoner energies are identical to the Bloch energies. We have therefore performed the above-mentioned $T=0$ band calculation for paramagnetic Ni. We believe that all interactions responsible for the magnetic behavior are then switched off, while all the other interactions contribute to a renormalization of the one-particle energies

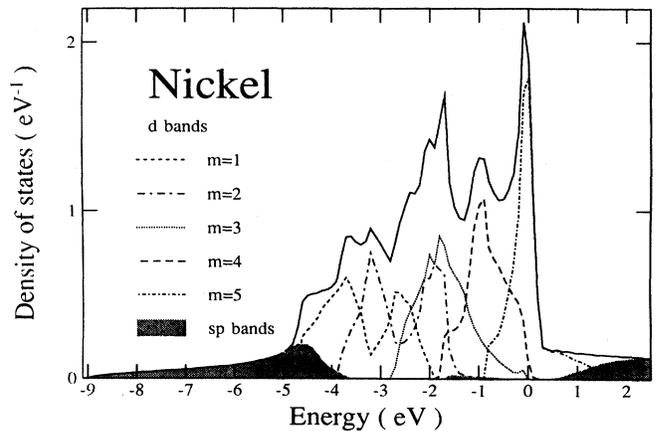


FIG. 1. Bloch density of states for paramagnetic nickel as function of energy and its decomposition into d and sp subbands.

$\varepsilon_m(\mathbf{k})$. As shown below, the actually required inputs for our many-body treatment are the Bloch densities of states (BDOS) of the five d bands ($m = 1, 2, \dots, 5$), which we obtain by a calculation of the energy eigenvalues at about 2 000 000 \mathbf{k} points—over 46 000 in an irreducible wedge of the first Brillouin zone—and sorting them into 0.1 eV wide energy intervals for the five subbands. Figure 1 shows the total density of states (solid line) which agrees very well with other calculations.^{61,48} We see that the sp bands (shaded regions) are almost completely pushed out of the d -band region, and that there is a significant part of the $m = 5$ subband well above the Fermi edge. An independent calculation using a combined interpolation scheme⁶² gave essentially the same results. The partial densities of states derived in Ref. 61 from an APW calculation, also agree very well with ours. We are aware that the distinction between d and sp bands is somewhat arbitrary. Our procedure, however, is well defined and assumes that the states with the highest d character show the strongest correlation effects. Except for the two coupling constants U and J , which are fixed at a later stage of our theory, our model Hamiltonian (2.15) is now completely established.

III. SELF-CONSISTENT MOMENT METHOD

The second term in the model Hamiltonian (2.15) turns out to be of crucial importance for the appearance of

spontaneous band ferromagnetism. The interband exchange term, which describes electron-magnon scattering, has a strong influence on the magnetic properties of the system, but *does not produce* the ferromagnetism. It provides the (\mathbf{k}, m, σ) electron with a certain self-energy contribution $M_{m\sigma}(\mathbf{k}, E)$. Let us assume for the moment that we have already determined this quantity—explicitly done in Sec. IV—and that we can express the influence of $M_{m\sigma}$ by a further renormalization of the Bloch energies [$\varepsilon_{m\sigma}(\mathbf{k}) \rightarrow \tilde{\varepsilon}_{m\sigma}(\mathbf{k})$]. We are then left with an effective Hamiltonian,

$$H_{\text{eff}} = \sum_{m=1}^5 H_{\text{eff}}(m), \quad (3.1)$$

which separates with respect to the band index m . Each additive term $H_{\text{eff}}(m)$ has the formal structure of the one-band Hubbard Hamiltonian:

$$H_{\text{eff}}(m) = \sum_{\mathbf{k}, \sigma} \tilde{\varepsilon}_{m\sigma}(\mathbf{k}) a_{\mathbf{k}m\sigma}^\dagger a_{\mathbf{k}m\sigma} + \frac{1}{2} U \sum_{i, \sigma} n_{im\sigma} n_{im-\sigma}. \quad (3.2)$$

As in Ref. 26 we solve the corresponding many-body problem by use of a self-consistent moment method. The central quantity of this procedure is the one-electron spectral density $S_{\mathbf{k}m\sigma}(E)$,

$$S_{\mathbf{k}m\sigma}(E) = (1/N) \sum_{i,j} e^{i\mathbf{k} \cdot (\mathbf{R}_i - \mathbf{R}_j)} \int_{-\infty}^{+\infty} d(t-t') e^{-(i/\hbar)E(t-t')} (1/2\pi) \langle [a_{im\sigma}(t), a_{jm\sigma}^\dagger(t')]_+ \rangle. \quad (3.3)$$

Previous investigations²⁴⁻²⁶ have convincingly demonstrated that a two-pole ansatz,

$$S_{\mathbf{k}m\sigma}(E) = \hbar \sum_{j=1}^2 \alpha_{jm\sigma}(\mathbf{k}) \delta(E + \mu - E_{jm\sigma}(\mathbf{k})), \quad (3.4)$$

represents a very realistic starting point for this fundamental function, at least as far as quasiparticle lifetime effects do not play a dominant role. It should be mentioned that the ansatz (3.4) is the only not exactly provable assumption of our method. The further treatment is rigorous. The spectral weights $\alpha_{jm\sigma}$, as well as the quasiparticle energies, are fixed by the first four spectral moments

$$Q_{\mathbf{k}m\sigma}^{(n)} = (1/\hbar) \int_{-\infty}^{+\infty} dE E^n S_{\mathbf{k}m\sigma}(E), \quad (3.5)$$

which can be calculated exactly and independently of the required spectral density by use of the following relationship:

$$Q_{\mathbf{k}m\sigma}^{(n)} = (1/N) \sum_{i,j} e^{-i\mathbf{k} \cdot (\mathbf{R}_i - \mathbf{R}_j)} \langle [[\dots [a_{im\sigma}, H_m], \dots, H_m]_-, a_{jm\sigma}^\dagger]_+ \rangle, \quad (3.6)$$

where $[[\dots [\dots], \dots], \dots]$ is an n -fold nested commutator. H_m is defined as

$$H_m = H_{\text{eff}}(m) - \mu \sum_{i, \sigma} n_{im\sigma}, \quad (3.7)$$

where μ denotes the chemical potential. After tedious but straightforward calculations (for more details see Ref. 26) we get, as quasiparticle energies,

$$E_{jm\sigma}(\mathbf{k}) = H_{m\sigma}(\mathbf{k}) + (-1)^j [K_{m\sigma}(\mathbf{k})]^{1/2}, \quad (3.8)$$

$$H_{m\sigma}(\mathbf{k}) = \frac{1}{2} [\tilde{\varepsilon}_{m\sigma}(\mathbf{k}) + U + B_{m-\sigma}], \quad (3.9)$$

$$K_{m\sigma}(\mathbf{k}) = \frac{1}{4} [U + B_{m-\sigma} - \tilde{\varepsilon}_{m\sigma}(\mathbf{k})]^2 + U \langle n_{m-\sigma} \rangle [\tilde{\varepsilon}_{m\sigma}(\mathbf{k}) - B_{m-\sigma}]. \quad (3.10)$$

The spectral weights are given by

$$\alpha_{jm\sigma}(\mathbf{k}) = \frac{1}{2}(-1)^j [E_{jm\sigma}(\mathbf{k}) - B_{m-\sigma} - U(1 - \langle n_{m-\sigma} \rangle)] / [K_{m\sigma}(\mathbf{k})]^{1/2}. \quad (3.11)$$

This set of equations still contains two equal time correlations, $B_{m-\sigma}$ and $\langle n_{m-\sigma} \rangle$, which must be expressed by the one-electron spectral density, in order to get a self-consistent solution. By use of the spectral theorem⁶³ the average occupation numbers $\langle n_{m\sigma} \rangle$ are uniquely determined by the spectral density,

$$\langle n_{m\sigma} \rangle = (1/N\hbar) \sum_{\mathbf{k}} \int_{-\infty}^{+\infty} dE f_{-}(E) S_{\mathbf{k}m\sigma}(E - \mu). \quad (3.12)$$

Because of translational symmetry they are, of course, site independent. $f_{-}(E)$ denotes the Fermi function,

$$f_{-}(E) = \{1 + \exp[(E - \mu)/k_B T]\}^{-1}. \quad (3.13)$$

The crucial term for the appearance of ferromagnetism is the ‘‘band correction’’ $B_{m-\sigma}$, which consists of higher equal-time correlation functions,

$$\langle n_{m-\sigma} \rangle (1 - \langle n_{m-\sigma} \rangle) (B_{m-\sigma} - T_{0m\sigma}) = (1/N) \sum_{\substack{i,j \\ (i \neq j)}} T_{ij-\sigma}^{(m)} \langle a_{im-\sigma}^{\dagger} a_{jm-\sigma} (2n_{im\sigma} - 1) \rangle. \quad (3.14)$$

$T_{0m\sigma}$ is the center of gravity of the renormalized (m, σ) Bloch band,

$$T_{0m\sigma} = (1/N) \sum_{\mathbf{k}} \bar{\epsilon}_{m\sigma}(\mathbf{k}). \quad (3.15)$$

Fortunately, the band correction is also expressible by the one-electron spectral density. This has been demonstrated in detail in Ref. 26. We therefore cite here only the final result for the ‘‘higher’’ expectation value in (3.14),

$$\langle a_{im-\sigma}^{\dagger} a_{jm-\sigma} n_{im\sigma} \rangle = (1/N\hbar) \sum_{\mathbf{k}} e^{-ik \cdot (\mathbf{R}_i - \mathbf{R}_j)} \int_{-\infty}^{+\infty} dE f_{-}(E) \frac{1}{U} [E - \bar{\epsilon}_{m-\sigma}(\mathbf{k})] S_{\mathbf{k}m-\sigma}(E). \quad (3.16)$$

This leads to the following expression for the important band correction:

$$\begin{aligned} \langle n_{m-\sigma} \rangle (1 - \langle n_{m-\sigma} \rangle) (B_{m-\sigma} - T_{0m\sigma}) \\ = (1/N\hbar) \sum_{\mathbf{k}} [\bar{\epsilon}_{m-\sigma}(\mathbf{k}) - T_{0m-\sigma}] \int_{-\infty}^{+\infty} dE \{(2/U)[E - \bar{\epsilon}_{m-\sigma}(\mathbf{k})] - 1\} f_{-}(E) S_{\mathbf{k}m-\sigma}(E). \end{aligned} \quad (3.17)$$

Eqs. (3.8)–(3.13), (3.15), and (3.17) constitute a closed system, which can be solved self-consistently for the average occupation numbers $\langle n_{m\sigma} \rangle$ and $\langle n_{m-\sigma} \rangle$, provided the renormalized energies $\bar{\epsilon}_{m\sigma}(k)$ are known. The latter are discussed in Sec. IV.

IV. EFFECTIVE MEDIUM APPROACH

Finally, we discuss the self-energy contribution $M_{m\sigma}(\mathbf{k}, E)$, which stems from the interband exchange term H_{e-m} (electron-magnon scattering) (2.17) of our model Hamiltonian. The operator H_{e-m} has exactly the same structure as the d - f exchange operator, which has been applied to the $4f$ ferromagnet EuO in Refs. 44–46. We therefore approximate $M_{m\sigma}(\mathbf{k}, E)$ by switching off the Hubbard term H_C for the moment and by solving the nontrivial many-body problem defined by the operator $H_0 + H_{e-m}$ (s - f or d - f model, Kondo lattice) strictly along the line exposed in Ref. 45. For details of the mathematical procedure, the reader is referred to Refs. 45 and 46. Here we present only the final result for the self-energy [see Eq. (2.33) in Ref. 46],

$$M_{m\sigma}(\mathbf{k}, E) \equiv M_{m\sigma}(E) = \sum_{\substack{m' \\ (m' \neq m)}} M_{mm'\sigma}(E), \quad (4.1)$$

$$M_{mm'\sigma}(E) = -\frac{1}{2} J z_{\sigma} \langle \sigma_{im'}^z \rangle + \frac{1}{4} J^2 \langle \sigma_{im'}^{-\sigma} \sigma_{im'}^{\sigma} \rangle G_{0-\sigma}^{mm'}(E) \{1 - [\frac{1}{2} J (1 + z_{\sigma} \langle \sigma_{im'}^z \rangle) - M_{mm'-\sigma}(E)] G_{0-\sigma}^{mm'}(E)\}^{-1}. \quad (4.2)$$

This is an implicit conditional equation for the electronic self-energy, which also enters the propagator $G_{0-\sigma}^{mm'}(E)$:

$$G_{0-\sigma}^{mm'}(E) = (1/N) \sum_{\mathbf{k}} [E - \epsilon_m(\mathbf{k}) - M_{mm'-\sigma}(E)]^{-1}. \quad (4.3)$$

The magnetization $\langle \sigma_{im}^z \rangle$ of the m th subband and the

spin correlation function $\langle \sigma_{im}^{-\sigma} \sigma_{im}^{\sigma} \rangle$ provide the self-energy with a characteristic temperature dependence. Both can be expressed by the one-electron spectral density. For the magnetization, this follows directly from (2.8) and (3.12):

$$\langle \sigma_m^z \rangle = (1/2N\hbar) \sum_{\mathbf{k}\sigma} z_{\sigma} \int_{-\infty}^{+\infty} dE f_{-}(E) S_{\mathbf{k}m\sigma}(E - \mu). \quad (4.4)$$

The spin correlation can be written

$$\begin{aligned} \langle \sigma_{im}^{-\sigma} \sigma_{im}^{\sigma} \rangle &= \langle a_{im-\sigma}^{\dagger} a_{im\sigma} a_{im\sigma}^{\dagger} a_{im-\sigma} \rangle \\ &= \langle n_{im-\sigma} \rangle - \langle n_{im-\sigma} n_{im\sigma} \rangle. \end{aligned} \quad (4.5)$$

We define

$$\langle n_{im-\sigma} n_{im\sigma} \rangle = (1/U) p_m(T) \quad (4.6)$$

and use (3.16) to express $p_m(T)$ by $S_{km-\sigma}(E)$,

$$\begin{aligned} p_m(T) &= (1/N\hbar) \sum_{\mathbf{k}} \int_{-\infty}^{+\infty} dE f_{-}(E) \\ &\quad \times [E - \tilde{\epsilon}_{m-\sigma}(\mathbf{k})] S_{km-\sigma}(E). \end{aligned} \quad (4.7)$$

Finally, the spin correlation reads

$$\langle \sigma_{im}^{-\sigma} \sigma_{im}^{\sigma} \rangle = \frac{1}{2} n_m - z_{\sigma} \langle \sigma_{im}^z \rangle - (1/U) p_m(T), \quad (4.8)$$

where $n_m = \langle \hat{n}_{im} \rangle$ is the average occupation of the m th d subband ($0 \leq n_m \leq 2$).

This completes our general theory. We see that after inserting (4.3), (4.4), and (4.8) in Eq. (4.2), the self-energy contribution $M_{m\sigma}(E)$ is determined by the one-electron spectral density only. In general, $M_{m\sigma}$ will be a complex quantity,

$$M_{m\sigma}(E) = r_{m\sigma}(E) + i i_{m\sigma}(E). \quad (4.9)$$

In accordance with our spectral density ansatz (3.4), which, from the very beginning, neglects quasiparticle damping, we have to determine the renormalized one-particle energies $\tilde{\epsilon}_{m\sigma}(\mathbf{k})$ as solution of the following equation:

$$\tilde{\epsilon}_{m\sigma}(\mathbf{k}) := \epsilon_m(\mathbf{k}) + r_{m\sigma}(E = \tilde{\epsilon}_{m\sigma}(\mathbf{k})). \quad (4.10)$$

In first order this equation is solved by

$$\tilde{\epsilon}_{m\sigma}^{(1)}(\mathbf{k}) = \epsilon_m(\mathbf{k}) - \frac{1}{2} J z_{\sigma} \sum_{m'} \langle \sigma_{m'}^z \rangle. \quad (4.11)$$

($m' \neq m$)

Via the very general expression for the one-electron Green's function,

$$G_{km\sigma}(E) = \hbar [E - \epsilon_m(\mathbf{k}) - \Sigma_{m\sigma}(\mathbf{k}, E)]^{-1}, \quad (4.12)$$

$$S_{km\sigma}(E) = -(1/\pi) \text{Im} G_{km\sigma}(E + i0^+), \quad (4.13)$$

we introduce the total self-energy $\Sigma_{m\sigma}(\mathbf{k}, E)$,

$$\Sigma_{m\sigma}(\mathbf{k}, E) = R_{m\sigma}(\mathbf{k}, E) + i I_{m\sigma}(\mathbf{k}, E), \quad (4.14)$$

which turns out to be \mathbf{k} independent. According to our ansatz it is, of course, a real quantity,

$$\Sigma_{m\sigma}(\mathbf{k}, E) \equiv R_{m\sigma}(E) = r_{m\sigma}(E) + U \langle n_{m-\sigma} \rangle [E - r_{m\sigma}(E) - B_{m-\sigma}] / [E - U(1 - \langle n_{m-\sigma} \rangle) - r_{m\sigma}(E) - B_{m-\sigma}]. \quad (4.15)$$

V. DISCUSSION OF THE RESULTS

A. Ferromagnetic ground state

We have self-consistently solved the closed system of equations, developed in Secs. III and IV, for the average occupation numbers $\langle n_{m\downarrow} \rangle$ and $\langle n_{m\uparrow} \rangle$. As already mentioned, it turns out that the question of whether or not the electron system orders ferromagnetically is mainly answered by the intraband correlation U and by the subband occupation n_m . In a previous paper²⁶ we have explicitly shown, for the one-band Hubbard model, that the Coulomb interaction U as well as the number of electrons (n_m) and the number of holes ($2 - n_m$), respectively, have to exceed certain critical values, otherwise a spontaneous ferromagnetic order becomes impossible. The lowest three subbands ($m = 1, 2, 3$) are fully occupied and therefore magnetically inactive. The number of holes in the $m = 4$ subband is far below the critical value. Thus the ferromagnetic ground state is exclusively due to the uppermost fifth subband, which is slightly more than half-filled. The interband exchange J enhances the ferromagnetism, but does not produce it. More strictly, the first term in (4.2) favors a ferromagnetic order, while the second term, arising from electron-magnon scattering, tends to destroy the order. However, the first term is dominating. Previous studies^{45,46} have shown that for temperatures below T_C , which we are mainly interested in, the electron-magnon contribution is sufficiently well

reproduced by the first term in (4.2), if one replaces J by a J^* being about 20% smaller than the original J . Since J is in any case an adjustable parameter within our model, we have done this replacement, which leads to a substantial simplification of the rather involved numerical evaluation of our theory. The renormalized one-particle energies $\epsilon_{m\sigma}(\mathbf{k})$ can then be used in the form (4.11) instead of (4.10). The self-consistent solution of our model yields a ferromagnetic ground state for Ni with the experimental value of $0.56\mu_B$ for the $T=0$ moment,⁶⁴ if we take

$$U = 6 \text{ eV}, \quad J^* = 0.8 \text{ eV}. \quad (5.1)$$

This finally determines our model. There is no further adjustable parameter.

B. Magnetization, susceptibility, and spin correlation

The total Ni magnetization m_{tot} shows, as a function of temperature, a typical Brillouin function-type behavior (Fig. 2). The main contribution to the magnetization stems from the moment m_5 of the magnetically active fifth d subband and a minor part from that of the polarized fourth subband. The first three completely occupied subbands are spin-split below T_C , but without resulting moment. The self-consistent solution of our model determines the Curie temperature of Ni to $T_C = 635 \text{ K}$ in striking agreement with the experiment [$T_C^{\text{exp}} = 631 \text{ K}$ (Ref.

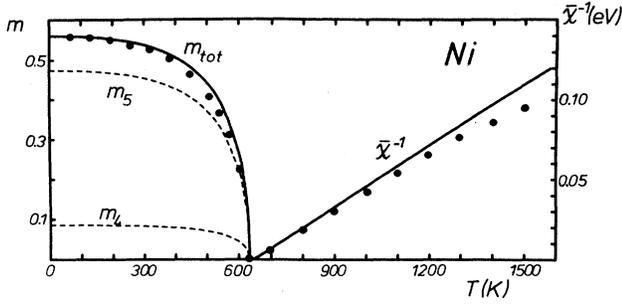


FIG. 2. Left: Magnetization m_{tot} of ferromagnetic nickel as function of temperature T . m_4 and m_5 are the partial magnetizations of the fourth and fifth d subbands, respectively. The solid line is from the present theory, the dots are experimental data from Ref. 65. Right: Static susceptibility $\bar{\chi}$ [see text, Eq. (5.2)] for paramagnetic Ni as function of temperature. The solid line is from the present theory, the dots are from the experiment (Ref. 66).

$$\bar{\chi}(T) = [\mu_0 / (N \hbar \mu_B)] \sum_{m, \mathbf{k}, \sigma} z_{\sigma} \int_{-\infty}^{+\infty} dE f_{-}(E) [\partial / \partial B_0 S_{\mathbf{k}m\sigma}(E - \mu)]_{T, B_0 \rightarrow 0}^{(0)}. \quad (5.4)$$

The result of a troublesome, but straightforward calculation for $\bar{\chi}(T)$ is exhibited in Fig. 2. This quantity is related to the so-called specific susceptibility,

$$\chi_s = \chi / \rho \quad (\rho \text{ is the mass density}), \quad (5.5)$$

by the following relation:

$$(\bar{\chi})^{-1} (\text{eV}) = 0.692 \times 10^{-5} \chi_s^{-1} (\text{cm}^3 / \text{g}). \quad (5.6)$$

The static susceptibility of paramagnetic Ni, as calculated within our model, shows an almost strict Curie-Weiss behavior, again in excellent agreement with the experiment.^{64,66} The phenomenological fit to the experimental data is frequently written as⁶⁶

$$\chi_{\text{tot}}^{\text{expt}}(T) = C / (T - T_C) + \chi_a, \quad (5.7)$$

where χ_a is assumed to be rather small and T independent. It may be caused by influences like paramagnetic susceptibility of sp electrons, orbital contribution of d electrons, s - d exchange interactions or similar effects, which are not considered by our model. For very high temperatures χ_a causes a slight deviation of $(\chi_{\text{tot}}^{\text{expt}})^{-1}$ from the Curie-Weiss line as can be seen in Fig. 2.

The results for the magnetization and for the static susceptibility clearly prove that our band model (2.1) excellently reproduces the localized aspects in the band magnetism of Ni. This is further supported by the behavior of the spin-flip correlation function $\langle \sigma_m^{\pm} \sigma_m^{\mp} \rangle$, which can be evaluated with the self-consistent solution of our model by use of Eq. (4.8). The result, plotted for the two highest d bands in Fig. 3, strikingly resembles corresponding correlations of localized spin systems. The main difference is the $T=0$ behavior. In the ferromagnetic saturation of a localized spin system, $\langle \sigma^{-} \sigma^{+} \rangle$ is, of

11]. The calculated magnetization curve (Fig. 2) fits the experimental data almost quantitatively.⁶⁵

Figure 2 shows also the temperature behavior of the static susceptibility of paramagnetic Ni,

$$\chi_{\text{tot}}(T) = (\mu_B^2 / \mu_0) (N/V) \bar{\chi}(T), \quad (5.2)$$

$$\bar{\chi}(T) = (\mu_0 / \mu_B) \sum_{m=1}^5 \sum_{\sigma} z_{\sigma} \langle \partial \langle n_{m\sigma} \rangle / \partial B_0 \rangle_{T, B_0 \rightarrow 0}^{(0)}. \quad (5.3)$$

μ_B is the Bohr magneton and μ_0 the vacuum permeability. The superscript "0" means "paramagnetic." In the presence of a magnetic field $B_0 = \mu_0 H$, we have to add a Zeeman term $z_{\sigma} \mu_B H$ to the one-particle energies $\epsilon_{m\sigma}(\mathbf{k})$. Furthermore, all expectation values $\langle \dots \rangle$ are then field dependent.

course, zero. In the $m=5$ subband it is, however, possible to flip the electron spin from \downarrow to \uparrow even at $T=0$, since the $(m=5, \sigma=\uparrow)$ subband is not completely filled. Thus, $\langle \sigma_5^{-} \sigma_5^{+} \rangle$ is finite at $T=0$ K. In the $m=4$ subband, on the other hand, there are no free \uparrow states available at $T=0$ K. The correlation $\langle \sigma_4^{-} \sigma_4^{+} \rangle$ therefore vanishes.

It is interesting to recognize that the local-spin magnitude $\langle \sigma_m \cdot \sigma_m \rangle$ is practically temperature independent. It is mainly determined by the double occupancy $\langle n_{im\sigma} n_{im-\sigma} \rangle$,

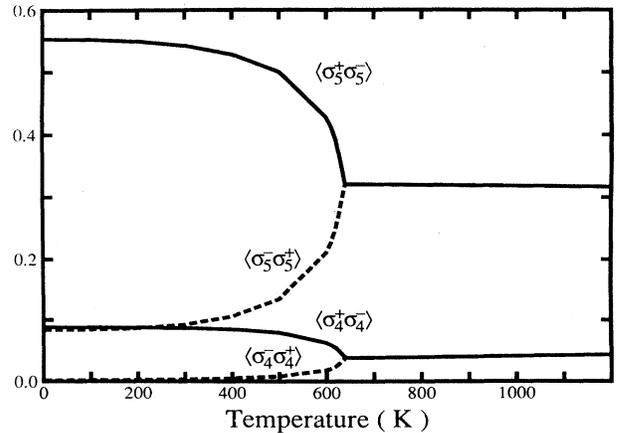


FIG. 3. Spin-flip correlation functions $\langle \sigma_m^{\pm} \sigma_m^{\mp} \rangle$ of the two uppermost Ni subbands ($m=4,5$) as function of temperature.

$$\langle \sigma_m \cdot \sigma_m \rangle = \frac{3}{2} \left(\frac{1}{2} n_m - \langle n_{im\sigma} n_{im-\sigma} \rangle \right), \quad (5.8)$$

which hardly changes with temperature, as can be seen in Fig. 4. In order to find out why the magnetic properties of the itinerant ferromagnet nickel are so similar to those of a typical Heisenberg ferromagnet, we have inspected the degree of effective moment localization, which we define in a similar manner as proposed in Ref. 67. In the "band limit" ($U=J=0$), the spin magnitude reads

$$\langle \sigma_m \cdot \sigma_m \rangle_{BL} = \frac{3}{4} n_m \left(1 - \frac{1}{2} n_m \right). \quad (5.9)$$

The opposite limit can be considered as a dilute local moment system with spin $\frac{1}{2}$. Because of the more than half-filled subbands, the holes are the spin carriers. Thus we have

$$\langle \sigma_m \cdot \sigma_m \rangle_{loc} = \frac{1}{2} \left(1 + \frac{1}{2} \right) (2 - n_m). \quad (5.10)$$

A proper measure for the degree of magnetic moment localization may be the following ratio, which varies between one for the local moment limit and zero for the band limit:

$$D_{LM}(m) = (\langle \sigma_m \cdot \sigma_m \rangle - \langle \sigma_m \cdot \sigma_m \rangle_{BL}) / (\langle \sigma_m \cdot \sigma_m \rangle_{loc} - \langle \sigma_m \cdot \sigma_m \rangle_{BL}). \quad (5.11)$$

Figure 4 shows that $D_{LM}(5)$ as well as $D_{LM}(4)$ are very much closer to the local moment limit than to the band limit. $D_{LM}(5)$ has a nearly temperature-independent value between 0.88 and 0.92; $D_{LM}(4)$ shows some structure below T_C , mainly because of a temperature-dependent band filling n_m .

C. Quasiparticle density of states and quasiparticle band structure

The magnetic Ni properties are direct consequences of the temperature-dependent quasiparticle density of states

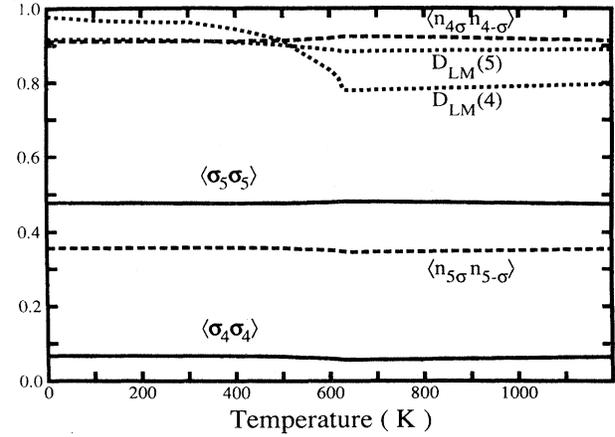


FIG. 4. Local spin magnitude $\langle \sigma_{-m} \cdot \sigma_{-m} \rangle$ (solid lines), double occupancy $\langle n_{im\sigma} n_{im-\sigma} \rangle$ (dashed lines), and degree of moment localization $D_{LM}(m)$ (dotted lines) as function of temperature for the $m=4,5$ subbands.

(QDOS) which is plotted in Fig. 5 for four different temperatures. We observe a spin splitting of the bands for all temperatures below T_C . This splitting is rigid ("Stoner-type") only in the low-energy part of the spectrum. In the upper, not fully occupied, d -band region the strong electron correlations have two different effects. On the one side they cause an exchange shift of the \downarrow spectrum to higher energies relatively to the \uparrow spectrum. On the other side they create a spin-dependent band narrowing, which is stronger for the \uparrow than for the \downarrow spectrum. This is especially evident in the uppermost $m=5$ subband

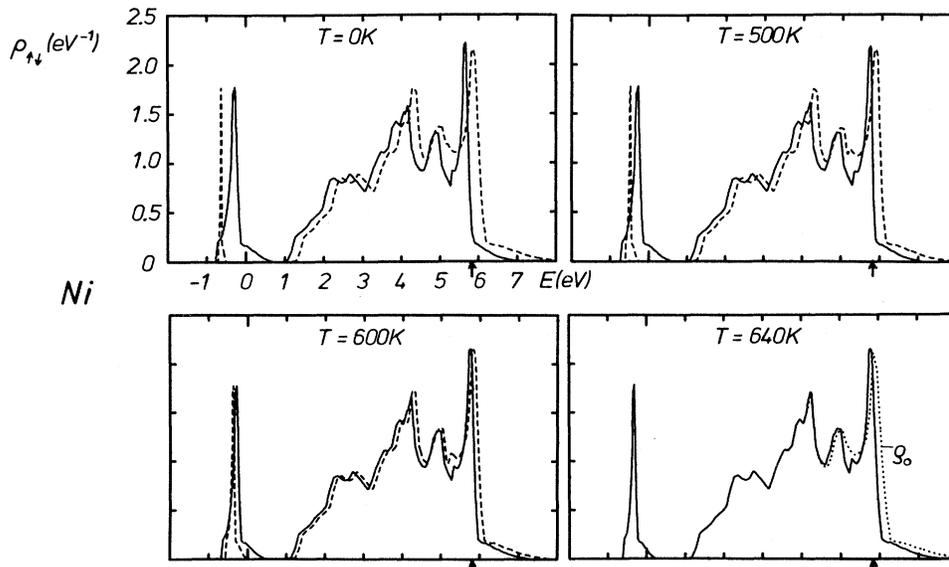


FIG. 5. Quasiparticle density of states $\rho_{\uparrow\downarrow}$ for ferromagnetic Ni as function of energy for four different temperatures ($T_C=635$ K) (solid line: $\sigma=\uparrow$; dashed line: $\sigma=\downarrow$). The arrow on the energy axis indicates the chemical potential μ . The dotted curve is the result of the one-electron band calculation for paramagnetic Ni as in Fig. 1.

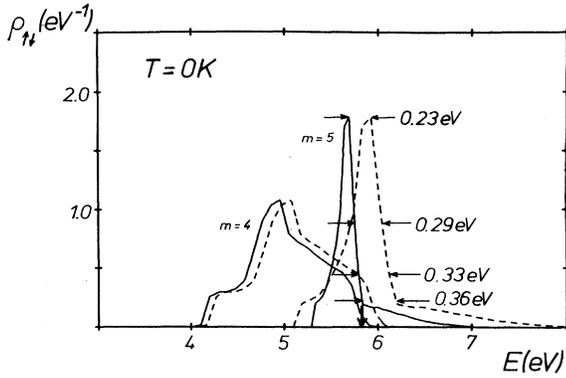


FIG. 6. Quasiparticle density of states of the two highest d subbands as function of energy for $T=0$ K. The solid lines are for the \uparrow states, the dashed lines are for \downarrow states. The arrow on the energy axis indicates the Fermi energy.

(Fig. 6). Our model, therefore, predicts an exchange splitting which may change its sign near the bottom of this subband as can be seen in Fig. 6, where we have plotted the QDOS of the two highest d subbands for $T=0$ K. This figure demonstrates that the exchange splitting is energy dependent and of order 0.2, . . . , 0.35 eV, exactly as observed in the experiment.⁹⁻¹³ The spin splitting of the QDOS maximum, e.g., amounts to 0.23 eV at $T=0$ K, being, of course, strongly temperature dependent, as shown in Fig. 7. There is no exchange splitting above T_C . For paramagnetic Ni the QDOS $\rho_\sigma(E)$ takes its maximum value of about 2.2 eV^{-1} just at the chemical potential μ . This value agrees very well with that given in Ref. 64. Upon cooling below T_C predominantly the \uparrow subband shifts to lower energies, $\rho_\uparrow(\mu)$ therefore decreases, while $\rho_\downarrow(\mu)$ remains (nearly) constant (Fig. 7). Figure 8 shows the quasiparticle band structure for two high-symmetry directions and for four different temperatures. The exchange splitting of the lower fully occupied d states is roughly proportional to the Ni magnetization (Fig. 2) and is rigid. However, this does not hold at all

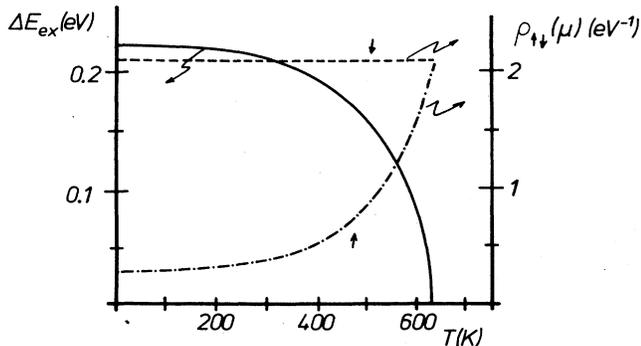


FIG. 7. Exchange splitting of the QDOS maximum and spin dependent QDOS ρ_σ at the chemical potential μ as functions of temperature.

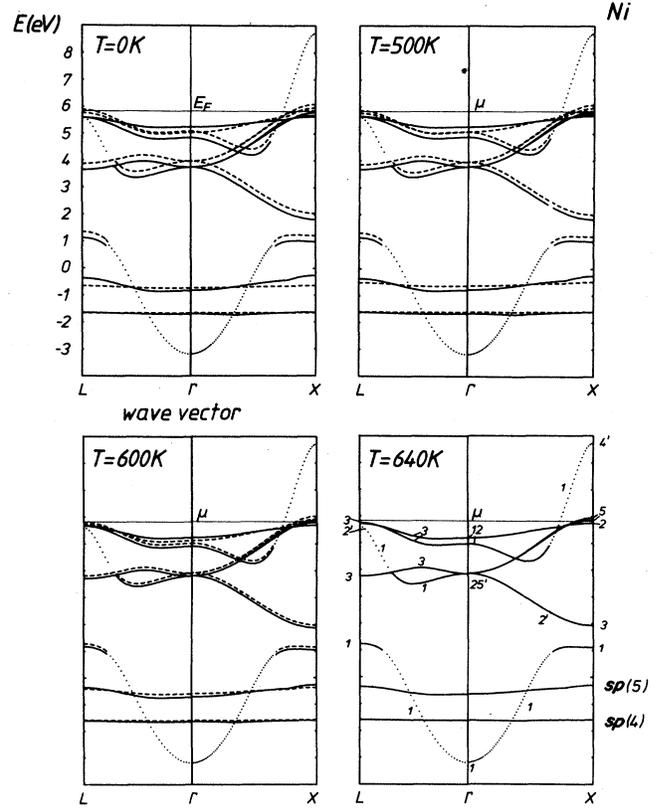


FIG. 8. Quasiparticle band structure for Ni as function of wave vector \mathbf{k} along the ΓL and ΓX directions for different temperatures. The solid lines are for \uparrow and the dashed lines are for \downarrow quasiparticles. Dotted lines mark sp -like states, not involved in our many-body treatment, therefore taken from a one-electron band calculation for paramagnetic Ni. $sp(4,5)$ are satellites belonging to the $m=4,5$ subbands.

for states near the chemical potential μ . The already-mentioned interplay between band shift and band narrowing may even cause a change in sign of the exchange splitting as function of the wave vector \mathbf{k} . The exchange splitting disappears in any case in the paramagnetic phase of Ni. The temperature behavior of the unoccupied quasiparticle d states has experimentally been investigated very recently⁶⁸ by the use of spin-resolved inverse photoemission. The data of this experiment are fully compatible with a vanishing exchange splitting upon approaching T_C . The sp -like states are inserted into Fig. 8 as dotted lines, although they are not affected by our model calculation. They are simply taken from the original one-electron band calculation for paramagnetic Ni (Fig. 2.). In reality they will, of course, also be spin split as a reaction on the $3d$ ferromagnetism.

D. Satellite peak

The most striking feature of the QDOS is the satellite peak some 6 eV below the chemical potential μ (Fig. 5), which has received extraordinary attention in the recent past.¹⁴⁻¹⁶ According to our theory, the satellite peak

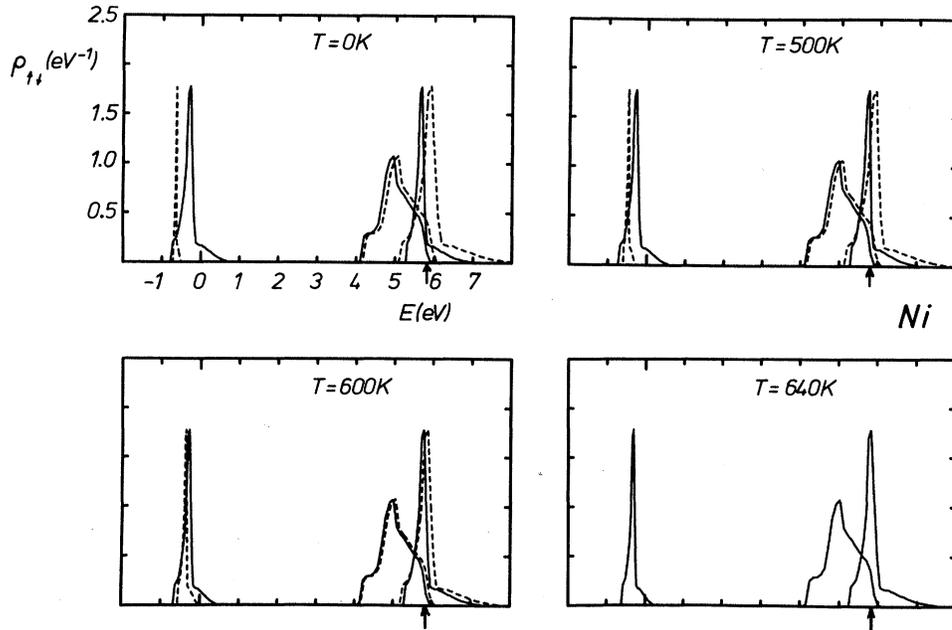


FIG. 9. Quasiparticle densities of states for the $m=4$ and $m=5$ subbands as functions of energy and for four different temperatures. The solid line is for $\sigma=\uparrow$, the dashed line is for $\sigma=\downarrow$. The low-energy satellite peak results from electron correlations in the $m=5$ subband. The chemical potential μ is indicated by an arrow on the E axis.

arises from electron correlations in the partially filled $m=5$ subband. The Coulomb interaction U splits the original Bloch band into two quasiparticle subbands.^{25,26} The only exceptions are completely filled and empty bands. The spectral weight of the upper quasiparticle subband scales with the probability that a propagating (m,σ) electron will meet a lattice site, where another m electron with opposite spin $(-\sigma)$ is already present ($\approx \langle n_{m-\sigma} \rangle$). The weight of the lower quasiparticle subband is determined by the probability [$\approx (1 - \langle n_{m-\sigma} \rangle)$] that the (m,σ) electron will find a site with no other electron from the same subband. The latter probability is zero for $m=1,2,3$ because these subbands are completely filled ($\langle n_{m-\sigma} \rangle = 1$). It is very small for $m=4$ because of the very few holes. It is, however, significant for the $m=5$ subband. A satellite structure is therefore possible only for the $m=4,5$ subbands, where the weight of the $m=4$ band is so small that the respective satellite does not appear in the QDOS. To demonstrate this more clearly we have plotted in Fig. 9 the QDOS of the two magnetically active d subbands only, and that for the same four temperatures as in Fig. 5 for the total QDOS. The satellite belongs to the $m=5$ subband, where the sum of the areas under the satellite and under the upper $m=5$ band is normalized to one for each spin direction. As a function of temperature a shift of weight occurs between the two parts of the $m=5$ subband, most clearly to be seen in the \downarrow spectrum. The weight of the lower $m=5$ quasiparticle subband is furthermore strongly spin dependent, which results in a high spin polarization P_s of the satellite in excellent agreement with the experiment.^{1,17} Our model predicts a temperature-dependent spin-

polarization P_s , starting at about 75% for $T=0$ K, decreasing with increasing temperature and disappearing for $T \geq T_C$ (Fig. 10). The reason for this behavior is a temperature-dependent rearrangement of spectral weight between the lower and the upper $m=5$ quasiparticle subband, which for $T < T_C$ is different for \uparrow and \downarrow spectra. The satellite exists, however, for $T > T_C$, too.

The appearance of the satellite can be understood by inspection of the electronic self-energy $R_{m\sigma}(E)$ (4.15) which is plotted in Fig. 11 for the $m=5$ subband. For

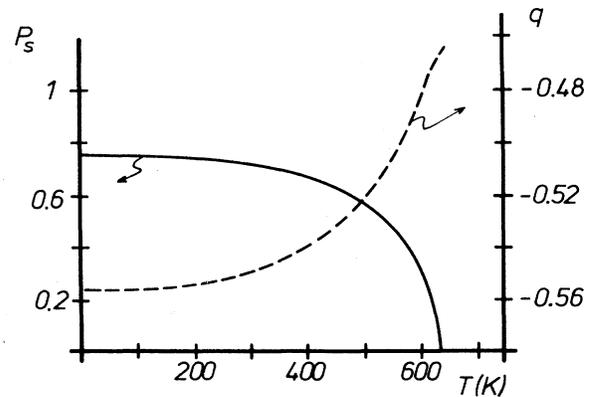


FIG. 10. Temperature dependence of the spin polarization P_s of the satellite peak and of the specific-heat enhancement factor q .

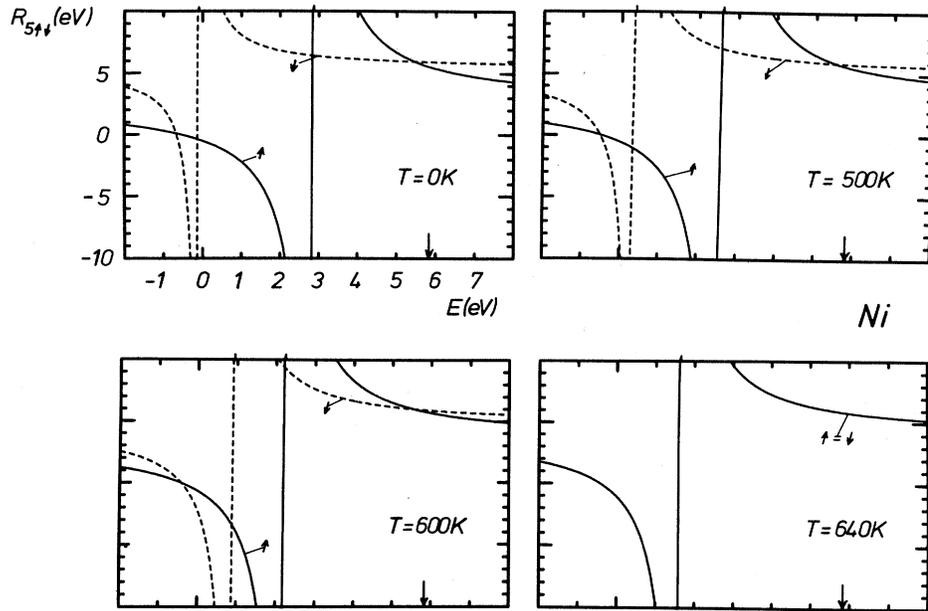


FIG. 11. Electronic self-energy $R_{5\sigma}$ of the $m=5$ subband as function of energy E for four different temperatures. The solid lines are for $\sigma=\uparrow$, the dashed lines are for $\sigma=\downarrow$. The arrow on the E axis marks the chemical potential.

both spins the self-energy exhibits a singularity, so that the equation

$$E - \varepsilon_m(\mathbf{k}) - R_{m\sigma}(E) = 0 \quad (5.12)$$

has two solutions. The low-energy one contributes to the satellite. According to Eq. (4.15) this singularity disappears for empty ($\langle n_{m-\sigma} \rangle = 0$) and for fully occupied ($\langle n_{m-\sigma} \rangle = 1$) bands, so that a satellite may exist for the

$m=4$ and $m=5$ subbands. In the quasiparticle band structure in Fig. 8 they appear as rather dispersionless curves $sp(4)$ and $sp(5)$, respectively, just in the middle of the sp -band region. The satellite $sp(4)$, however, is only formally a solution of (5.12), because it has such a small spectral weight, as explained above, that it will not be observable in a photoemission experiment.

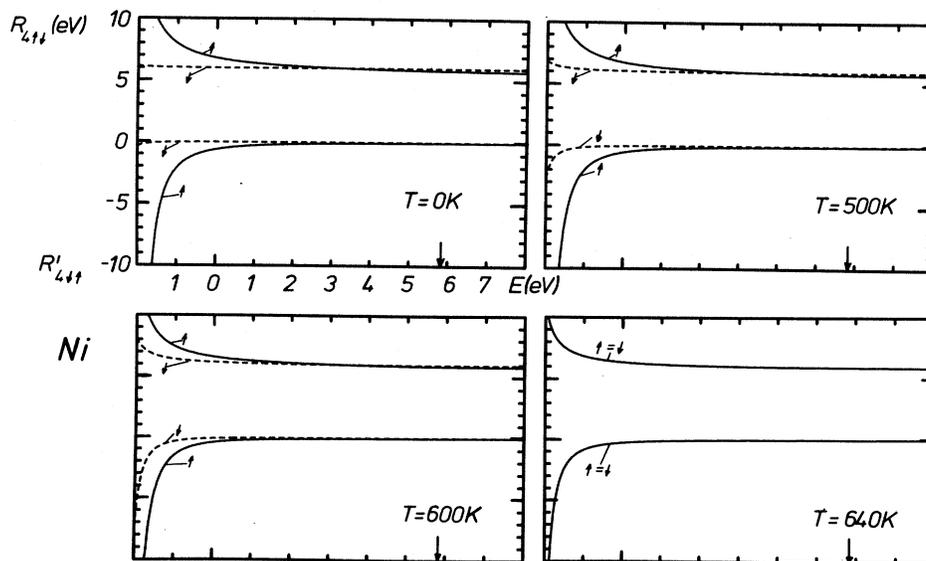


FIG. 12. Electronic self-energy $R_{4\sigma}$ and its derivative $R'_{4\sigma}$ of the $m=4$ subband as functions of energy for four different temperatures. The solid lines are for $\sigma=\uparrow$, the dashed lines are for $\sigma=\downarrow$. The arrow on the E axis marks the chemical potential.

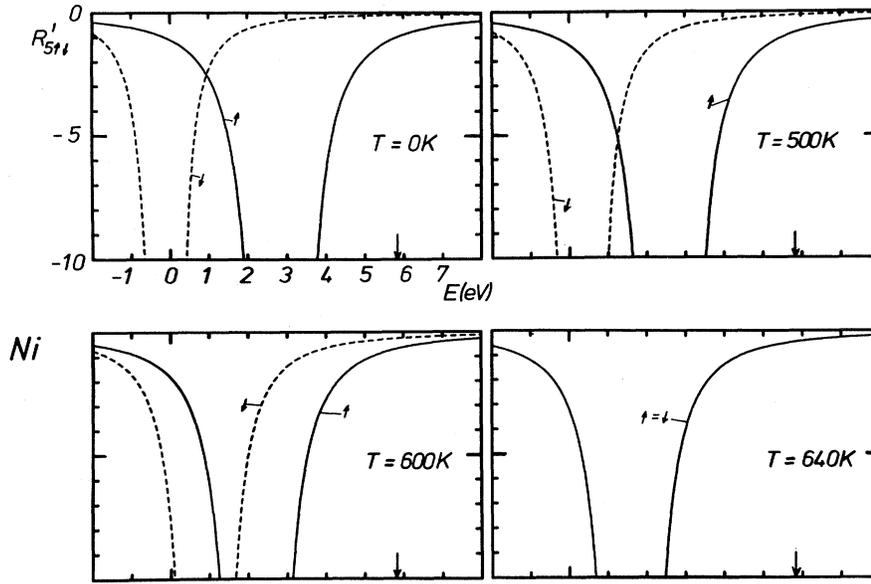


FIG. 13. The derivative $R'_{5\sigma}$ of the electronic self-energy of the $m=5$ subband as function of energy for four different temperatures. The solid lines are for $\sigma=\uparrow$, the dashed lines are for $\sigma=\downarrow$. The arrow on the E axis marks the chemical potential.

E. Specific heat

The electronic part of the low-temperature specific heat is usually written as

$$C_V = \gamma T, \quad \gamma = \gamma_0(1 + \lambda), \quad (5.13)$$

where γ_0 is the well-known free-electron coefficient of the "Sommerfeld model." The enhancement factor λ accounts for electron-electron and electron-phonon interactions, which is completely neglected in the Sommerfeld model. Strictly speaking, one replaces in a rough approximation the bare free-electron mass in the Sommerfeld expression for γ by the many-body effective mass $m_\sigma^*(T)$. This consists in the case of Ni of two contributions ($\lambda = p - q$) from electron-electron ($-q$) and electron-phonon (p) interactions. The experimental Ni value for λ is $\simeq 0.77$,^{4,5} while p has been estimated in Ref. 69 to about 0.17. Therefore, q is expected to be of order -0.6 . It is defined as the derivative of the real part of the self-energy at $E = \mu$:

$$q = -\frac{1}{2} \sum_{m,\sigma} (\partial R_{m\sigma} / \partial E)_{E=\mu}. \quad (5.14)$$

There is no contribution from the fully occupied $m=1,2,3$ subbands. The derivative of $R_{4\sigma}(E)$ at $E = \mu$ is also practically zero (Fig. 12). The main contribution stems from the $m=5$ subband (Fig. 13), and that for temperatures below T_C , in particular, from the majority spin ($\sigma = \uparrow$) carriers. Figure 10 shows that in our model the enhancement factor is rather constant ($q \simeq -0.56$). For $T < 400$ K. For higher temperatures, however, q becomes strongly temperature dependent. This is not

surprising because the ansatz (5.10) is, of course, acceptable only for very low temperatures.

VI. SUMMARY

We have implemented the results of a realistic one-electron band-structure calculation for the $3d$ transition-metal nickel into a reliable many-body procedure on a generalized Hubbard model, in order to get the full temperature dependence of all important quasiparticle quantities of the band ferromagnet Ni. The self-consistent solution of our model yields a ferromagnetic ground state, which in the last analysis is caused by the uppermost of the five d subbands. Our model contains two parameters, the direct Coulomb interaction U and the interband exchange J , which are fixed by fitting the experimental $T=0$ moment. The further evaluation leads to a highly realistic Curie temperature $T_C = 635$ K, and to a magnetization curve which fits almost quantitatively the experimental data. The static susceptibility of paramagnetic Ni shows a strict Curie-Weiss behavior, again in excellent agreement with the experiment. In this respect our band model reproduces in an almost quantitative manner all the "localized" aspects of the band ferromagnetism in Ni. In addition, the very often, controversially discussed, discrepancies between one-electron band-structure calculations and valence-band photoemission data are removed to a great portion by our model. In particular, the resonant satellite structure some 6 eV below the chemical potential turns out to be a consequence of strong electron correlations in the only partially filled uppermost d subband. These split the original Bloch band into two quasiparticle subbands. The lower

one leads to the satellite structure. We consider it as a weighty argument for our model that it is able to explain all of the outstanding and intensely discussed problems connected with the band ferromagnet nickel, and that with a minimum of adjustable parameters. Corresponding investigations on iron are in progress.

ACKNOWLEDGMENTS

We thank G. Borstel and M. Donath for instructive discussions. Financial support of the Deutsche Forschungsgemeinschaft (Bonn, Germany) is gratefully acknowledged.

- ¹For a recent review, see *Metallic Magnetism*, edited by H. Capellmann (Springer-Verlag, Berlin, 1987).
- ²J. Friedel and C. M. Sayers, *J. Phys. (Paris)* **38**, 697 (1977).
- ³F. Kajzar and J. Friedel, *J. Phys. (Paris)* **39**, 397 (1978).
- ⁴N. E. Phillips, *Crit. Rev. Solid State Sci.* **2**, 467 (1972).
- ⁵R. Caudron, J. J. Mennier, and P. Costa, *Solid State Commun.* **14**, 975 (1974).
- ⁶C. S. Wang and J. Callaway, *Phys. Rev. B* **15**, 298 (1977).
- ⁷D. A. Papaconstantopoulos, *Handbook of the Band Structure of Elemental Solids* (Plenum, New York, 1986).
- ⁸L. C. Davis, *J. Appl. Phys.* **59**, R25 (1986), and references therein.
- ⁹D. E. Eastman, F. J. Himpsel, and J. A. Knapp, *Phys. Rev. Lett.* **40**, 1514 (1978).
- ¹⁰E. Dietz, U. Gerhardt, and C. Maetz, *Phys. Rev. Lett.* **40**, 892 (1978).
- ¹¹F. J. Himpsel, J. A. Knapp, and D. E. Eastman, *Phys. Rev. B* **19**, 2919 (1979).
- ¹²D. E. Eastman, F. J. Himpsel, and J. A. Knapp, *Phys. Rev. Lett.* **44**, 95 (1980).
- ¹³W. Eberhardt and E. W. Plummer, *Phys. Rev. B* **21**, 3245 (1980).
- ¹⁴C. Guillot, Y. Ballu, J. Paigne, J. Lecante, K. P. Jain, P. Thiry, R. Pinchaux, Y. Petroff, and L. M. Falicov, *Phys. Rev. Lett.* **39**, 1632 (1977).
- ¹⁵Y. Sakisaki, T. Komeda, M. Ouchi, H. Kato, S. Masuda, and K. Yagi, *Phys. Rev. Lett.* **58**, 733 (1987).
- ¹⁶S. Raaen and V. Murgai, *Phys. Rev. B* **36**, 887 (1987).
- ¹⁷R. Clauberg, W. Gudat, E. Kisker, E. Kuhlmann, and G. M. Rothberg, *Phys. Rev. Lett.* **47**, 1314 (1981).
- ¹⁸J. Hubbard, *Proc. Soc. London, Ser. A* **276**, 238 (1963).
- ¹⁹J. Hubbard, *Proc. R. Soc. London, Ser. A* **277**, 237 (1964).
- ²⁰J. Hubbard, *Proc. R. Soc. London, Ser. A* **281**, 401 (1964).
- ²¹D. Penn, *Phys. Rev.* **142**, 350 (1966).
- ²²W. Schumacher, U. Lindner, and R. Jauch, *Phys. Status Solidi B* **86**, 621 (1978).
- ²³L. M. Roth, *Phys. Rev.* **184**, 451 (1969).
- ²⁴W. Nolting, *Z. Phys.* **265**, 173 (1973).
- ²⁵G. Geipel and W. Nolting, *Phys. Rev. B* **38**, 2608 (1988).
- ²⁶W. Nolting and W. Borgiel, *Phys. Rev. B* **39**, 6962 (1988).
- ²⁷M. Cyrot, *J. Phys. (Paris)* **33**, 125 (1972).
- ²⁸J. Hubbard, *Phys. Rev. B* **19**, 2626 (1979).
- ²⁹J. Hubbard, *Phys. Rev. B* **20**, 4584 (1979).
- ³⁰J. Hubbard, *Phys. Rev. B* **23**, 5970 (1981).
- ³¹H. Hasegawa, *J. Phys. Soc. Jpn.* **46**, 1504 (1979).
- ³²H. Hasegawa, *J. Phys. Soc. Jpn.* **49**, 178 (1980).
- ³³T. Moriya and H. Hasegawa, *J. Phys. Soc. Jpn.* **48**, 1490 (1980).
- ³⁴Y. Kakehashi and P. Fulde, *Phys. Rev. B* **32**, 1595 (1985).
- ³⁵M. C. Gutzwiller, *Phys. Rev. A* **137**, 1726 (1965).
- ³⁶Y. Kakehashi and H. Hasegawa, *Phys. Rev. B* **36**, 4066 (1987).
- ³⁷K. Kubo, *Prog. Theor. Phys.* **64**, 758 (1980).
- ³⁸B. H. Zhao, H. Q. Nie, K. Y. Zhang, K. A. Chao, and R. Micnas, *Phys. Rev. B* **36**, 2321 (1987).
- ³⁹H. Shiba and P. Pincus, *Phys. Rev. B* **5**, 1966 (1972).
- ⁴⁰Z. G. Soos and S. Ramasesha, *Phys. Rev. B* **29**, 5410 (1984).
- ⁴¹J. E. Hirsch, *Phys. Rev. B* **31**, 4403 (1985).
- ⁴²J. E. Hirsch, *Phys. Rev. B* **35**, 1851 (1987).
- ⁴³J. Callaway, D. P. Chen, and Y. Zhang, *Phys. Rev. B* **36**, 2804 (1987).
- ⁴⁴W. Nolting, G. Borstel, and W. Borgiel, *Phys. Rev. B* **35**, 7015 (1987).
- ⁴⁵W. Nolting, W. Borgiel, and G. Borstel, *Phys. Rev. B* **35**, 7025 (1987).
- ⁴⁶W. Nolting, W. Borgiel, and G. Borstel, *Phys. Rev. B* **37**, 7663 (1988).
- ⁴⁷G. Treglia, F. Ducastelle, and D. Spanjaard, *J. Phys. (Paris)* **43**, 341 (1982).
- ⁴⁸V. Moruzzi, J. F. Janak, and A. R. Williams, *Calculated Electronic Properties of Metals* (Pergamon, New York, 1978).
- ⁴⁹O. Gunnarson, *Physica B* **91**, 329 (1977).
- ⁵⁰R. Taranko, E. Taranko, and J. Malek, *J. Phys. F* **18**, L87 (1988).
- ⁵¹L. C. Davis and L. A. Feldkamp, *Solid State Commun.* **34**, 141 (1980).
- ⁵²D. G. Dempsey, W. R. Grise, and L. Kleinmann, *Phys. Rev. B* **18**, 1270 (1978).
- ⁵³S. Doniach and E. H. Sondheimer, *Green's Functions for Solid State Physicists* (Benjamin and Cummings, Reading, 1974).
- ⁵⁴W. Nolting, *Quantentheorie des Magnetismus 2* (Teubner-Verlag, Stuttgart, 1986), Chap. 8.4.1.
- ⁵⁵A. Liebsch, *Phys. Rev. Lett.* **43**, 1431 (1979).
- ⁵⁶A. Liebsch, *Phys. Rev. B* **23**, 5203 (1981).
- ⁵⁷D. R. Penn, *Phys. Rev. Lett.* **42**, 921 (1979).
- ⁵⁸J. Kanamori, *Prog. Theor. Phys.* **30**, 275 (1963).
- ⁵⁹H. Capellmann, *Z. Phys. B* **34**, 29 (1979).
- ⁶⁰A. M. Oleś and G. Stollhoff, *Phys. Rev. B* **29**, 314 (1984).
- ⁶¹F. Szmulowicz and D. M. Pease, *Phys. Rev. B* **17**, 3341 (1978).
- ⁶²N. V. Smith, *Phys. Rev. B* **19**, 5019 (1979).
- ⁶³W. Nolting, *Quantentheorie des Magnetismus 2*, Ref. 54, p. 289.
- ⁶⁴S. Hirooka and M. Shimizu, *Phys. Lett.* **46A**, 209 (1973).
- ⁶⁵M. I. Darby, *Brit. J. Appl. Phys.* **18**, 1415 (1967).
- ⁶⁶S. Arajs and R. V. Colvin, *J. Phys. Chem. Solids* **24**, 1233 (1963).
- ⁶⁷J. Spałek, A. M. Oleś, and J. M. Honig, *Phys. Rev. B* **28**, 6802 (1983).
- ⁶⁸M. Donath and V. Dose, *Europhys. Lett.* (to be published).
- ⁶⁹D. A. Papaconstantopoulos, L. L. Boyer, B. M. Klein, A. R. Williams, V. L. Moruzzi, and J. F. Janak, *Phys. Rev. B* **15**, 4221 (1977).