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# On a Simple Functional Moment Approach to Itinerant Magnetism - Application to Ni

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The modern theories of itinerant magnetism are usually /1 to 5/ based on functional integral representations of the Hubbard model /6/. Those so-called spin fluctuation approaches yield a satisfactory theoretical description of the major magnetic phenomena which are observed in transition metals and their alloys, for instance the low Curie temperatures $T_C$ of Ni, Co, and Fe in spite of the large exchange splitting energies, the temperature dependence of the magnetization, as well as the existence of temperature dependent local moments even above $T_C$. However, these theories require an expensive numerical analysis, particularly, if a realistic band structure is taken into account.

In this note we present a simple self-consistent calculation scheme by combination of functional moment relations with the spin fluctuation theory proposed by Hasegawa /2/, avoiding the explicit determination of the distribution function for the spin fluctuations. Furthermore, we use differently from /2, 3, 5, 7/ a Chebyshev polynomial expansion for the representation of a realistic density of states (DOS).

Starting from the Hubbard model, via a functional integral formulation of the partition function (adopting the static and the single site approximations, as well as the saddle point approximation for the charge fields), one gets the following expression for the free energy in terms of the fluctuating local exchange field $\xi_i$:

$$F_{stat} = \tilde{F} - \frac{1}{\beta}\sum_i \ln \sqrt{\frac{\beta U}{4\pi}} \int d\xi_i \exp\left(-\beta\Omega_i(\xi_i)\right) \tag{1}$$

with

$$\Omega_i(\xi_i) = \frac{U}{4}\xi_i - n_i u_i(\xi_i) + \int_{-\infty}^{\infty} dE\, f(E-\mu)\,\frac{1}{\pi}\,\mathrm{Im}\left\{\sum_\sigma \ln\left(1-\Delta_\sigma(\xi_i;E^+)F_{0\sigma}(E^+)\right)\right\} \tag{2}$$

and $\Delta_\sigma(\xi_i; z) = u_i(\xi_i) - \frac{U}{2}\sigma\xi_i - \Sigma_\sigma(z)$ (cf. /5/). Here U and $n_i$ denote the intra-atomic Coulomb repulsion and the electron number at site i, respectively. f(E)

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is the Fermi function with the chemical potential $\mu$, $\beta = 1/k_B T$, $E^+ = +i0$, $\tilde{F}$ is an irrelevant quantity; and the charge potential $u_i(\xi_i)$ arising from the charge neutrality limit /1/ at each site. The coherent potential $\Sigma_\sigma(z)$ and the site-diagonal coherent Green function

$$F_{oo\sigma}(z) = \frac{1}{N}\sum_{\vec{k}}\left[z - \varepsilon^o(\vec{k}) - \Sigma_\sigma(z)\right]^{-1} \tag{3}$$

will be determined by CPA, where $\varepsilon^o(\vec{k})$ is related to the band structure of the crystal. To calculate electronic quantities one has to perform the average $\langle \ldots \rangle = \int d\xi_i \ldots \exp(-\beta\Omega_i(\xi_i)) \Big/ \left[\int d\xi_i \exp(-\beta\Omega_i(\xi_i))\right]$ with respect to the auxiliary fields. If we use Hasegawa's /2/ decoupling procedure exact up to second-order moments $\langle \xi^{in+k} \rangle$ $\langle \xi^2 \rangle^n \langle \xi^k \rangle$ (k = 0, 1), it can be easily shown that the self-energy $\Sigma_\sigma$ results from the simplified scattering matrix equation

$$\sum_{s=\pm 1} w_s \Delta_\sigma(s\sqrt{\langle \xi^2 \rangle}; z)\left[1 - \Delta_\sigma(s\sqrt{\langle \xi^2 \rangle}; z)\, F_{oo\sigma}(z)\right]^{-1} = 0 \tag{4}$$

with the probabilities $w_s = \frac{1}{2}\left(1 + s\frac{\langle \xi \rangle}{\sqrt{\langle \xi^2 \rangle}}\right)$. Then $\eta = w_+ - w_-$ plays the role of a long-range order parameter that becomes zero at $T_C$, and we have $\langle K(\xi) \rangle = \sum_s w_s K(s\sqrt{\langle \xi^2 \rangle})$ for the average of some quantity K. Introducing the local Green function

$$F^s_{oo\sigma}(z) = F_{oo\sigma}(z)\left[1 - \Delta_\sigma(s\sqrt{\langle \xi^2 \rangle}; z)\, F_{oo\sigma}(z)\right]^{-1} \tag{5}$$

at sites with moment $\langle \xi^2 \rangle$ in s-direction the partial averaged electron numbers are obtained as

$$n^s_\sigma = -\int_{-\infty}^{\infty} dE\, f(E - \mu)\, \frac{1}{\pi}\, \mathrm{Im}\left\{F^s_{oo\sigma}(E^+)\right\}. \tag{6}$$

Hence, the magnetization m and the root-mean-square local moment $m_{loc}$ are given by

$$m = \sum_s w_s \sum_\sigma \sigma n^s_\sigma \; ; \qquad m^2_{loc} = \sum_s w_s \left[\sum_\sigma \sigma n^s_\sigma\right]^2 \tag{7a}$$

or, using general relations of functional technique, by

$$m = \langle \xi \rangle \; ; \qquad m^2_{loc} = \langle \xi^2 \rangle - \frac{2}{\beta U}. \tag{7b}$$

The charge potentials and the chemical potential are fixed by the requirements

$$n = \sum_\sigma n^s_\sigma \tag{8}$$

and

$$n = -\int_{-\infty}^{\infty} dE\, f(E - \mu)\, \frac{1}{\pi}\, \mathrm{Im}\left\{F_{oo\sigma}(E^+)\right\}, \tag{9}$$

respectively. Note, that it is now possible to evaluate the self-consistent loop

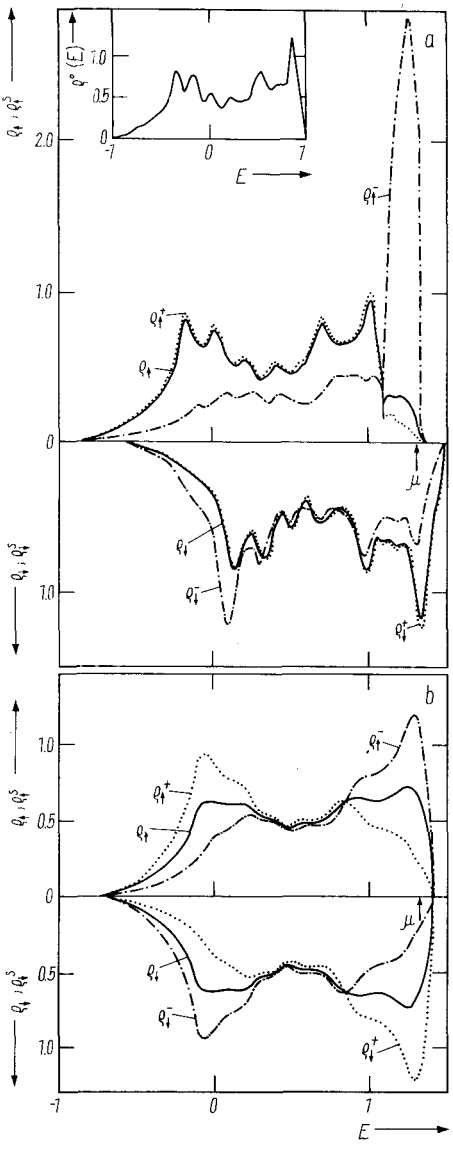


Fig. 1. Partially and totally averaged DOS $\varrho_\sigma^+(E)$ ( $\cdots$ ), $\varrho_\sigma^-(E)$ (—·—), and $\varrho_\sigma(E)$ (——), respectively, of Ni with $n = 1.88$ and $U = 2.5$ W (W is the half-bandwidth); a) at temperature $T = 0.3\ T_C$ and b) at the transition point $T = T_C$; where $\mu$ denotes the chemical potential and the inset in a) shows the unperturbed DOS $\varrho^0(E)$ according to /8/

(3), (4), (7a), (7b), (8), and (9) for the determination of $\Sigma_\sigma$, $\langle \xi \rangle$, and $\langle \xi^2 \rangle$, i.e. it is not necessary to perform the functional average by means of $\Omega_i(\xi_i)$ explicitly.

As already mentioned the band structure of the unperturbed crystal enters through $\varepsilon^0(\vec{k})$ into the numerical work. Adopting $\varrho^0(E) = \frac{1}{N} \sum_{\vec{k}} \delta(E - \varepsilon^0(\vec{k}))$ equation (3) becomes

$$F_{0\sigma}(z) = \int \frac{\varrho^0(E)}{z - \Sigma_\sigma(z) - E}\, dE \ . \qquad (10)$$

A powerful method, avoiding the numerical calculation of (10), was proposed by Riedinger and Nauciel-Bloch /8/. They expanded the unperturbed DOS into polynomial series $\varrho^0(E) = \frac{1}{N} \sum_{n=0}^{\infty} c_n \sqrt{1 - E^2}\, \tilde{U}_n(E)$, where $\tilde{U}_n(x)$ are Chebyshev polynomials of second kind and the $c_n$ are determined to fit a realistic band structure in a certain order. Then the integration in (10) can be done analytically and one has

$$F_{0\sigma}(z) = \sum_{n=0}^{\infty} c_n P_{n\sigma}(z) \qquad (11)$$

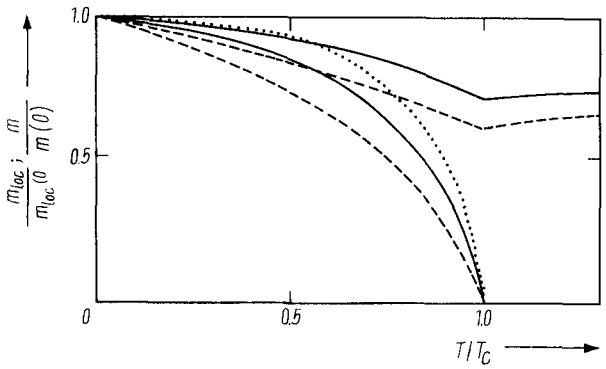


Fig. 2. Temperature dependence of the reduced magnetization m/m(0) and the local magnetic moment $m_{loc}/m_{loc}(0)$ of Ni with n = 1.88, U = 2.5 W and $\varrho^0(E)$ from Fig. 1a (——) in comparison to the results using the semielliptic DOS and U = 4 W (– – –); (- - - -) shows the Brillouin function $B_{1/2}(x)$ for spin 1/2

with

$$P_{n\sigma}(z) = \pi \left[ z - \Sigma_\sigma(z) - \sqrt{(z - \Sigma_\sigma(z))^2 - 1} \right]^{n+1} . \qquad (12)$$

The numerical results for the case of Ni (within the equivalent d-band approximation) are presented in the figures, where the $c_n$ (n = 0, 1, ...., 38) are taken from /8/. Fig. 1 shows the partial DOS $\varrho^s_\sigma = -\frac{1}{\pi} \mathrm{Im} \left\{ F^s_{o\sigma} \right\}$ in the vicinity of the saturation region ($w_+ = 0.94$ (a)) and at the phase transition to the paramagnetic regime ($w_+ = w_- = 0.5$ (b)). At low temperatures we have $\varrho_\sigma \approx \varrho^+_\sigma$ and a deformation of the majority spin band only. With increasing T the structure of the DOS becomes obliterated and at $T_C$ ($T_C$ = 350 K if W = = 2.38 eV) the relation $\varrho^s_\sigma = \varrho^{-s}_{-\sigma}$ is fulfilled. Analogous results are obtained for Fe in /7, 9/, but these theories are not applicable to Ni, because (2) exhibits only one local minimum in this case.

To investigate the influence of the model DOS we have calculated m(T) and $m_{loc}(T)$ (see Fig. 2) using both the simple semielliptic (n = 0 in (12)!) and the more realistic DOS according to Fig. 1a. Obviously, in the latter case m(T) follows more closely the experimental curve (approximated by $B_{1/2}(x)$ in Fig. 2), showing the importance of the DOS structure especially in the vicinity of $\mu$. In qualitative agreement with experimental /10, 11/ and other theoretical/3, 5/ results $m_{loc}(T)$ of Ni increases slightly with T above $T_C$ and we have $m_{loc}(T_C)/m_{loc}(0) \approx 72\%$.

References

/1/ J. HUBBARD, Phys. Rev. B 20, 4584 (1979).

/2/ H. HASEGAWA, J. Phys. Soc. Japan 49, 178 (1980).

/3/ H. HASEGAWA, J. Phys. Soc. Japan 49, 963 (1980).

/4/ J. HUBBARD, Phys. Rev. B 23, 5974 (1981).

/5/ Y. KAKEHASHI, J. Phys. Soc. Japan 50, 1505, 2251 (1981).

/6/ J. HUBBARD, Proc. Roy. Soc. A276, 238 (1963).

/7/ J.L. MORÁN-LÓPEZ and K.H. BENNEMANN, Phys. Rev. B 23, 5978 (1981).

/8/ R. RIEDINGER and M. NAUCIEL-BLOCH, J. Phys. F 5, 732 (1975).

/9/ H. HASEGAWA, J. Phys. Soc. Japan 46, 1504 (1979).

/10/ D.E. EASTMAN, F.J. HIMPSEL, and J.A. KNAPP, Phys. Rev. Letters 40, 1514 (1973).

/11/ M. CAMPAGNA and B.L. GYORFFY, Phys. Bl. 40, 95 (1984).

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