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**ELECTRON CORRELATIONS
AND FERROMAGNETISM
IN DISORDERED ALLOYS**

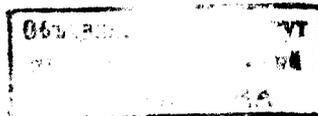
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**ELECTRON CORRELATIONS
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Электрон-электронные корреляции и ферромагнетизм
в неупорядоченных сплавах

В рамках неупорядоченной модели Хаббарда исследуются магнитные свойства неупорядоченных сплавов. В расчетах используется комбинация локального лестничного приближения и ПКП. Для нескольких параметров сплавов вычислены электронная плотность состояний и магнетизация. Проведено сравнение с результатами, полученными в приближении Хартри-Фока.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Препринт Объединенного института ядерных исследований. Дубна 1977

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Electron Correlations and Ferromagnetism
in Disordered Alloys

The magnetic properties of disordered alloys are investigated using a disordered Hubbard model. The calculation is based on a combination of a local ladder approximation and the CPA. The electronic density of states and the magnetization are calculated numerically for several alloy parameters. A comparison with the Hartree-Fock results is given.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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1. INTRODUCTION

In recent years the problem of itinerant magnetism of disordered substitutional alloys has been discussed within the framework of the Coherent Potential Approximation (CPA)^{/1-3/}. In order to describe the magnetic properties of such alloys the electron correlation must be taken into account in an appropriate way. Previous calculations are based on a local Hartree-Fock approximation^{/1/} of the Hubbard Hamiltonian, which is correct in first order of the interaction but which is not justified generally if the Coulomb repulsion is strong. Nevertheless, this scheme provides magnetic solutions in the regime of strong correlations. Other approximations as the so-called Hubbard-I decoupling, the Hubbard-III decoupling, and the alloy analogy permit at finite correlation strength only nonmagnetic solutions^{/2,3,8/}. Therefore they are not suitable for the description of magnetic properties.

In this paper we apply the so-called ladder approximation, which is justified for arbitrary correlation energy in the limit of small electron concentrations. This approximation was applied in a local form to the Hubbard model^{/4/} and it has been recently extended to the treatment of disordered alloys^{/5,6/}. In the preceding paper^{/6/} only paramagnetic solutions are investigated, in this paper we present magnetic solutions of this theory.

2. THEORY*

The disordered $A_x B_{1-x}$ alloy is described by the Hamiltonian

$$\left. \begin{aligned} H^{\{\nu\}} &= H_0^{\{\nu\}} + W^{\{\nu\}} \\ H_0^{\{\nu\}} &= \sum_{i,\sigma} \epsilon_i^\nu n_{i\sigma} + \sum_{i,j,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} \\ W^{\{\nu\}} &= \frac{1}{2} \sum_{i,\sigma} U_i^\nu n_{i\sigma} n_{i-\sigma} \end{aligned} \right\} \quad (1)$$

$H^{\{\nu\}}$ is the Hamiltonian of a fixed configuration $\{\nu\}$, $H_0^{\{\nu\}}$ is the usual one-band-tight-binding Hamiltonian of a disordered binary alloy, $W^{\{\nu\}}$ is the correlation term as in the Hubbard model. The atomic energies ϵ_i^ν and the Coulomb energies U_i^ν depend on the occupation of the lattice site i , they may take the values $\epsilon_A^\nu, \epsilon_B^\nu$ and U_A^ν, U_B^ν , respectively. The transfer integrals t_{ij} are assumed to be independent of the occupation of the lattice sites (diagonal disorder). An extension to off-diagonal disorder is possible without difficulties (see refs. /5,6/). In the present investigation we combine the local ladder approximation (LLA)^{/4/} for the treatment of correlations with the CPA^{/7/} for the treatment of disorder. In the LLA the effects of the electron correlation are described by a local self-energy (the index c denotes the correlation part)

$$\Sigma_{c\sigma}^{\{\nu\}}(E) = \sum_i \sigma_c^\nu \rho_{i\sigma}^\nu(E) n_{i\sigma} \quad (2)$$

where the correlation strength U_i^ν and the electron density $n_{i\sigma}^\nu$ as parameters enter into the calculation. Both quantities and accordingly σ_c^ν depend on the

*The theory is described in detail in the paper /6/. Therefore we will give here only a short summary.

occupation of the site i . Therefore the problem is reduced to a disordered alloy problem without electron interaction and with the random external potential

$$V_\sigma^{\{\nu\}}(E) = \sum_i V_{i\sigma}^\nu = \sum_i \{ \epsilon_i^\nu + \sigma_c^\nu \rho_{i\sigma}^\nu(E) \} n_{i\sigma} \quad (3)$$

The electron correlation leads only to an energy-dependent renormalization of the diagonal elements of the scattering potential. So we can apply the CPA as usual. We obtain the CPA-equation

$$\begin{aligned} \langle T_{i\sigma}^\nu \rangle &= \langle (V_{i\sigma}^\nu - \Sigma_{i\sigma}^\nu(z)) [1 - \langle G_\sigma(z) \rangle \times \\ &\quad \times (V_{i\sigma}^\nu - \Sigma_{i\sigma}^\nu(z))]^{-1} \rangle = 0, \end{aligned} \quad (4)$$

from which we can determine the self-energy

$$\Sigma_\sigma(z) = \sum_i \Sigma_{i\sigma}(z) = \sum_i \sigma_\sigma(z) n_{i\sigma}$$

and the averaged Green function (K : periodic part of $H^{\{\nu\}}$)

$$\langle G_\sigma(z) \rangle = (z - K - \Sigma_\sigma(z))^{-1} \quad (5)$$

The LLA and the CPA are connected by the equations determining the component electron densities n^ν

$$n = \sum_\sigma \langle n_\sigma^\nu \rangle = \sum_\sigma \langle \int_{-\infty}^{\mu} dE \rho_\sigma^\nu(E) \rangle = -\frac{1}{\pi} \sum_\sigma \langle \int_{-\infty}^{\mu} dE \text{Im} G_\sigma^\nu(E) \rangle, \quad (6)$$

where n is the averaged number of electrons per lattice site, and $\rho_\sigma^\nu(E)$ is the component density of states calculated from the partial averaged Green function

$$G_\sigma^\nu = \langle G_\sigma \rangle + \langle G_\sigma \rangle T_{i\sigma}^\nu \langle G_\sigma \rangle \quad (7)$$

The n^ν and the G^ν , respectively, enter into the set of the corresponding LLA equations for A- and B-sites. Therefore we have to solve simultaneously the LLA equations

$$\begin{aligned}
\text{Re} \sigma_{c\sigma}^{\nu} (E) &= -\frac{1}{\pi} \int_{-\infty}^{\mu} dE' \text{Im} G_{-\sigma}^{\nu} (E') \text{Re} \Gamma^{\nu} (E+E') - \\
&\quad - \frac{1}{\pi} \int_{-\infty}^{2\mu-E} dE' \text{Re} G_{-\sigma}^{\nu} (E') \text{Im} \Gamma^{\nu} (E+E'), \\
\text{Im} \sigma_{c\sigma}^{\nu} (E) &= -\frac{1}{\pi} \int_{-\infty}^{\mu} dE' \text{Im} G_{-\sigma}^{\nu} (E') \text{Im} \Gamma^{\nu} (E+E'), \\
&\quad + \frac{1}{U^{\nu}} + \text{Re} D^{\nu} (E) \\
\text{Re} \Gamma^{\nu} (E) &= \frac{1}{\left\{ \frac{1}{U^{\nu}} + \text{Re} D^{\nu} (E) \right\}^2 + \left\{ \text{Im} D^{\nu} (E) \right\}^2}, \\
\text{Im} \Gamma^{\nu} (E) &= \frac{\text{Im} D^{\nu} (E)}{\left\{ \frac{1}{U^{\nu}} + \text{Re} D^{\nu} (E) \right\}^2 + \left\{ \text{Im} D^{\nu} (E) \right\}^2}, \quad \nu = (A, B)
\end{aligned} \tag{8}$$

with

$$\begin{aligned}
\text{Re} D^{\nu} (E) &= \frac{1}{\pi} \int_{-\infty}^{E-\mu} dE' \text{Re} G_{\sigma}^{\nu} (E') \text{Im} G_{-\sigma}^{\nu} (E-E') - \\
&\quad - \frac{1}{\pi} \int_{-\infty}^{\mu} dE' \text{Im} G_{\sigma}^{\nu} (E') \text{Re} G_{-\sigma}^{\nu} (E-E'), \\
\text{Im} D^{\nu} (E) &= -\frac{1}{\pi} \int_{-\infty}^{E-\mu} dE' \text{Im} G_{\sigma}^{\nu} (E') \text{Im} G_{-\sigma}^{\nu} (E-E'),
\end{aligned}$$

and the CPA equations (4)-(7).

3. NUMERICAL EXAMPLES AND DISCUSSION

The numerical calculations have been carried out by the technique described in^{6/}.

In this paper we restrict ourselves to the split band regime. In this case we replace in the calculation of the correlation part of the self energy (8) G_{σ}^{ν} by a sim-

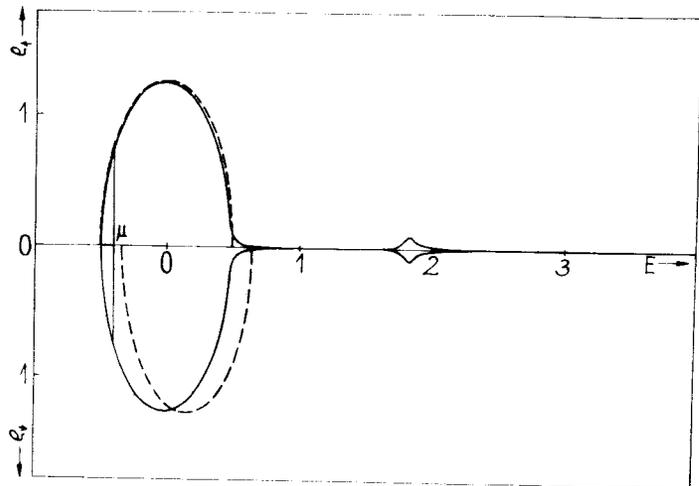
plified \tilde{G}_{σ}^{ν} which describes a correlated electron in a ν -lattice (i.e., the influence of disorder on the electron correlation at a given site via the occupation of the neighbouring sites is neglected). Since the LLA is a local theory this additional approximation should cause no important effects, at least in the split band regime. Then the equations determining the correlation part and the coherent self-energy are still coupled by the equation (6), from which the chemical potential is fixed.

For the unperturbed density of states (i.e., perfect B-crystal without interaction) we use an elliptical shape

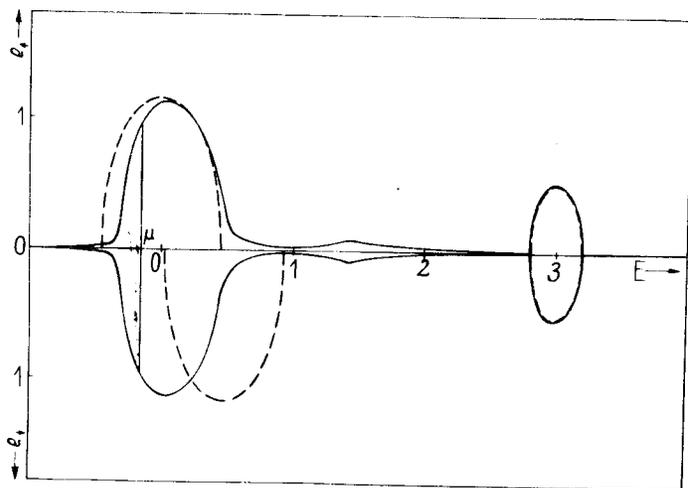
$$\rho_0^B (E) = \frac{8}{\pi} \sqrt{\frac{1}{4} - E^2} \theta\left(\frac{1}{4} - E^2\right),$$

whose bandwidth is equal to unity. Input parameters are the Coulomb energies U_A, U_B , the atomic energies ϵ_A, ϵ_B , the number of electrons per A-atom and per B-atom N_A, N_B , and the concentration x . The density of states $\rho(E)$ and the magnetization $m = n_{\uparrow} - n_{\downarrow}$ are calculated. A characteristic feature of the alloy problem is the possibility to change the electron concentrations n_{\uparrow} and n_{\downarrow} in consequence of the alloying. In the presence of diagonal disorder a change of x has different consequences on the electron concentrations at the A- and B-sites. In the investigated split band example (Fig. 1) with increasing x the filling of the lower band increases. At a critical electron concentration the alloy becomes ferromagnetic (Fig. 2). We can see that the magnetization rises steeply to the saturation value.

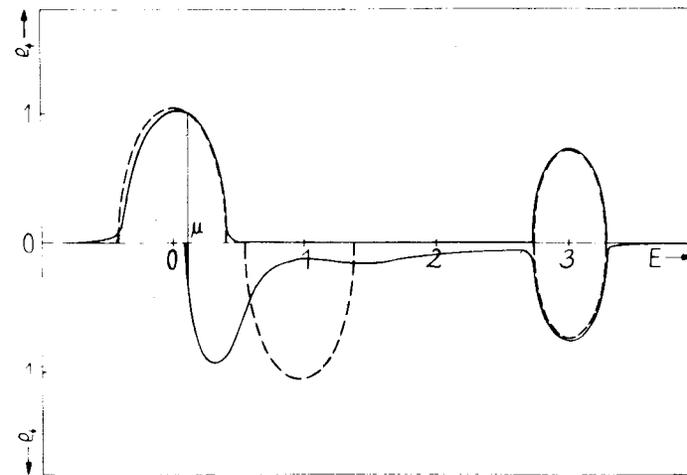
For comparison we have shown in all figures the Hartree-Fock results, too. For such a great correlation strength one obtains already saturated ferromagnetic solutions in the whole concentration range, whereas a transition to the paramagnetic state appears at smaller U -values. Therefore the Hartree-Fock approximation shows in these cases an overestimation of the correlation effects, too.



a



b



c

Fig. 1. Electronic density of states $\rho(E)$ for both spin directions. Parameter: $\epsilon_B=0$, $\epsilon_A=3$, $N_B=0.1$, $N_A=1$, $U_A=U_B=1.6$, a) $x=0$, b) $x=0.166$, c) $x=0.333$. The dashed line shows the Hartree-Fock results.

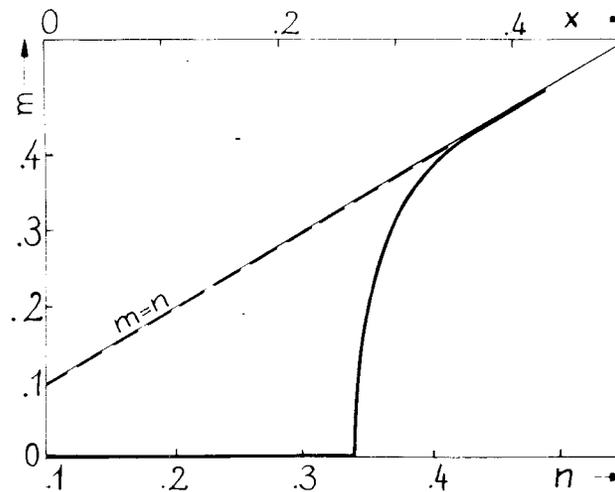


Fig. 2. Magnetization as a function of x and n , respectively. The dashed line shows the Hartree-Fock result.

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