phys. stat. sol. (b) **123**, 533 (1984)

Subject classification: 18; 13; 21

Sektion Physik der Karl-Marx-Universität Leipzig[1])

Spin-Glass Behaviour in Disordered Hubbard Alloys

By

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The paramagnetism to spin glass transition in concentrated itinerant alloys A_cB_{1-c} is studied on the basis of the random Hubbard model. Kakehashi's treatment of nonlocal spin fluctuations mapped onto an effective random-site Ising model is combined with Nambu's Landau-type order parameter expansion of the quenched averaged free energy based on the replica method. The temperature- and concentration-dependence of the exchange couplings is determined by a self-consistent CPA calculation. Numerical results are presented for nearest-neighbour pair interactions, freezing temperature, specific heat, single-site distribution functions, densities of states, and spin glass order parameters.

Der Übergang von Paramagnetismus zu Spinglas in konzentrierten itineranten A_cB_{1-c}-Legierungen wird auf der Basis des ungeordneten Hubbard-Modells untersucht. Kakehashis Behandlung nichtlokaler Spinschwankungen, abgebildet auf ein effektives „random-site" Ising-Modell, wird kombiniert mit Nambus Landau-Typ-Ordnungsparameterentwicklung der „quenched" gemittelten freien Energie, die auf der Replika-Methode basiert. Die Temperatur- und Konzentrationsabhängigkeit der Austauschkopplungen wird durch eine selbstkonsistente CPA-Rechnung bestimmt. Für Paarwechselwirkungen zwischen nächsten Nachbarn, Übergangstemperatur, spezifische Wärme, lokale Verteilungsfunktionen, Zustandsdichten und Spinglas-Ordnungsparameter werden numerische Resultate angegeben.

1. Introduction

Spin fluctuation approaches to itinerant-electron magnetism in narrow-band systems, such as transition metals and their alloys, are usually [1 to 5] based on the Hubbard model in functional-integral formulation. One has to distinguish between single-site theories for pure substances [1] and alloys [2], and theories which take into account non-local spin fluctuation effects in the pure [3] and alloy [4, 5] cases. The spin-glass phase was treated in [4, 5] in terms of an effective Ising model by the method of the distribution function.

In the presence of well-defined local moments, spin-glass order parameter expansions for the free energy of a quenched random system are usually based [6 to 8] on the replica method. The concept of a quasi-free energy [6] is convenient to investigate both the random bond [7] and random site [8] models. The latter one (although more involved) is very natural to describe the mixture of two kinds of atoms A and B in contrast to the ad hoc ansatz for the variance of the exchange integral in the bond model. Standard replica procedures for random bond Ising spin glasses are given in [9, 10]. Without well-developed local moments, the Stoner glass theories [11, 12], based on the Wolff or Anderson models, work perturbatively with random intersite susceptibilities in diluted situations.

In this paper we try to combine Kakehashi's [5] spin fluctuation approach with Nambu's [8] Landau-type order parameter expansion to describe the paramagnetic

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to spin-glass transition in concentrated itinerant alloys (Section 2). Hence, the exchange coupling of effective Ising spins is founded microscopically as in [5], i.e. without having to insert it by hand as in [8]. Here the propagator (instead of the locator [5]) formalism of the coherent potential approximation (CPA) is chosen. In Section 3 numerical results are presented for exchange pair interactions, freezing temperature, specific heat, single-site distribution functions, densities of states, and spin-glass order parameters.

2. Theoretical Background

2.1 Effective random-site Ising model

To describe narrow-band alloys A_cB_{1-c} we start with the site-diagonally disordered Hubbard model

$$H = \sum_{i\sigma} \varepsilon_i n_{i\sigma} + \sum_{\substack{ij\sigma \\ (i \neq j)}} t_{ij} c_{i\sigma}^{+} c_{j\sigma} + \sum_i U_i n_{i\uparrow} n_{i\downarrow} , \tag{1}$$

where the atomic energy ε_i and the electron–electron interaction strength U_i are random parameters taking the values ε_ν and U_ν (ν = A, B) according to the atom species at the i-th site. The hopping integral t_{ij} is assumed to be configuration-independent.

Adopting functional integral technique to (1) and performing the Stratonovich-Hubbard transformation within the scalar two-field scheme the following approximations are made: static fields, saddle point for the charge fields, Hasegawa's [1, 2] decoupling procedure up to second-order moments of the exchange fields, and the pair approximation [3, 5]. From the beginning we restrict ourselves to paramagnetic and spin-glass states, i.e. long-range magnetic order is not considered. Then the free energy F for an arbitrary configuration of the lattice can be written as

$$\beta F = \beta F_0 - \sum_i \ln \sqrt{\frac{\beta U_i}{4\pi}} \int \mathrm{d}\zeta_i \, \mathrm{e}^{-\beta \Omega_{\mathrm{I}i}(\zeta_i)} - \ln \sum_{\{s\}} \mathrm{e}^{-\beta H_{\mathrm{II}}} , \tag{2}$$

where $\beta = 1/kT$, and F_0 is an irrelevant quantity.

The single-site contribution to (2) associated with the CPA is expressed by

$$\Omega_{\mathrm{I}}[\zeta] = \sum_i \Omega_{\mathrm{I}i}(\zeta_i) = \sum_i \left\{ \frac{U_i}{4} \zeta_i^2 - n_i w_i(\zeta_i) + \right.$$

$$\left. + \frac{1}{\pi} \int \mathrm{d}E \, f(E) \, \mathrm{Im} \sum_\sigma \ln \left(1 - \mathcal{F}_\sigma(E^+) \left(V_{i\sigma}(\zeta_i) - \Sigma_\sigma(E^+)\right)\right) \right\} \tag{3}$$

in terms of the fluctuating local exchange field ζ_i, the electron number n_i at site i, the charge potential $w_i(\zeta_i)$ arising from the charge neutrality limit [5] at each site, the Fermi function $f(E) = (1 + \mathrm{e}^{\beta(E-\mu)})^{-1}$ with the chemical potential μ, and $E^+ = E + i0$. Σ_σ denotes the coherent potential which will be determined by the CPA. $\mathcal{F}_\sigma = \mathcal{G}_{ii\sigma}$ is the site-diagonal element of the coherent Green function

$$\mathcal{G}_{ij\sigma}(z) = \frac{1}{N} \sum_{\boldsymbol{k}} \frac{\mathrm{e}^{i\boldsymbol{k}(\boldsymbol{R}_i - \boldsymbol{R}_j)}}{z - \varepsilon_{\mathrm{B}} - ts(\boldsymbol{k}) - \Sigma_\sigma(E)} \tag{4}$$

with $s(\boldsymbol{k}) = \sum_{\substack{j \\ (j \neq i:\,\text{n.n.})}} e^{i\boldsymbol{k}(\boldsymbol{R}_i - \boldsymbol{R}_j)}$ and the nearest-neighbour (n.n.) hopping integral t. N denotes the number of lattice sites with the position vectors $\boldsymbol{R}_i$. The local perturbation reads

$$V_{i\sigma}(\zeta_i) = \varepsilon_i - \varepsilon_B + w_i(\zeta_i) - \frac{U_i}{2}\sigma\zeta_i \,. \tag{5}$$

Beyond the single-site approximation, on the pair interaction level, the present problem can be mapped onto an effective Ising model [5]. Hence the third term of (2) involves the Ising Hamiltonian

$$H_{II} = -\sum_{(ij)} J_{ij} s_i s_j \tag{6}$$

summed over pairs (ij), with the fictitious spin $s_i = \pm 1$ at site i. Note that pair effects on $w_i[\zeta]$ are neglected. The effective exchange interaction is given by

$$J_{ij}(x_i, x_j) = -\tfrac{1}{4} \sum_{\lambda_i = \pm 1} \sum_{\lambda_j = \pm 1} \lambda_i \lambda_j \Phi_{ij}(\lambda_i x_i, \lambda_j x_j) \,, \tag{7}$$

$$x_i = \sqrt{\langle \zeta_i^2 \rangle_I} = \left(\frac{\int \mathrm{d}\zeta_i \zeta_i^2 \, e^{-\beta \Omega_{Ii}(\zeta_i)}}{\int \mathrm{d}\zeta_i \, e^{-\beta \Omega_{Ii}(\zeta_i)}} \right)^{1/2} . \tag{8}$$

It is pointed out that on assuming $\langle \zeta_i^{2m+k} \rangle_I = \langle \zeta_i^2 \rangle_I^m \langle \zeta_i^k \rangle_I$ $(k = 0, 1)$ [2] only x_i survives because of $\langle \zeta_i \rangle_I = 0$. The pair interaction

$$\Phi_{ij}(\zeta_i, \zeta_j) = \frac{1}{\pi} \int \mathrm{d}E \, f(E) \, \mathrm{Im} \sum_{\sigma} \ln \left(1 - t_{i\sigma}(\zeta_i) \, \tilde{\mathcal{G}}_{ij\sigma} t_{j\sigma}(\zeta_j) \, \tilde{\mathcal{G}}_{ji\sigma} \right)_{E^+} \tag{9}$$

with $\tilde{\mathcal{G}}_{ij\sigma} = \mathcal{G}_{ij\sigma}(1 - \delta_{ij})$, is expressed by the single-site scattering matrix

$$t_{i\sigma}(\zeta_i) = \frac{V_{i\sigma}(\zeta_i) - \Sigma_\sigma}{1 - \mathcal{F}_\sigma\left(V_{i\sigma}(\zeta_i) - \Sigma_\sigma\right)} \tag{10}$$

which has to satisfy the CPA requirements

$$\overline{\langle t_{i\sigma}(\zeta_i) \rangle_I} = \tfrac{1}{2} \sum_{\nu = A, B} c_\nu \left(t_{\nu\sigma}(x_\nu) + t_{\nu\sigma}(-x_\nu) \right) = 0 \,, \tag{11a}$$

$$\overline{\langle t_{i\sigma}(\zeta_i) \rangle_{II}} = 0 \,, \tag{11b}$$

where the bar refers to configurational averaging, and $c_A = 1 - c_B = c$. Further, the notation $\langle A\{\zeta\} \rangle_{II} = \sum_{\{s\}} A\{sx\} \, e^{-\beta H_{II}} / \sum_{\{s\}} e^{-\beta H_{II}}$ is used. The configuration average in (11b) will be realized below.

2.2 Order parameter expansion

The third, nonlocal part of (2) will be treated as a quenched random spin system. The calculation of the configurationally averaged free energy for a random site n.n. Ising model can be embedded into the replication approach proposed in [8]. In contrast to [8] the randomness of the coupling J_{ij} is here originated from the variable "spin length" x_i and via $t_{i\sigma}(\zeta_i)\, t_{j\sigma}(\zeta_j)$ from Φ_{ij}. The treatment of such site-disorder is fundamentally different from the random bond problem [7].

The averaged free energy $\bar{f}_{\mathrm{II}}$ per site is obtained by means of the replica trick

$$\beta\bar{f}_{\mathrm{II}} = -\frac{1}{N}\lim_{n\to 0}\frac{1}{n}\left(\overline{Z_{\mathrm{II}}^{n}} - 1\right) \tag{12}$$

which may be rewritten as $\beta\bar{f}_{\mathrm{II}} = -\lim_{n\to 0}\lim_{N\to\infty}\frac{1}{nN}\ln\overline{Z_{\mathrm{II}}^{n}}$ in the thermodynamic limit $N \to \infty$. More explicitly, we have

$$\overline{Z_{\mathrm{II}}^{n}} = \int\prod_{i}\left(\mathrm{d}p_i P(p_i)\right)\mathrm{Tr}^{(n)}\,\mathrm{e}^{\beta\sum_{(ij)}\sum_{\alpha=1}^{n}\tilde{J}_{ij}x_i x_j s_i^{\alpha}s_j^{\alpha}}\Big/\mathrm{Tr}^{(n)}\,1 \tag{13}$$

in which the Hamiltonian (6) enters in the n-replicated version, where "$\mathrm{Tr}^{(n)}$" runs over the set of spin variables $\{s_i^{\alpha}\}$ with the replica label α. The random site variable p_i takes the values 1 and 0 according to the site i is occupied by an A or B atom, respectively. p_i is subject to the probability distribution

$$P(p_i) = c_{\mathrm{A}}\,\delta(p_i - 1) + c_{\mathrm{B}}\,\delta(p_i)\,, \tag{14}$$

thus having assumed in (13) that the sites are statistically independent. Therefore, the renormalized n.n. exchange interaction $\tilde{J}_{ij} = J_{ij}/x_i x_j$ reads

$$\tilde{J}_{ij} = \tilde{J}_{\mathrm{AA}}p_i p_j + \tilde{J}_{\mathrm{AB}}\big(p_i(1-p_j) + p_j(1-p_i)\big) + \tilde{J}_{\mathrm{BB}}(1-p_i)\,(1-p_j)\,. \tag{15}$$

The aim is an order parameter expansion of the averaged free energy. Define the quasi-free energy $\overline{f_{\mathrm{II}}^{(n)}}\{q\}$ by $\overline{Z_{\mathrm{II}}^{n}} = \int \mathrm{d}q_{\mathrm{A}}\,\mathrm{d}q_{\mathrm{B}}\,\mathrm{e}^{-nN\beta\overline{f_{\mathrm{II}}^{(n)}}\{q_{\mathrm{A}},\,q_{\mathrm{B}}\}}$ in terms of the partial spin-glass order parameters $q_\nu(\nu = \mathrm{A}, \mathrm{B})$. Following [8] one finds, in the limit $N \to \infty$, the Landau-type expansion for spin glasses as

$$\beta\overline{f_{\mathrm{II}}^{(n)}}\{q\} = b_0 + \sum_{\nu\nu'} b_2^{\nu\nu'}q_\nu q_{\nu'} + \sum_{\nu} b_3^{\nu}q_\nu^3 + \ldots \tag{16}$$

with $b_0 = -\frac{\beta^2 z_{\mathrm{c}}}{4}\sum_{\nu\nu'} c_\nu c_{\nu'}J_{\nu\nu'}^2$, and the coefficients

$$b_2^{\nu\nu'} = \frac{1}{4}(n-1)\left(\frac{c_\nu}{x_\nu^4}\,\delta_{\nu\nu'} - \beta^2 z_{\mathrm{c}}c_\nu c_{\nu'}\tilde{J}_{\nu\nu'}^2\right), \tag{17}$$

$$b_3^{\nu} = -\frac{1}{3!}(n-1)(n-2)\frac{c_\nu}{x_\nu^6}, \tag{18}$$

where z_{c} is the coordination number. In getting (16) the average with respect to p_i was carried out approximately up to second-order cumulants. The lowest-order expansion (16) was given in [6] phenomenologically, in [8] the coefficients were derived explicitly. The main difference to [8] consists here in the additional microscopic foundation of $J_{\nu\nu'}$ concerning random Hubbard alloys. In particular, the $J_{\nu\nu'}$ rely on the CPA; they actually depend on c and T. By means of the replica technique one can prove that (11 b) coincides explicitly with (11 a); this does not hold in the ferromagnetic case.

On the basis of (16) at $n = 0$ we can draw some conclusions about the paramagnetism to spin-glass transition. The spin-glass transition temperature T_{SG} is determined via $[b_2^{\mathrm{AA}}b_2^{\mathrm{BB}} - (b_2^{\mathrm{AB}})^2]_{n=0} = 0$ by

$$T_{\mathrm{SG}} = \frac{1}{k}\sqrt{\frac{z_{\mathrm{c}}}{2}}\left\{c_{\mathrm{A}}J_{\mathrm{AA}}^2 + c_{\mathrm{B}}J_{\mathrm{BB}}^2 + \sqrt{(c_{\mathrm{A}}J_{\mathrm{AA}}^2 - c_{\mathrm{B}}J_{\mathrm{BB}}^2)^2 + 4c_{\mathrm{A}}c_{\mathrm{B}}J_{\mathrm{AB}}^4}\right\}^{1/2}. \tag{19}$$

Formally, (19) agrees with the results in [4, 5, 8], but here (19) is understood as an implicit equation in order to find T_{SG}. Near T_{SG} one gets $q_A = (x_A/x_B)^2 \sqrt{c_B/c_A}\, r^{-1} q_B$. Going a step further, from (16) one finds

$$q_A = \frac{x_A^2}{2}\left(\frac{1+r^2}{1+r^3\sqrt{c_A/c_B}}\right)\left(\left(\frac{T_{SG}}{T}\right)^2 - 1\right) \qquad (T \lessapprox T_{SG}) \tag{20}$$

with the abbreviations $\delta = J_{AB}/J_{AA}$, $\gamma = J_{BB}/J_{AA}$, and $r = [-c_A + c_B\gamma^2 + \sqrt{(c_A - c_B\gamma^2)^2 + 4c_Ac_B\delta^4}]/2\sqrt{c_Ac_B}\,\delta^2$. By using (20) and the analog for $q_B(T)$ the result of the specific heat C_V in the critical region is quoted as [8]

$$\frac{C_V}{k} = \begin{cases} C_0\left(\dfrac{T_{SG}}{T}\right)^2 & (T > T_{SG}), \qquad (21\,a) \\ C_0\left(\dfrac{T_{SG}}{T}\right)^2 - \dfrac{c_Ac_B(1+r^2)^3}{8\,(r^3\sqrt{c_A}+\sqrt{c_B})^2}\left(\dfrac{T_{SG}}{T}\right)^2\left\{1 - 6\left(\dfrac{T_{SG}}{T}\right)^2 + 5\left(\dfrac{T_{SG}}{T}\right)^4\right\} & (T \lessapprox T_{SG}), \qquad (21\,b) \end{cases}$$

where $C_0 = (c_A^2 + c_B^2\gamma^2 + 2c_Ac_B\delta^2)/(\gamma^2 + (1-\gamma^2)\,c_A + \sqrt{(c_A - c_B\gamma^2)^2 + 4c_Ac_B\delta^4})$.

Alternatively, the extremum value of the quasi-free energy defined by $\overline{f_{II,\,extr}^{(0)}} = \lim_{n\to 0} \overline{f_{II}^n}\{q = q_{extr}\}$, with $q_{\nu\,extr}$ arising from $\partial\overline{f_{II}^{(n)}}/\partial q_{\nu\,extr} = 0$ provided that $\overline{f_{II}^{(n)}}$ is taken in saddle-point approximation [8] (cf. [9]), can be given in the analytic form

$$\beta\overline{f_{II,\,extr}^{(0)}} = -\frac{z_c\beta^2}{4}\sum_{\nu\nu'} c_\nu c_{\nu'} J_{\nu\nu'}^2\left(1 - \frac{q_\nu}{x_\nu^2}\right)\left(1 - \frac{q_{\nu'}}{x_{\nu'}^2}\right) - \\ - \frac{1}{\sqrt{2\pi}}\int \mathrm{d}y\, \mathrm{e}^{-y^2/2} \sum_\nu c_\nu \ln\cosh\left(y\beta\sqrt{z_c\sum_{\nu'} c_{\nu'} J_{\nu\nu'}^2 \frac{q_{\nu'}}{x_{\nu'}^2}}\right), \tag{22}$$

where the q_ν satisfy the coupled system of equations

$$q_A = \frac{x_A^2}{\sqrt{2\pi}}\int \mathrm{d}y\, \mathrm{e}^{-y^2/2} \tanh^2\left(y\beta\sqrt{z_c\left(c_A J_{AA}^2 \frac{q_A}{x_A^2} + c_B J_{AB}^2 \frac{q_B}{x_B^2}\right)}\right), \tag{23}$$

$$q_B = \frac{x_B^2}{\sqrt{2\pi}}\int \mathrm{d}y\, \mathrm{e}^{-y^2/2} \tanh^2\left(y\beta\sqrt{z_c\left(c_A J_{AB}^2 \frac{q_A}{x_A^2} + c_B J_{BB}^2 \frac{q_B}{x_B^2}\right)}\right). \tag{24}$$

The connection of the spin fluctuation theory with the replica method can be also expressed by the weighted mean of q_ν: $\bar{q} = \overline{\langle\zeta_i\rangle_{II}^2} = \lim_{n\to 0}\{\overline{\langle p_i x_A^2 s_i^\alpha s_i^{\alpha'}\rangle_{II}^{(n)}} + \overline{\langle(1-p_i)\,x_B^2 s_i^\alpha s_i^{\alpha'}\rangle_{II}^{(n)}}\}_{\alpha\neq\alpha'}$, where $\langle\ldots\rangle_{II}^{(n)}$ indicates the average with respect to the replicated Hamiltonian $H_{II}^{(n)}$.

3. Numerical Results and Discussion

Let us list some details of the numerical model calculation. We choose a semielliptic shape of the unperturbed band entering (4), namely $\varrho_0(E) = (1/N)\sum_{\boldsymbol{k}} \delta(\varepsilon - \varepsilon_B - ts(\boldsymbol{k})) = (2/\pi)\sqrt{1-(E-\varepsilon_B)^2}\,\theta(1-|E-\varepsilon_B|)$ with the half-band width $w = z_c t = 1$

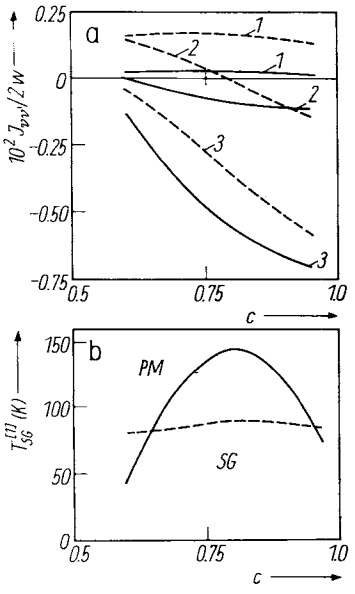

Fig. 1

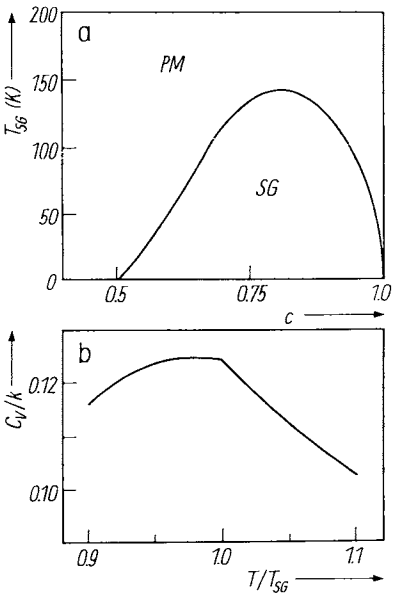

Fig. 2

Fig. 1. a) Effective exchange n.n. pair interactions J_{AA} (1), J_{AB} (2), and J_{BB} (3) (scaled by the unperturbed band width $2w$) in dependence on the concentration c of A atoms at the temperatures 10^2 K (———) and 10^3 K (– – –); b) spin-glass transition temperature $T_{SG}^{[1]}$ versus c obtained from (19) after the first iteration step with the values $J_{\nu\nu'}(T)$ of a)

Fig. 2. a) Transition temperature T_{SG} versus concentration c as phase boundary line between paramagnetism (PM) and spin glass (SG); b) specific heat C_V/k plotted against the reduced temperature T/T_{SG} near T_{SG} at $c = 0.8$

(in units of eV), $z_c = 6$. The local density of states $\varrho_{\nu\sigma}(E;\zeta_i)$ is related to the conditionally CPA averaged Green function $G_{\nu\sigma}$ through

$$\varrho_{\nu\sigma}(E;\zeta_i) = -\frac{1}{\pi}\,\mathrm{Im}\,G_{\nu\sigma}(E^+;\zeta_i) = \\ = -\frac{1}{\pi}\,\mathrm{Im}\left(\frac{\mathcal{F}_\sigma(E^+)}{1-\mathcal{F}_\sigma(E^+)\left(V_{\nu\sigma}(\zeta_i)-\Sigma_\sigma(E^+)\right)}\right). \tag{25}$$

Then $w_\nu(\zeta_i)$ is evaluated from the charge neutrality condition $n_\nu(\zeta_i) = \sum_\sigma \int \mathrm{d}E\, f(E) \times \varrho_{\nu\sigma}(E;\zeta_i) = n_\nu$ with the mean electron number at ν-sites $n_\nu = \langle n_\nu(\zeta_i)\rangle_{\mathrm{I}} = \int \mathrm{d}\zeta_i \varphi_\nu(\zeta_i)\, n_\nu(\zeta_i)$. Recall, in view of (8), the single-site distribution function

$$\varphi_\nu(\zeta_i) = \frac{\mathrm{e}^{-\beta\Omega_{\mathrm{I}\nu}(\zeta_i)}}{\int \mathrm{d}\zeta_i\, \mathrm{e}^{-\beta\Omega_{\mathrm{I}\nu}(\zeta_i)}}. \tag{26}$$

The chemical potential μ is determined by the mean particle number per site $n = \sum_\nu c_\nu n_\nu$. Moreover, the second moment relation $\langle m_\nu^2(\zeta_i)\rangle_{\mathrm{I}} = x_\nu^2 - 2/\beta U_\nu$ is employed in the numerical work, where $m_\nu(\zeta_i) = \sum_\sigma \sigma \int \mathrm{d}E\, f(E)\, \varrho_{\nu\sigma}(E;\zeta_i)$.

The parameters U_ν and n are chosen so that no long-range magnetic order may appear for $T = 0$ in the Hartree-Fock approximation. Note that n is fixed here, but

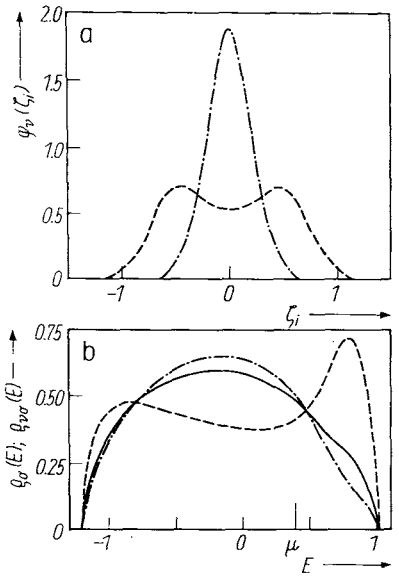

Fig. 3

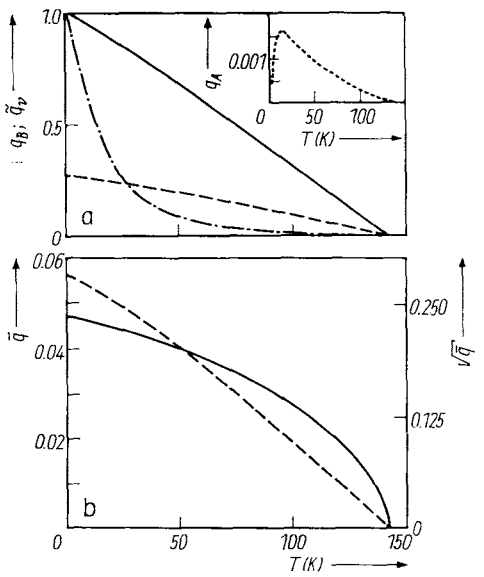

Fig. 4

Fig. 3. a) Single-site distribution functions $\varphi_A(\zeta_i)$ (—·—·) and $\varphi_B(\zeta_i)$ (— — —) in dependence on the local exchange field ζ_i; b) $\varrho_{A\sigma}(E)$ (—·—·), $\varrho_{B\sigma}(E)$ (— — —), and $\varrho_\sigma(E)$ (———) as partially and totally averaged densities of states, μ denotes the chemical potential; a) and b) at concentration $c = 0.8$ and temperature $T = T_{SG}$

Fig. 4. Spin-glass order parameters $\tilde{q}_\nu$ (renormalized), q_ν (partial at ν sites), and $\bar{q}$ (total) versus temperature T at concentration $c = 0.8$; a) $\tilde{q}_A$(—·—·), $\tilde{q}_B$ (———), q_A (·····), q_B (— — —); b) $\bar{q}$ (— — —), $\sqrt{\bar{q}}$ (———)

n_ν is calculated self-consistently. In the following the numerical examples of A_cB_{1-c} alloys belong to the parameter set: $\varepsilon_A = \varepsilon_B = -1$, $w = 1$, $U_A = 1$, $U_B = 1.5$, and $n = 1.6$.

Fig. 1a shows the concentration and temperature dependence of the n.n. exchange interaction energies $J_{\nu\nu'}$ in contrast to the simple Ising model [8]. This is a peculiarity of the itinerant system. There is a concentration region with $J_{AA} > 0$ and $J_{BB} < 0$, being necessary for the occurrence of a glass-like phase (competing interactions). One recognizes a reasonable order of magnitude of the $J_{\nu\nu'}$ (cf. [5]). Inserting $J_{\nu\nu'}(c, T)$ from Fig. 1a into the right-hand side of (19) the first iterative $T_{SG}^{[1]}$ in Fig. 1b refers to the phase separation between paramagnetism (PM) and spin glass (SG). Obviously, the self-consistency of T_{SG} is needed.

The self-consistent calculation of the transition temperature T_{SG} leads to the phase diagram in Fig. 2a. There exists a critical concentration c_{crit} so that for $c < c_{crit}$ no glass-like phase appears as predicted qualitatively in [11, 12]. Fig. 2b exhibits a weak (cusp-like) singularity of the specific heat C_V at the transition point, but here $C_V'(T)$ alters its sign near T_{SG} in difference to [8].

Fig. 3a demonstrates the consistency of the pair correlation problem with the single-site spin fluctuation picture by means of the distribution functions $\varphi_\nu(\zeta_i)$ defined in (26). The single and two maxima of φ_A and φ_B, respectively, correspond to the ferromagnetic (J_{AA}) and antiferromagnetic (J_{BB}) couplings in Fig. 1a. Note that the local free energy functionals $\Omega_{I\nu}(\zeta_i)$ have single- or double-minimum structures. In Fig. 3b

the partially and totally averaged densities of states $\varrho_{\nu\sigma}(E) = \int \mathrm{d}\zeta_i \varphi_\nu(\zeta_i)\, \varrho_{\nu\sigma}(E;\zeta_i)$ defined on the basis of (25) and $\varrho_\sigma(E) = -(1/\pi)\ \mathrm{Im}\ \mathcal{F}_\sigma(E^+)$, respectively, are presented. The partial electron numbers are found to be $n_\mathrm{A} = 1.675$ and $n_\mathrm{B} = 1.3$.

The solutions $\tilde{q}_\nu = q_\nu/x_\nu^2$ of the coupled system (23) and (24) as well as the q_ν are drawn in Fig. 4a. Fig. 4b gives the mean value $\bar{q} = \sum_\nu c_\nu q_\nu$ and $\sqrt{\bar{q}}$, where the latter one behaves similarly as the equivalent quantity in the Sherrington-Kirkpatrick random bond model [9, 10]. Physically, $\bar{q}$ or q_ν play the role of suitable spin-glass order parameters rather than $\tilde{q}_\nu$.

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(Received February 9, 1984)