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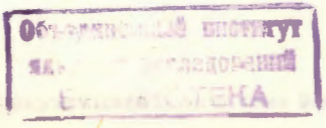

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Особенности парамагнитной восприимчивости модели Хаббарда для неупорядоченных сплавов

Вычислена парамагнитная восприимчивость неупорядоченного сплава. Для описания сильно связанных электронов при нулевой температуре используется микроскопический ферми-жидкостный подход. Эффективные вершины для рассеяния "частица-частица" и "частица-дырка" вычисляются в рамках когерентного локального лестничного приближения. Оказывается, что полученные выражения для восприимчивостей компонент и сплава, при учете корреляционных эффектов в лестничном приближении, обладают парамагнитной неустойчивостью. Представлены численные результаты для усредненных по конфигурациям полных и парциальных статических восприимчивостей, намагниченностей и зависящих от спина плотностей состояний.

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Singularities in the Paramagnetic Susceptibility of Random Hubbard Alloys

The paramagnetic susceptibility of disordered alloys is derived from a microscopic Fermi liquid approach to tightly bound electrons at zero temperature. Particle-particle and particle-hole effective vertices are calculated within the coherent local ladder approximation. The correlation-enhanced expressions for component and alloy susceptibilities refer to paramagnetic instabilities. Numerical results are presented for partial and total CPA averages of static susceptibilities, magnetizations, and spin-dependent densities of states.

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

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1. INTRODUCTION

A central problem of the theory of itinerant magnetism in transition metals and their alloys is surely which role play electron-electron correlations. One of the standard answers is that dynamical correlations suppress magnetism. To modify this quantitatively is a matter of more accurate self-consistent calculations. Specifically, the microscopic derivation of the boundaries between magnetic phases for the itinerant electron system in narrow-band alloys A_cB_{1-c} is usually based [1-7] on the "bare" Hubbard model [8] in the random version

$$H^{\{\nu\}} = \sum_{ij\sigma\,(i\neq j)} t_{ij}\, c^{+}_{i\sigma} c_{j\sigma} + \sum_{i\sigma} \epsilon_i^{\nu} n_{i\sigma} + \tfrac{1}{2}\sum_{i\sigma} U_i^{\nu} n_{i\sigma} n_{i-\sigma} = H_{\Delta}^{\{\nu\}} + H_{U}^{\{\nu\}} . \quad (1)$$

Here $c^{+}_{i\sigma}(c_{i\sigma})$ is the creation (annihilation) operator for a spin σ electron in the Wannier state at lattice site i, and $n_{i\sigma} = c^{+}_{i\sigma} c_{i\sigma}$. The atomic energy ϵ_i^{ν} and the strength of the intra-atomic Coulomb repulsion U_i^{ν} take the random values ϵ^{ν} and U^{ν} ($\nu = A, B$), respectively, according to whether an A or B atom occupies the site i. The hopping integrals t_{ij} are assumed to be independent of the atomic arrangement. The superscript $\{\nu\} = \{\nu_1, \ldots, \nu_i, \ldots, \nu_N\}$ with $\nu_i = A, B$ refers to the whole configuration.

Spin susceptibility calculations allow one to derive an explicit criterion for magnetism. Having used the coherent potential approximation (CPA) to treat the disorder, Hartree-Fock theories [1,2] overesti-

mate the magnetic state, whereas the Hubbard-III decoupling [4] yields no magnetism. The T-matrix approximation (ladder summation in the particle-particle channel) as, e.g., applied to the Anderson model for dilute alloys [9] and, combined with the CPA, to the disordered Hubbard model [10,11] is a good candidate to describe effective quasiparticle interaction of short range and at low density of electrons. Adopting it to calculate the susceptibility means solving Bethe-Salpeter-type equations for effective vertex functions. In some cases it is possible to replace the energy-dependent T-matrix by an appropriate constant value [9,11] (see also [12]). This has been done [11] in evaluating the paramagnetic susceptibility at finite temperatures.

The aim of the present paper is to calculate the paramagnetic susceptibility for the model (1) at zero temperature in the static limit, but with retaining the dynamical character of the effective interaction involved in a completely self-consistent scheme. In Sect. 2 the magnetic response is derived from a microscopic Fermi liquid approach to disordered systems [13] According to the local ladder approximation particle-particle and particle-hole vertices averaged partially in CPA are given in Sect. 3. In Sect. 4 the static paramagnetic susceptibility is evaluated explicitly. Numerical results for partial (component) and total (alloy) averages of spin-dependent densities of states, magnetizations, and susceptibilities are presented in Sect. 5.

2. MAGNETIC RESPONSE OF AN INHOMOGENEOUS FERMI LIQUID

In this Section we give a microscopic justification for some relations concerning the linear magnetic response. Working within a fixed configuration $\{\nu\}$ the lattice-space description is favoured owing to lack of transitional symmetry.

Following the nonuniform Fermi liquid approach [13] the longitudinal (nonlocal and dynamic) spin susceptibility $\chi_{ij}^{\{\nu\}}(\omega)$ at T=0 can be written in terms of the causal response function $L^{\{\nu\}}$ as

$$\chi_{ij}^{\{\nu\}}(\omega) = -\mu_B^2 \sum_{\sigma\sigma'} \int \frac{dE\, dE'}{(2\pi)^2} iL^{\{\nu\}}_{ij\,ij\,\sigma\sigma'\sigma\sigma'}(E,E';E-\omega,E+\omega)\sigma\sigma', \quad (2)$$

where μ_B is the Bohr magneton. This expression reflects the linear response to a space- and time-varying magnetic field applied parallel to the z-axis. The two-particle correlation function $L^{\{\nu\}}$ satisfies the integral equation

$$L^{\{\nu\}}_{ij\,ij\,\sigma\sigma'\sigma\sigma'}(E,E';\omega) = -2\pi\delta(E-E'+\omega) G^{\{\nu\}}_{ij\sigma}(E) G^{\{\nu\}}_{ji\sigma}(E')\delta_{\sigma\sigma'} - \sum_{\ell\bar{\sigma}} G^{\{\nu\}}_{i\ell\sigma}(E) G^{\{\nu\}}_{\ell i\sigma}(E+\omega) \int \frac{d\bar{E}}{2\pi} i I^{\{\nu\}}_{\ell\sigma\bar{\sigma}}(E,\bar{E}+\omega;\omega) L^{\{\nu\}}_{\ell j\ell j\,\bar{\sigma}\sigma'\bar{\sigma}\sigma'}(\bar{E},E';\omega), \quad (3)$$

where the energy transfer ω in all two-particle quantities is abbreviated by, e.g., $L^{\{\nu\}}(E,E';E+\omega,E'-\omega) \equiv L^{\{\nu\}}(E,E';\omega)$, hereafter. Note that in (3) only spin-diagonal one-particle Green functions $G^{\{\nu\}}$ are taken into account. Assuming a site-diagonal self-energy $\Sigma^{\{\nu\}}_{Uii\sigma}$ the dressed $G^{\{\nu\}}$ has to fulfil the Dyson equation

$$(G^{\{\nu\}-1}(E))_{ij\sigma} = (G^{\{\nu\}-1}_{\Delta}(E))_{ij} - \Sigma^{\{\nu\}}_{Uii\sigma}(E)\delta_{ij}, \quad (4)$$

where $G^{\{\nu\}}_{\Delta}$ is the propagator related with the non-interacting part $H^{\{\nu\}}_{\Delta}$ from (1). Moreover, we suppose a local self-consistent approximation to determine $\Sigma^{\{\nu\}}_{U}$ via the functional

$$\Sigma^{\{\nu\}}_{Uii\sigma} = F[G^{\{\nu\}}_{ii\sigma}, G^{\{\nu\}}_{ii-\sigma}]. \quad (5)$$

To maintain consistent approximations one has to apply the Baym and Kanadoff technique [14] by setting (here the source field is omitted)

$$\frac{\delta\Sigma^{\{\nu\}}_{Uii\sigma}(E)}{\delta G^{\{\nu\}}_{ii\sigma'}(E')} = -I^{\{\nu\}}_{iiii\,\sigma\bar{\sigma}\bar{\sigma}\sigma'}(E,E';E,E') \equiv -iI^{\{\nu\}}_{i\sigma\sigma'}(E,E') \qquad (6)$$

to get a local irreducible particle-hole vertex $I^{\{\nu\}}$ entering into (3). The full vertex $\Gamma^{\{\nu\}}$ corresponding to (3) is reduced in the particle-hole channel, yielding the Bethe–Salpeter equation (see Fig. 1)

$$\Gamma^{\{\nu\}}_{ijik\,\sigma\bar{\sigma}\bar{\sigma}\sigma'}(E,E';\omega) = I^{\{\nu\}}_{i\sigma\sigma'}(E,E';\omega)\delta_{ij}\delta_{ik} -$$
$$- i\sum_{\ell\bar{\sigma}}\int\frac{d\bar{E}}{2\pi}I^{\{\nu\}}_{i\sigma\bar{\sigma}}(E,\bar{E}+\omega;\omega)G^{\{\nu\}}_{i\ell\bar{\sigma}}(\bar{E})G^{\{\nu\}}_{\ell i\bar{\sigma}}(\bar{E}+\omega)\Gamma^{\{\nu\}}_{\ell j\ell k\,\bar{\sigma}\sigma\bar{\sigma}\sigma'}(\bar{E},E';\omega). \qquad (7)$$

Note that for small ω one can set $\omega=0$ in $I^{\{\nu\}}$ in (3) and (7) as in the uniform Fermi liquid theory of Landau [15].

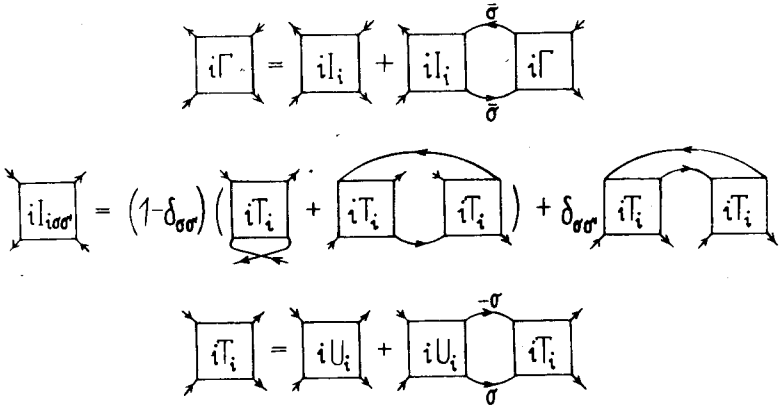

Fig. 1. Diagrammatic representation of the coupled system of vertex equations (7), (15), and (21).

In the following we are interested in the local spin susceptibility $\chi^{\{\nu\}}_i$ introduced by

$$\frac{1}{N}\sum_{ij}\chi^{\{\nu\}}_{ij}(\omega) = \frac{\mu_B^2}{N}\sum_{ij\sigma}\sigma\int\frac{dE}{2\pi}G^{\{\nu\}}_{ij\sigma}(E+\omega)\,i\Lambda^{\{\nu\}}_{j\sigma}(E+\omega,E)G^{\{\nu\}}_{ji\sigma}(E) \equiv \qquad (8)$$
$$\equiv \frac{1}{N}\sum_i\chi^{\{\nu\}}_i(\omega),$$

where the effective spin vertex $\Lambda^{\{\nu\}}_{i\sigma}$ is defined simultaneously. Despite locality, both $\chi^{\{\nu\}}_i$ and $\Lambda^{\{\nu\}}_i$ depend, in principle, on the whole configuration $\{\nu\}$. On combining (2), (3), and (8) one derives the integral equation for the spin vertex as

$$\Lambda^{\{\nu\}}_{i\sigma}(E+\omega,E) = \sigma - \sum_{j\bar{\sigma}}\int\frac{d\bar{E}}{2\pi}iI^{\{\nu\}}_{i\sigma\bar{\sigma}}(E+\omega,\bar{E};-\omega)\times \qquad (9)$$
$$\times G^{\{\nu\}}_{ij\sigma}(\bar{E}+\omega)\,G^{\{\nu\}}_{ji\bar{\sigma}}(\bar{E})\Lambda^{\{\nu\}}_{j\bar{\sigma}}(\bar{E}+\omega,\bar{E}).$$

On the other hand, in the limit of a uniform and static magnetic field h a Ward identity must hold of the type (in the ordered case cf. [16])

$$\left(\frac{\partial\Sigma^{\{\nu\}}_{Uii\sigma}(E;h)}{\partial h}\right)_{h=0} = \mu_B\sum_{j\sigma'}\int\frac{d\bar{E}}{2\pi}\Gamma^{\{\nu\}}_{ijij\,\sigma\bar{\sigma}\bar{\sigma}\sigma'}(E,\bar{E};E,\bar{E})(G^{\{\nu\}}_{\sigma'}(\bar{E})\sigma' G^{\{\nu\}}_{\sigma'}(\bar{E}))_{jj}, \qquad (10)$$

which can be found [13] from the first order variation of the self-energy $\Sigma^{\{\nu\}}_U$ with respect to h. Note that this limiting procedure coincides with the case of physical interest, see also below. Substituting (7) at $\omega=0$ into (10) we obtain

$$\left(\frac{\partial\Sigma^{\{\nu\}}_{Uii\sigma}(E;h)}{\partial h}\right)_{h=0} = \mu_B\sum_{\sigma'}\int\frac{d\bar{E}}{2\pi}iI^{\{\nu\}}_{i\sigma\sigma'}(E,\bar{E})(G^{\{\nu\}}_{\sigma'}(\bar{E})\sigma' G^{\{\nu\}}_{\sigma'}(\bar{E}))_{ii} -$$

$$-\sum_{j\sigma'}\int\frac{d\bar{E}}{2\pi}iI^{\{\nu\}}_{i\sigma\sigma'}(E,\bar{E})(G^{\{\nu\}}_{ij\sigma'}(\bar{E})G^{\{\nu\}}_{ji\sigma'}(\bar{E})(\frac{\partial\Sigma^{\{\nu\}}_{Ujj\sigma'}(\bar{E};h)}{\partial h})_{h=0}. \quad (11)$$

Comparison of (11) and (9) yields

$$(\frac{\partial\Sigma^{\{\nu\}}_{Uii\sigma}(E;h)}{\partial h})_{h=0} = \mu_B(\sigma - \Lambda^{\{\nu\}}_{i\sigma}(E,E)). \quad (12)$$

By inserting $\Lambda^{\{\nu\}}_{i\sigma}$ from (12) into (8) one verifies the static local susceptibility $\chi^{\{\nu\}}_i \equiv \chi^{\{\nu\}}_i(\omega=0)$ to be

$$\chi^{\{\nu\}}_i = \mu_B i\sum_{j\sigma}\sigma\int\frac{dE}{2\pi}G^{\{\nu\}}_{ij\sigma}(E)(\mu_B\sigma-(\frac{\partial\Sigma^{\{\nu\}}_{Ujj\sigma}(E;h)}{\partial h})_{h=0})G^{\{\nu\}}_{ji\sigma}(E) \quad (13)$$

$$= -\mu_B i\sum_\sigma\sigma\int\frac{dE}{2\pi}(\frac{\partial G^{\{\nu\}}_{ii\sigma}(E;h)}{\partial h})_{h=0},$$

where in getting the last term we have used (4) with h included.

3. CONDITIONALLY AVERAGED VERTICES IN LADDER APPROXIMATION

Next we determine the irreducible particle-hole vertex in a consistent way based on the local ladder approximation. Moreover, configuration-dependent quantities are partially CPA averaged, provided a ν atom is fixed at some site. In the single-site version multiple scatterings in the particle-particle channel yield [10], instead of (5), (in terms of conditionally averaged causal functions)

$$\Sigma^\nu_{Uii\sigma}(E) = \int\frac{dE'}{2\pi i}G^\nu_{ii-\sigma}(E')T^\nu_i(E+E'), \quad (\nu = A,B) \quad (14)$$

$$T^\nu_i(E) = [\frac{1}{U^\nu_i} + \int\frac{dE'}{2\pi i}G^\nu_{ii\sigma}(E')G^\nu_{ii-\sigma}(E-E')]^{-1}, \quad (15)$$

where T^ν_i (see Fig. 1) is the effective two-particle vertex. Such a form was proposed for the ordered case by Babanov et al. [17]. The dressed local Green function $G^\nu_{ii\sigma}$ written as resolvent (z being the complex energy) is determined by

$$G^\nu_{ii\sigma}(z) = \frac{F_\sigma(z)}{1-(\tilde{\epsilon}^\nu_{i\sigma}(z) - \Sigma_\sigma(z))F_\sigma(z)}, \quad (16)$$

$$\tilde{\epsilon}^\nu_{i\sigma}(z) = \epsilon^\nu_i + \Sigma^\nu_{Uii\sigma}(z), \quad (17)$$

$$F_\sigma(z) = \frac{1}{N}\sum_{\vec{k}}\frac{1}{z-\epsilon(\vec{k})-\Sigma_\sigma(z)} \equiv \frac{1}{N}\mathrm{tr}\,\mathcal{G}_\sigma(z), \quad (18)$$

$$\Sigma_\sigma(z) = c\tilde{\epsilon}^A_\sigma(z)+(1-c)\tilde{\epsilon}^B_\sigma(z)-[\tilde{\epsilon}^A_\sigma(z)-\Sigma_\sigma(z)]F_\sigma(z)[\tilde{\epsilon}^B_\sigma(z)-\Sigma_\sigma(z)]. \quad (19)$$

Here Σ_σ is the coherent potential obeying (19) based on the CPA [18], $\mathcal{G}_\sigma$ denotes the totally averaged Green function, and $\epsilon(\vec{k}) = t\sum'_{j(\neq i)}\exp\{\vec{k}(\vec{R}_j - \vec{R}_i)\}$ provided that only the nearest-neighbour hopping integral t is taken into account, $\vec{k}$ is the wave-vector, and $\vec{R}_i$ is the lattice vector. Note that the site index i in $\tilde{\epsilon}^\nu_{i\sigma}$ is dropped in (19). The set of self-consistent equations is closed by adding

$$n = \sum_\sigma n_\sigma = -\frac{1}{\pi}\sum_\sigma\int_{-\infty}^{\mu}dE\ \mathrm{Im}\,F_\sigma(E+i0), \quad (20)$$

which connects the average number of electrons n per site with the chemical potential μ.

From (14) and (15) one derives in the sense of (6) the irreducible particle-hole vertex at zero energy transfer as (see Fig. 1)

$$I^\nu_{i\sigma\sigma'}(E,E') \equiv i\frac{\delta\Sigma^\nu_{Uii\sigma}(E)}{\delta G^\nu_{ii\sigma'}(E')} = -\int\frac{d\bar{E}}{2\pi i}G^\nu_{ii-\sigma}(\bar{E})G^\nu_{ii-\sigma}(E+\bar{E}-E')[T^\nu_i(E+\bar{E})]^2\delta_{\sigma\sigma'} +$$

$$+(T^\nu_i(E+E') - \int\frac{d\bar{E}}{2\pi i}G^\nu_{ii-\sigma}(\bar{E})G^\nu_{ii\sigma}(E+\bar{E}-E')[T^\nu_i(E+\bar{E})]^2)(1-\delta_{\sigma\sigma'}). \quad (21)$$

As a first step of partial averaging, this expression can serve as the kernel of (9).

Now we pass to the paramagnetic phase. Hence, substituting (21) into (9) and using $G^{\nu}_{ii\sigma} = G^{\nu}_{ii-\sigma} = G^{\nu}_{ii}$ one can reduce (9) via the ansatz $\Lambda^{\{\nu\}}_{i\sigma}(E+\omega, E) = \sigma\Lambda^{\{\nu\}}_{i}(E+\omega,E)$ to

$$\Lambda^{\{\nu\}}_{i}(E+\omega,E)=1+\sum_{j}\int\frac{d\bar{E}}{2\pi}iT^{\nu}_{i}(E+\bar{E})G^{\{\nu\}}_{ij}(\bar{E}+\omega)G^{\{\nu\}}_{ji}(\bar{E})\Lambda^{\{\nu\}}_{j}(\bar{E}+\omega,\bar{E}), \tag{22}$$

where spin indices are hereafter neglected unless they are explicitly required.

Following arguments of /19/ we approximate in (22) the energy dependence of T^{ν}_{i} by replacing $T^{\nu}_{i}(E+\bar{E}) \to \tilde{T}^{\nu}_{i}(E)=\Sigma^{\nu}_{Uii}(E)/n^{\nu}_{i}$, where $n^{\nu}_{i}=\int\frac{dE}{2\pi i}G^{\nu}_{ii}(E)$ is the average electron number (per spin) at site i occupied by a ν atom in an otherwise effective CPA medium. Such a step is best judged by looking at (14) in the paramagnetic case. Combining (22) and (8) at $\omega=0$ with the approximated $\tilde{T}^{\nu}_{i}(E)$ we obtain

$$\Lambda^{\{\nu\}}_{i}(E,E) = 1 + \frac{\Sigma^{\nu}_{Uii}(E)}{2\mu^{2}_{B}n^{\nu}_{i}}\chi^{\{\nu\}}_{i} . \tag{23}$$

From (23) and (12) in the paramagnetic state, it follows after partial averaging that

$$\left(\frac{\partial\Sigma^{\nu}_{Ui\sigma}(E;h)}{\partial h}\right)_{h=0} = -\sigma\frac{\Sigma^{\nu}_{Uii}(E)}{2\mu_{B}n^{\nu}_{i}}\chi^{\nu}_{i} . \tag{24}$$

This relation describes the h-field dependence of the correlation part needed in the following.

4. INSTABILITIES OF THE PARAMAGNETIC PHASE

Within a treatment similar to /1/ we now derive explicit expressions for the local paramagnetic susceptibilities. Start from the conditionally averaged form of (13) (for brevity, we drop the site index i)

$$\chi^{\nu} = \mu_{B}\sum_{\sigma}\sigma\left(\frac{\partial n^{\nu}_{\sigma}(h)}{\partial h}\right)_{h=0}, \qquad (\nu = A,B) \tag{25}$$

with (16) rewritten as

$$\eta^{\nu}_{\sigma}(h) = -\frac{1}{\pi}\mathrm{Im}\int_{-\infty}^{\mu}dE\frac{F_{\sigma}(z;h)}{1-(\tilde{\epsilon}^{\nu}_{\sigma}(z;h)-\Sigma_{\sigma}(z;h))F_{\sigma}(z;h)}\Bigg|_{z=E+i0} . \tag{26}$$

Here the Zeeman energy is added to (17), yielding $\tilde{\epsilon}^{\nu}_{\sigma}(z;h)=\epsilon^{\nu}+\Sigma^{\nu}_{U\sigma}(z;h) - \mu_{B}\sigma h$ and implying a field-dependent $F_{\sigma}(z;h)$ instead of (18) via $\Sigma_{\sigma}(z;h)$ from (19). Thus, having introduced the h-field in (17) to (19) the differentiation with respect to h gives rise to

$$\left(\frac{\partial\Sigma_{\sigma}(z;h)}{\partial h}\right)_{h=0} = K^{A}(z)\left[\left(\frac{\partial\Sigma^{A}_{U\sigma}(z;h)}{\partial h}\right)_{h=0} - \mu_{B}\sigma\right] + K^{B}(z)\left[\left(\frac{\partial\Sigma^{B}_{U\sigma}(z;h)}{\partial h}\right)_{h=0} - \mu_{B}\sigma\right], \tag{27}$$

where

$$K^{A}(z)=[c-(\tilde{\epsilon}^{B}(z)-\Sigma(z))F(z)]/K(z), \tag{28}$$

$$K^{B}(z)=[1-c-(\tilde{\epsilon}^{A}(z)-\Sigma(z))F(z)]/K(z), \tag{29}$$

$$K(z)=1-(\tilde{\epsilon}^{A}(z)+\tilde{\epsilon}^{B}(z)-2\Sigma(z))F(z)+(\tilde{\epsilon}^{A}(z)-\Sigma(z))(\tilde{\epsilon}^{B}(z)-\Sigma(z))\bar{F}(z), \tag{30}$$

$$\bar{F}(z) = \frac{1}{N}\sum_{\vec{k}}\left(\frac{1}{z-\epsilon(\vec{k})-\Sigma(z)}\right)^{2} \equiv \frac{1}{N}\,\mathrm{tr}\,\mathcal{G}^{2}(z). \tag{31}$$

Altogether, from (25) and (26) by means of (27) one gets

$$\chi^{\nu} = \chi^{\nu}_{1} - \frac{\mu_{B}}{\pi}\sum_{\sigma}\sigma\,\mathrm{Im}\int_{-\infty}^{\mu}dE\ \times \tag{32}$$

$$\times\frac{[\bar{F}(z)-F^{2}(z)][K^{A}(z)\left(\frac{\partial\Sigma^{A}_{U\sigma}(z;h)}{\partial h}\right)_{h=0}+K^{B}(z)\left(\frac{\partial\Sigma^{B}_{U\sigma}(z;h)}{\partial h}\right)_{h=0}]+F^{2}(z)\left(\frac{\partial\Sigma^{\nu}_{U\sigma}(z;h)}{\partial h}\right)_{h=0}}{[1-(\tilde{\epsilon}^{\nu}(z)-\Sigma(z))F(z)]^{2}}\Bigg|_{z=E+i0},$$

where

$$\chi_1^\nu = -\frac{2\mu_B^2}{\pi}\,\mathrm{Im}\int_{-\infty}^{\mu} dE\,\frac{(F^2(z)-F(z))(K^A(z)+K^B(z))-F^2(z)}{[1-(\tilde{\epsilon}^\nu(z)-\Sigma(z))F(z)]^2}\Big|_{z=E+i0}, \tag{33}$$

which can be rewritten as

$$\chi_1^\nu = \chi_0^\nu + \frac{2\mu_B^2}{\pi}\,\mathrm{Im}\int_{-\infty}^{\mu} \frac{[\bar{F}(z)-F^2(z)][K^A(z)\frac{\partial\Sigma_U^A(z)}{\partial z}+K^B(z)\frac{\partial\Sigma_U^B(z)}{\partial z}]+F^2(z)\frac{\partial\Sigma_U^\nu(z)}{\partial z}}{[1-(\tilde{\epsilon}^\nu(z)-\Sigma(z))F(z)]^2}\Big|_{z=E+i0} \tag{34}$$

with

$$\chi_0^\nu = -\frac{2\mu_B^2}{\pi}\,\mathrm{Im}\int_{-\infty}^{\mu} dE\,\frac{\partial G^\nu(z)}{\partial z}\Big|_{z=E+i0} = 2\mu_B^2\rho^\nu(\mu). \tag{35}$$

Here ρ^ν is the component density of states (per spin) associated with a ν atom. Finally, we insert (24) into (32) and solve the system of algebraic equations, yielding the partial susceptibilities

$$\chi^A = \frac{1}{D}[\chi_1^A(1+\frac{1}{\pi n^B}\,\mathrm{Im}\int_{-\infty}^{\mu} dE M^B(z)\Sigma_U^B(z)|_{z=E+i0}) - \tag{36}$$
$$-\chi_1^B\frac{1}{\pi n^B}\,\mathrm{Im}\int_{-\infty}^{\mu} dE M^{AB}(z)\Sigma_U^B(z)|_{z=E+i0}],$$

$$\chi^B = \frac{1}{D}[\chi_1^B(1+\frac{1}{\pi n^A}\,\mathrm{Im}\int_{-\infty}^{\mu} dE M^A(z)\Sigma_U^A(z)|_{z=E+i0}) - \tag{37}$$
$$-\chi_1^A\frac{1}{\pi n^A}\,\mathrm{Im}\int_{-\infty}^{\mu} dE M^{BA}(z)\Sigma_U^A(z)|_{z=E+i0}],$$

where

$$D = (1+\frac{1}{\pi n^A}\,\mathrm{Im}\int_{-\infty}^{\mu} dE M^A(z)\Sigma_U^A(z)|_{z=E+i0})\times$$
$$\times(1+\frac{1}{\pi n^B}\,\mathrm{Im}\int_{-\infty}^{\mu} dE M^B(z)\Sigma_U^B(z)|_{z=E+i0}) -$$

$$-\frac{1}{\pi^2 n^A n^B}(\mathrm{Im}\int_{-\infty}^{\mu} dE M^{AB}(z)\Sigma_U^B(z)|_{z=E+i0})(\mathrm{Im}\int_{-\infty}^{\mu} dE M^{BA}(z)\Sigma_U^A(z)|_{z=E+i0}), \tag{38}$$

$$M^\nu(z) = [(F^2(z)-\bar{F}(z))K^\nu(z)-F^2(z)]/[1-(\tilde{\epsilon}^\nu(z)-\Sigma(z))F(z)]^2, \tag{39}$$

$$M^{\nu\nu'}(z) = (F^2(z)-\bar{F}(z))K^{\nu'}(z)/[1-(\tilde{\epsilon}^\nu(z)-\Sigma(z))F(z)]^2, (\nu,\nu' = A,B). \tag{40}$$

Then, the totally averaged susceptibility becomes

$$\chi = \langle\chi^\nu\rangle = c\chi^A + (1-c)\chi^B. \tag{41}$$

It is pointed out that the correlation-enhanced result (36) and (37) involves the dynamics in terms of $\Sigma_U(E)$, which must be calculated from the self-consistent cycle (14) to (20). Instabilities of the paramagnetic phase can arise from the condition D=0 (criterion for magnetism) imposed on the determinant (38).

Let us discuss some limiting cases.

(i) First consider the Hartree-Fock approximation defined by $\Sigma_{UHF}^\nu = U^\nu n^\nu$. Then, one recovers immediately the result of Hasegawa and Kanamori /1/ at T=0 by looking at (36) to (40) with χ_1^ν in (34) reduced to $\chi_0^\nu = 2\mu_B^2\rho^\nu(\mu)$.

(ii) At zero Coulomb energy ($U^\nu=0$) the static spin susceptibilities (36) and (37) simplify to $\chi_{CPA}^\nu \equiv \chi_0^\nu = 2\mu_B^2\rho^\nu(\mu)$, implying the total $\chi_{CPA} = 2\mu_B^2\rho(\mu)$ (cf. (41)), where $\rho(\mu)$ is the alloy density of states at the Fermi level. This "pure" CPA result can be confirmed by looking at the more general expression $K(\vec{k},\omega) = \rho(\mu)iD(\mu)\vec{k}^2/(\omega+iD(\mu)\vec{k}^2)$ derived in /20/, see also /21/, where $K(\vec{k},\omega)$ is the retarded two-particle correlation function for small ω and $\vec{k}$, and D is the diffusion constant. Hence in the so-called $\vec{k}$-limit /22/ the dynamic response $\chi(\vec{k},\omega) = 2\mu_B^2 K(\vec{k},\omega)$ turns into $\lim_{\vec{k}\to 0}\lim_{\omega\to 0}\chi(\vec{k},\omega) = 2\mu_B^2\rho(\mu) \equiv \chi_{CPA}$, emphasizing that the present χ corresponds to the retarded response.

(iii) In the dilute alloy limit $c \to 0$, $\Sigma(z)$ in (19) can be replaced by $\tilde{\epsilon}^B(z) = \epsilon^B - \Sigma_U^B(z)$ giving rise to $K^A \to 0$ and $K^B \to 1$ in (28) to (30), and $M^{BA} \to 0$ in (40). With these simplifications, from (33) and (37) to (41) we get

$$D_{c\to 0} = (1 - \frac{1}{\pi n^A} \mathrm{Im} \int_{-\infty}^{\mu} dE \frac{F^2(z)\Sigma_U^A(z)}{[1-(\tilde{\epsilon}^A(z)-\tilde{\epsilon}^B(z))F(z)]^2}|_{z=E+i0}) \times$$

$$\times (1 - \frac{1}{\pi n^B} \mathrm{Im} \int_{-\infty}^{\mu} dE \bar{F}(z)\Sigma_U^B(z)|_{z=E+i0}), \qquad (42)$$

$$\chi_{c\to 0} - \chi^B = (\frac{2\mu_B^2}{\pi} \mathrm{Im} \int_{-\infty}^{\mu} dE \bar{F}(E+i0))/(1 - \frac{1}{\pi n^B} \mathrm{Im} \int_{-\infty}^{\mu} dE\, \bar{F}(z)\Sigma_U^B(z)|_{z=E+i0}), \qquad (43)$$

where $\bar{F}(z) = \frac{1}{N}\sum_{\vec{k}} 1/(z - \epsilon(\vec{k}) - \epsilon_B^B - \Sigma_U^B(z))^2 = (G^{B^2}(z))_{ii}$ instead of (31), and $F(z) \equiv G_{ii}(z)$ instead of (18). Analogously, the limit $c \to 1$ is obtained by interchanging A and B. The formula (43) coincides with the result[23] for pure systems. The condition $D_{c\to 0} = 0$ put on the first factor of (42) signals the occurence of a localized magnetic moment on the impurity atom A embedded in an otherwise pure B system (compare[1]).

Note that χ from (41), restoring translational symmetry, can be interpreted as the $\vec{k}$-limit result caused by the Ward relation (10) and the magnetic field coupling in the context of (26). Thus, singularities of χ refer towards ferromagnetic ordering.

5. NUMERICAL ANALYSIS

For the numerical study the unperturbed density of states (per site per spin) reflecting the hopping term in (1) is chosen as

$$\rho_0(E) = \frac{1}{N}\sum_{\vec{k}} \delta(E - \epsilon(\vec{k})) = \begin{cases} \frac{2}{\pi w}[1-(\frac{E}{w})^2]^{1/2}, & |E| \le w \\ 0, & |E| > w \end{cases} \qquad (44)$$

where w is the half-bandwidth. Then, without van Hove singularities, F_σ and $\bar{F}$ defined in (18) and (31) are calculated analytically. Let us list the input parameters $w, \epsilon^A, \epsilon^B = 0$ fixed, U^A, U^B, c, n; output quantities are the component and alloy densities of states $\rho_\sigma^\nu(E) = -(1/\pi)\,\mathrm{Im}\,G_\sigma^\nu(E + i0)$ $(\nu = A,B)$ and $\rho_\sigma(E) = -(1/\pi)\,\mathrm{Im}\,F_\sigma(E + i0)$, resp., the average electron number with spin σ at ν sites $n_\sigma^\nu = \int_{-\infty}^{\mu} dE \rho_\sigma^\nu(E)$, the component and average magnetizations $m^\nu = n_\uparrow^\nu - n_\downarrow^\nu$ and $m = n_\uparrow - n_\downarrow$, resp., and the susceptibilities χ^ν and χ.

The procedure for getting solutions is as follows: Choose a set of parameter values and solve the system of equations (14) to (20) numerically up to self-consistency (as outlined in[10]) in order to deduce immediately ρ_σ^ν, ρ_σ, m^ν, m in the ferromagnetic case or to lay out all quantities needed in the paramagnetic phase; and substitute these into (33) and (36) to (41), and carry out the integrals to obtain χ^ν and χ. Here we have chosen parameters so that the case $n_\sigma^\nu \ge 1$ is not attained for any ν.

Now we turn to the discussion of the numerical results. The densities of states $\rho_\sigma(E)$ in Fig. 2 exhibit the transition from paramagnetic via ferromagnetic to saturated ferromagnetic behaviour with increasing electron concentration n. Note that the magnetization changes its sign from n=0.28 to n=0.4. Such an effect was also found in the Hartree-Fock treatment[5]. The shapes of the up- and down-spin bands greatly differ in the saturated case. Here the absence of the two-particle region (large tailing with small humps) in the down-spin band is due to the fact that only electrons with opposite spins are scattered mutually.

In the split-band case of Fig. 3 the spin-dependent shift of the spectrum appears especially for the B component, since the self-consistency of n^ν gives rise to $n^A \ll n^B$ in the present example. This is confirmed if looking at the magnetization. Moreover, the m (or m^ν) curve shows a gradual (hyste-

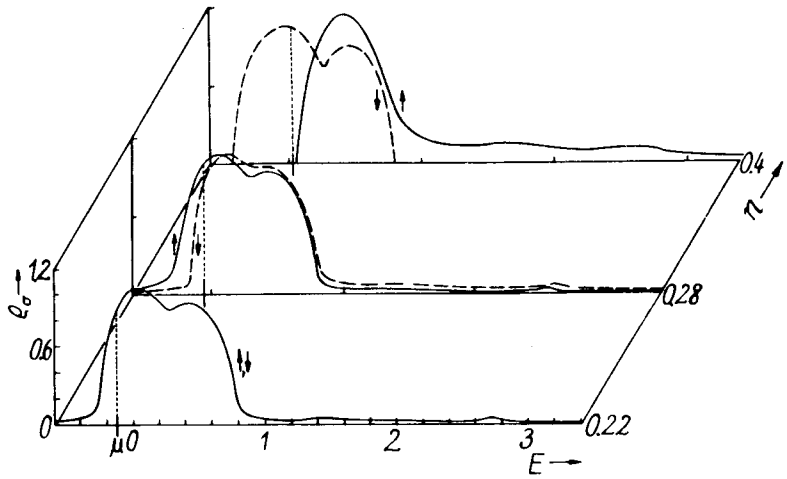

Fig. 2. Spin-dependent densities of states $\rho_\sigma(E)$ at various values of the electron density n for an alloy with $(w, \epsilon^A, \epsilon^B, U^A, U^B, c) = (0.5, 0.4, 0, 1.9, 2, 0.4)$. Dotted vertical lines refer to the Fermi energy.

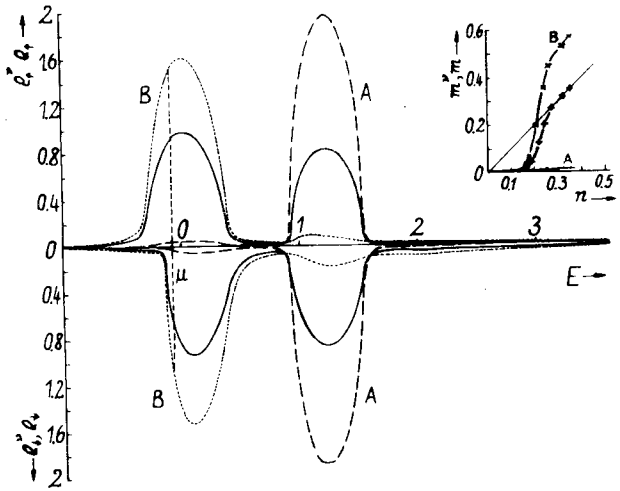

Fig. 3. Spin-dependent densities of states averaged partially $\rho^\nu_\sigma(E)$ $(\nu = A, B)$ and totally $\rho_\sigma(E)$, respectively, at $n = 0.23$, magnetizations $m^\nu(\cdot, \times)$ and $m(+)$ versus n for the set $(w, \epsilon^A, \epsilon^B, U^A, U^B, c) = (0.5, 1.2, 0, 1.5, 2.2, 0.4)$.

resis-like) transition from the paramagnetic to the ferromagnetic state, in contrast to the "nearly" (owing to approximated G^ν_σ) self-consistent calculation [7]. The case of saturated ferromagnetism corresponding to the alloy parameters of Fig. 3 is presented in Fig. 4.

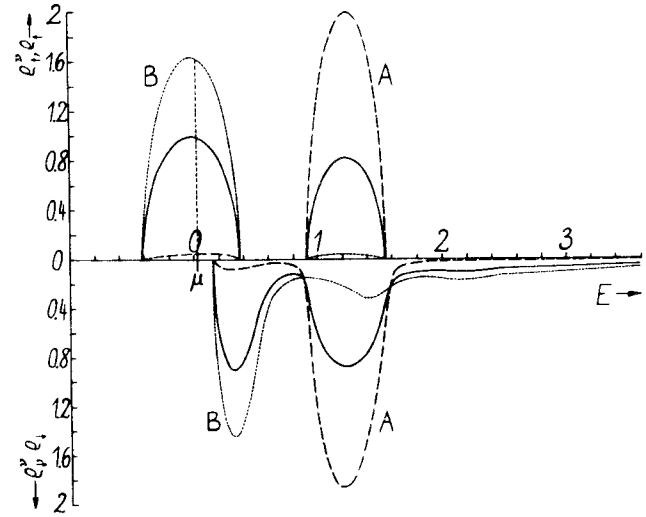

Fig. 4. Spin-dependent densities of states averaged partially $\rho^\nu_\sigma(E)$ $(\nu = A, B)$ and totally $\rho_\sigma(E)$, respectively, for the set $(w, \epsilon^A, \epsilon^B, U^A, U^B, c, n) = (0.5, 1.2, 0, 1.5, 2.2, 0.4, 0.35)$.

The influence of electron correlations on the partial susceptibilities χ^ν is shown in Fig. 5 for the special cases $U^B = 0$ (a) and $U^A = 0$ (b). Correlations to minority sites (a) cause only small enhanced paramagnetism. Singularities in χ^ν can occur with increasing U^B(b) acting on majority sites. Notice that χ^ν can be qualitatively approximated by $2\rho^\nu(\mu)$ in the case a) and for small U^B in b).

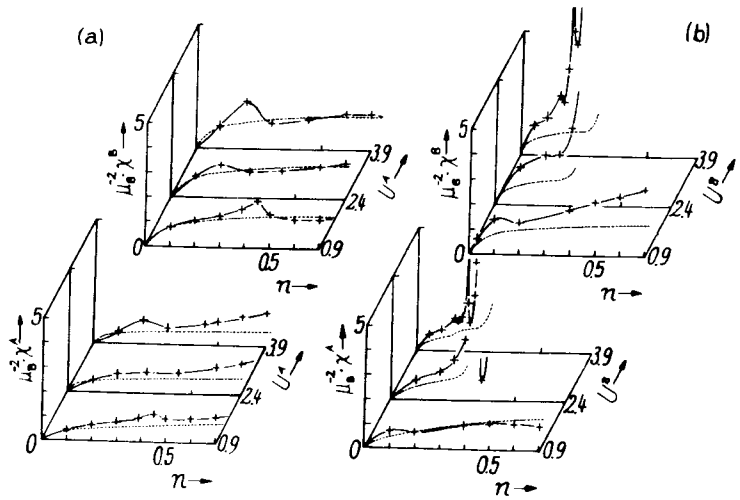

Fig. 5. Partial static paramagnetic susceptibilities $\chi^{\nu}(+)$ (ν=A,B) and densities of states $2\rho^{\nu}(\mu)$ (---) at the Fermi energy μ versus n for various strengths of the intra-atomic repulsion U^{ν}, a) $U^{B}=0$ and b) $U^{A}=0$, in the case $(w, \epsilon^{A}, \epsilon^{B}, c) = (1, 0.2, 0, 0.25)$.

Numerical results of the inverse susceptibility χ^{-1} obtained in the ladder and Hartree-Fock approximations are in good agreement for small repulsion strengths, i.e., at $U^{B}=0$ and $U^{B}=1$ in Fig. 6a. However, both treatments differ essentially with increasing U^{B}; in particular, Hartree-Fock results overestimate the magnetic state. Note that several zeroes of χ^{-1} typify alloys with strong correlation strengths, e.g., for $U^{B}=3$. In Fig. 6b susceptibility results determine the critical curve which is the locus of $\chi^{-1}=0$.

There is an apparent relationship between partial susceptibilities χ^{ν} and electron concentrations n^{ν} as shown by two parameter sets in Fig. 7. For smaller U^{ν} values we have no singularities, whereas in the case $U^{A}=1$ and $U^{B}=2$ zeroes of the inverse susceptibilities refer to ferromagnetic ordering. Dis-

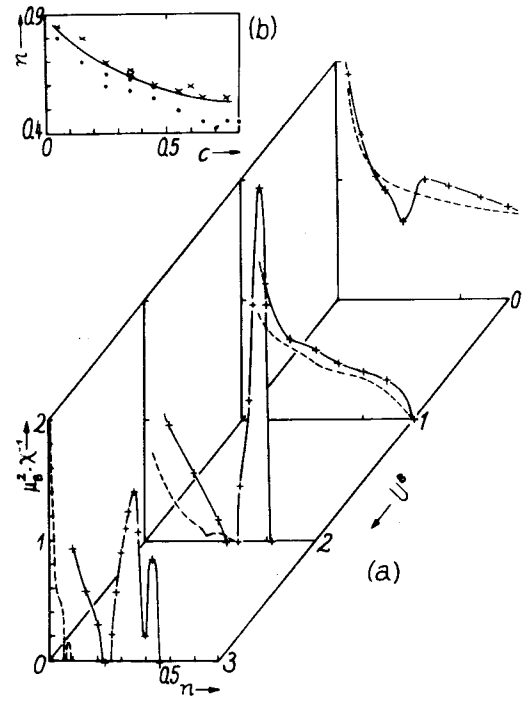

Fig. 6. a) Inverse static paramagnetic susceptibility $\chi^{-1}(+)$ versus n for several values U^{B} at c=0.25 in comparison with Hartree-Fock results (---), and b) dividing line between paramagnetism (·) and ferromagnetism (×) in n versus c plot at $U^{B}=1$ for the set $(w, \epsilon^{A}, \epsilon^{B}, U^{A}) = (1, 0.2, 0, 1.9)$.

order favours paramagnetic instabilities in comparison with the result for the pure B component in Fig. 7b. Note that a crossing of the n^{ν} values is found in the transition region.

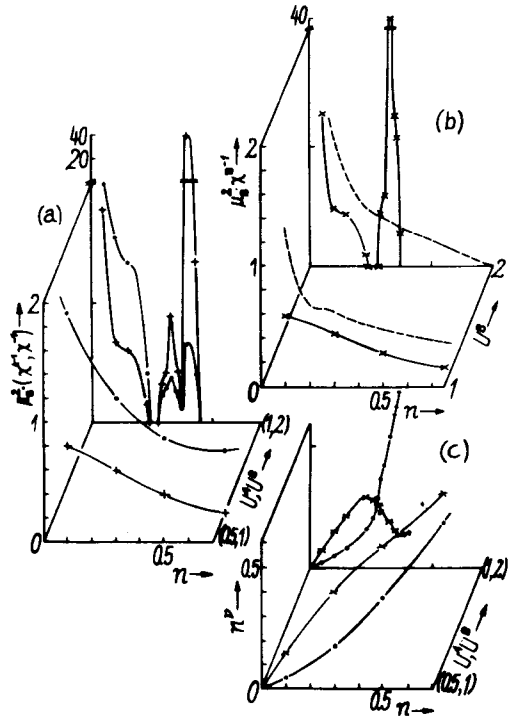

Fig. 7. Inverse static paramagnetic susceptibilities $\chi^{-1}, (\chi^{\nu})^{-1}$, and partial electron densities n^{ν} versus n for various values U^{ν} in the case $(w, \epsilon^{A}, \epsilon^{B}, c) = (1, 0.4, 0, 0.4)$; a) total χ^{-1} (+) and partial $(\chi^{A})^{-1}$ (·), b) partial $(\chi^{B})^{-1}$ (×) at the same U^{A} values as in a) compared with $(\chi^{B})^{-1}$(---)for the pure B system, and c) n^{A} (·), n^{B} (×).

6. CONCLUSION

It has been proved that the coherent local ladder approximation applied to the random Hubbard model is a practicable method to derive correlation-enhanced paramagnetic susceptibilities of disordered alloys, giving rise to a criterion for ferromagnetism.

The magnetic response is verified to be consistent with a Ward relation. Despite of some simplifying assumptions the present scheme is, with respect to the dynamics, beyond CPA-RPA treatment. Numerical calculations have been performed for an elliptical shape of the unperturbed state density and, in most cases, alloy parameter values were chosen corresponding to the adequacy of the ladder approximation. Instabilities of the paramagnetic phase are found which preclude some artificial overestimation or suppression of magnetism.

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