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Межэлектронные корреляции в "случайных недиагональных" сплавах

Динамическая природа хаббардовского электрон-электронного взаимодействия в неупорядоченных сплавах выражена на языке случайного энергетического поля. Локальные собственно-энергетические части для электронов чистых компонент вычислены в рамках самосогласованного лестничного приближения и учтены в обобщенном недиагональном приближении когерентного потенциала. В отличие от других приближений, численные расчёты в рамках нашего подхода приводят к бесщелевой плотности состояний с хвостами и к сильно затухающему двухчастичному всплеску.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

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Electron Correlations in Random Off-Diagonal Alloys

The dynamic nature of Hubbard's electron-electron interaction in disordered alloys is expressed by an energy-dependent random field. Local electronic self-energies for the pure components calculated within a self-consistent ladder approximation are included into a generalized off-diagonal CPA. Numerical results exhibit in contrast to other approximations a gapless and tailed density of states with strongly damped two-particle humps.

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

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1. INTRODUCTION

The dynamical aspect of the electron-electron interaction in disordered narrow-band systems is of a special interest for the combined study of correlation and randomness effects. In particular, the problem consists in taking into account dynamic solutions for the random Hubbard model which must be subjected to any version of the coherent potential approximation (CPA). The decoupling procedure adopted by Tsukada /1/ leads to complete Hubbard-III-type solutions /2/ including resonance broadening corrections; moreover, off-diagonal randomness of the Shiba type /3/ is treated within an extended CPA /1/.

In this paper we choose a diagrammatic approach which is based on the ladder approximation suggested by Babanov et al. /4,5/ for the pure Hubbard model /6/. In a self-consistent manner one can calculate the damping of electron states due to dynamical correlations, and some shortcomings of Hubbard's decoupling schemes as the violation of the Luttinger theorem /7/ are avoided. An effective energy-dependent Hamiltonian is used as the starting point for applying the modified CPA /8/ developed for the additive type of off-diagonal randomness.

2. LADDER APPROXIMATION AND CPA

The CPA treatment of the electronic behaviour of substitutionally random systems, such as alloys of the type A_cB_{1-c}, is aug-

mented by including electron correlation effects. Starting from the Hubbard model /6/

$$H^{\{\nu\}} = \sum_{i\sigma} \varepsilon_i^{\nu} n_{i\sigma} + \sum_{\substack{ij\sigma \\ (i\neq j)}} t_{ij}^{\nu\mu} c_{i\sigma}^{+} c_{j\sigma} + \frac{1}{2} \sum_{i\sigma} U_i^{\nu} n_{i\sigma} n_{i-\sigma} \qquad (1)$$

for some configuration $\{\nu\}$, we can approximately describe the one-particle properties by the effective energy-dependent Hamiltonian $H_{eff\sigma}^{\{\nu\}}$ for electrons with spin σ as

$$H_{eff\sigma}^{\{\nu\}}(z) = \sum_{i} \left(\varepsilon_i^{\nu} + \Sigma_{Ui\sigma}^{\nu}(z)\right) n_{i\sigma} + \sum_{\substack{ij \\ (i\neq j)}} t_{ij}^{\nu\mu} c_{i\sigma}^{+} c_{j\sigma} \ , \qquad (2)$$

where $c_{i\sigma}^{+}(c_{i\sigma})$ creates (destroys) a Wannier electron with spin σ at lattice site i, and $n_{i\sigma} = c_{i\sigma}^{+} c_{i\sigma}$; note that $H_{eff\sigma}^{\{\nu\}+}(z) = H_{eff\sigma}^{\{\nu\}}(z^{*})$. The random parameters ε_i^{ν}, $t_{ij}^{\nu\mu}$, U_i^{ν} take the values ε^{ν}, $t^{\nu\mu}$, U^{ν} ($\nu, \mu = A, B$), resp., according to whether an A or B atom occupies the site i (j). The off-diagonal randomness is restricted to the additive limit /8,9/

$$t^{AB} = \frac{1}{2}\left(t^{AA} + t^{BB}\right) \ , \qquad (3)$$

where only nearest-neighbour hopping integrals are taken into account. The self-energy $\Sigma_{Ui\sigma}^{\nu}(z)$ caused by the intra-atomic Coulomb repulsion U_i^{ν} ($\nu = A, B$) plays the role of a local and energy-dependent stochastic potential within the CPA scheme.

To calculate $\Sigma_{Ui\sigma}^{\nu}$ we apply the horizontal ladder approximation proposed by Babanov et al. /4/ for studying electron-electron correlations in pure metallic systems at low density of electrons. For the pure Hubbard Hamiltonian $H^{\nu} = H^{\nu}(\varepsilon^{\nu}, t^{\nu\nu}, U^{\nu})$, the self-consistency equations resulting from a zero-temperature diagram analysis can be expressed in terms of retarded functions as (cf. /4/)

$$Re\,\Sigma_{U\sigma}^{\nu}(E) = -\frac{1}{\pi}\int_{-\infty}^{\mu^{\nu}} dE'\, Im\,G_{-\sigma}^{\nu}(E')\,Re\,\Gamma^{\nu}(E+E') - \frac{1}{\pi}\int_{-\infty}^{2\mu^{\nu}-E} dE'\, Re\,G_{-\sigma}^{\nu}(E')\,Im\,\Gamma^{\nu}(E+E') \ , \qquad (4)$$

$$Im\,\Sigma_{U\sigma}^{\nu}(E) = \frac{1}{\pi}\int_{\mu^{\nu}}^{2\mu^{\nu}-E} dE'\, Im\,G_{-\sigma}^{\nu}(E')\,Im\,\Gamma^{\nu}(E+E') \ , \qquad (5)$$

$$Re\,\Gamma^{\nu}(E) = \frac{\frac{1}{U^{\nu}} + Re\,D^{\nu}(E)}{\left[\frac{1}{U^{\nu}} + Re\,D^{\nu}(E)\right]^2 + \left[Im\,D^{\nu}(E)\right]^2} \ , \qquad (6)$$

$$Im\,\Gamma^{\nu}(E) = -\frac{Im\,D^{\nu}(E)}{\left[\frac{1}{U^{\nu}} + Re\,D^{\nu}(E)\right]^2 + \left[Im\,D^{\nu}(E)\right]^2} \ , \qquad (7)$$

where

$$Re\,D^{\nu}(E) = -\frac{1}{\pi}\int_{-\infty}^{\mu^{\nu}} dE'\, Im\,G_{\sigma}^{\nu}(E')\,Re\,G_{-\sigma}^{\nu}(E-E') + \frac{1}{\pi}\int_{-\infty}^{E-\mu^{\nu}} dE'\, Re\,G_{\sigma}^{\nu}(E')\,Im\,G_{-\sigma}^{\nu}(E-E') \ , \qquad (8)$$

$$Im\,D^{\nu}(E) = \frac{1}{\pi}\int_{\mu^{\nu}}^{E-\mu^{\nu}} dE'\, Im\,G_{\sigma}^{\nu}(E')\,Im\,G_{-\sigma}^{\nu}(E-E') \ , \quad (\nu = A, B) \ . \qquad (9)$$

This completely local approximation means that $\Sigma_{U\sigma}^{\nu}$, G_{σ}^{ν}, Γ^{ν}, D^{ν} are the diagonal elements (at site i, indices i are omitted) of the self-energy, one-particle Green function, effective vertex, renormalization contribution to the bare vertex U^{ν}, respectively. The chemical potential μ^{ν} is determined by the relation

$$n^{\nu} = \sum_{\sigma} n_{\sigma}^{\nu} = -\frac{1}{\pi}\sum_{\sigma}\int_{-\infty}^{\mu^{\nu}} dE\ Im\,G_{\sigma}^{\nu}(E) \ , \quad (\nu = A, B) \ , \qquad (10)$$

where n^{ν} is the total electron number per site of the pure ν-system. The Green function G_{σ}^{ν} is found from the Dyson equation as

$$G_{\sigma}^{\nu}(z) = G_{\Delta}^{\nu}\left(z - \Sigma_{U\sigma}^{\nu}(z)\right) \ , \qquad (11)$$

where G_{Δ}^{ν} denotes the Green function for noninteracting electrons ($U^{\nu} = 0$). By assuming for simplicity a semielliptical ν-band given by the unperturbed density of states (per site per spin)

$$\rho_{\Delta}^{\nu}(E) = \begin{cases} \frac{2}{\pi W^{\nu}}\left[1 - \left(\frac{E-\varepsilon^{\nu}}{W^{\nu}}\right)^2\right]^{\frac{1}{2}}, & |E-\varepsilon^{\nu}| \le W^{\nu} \\ 0 \ , & |E-\varepsilon^{\nu}| > W^{\nu} \ , \end{cases} \qquad (12)$$

one gets

$$G_{\Delta}^{\nu}(z) = \frac{2}{w^{\nu}}\left(\frac{z-\varepsilon^{\nu}}{w^{\nu}} - i\left[1 - \left(\frac{z-\varepsilon^{\nu}}{w^{\nu}}\right)^2\right]^{\frac{1}{2}} \right), \qquad (13)$$

where w^{ν} is the half-band width; obviously, this means putting $w^{\nu} = 6\,t^{\nu\nu}$ for a s.c. lattice. Then we have with (11) and (13) an analytic expression for G_{σ}^{ν} ($\nu = A,B$) which enters into the self-consistent correlation problem (4) to (10). For comparison the corresponding Green function in /5/ was calculated numerically without assuming the model form (12).

Having determined $\Sigma_{U\sigma}^{\nu}$ we adopt the modified CPA /8/ to the effective Hamiltonian (2). The averaged Green function we are looking for can be defined as resolvent

$$\mathcal{G}_{\sigma}(z) = \left\langle \left(z - H_{eff\,\sigma}^{\{\omega\}}(z)\right)^{-1} \right\rangle = \left[\left(G_{\Delta}^{B}(z)\right)^{-1} - \Sigma_{\sigma}(z) \right]^{-1}, \qquad (14)$$

and, more explicitly, in the Bloch representation one gets

$$\mathcal{G}_{\vec{k}\sigma}(z) = \left[z - \varepsilon^{B} - t^{BB} s(\vec{k}) - \Sigma_{\sigma}(\vec{k},z) \right]^{-1}, \qquad (15)$$

where the nearest-neighbour structure factor $s(\vec{k})$ is given by

$$s(\vec{k}) = \sum_{j(\neq i)} e^{i\vec{k}\,(\vec{R}_j - \vec{R}_i)} . \qquad (16)$$

Expanding the coherent potential as

$$\Sigma_{\sigma}(\vec{k},z) = \sigma_{0\sigma}(z) + 2\,\sigma_{1\sigma}(z)\,s(\vec{k}) + \sigma_{2\sigma}(z)\,s^2(\vec{k}) \qquad (17)$$

means precisely computing the contributions $\sigma_{0\sigma}$, $\sigma_{1\sigma}$, $\sigma_{2\sigma}$ from CPA conditions of the type (cf. /8,9/)

$$\left\langle \tau_{l\sigma}^{\nu}(z,\Sigma_{U\sigma}^{\nu}(z);\delta_0^{\nu},\delta_1^{\nu}) \right\rangle = c\,\tau_{l\sigma}^{A}(z,\Sigma_{U\sigma}^{A}(z);\varepsilon^{A}-\varepsilon^{B},\tfrac{1}{6}(t^{AA}-t^{BB})) + (1-c)\,\tau_{l\sigma}^{B}(z,\Sigma_{U\sigma}^{B}(z);0,0) = 0, \qquad (18)$$

$$(l = 0,1,2).$$

Essentially, the scattering-matrix parts $\tau_{l\sigma}^{\nu}$ become algebraic functions of $\sigma_{0\sigma}$, $\sigma_{1\sigma}$, $\sigma_{2\sigma}$ via the coherent Green functions (appearing in (18))

$$F_{l\sigma}(z) = \frac{1}{N}\sum_{\vec{k}} \mathcal{G}_{\vec{k}\sigma}(z)\left[s(\vec{k})\right]^{l}, \quad (l = 0,1,2), \qquad (19)$$

which can be calculated analytically with (12) /9/.

Given the self-consistency cycles (4) to (11) (closed set) and (18), (19) (associated with the output $\Sigma_{U\sigma}^{\nu}$ of the former set) for the correlation and CPA problems, respectively, the coherent density of states ρ_{σ} (per site) for electrons with spin σ is obtained as

$$\rho_{\sigma}(E) = -\frac{1}{\pi}\,\mathrm{Im}\,F_{0\sigma}(E). \qquad (20)$$

For comparison the state density associated with the pure ν-system reads

$$\rho_{\sigma}^{\nu}(E) = -\frac{1}{\pi}\,\mathrm{Im}\,G_{\sigma}^{\nu}(E), \quad (\nu = A,B). \qquad (21)$$

The chemical potential μ of the coherent system can be determined by

$$n = \sum_{\sigma} n_{\sigma} = \sum_{\sigma} \int_{-\infty}^{\mu} dE\,\rho_{\sigma}(E), \qquad n = \langle n^{\nu} \rangle, \qquad (22)$$

where the average electron number n per site comes from the particle-number conservation.

3. NUMERICAL RESULTS AND DISCUSSION

Before going over to numerical calculations, it should be noted that c, Δ_0, Δ_1, U^A, U^B, n^A, n^B are the input parameters needed, where

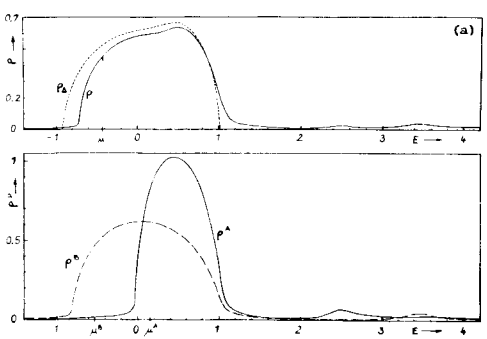
$$\Delta_0 = \varepsilon^{A} - \varepsilon^{B}, \quad \Delta_1 = 6\,(t^{AA} - t^{BB}) \qquad (23)$$

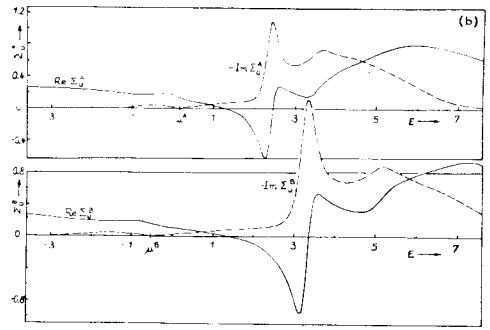
are associated with the diagonal and off-diagonal randomness, respectively. Now we define the energy origin $\varepsilon^B = 0$ and express the energy in units of the half-width of the unperturbed B-band ($6t^{BB} = 1$, except one example designated). The nonmagnetic solution-type obtained for suitable choices of the parameters can be characterized by

$$\Sigma_U^\nu = \Sigma_{U\sigma}^\nu = \Sigma_{U-\sigma}^\nu \quad , \quad (\nu = A, B). \tag{24}$$

Since in the following we shall be concerned only with the nonmagnetic case let us omit the spin indices of G_σ^ν , $\mathcal{G}_\sigma$, Σ_σ , $\sigma_{l\sigma}$, $\tau_{l\sigma}^\nu$, $F_{l\sigma}$, ρ_σ^ν , and ρ_σ .

The numerical procedure begins with solving the self-consistent chain (4) to (11) by the iteration method. Starting with the Hartree-Fock result $\Sigma_U^\nu = U^\nu \frac{n^\nu}{2}$ ($\nu = A, B$) corresponding to the asymptotic solution we calculate in sequence G^ν via (11) and (13), μ^ν from (10), D^ν from (8) and (9), Γ^ν via (6) and (7), and again Σ_U^ν based on (4) and (5), etc., by repeating this cycle. After incorporating the convergent Σ_U^ν values into the CPA equations (18), the coherent potential terms σ_0 , σ_1 , σ_2 are computed by using a modified iteration scheme /8/ beginning from the virtual-crystal limit.





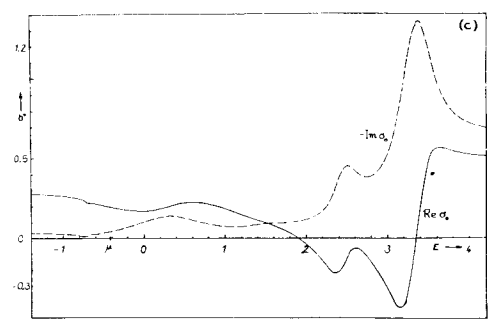


Fig. 1. (a) Electron densities of states ρ^ν and ρ (ρ_Δ without electron-electron interaction), real and imaginary parts of the self-energies (b) Σ_U^ν and (c) σ_0 for pure ν -components and the alloy, resp., with c=0.25, Δ_0 =0.4, Δ_1 =-0.4, U^A =3, U^B =4, n^A =0.25, n^B =0.2.

In Fig. 1 the electron densities of states and self-energies of disordered and pure systems are compared in the unsplit ρ_Δ - band case. At zero Coulomb energy the coherent density of states ρ_Δ was discussed in detail [9] on the basis of two impurity-scattering mechanisms associated with Δ_0 and Δ_1. In addition to the one-particle region defined by $\rho_\Delta(E) \neq 0$, the coherent ρ in Fig. 1a displays a two-particle region with two humps ascribed to electron pair states in the alloy. In contrast to Hubbard-like treatments of alloys, no gaps arise from dynamic correlations. Roughly speaking, the shape of ρ can be explained as the superposition of ρ^ν ($\nu = A, B$) for pure ν-systems. Such a type of continuous ρ^ν spectrum with a small correlation maximum and large tails as shown in Fig. 1a (compare also [5]) differs strongly from results obtained by using Hubbard$s decoupling scheme [10]. The smallness of the two-particle humps in ρ^ν is caused by a strong damping, i.e. the imaginary parts of Σ_U^ν have peaks in the corresponding energy regions in Fig. 1b; an analogous behaviour was found for Γ^ν (see also [5]). Within the pure components, the quasi-particle conditions [5] $\mathrm{Im}\,\Sigma_U^\nu(\mu^\nu) = 0$, $\mathrm{Im}\,\Sigma_U^\nu(E) \propto (E - \mu^\nu)^2$ near $E = \mu^\nu$ (local version of the Luttinger theorem [7]), and $(\partial\,\mathrm{Re}\,\Sigma_U^\nu(E)/\partial E)_{E=\mu^\nu} \leq 0$ can be confirmed numerically. The asymptotic limit is given by $\mathrm{Re}\,\Sigma_U^\nu(\pm\infty) = U^\nu n^\nu/2$, $\mathrm{Re}\,\Gamma^\nu(\pm\infty) = U^\nu$, $\mathrm{Re}\,G^\nu$ and the imaginary parts of all functions tend to zero asymptotically. Resulting from the interplay of correlations and disorder, the correlation peaks of Σ_U^ν entering into the coherent σ_0 in Fig. 1c are diminished by the randomness. As is expected, the impurity-scattering associated with Δ_0 especially leads to a damping of electron states at the Fermi energy, i.e.,to a finite value of $\mathrm{Im}\,\sigma_0(\mu)$.

Fig. 2 shows the dependence of the state densities ρ and ρ^ν on carrier concentration in the split ρ_Δ -band case. With decreasing n^ν (U^ν fixed) the two-particle humps in ρ^ν ($\nu = A, B$) become sharper and are shifted to higher energies. These humps are smeared out in the coherent density of states ρ. The gap in ρ_Δ arising from strong diagonal disorder ($\Delta_0 > 1$) is closed due to electron-electron correlations (compare alloys with electron-phonon interaction [9]). The band deepening between majority and minority parts of ρ depends sensitively on the set n^ν. Maxima of ρ^ν and ρ within the one-particle region are shifted

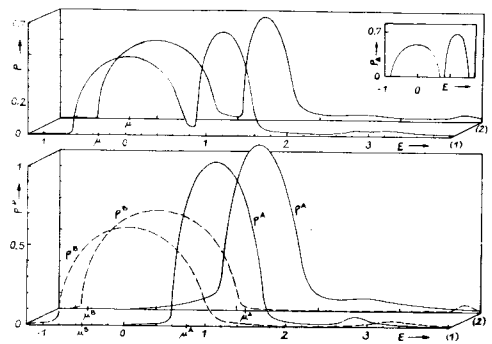


Fig. 2. Pure ν -component and alloy densities of states ρ^ν and ρ, resp., for the sets c=0.4, Δ_0 =1.1, Δ_1 =-0.4, U^A =1.5, U^B =3.5 with (1) n^A =0.2, n^B =0.2 and (2) n^A =0.5, n^B =0.1. Split band for the coherent ρ_Δ without electron-electron interaction.

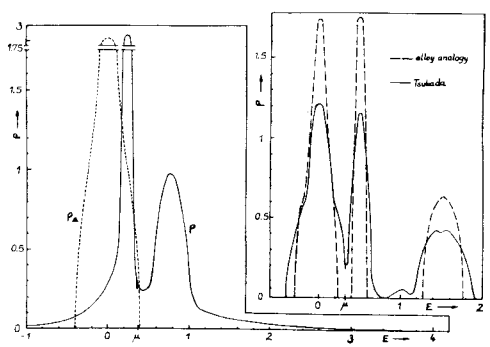


Fig. 3. Density of states ρ (ρ_Δ without electron-electron interaction) for an alloy with c=0.5, Δ_0 =0, Δ_1 =-0.32 ($6t^{BB} = 0.5$), U^A =0.5, U^B =1.5, $n^A = n^B$ =1 compared with results of Tsukada [1] (note the other type of parameters in [1]).

by correlations into the energy interval between ε^ν and $\tilde{\varepsilon}^\nu = \varepsilon^\nu + \frac{U^\nu n^\nu}{2}$ (maxima of the Hartree-Fock approximation).

In Fig. 3 the coherent densities of states ρ_Δ and ρ are exhibited in comparison to results obtained by Tsukada /1/ for a half-filled band in the case of pure off-diagonal randomness. Note that we can compare only on principle, because the ladder approximation is more trustworthy at small n^ν, and we have taken into account another type of off-diagonal randomness. As a result of our treatment the density of states ρ takes considerable tails (without humps) at low and high energies. Furthermore, the maxima of $\rho(E)$ arise near the Hartree-Fock points $U^\nu n^\nu/2$ in contrast to Hubbard-like schemes, where maxima occur at ε^ν and $\tilde{\varepsilon}^\nu = \varepsilon^\nu + U^\nu$ ($\nu = A, B$). Concerning /1/ it is pointed out that the positions of the ρ maxima persist in going over from the alloy analogy (Hubbard-III with scattering corrections) to the dynamic Hubbard-III solution including resonance broadening corrections.

4. CONCLUSION

Having adopted a local ladder approximation to the electron-electron interaction in disordered alloys one can treat the randomness in a single-site approximation. In this paper, we have performed calculations within two different (but not independent) self-consistent chains describing the correlation and randomness problems, respectively. The numerical results show that gaps in the spectrum predicted by other approximations disappear by taking into account more accurately the dynamic nature of electron-electron correlations. The self-consistent connection between the correlation and CPA calculation-cycles is proposed in a subsequent paper.

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