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Когерентное лестничное приближение для неупорядоченной модели Хаббарда

Обсуждаются динамические эффекты электрон-электронного взаимодействия в бинарных сплавах с недиагональным беспорядком на основе самосогласованной теории, полученной обобщением локального лестничного приближения для неупорядоченной модели Хаббарда и модификацией метода когерентного потенциала. На основе численных расчётов получены результаты для частично усредненной плотности состояний, массового оператора, удовлетворяющего теореме Латтинжера, и эффективного двухчастичного взаимодействия. Наблюдается увеличение плотности состояний в виде сильно демпфированных корреляционных всплесков на хвостах полностью усредненной плотности состояний.

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Coherent Ladder Approximation for the Random Hubbard Model

Dynamical effects of the electron-electron interaction in binary alloys with off-diagonal disorder are described in a self-consistent theory obtained by unifying a local ladder approximation for the random Hubbard model and a modified CPA. Numerical results are presented for partially averaged densities of states, self-energies which fulfil the Luttinger theorem, and effective two-particle vertices. The totally averaged density of states exhibits tails with strongly damped correlation humps.

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

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1. Introduction

Self-consistent calculations for the electronic structure of substitutionally disordered narrow-band systems become more realistic by taking into account dynamical correlation effects and random hopping integrals. To describe the electron-electron and impurity scattering simultaneously a useful method should be the combination of dynamical solutions for the random Hubbard model with an extended version of the coherent potential approximation (CPA) aimed at finite-ranged disorder. Differences between decoupling and diagrammatic techniques for solving Hubbard's correlation problem arise especially from the extent to which the approximations include the dynamical character of the interaction.

Decoupling procedures mostly performed on the basis of Hubbard III [1] (for other decouplings see [2]) provide a static solution-type within the alloy analogy approximation [3-5] (i.e., Hubbard III with only scattering corrections) and a dynamical one by adding resonance-broadening terms [6]. In Tsukada's scheme [6] complete Hubbard-III-type solutions including resonance-broaden-

ing corrections are subjected to an extended CPA to treat off-diagonal randomness of the Shiba type [7].

The perturbative approach was chosen by Drchal and Velický [8] in solving the random alloy problem for a pair of interacting electrons. At low carrier concentration, the local version of the ladder approximation proposed by Babanov, Naish, Sokolov, Finashkin (BNSF) [9,10] for the pure Hubbard model [11] can be extended to alloys, too. Work along this line was done in the case of purely diagonal randomness [12] and for off-diagonal randomness [13]. The latter consists of two separated (but not independent) self-consistent chains describing correlation and randomness problems, respectively.

In this paper we unify the BNSF scheme [9] adapted to the random Hubbard model and the off-diagonal CPA [14] for the additive limit into a completely self-consistent theory (Section 2). This approach fulfils the Luttinger theorem [15] contrary to Hubbard's decoupling procedures. Numerical results for partial (or component) and total (alloy) averages of densities of states, self-energies, and effective vertices are presented in Section 3.

2. Self-Consistent Coherent Ladder Approximation

Consider the electron-electron interaction in substitutionally disordered narrow-band systems of the binary alloy-type A_cB_{1-c}. The Hubbard model Hamiltonian [11] depending on the configuration $\{\nu\}$ is

$$H^{\{\nu\}} = H_\Delta^{\{\nu\}} + H_U^{\{\nu\}} = H_\Delta^B + V_\Delta^{\{\nu\}} + H_U^{\{\nu\}} , \qquad (1)$$

where

$$H_\Delta^{\{\nu\}} = \sum_{i\sigma} \epsilon_i^\nu n_{i\sigma} + \sum_{\substack{ij\sigma \\ (i\neq j)}} t_{ij}^{\nu\mu} c_{i\sigma}^+ c_{j\sigma} , \qquad (2)$$

$$H_U^{\{\nu\}} = \frac{1}{2} \sum_{i\sigma} U_i^\nu n_{i\sigma} n_{i-\sigma} . \qquad (3)$$

Here $c_{i\sigma}^+ (c_{i\sigma})$ is the creation (annihilation) operator for an electron of spin σ in the Wannier state at lattice site i, and $n_{i\sigma} = c_{i\sigma}^+ c_{i\sigma}$. The atomic energy ϵ_i^ν, the hopping integrals $t_{ij}^{\nu\mu}$ as well as the intra-atomic Coulomb repulsion U_i^ν are random variables which take the values $\epsilon^\nu, t^{\nu\mu}$ and U^ν, respectively; the superscript $\nu(\mu)$ refers to the atomic species ($\nu, \mu = A, B$) located at site i(j). Only nearest-neighbour (n.n.) hopping integrals are included. Specialize the off-diagonal randomness by assuming the additive condition [14]

$$t^{AB} = \frac{1}{2}(t^{AA} + t^{BB}) . \qquad (4)$$

H_Δ^B is the one-electron Hamiltonian (2) for a perfect B-crystal.

The basic problem of treating electron-electron correlations and randomness simultaneously can be formulated as follows. The electron self-energy $\Sigma_U^{\{\nu\}}$ defined by the Dyson equation

$$G^{\{\nu\}} = G_{\Lambda}^{\{\nu\}} + G_{\Lambda}^{\{\nu\}} \Sigma_{U}^{\{\nu\}} G^{\{\nu\}} \qquad (5)$$

can be determined in principle by diagram analysis in a self-consistent approximation chain of the type

$$\Sigma_{U}^{\{\nu\}} = f(\Gamma^{\{\nu\}}, G^{\{\nu\}}), \qquad (6)$$

$$\Gamma^{\{\nu\}} = g(\Gamma^{\{\nu\}}, G^{\{\nu\}}). \qquad (7)$$

Here $G_{\Lambda}^{\{\nu\}}$ is the Green function for noninteracting electrons related to $H_{\Lambda}^{\{\nu\}}$, $G^{\{\nu\}}$ is the full one-particle Green function, and $\Gamma^{\{\nu\}}$ denotes the effective vertex within $\{\nu\}$. The randomness problem is expressed in terms of the total scattering operator $T^{\{\nu\}}$ introduced via

$$G^{\{\nu\}} = \mathcal{G} + \mathcal{G} T^{\{\nu\}} \mathcal{G}, \qquad (8)$$

where the totally averaged Green function $\mathcal{G}$ is given by

$$\mathcal{G} = \langle G^{\{\nu\}} \rangle = ((G_{\Lambda}^{B})^{-1} - \Sigma)^{-1}. \qquad (9)$$

$\langle \ldots \rangle$ implies the configurational averaging, G_{Λ}^{B} is the Green function related to H_{Λ}^{B}. The coherent potential Σ can be found from the CPA self-consistency condition

$$\langle T^{\{\nu\}} \rangle = \langle (V_{\Delta}^{\{\nu\}} + \Sigma_{U}^{\{\nu\}} - \Sigma)(1 - \mathcal{G}(V_{\Delta}^{\{\nu\}} + \Sigma_{U}^{\{\nu\}} - \Sigma))^{-1} \rangle = 0. \qquad (10)$$

By means of additional assumptions the equations (5) to (7) and (10) can be made more practicable. Obviously, the complete information about $\{\nu\}$ incorporated in $G^{\{\nu\}}$ and $\Sigma_{U}^{\{\nu\}}$, for instance, is not necessary to calculate $\mathcal{G}$ and Σ finally; accordingly, we have to modify the CPA problem (10), too. Both the correlation and randomness must be treated within a unified approximation.

There are arguments for restricting the considerations to the single-site approximation. $V_{\Delta}^{\{\nu\}}$ and $H_{U}^{\{\nu\}}$ are additive random operators; moreover, a local bare interaction term is taken into account. This allows one to decompose $V_{\Lambda}^{\{\nu\}}$, $\Sigma_{U}^{\{\nu\}}$ and Σ into sums

$$V_{\Lambda}^{\{\nu\}} = \sum_i V_{\Lambda i}^{\nu}, \quad \Sigma_{U}^{\{\nu\}} = \sum_i \Sigma_{Ui}^{\nu}, \quad \Sigma = \sum_i \Sigma_i. \qquad (11)$$

Note that $V_{\Lambda i}^{\nu}$ and Σ_i are finite-ranged quantities in the Wannier space due to the off-diagonal randomness, whereas Σ_{Ui}^{ν} is assumed to be local corresponding to a local effective vertex for the electron-electron interaction.

Let us introduce the partially averaged Green function G_i^{ν} as

$$G_i^{\nu} = \mathcal{G} + \mathcal{G}(V_{\Delta i}^{\nu} + \Sigma_{Ui}^{\nu} - \Sigma_i) G_i^{\nu} = \mathcal{G} + \mathcal{G} T_i^{\nu} \mathcal{G}, \qquad (12)$$

which is associated with the perturbation $(V_{\Delta i}^{\nu} + \Sigma_{Ui}^{\nu} - \Sigma_i)$ at some site i embedded in an otherwise effective medium given by $(H_{\Delta}^{B} + \Sigma)$. The single-site scattering operator T_i^{ν} taking finite range in the Wannier space is

$$T_i^\nu = (V_{\Delta i}^\nu + \Sigma_{Ui}^\nu - \Sigma_i)(1-\mathcal{G}(V_{\Delta i}^\nu + \Sigma_{Ui}^\nu - \Sigma_i))^{-1} \quad . \qquad (13)$$

Recalling (6), (7), (9) and (10) on the basis of (11) to (13), the completely self-consistent formulation of the random Hubbard problem in single-site approximation can be given by

$$\Sigma_{Ui|d}^\nu = f(\Gamma_{i|d}^\nu, G_{i|d}^\nu), \qquad (14)$$

$$\Gamma_{i|d}^\nu = g(\Gamma_{i|d}^\nu, G_{i|d}^\nu), \quad (\nu = A, B) \qquad (15)$$

$$\langle T_i^\nu \rangle = 0, \qquad (16)$$

where the CPA condition (16) corresponds now to $\langle G_i^\nu \rangle = \mathcal{G}$. $\Gamma_{i|d}^\nu$ denotes the local effective vertex; the subscript "|d" means including only diagonal elements of Σ_{Ui}^ν, G_i^ν, Γ_i^ν in Wannier representation at site i.

To describe the electron-electron interaction we use the local version of the horizontal ladder approximation developed by Babanov et al. [9,10] for pure metallic systems. This approximation results from a zero-temperature diagram analysis at low density of electrons. Adapting the BNSF self-consistency scheme [9] to the random Hubbard model, the relations (14) and (15) expressed in terms of causal functions take the form (see Fig. 1)

$$\Sigma_{Ui|d\sigma}^{(c)\nu}(E) = \int_{-\infty}^{\infty} \frac{dE'}{2\pi i} G_{i|d-\sigma}^{(c)\nu}(E') \Gamma_{i|d}^{(c)\nu}(E+E'), \qquad (17)$$

$$\Gamma_{i|d}^{(c)\nu}(E) = \left(\frac{1}{U_i^\nu} + \int_{-\infty}^{\infty} \frac{dE'}{2\pi i} G_{i|d\sigma}^{(c)\nu}(E') G_{i|d-\sigma}^{(c)\nu}(E-E')\right)^{-1}, (\nu = A, B). \qquad (18)$$

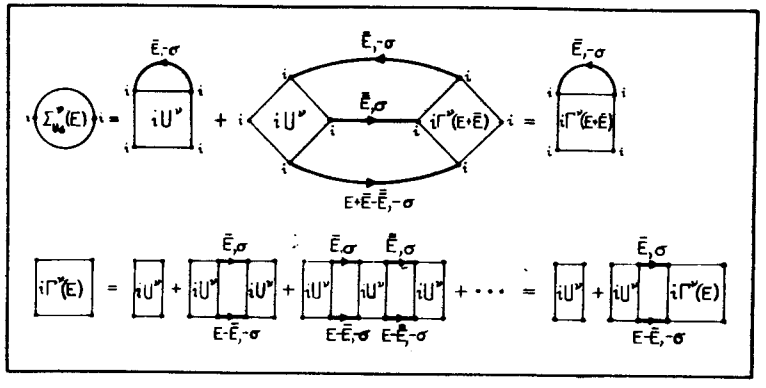

Fig. 1. Local ladder approximation for random self-energy and vertex parts. The arrowed lines denote partially averaged one-particle Green functions.

Here the total Green function $G^{(c)\nu}_{i|d\sigma}$, which must be determined from (12), represents the link between the correlation and CPA problems.

Adopting the extended CPA [14] we go over to the momentum representation. The translationally invariant Green function (9) written as resolvent takes the $\vec{k}$-transform

$$\mathcal{G}_{\vec{k}\sigma}(z) = (z - \epsilon^{B} - t^{BB} s(\vec{k}) - \Sigma_{\sigma}(\vec{k}, z))^{-1}, \qquad (19)$$

where the nearest-neighbour structure factor

$$s(\vec{k}) = \sum_{j(\neq i)} e^{i\vec{k}(\vec{R}_j - \vec{R}_i)} \qquad (20)$$

is associated with the lattice type. The coherent potential

$$\Sigma_{\sigma}(\vec{k}, z) = \sigma_{0\sigma}(z) + 2\sigma_{1\sigma}(z) s(\vec{k}) + \sigma_{2\sigma}(z) s^2(\vec{k}) \qquad (21)$$

is expressed in terms of $\sigma_{0\sigma}$, $\sigma_{1\sigma}$, $\sigma_{2\sigma}$ which satisfy the CPA conditions $\langle \tau^{\nu}_{\ell i\sigma} \rangle = 0$ $(\ell = 0,1,2)$ arising from (16) with the T^{ν}_{i} operator (13) in the $\vec{k}$-transformed version

$$\langle \vec{k}|T^{\nu}_{i\sigma}|\vec{k}'\rangle = \frac{1}{N} e^{-i(\vec{k}-\vec{k}')\vec{R}_i} [\tau^{\nu}_{0i\sigma} + \tau^{\nu}_{1i\sigma}(s(\vec{k}) + s(\vec{k}')) + \tau^{\nu}_{2i\sigma} s(\vec{k}) s(\vec{k}')]. \qquad (22)$$

The explicit expressions for $\tau^{\nu}_{\ell i\sigma}$ $(\ell = 0,1,2)$ are given below.

Combining (19) to (22) with (12) in the $\vec{k}$-representation, one can exactly derive the site-diagonal element of G^{ν}_{i} within the modified CPA as

$$G^{\nu}_{i|d\sigma} = F_{0\sigma} + F^{2}_{0\sigma} \tau^{\nu}_{0i\sigma} + 2F_{0\sigma} F_{1\sigma} \tau^{\nu}_{1i\sigma} + F^{2}_{1\sigma} \tau^{\nu}_{2i\sigma}, \qquad (23)$$

where

$$F_{\ell\sigma}(z) = \frac{1}{N} \sum_{\vec{k}} \mathcal{G}_{\vec{k}\sigma}(z) [s(\vec{k})]^{\ell}, \quad (\ell = 0,1,2). \qquad (24)$$

In the case of only diagonal randomness the usual CPA expression for (23) is recovered immediately (cf. [16]).

Let us summarize the basic equations introduced above in a more convenient and explicit form for practical calculations. Accordingly, the system of equations is classified into three parts.

a) With respect to the correlation problem, the relations (17) and (18) are rewritten by replacing the causal by retarded functions on the basis of spectral theorems. After separating real and imaginary parts one gets (compare [9])

$$\mathrm{Re}\Sigma^{\nu}_{U\sigma}(E) = -\frac{1}{\pi} \int_{-\infty}^{\mu} dE' \mathrm{Im}G^{\nu}_{-\sigma}(E') \mathrm{Re}\Gamma^{\nu}(E+E') - \frac{1}{\pi} \int_{-\infty}^{2\mu-E} dE' \mathrm{Re}G^{\nu}_{-\sigma}(E') \mathrm{Im}\Gamma^{\nu}(E+E'), \qquad (25)$$

$$\mathrm{Im}\Sigma^{\nu}_{U\sigma}(E) = \frac{1}{\pi} \int_{\mu}^{2\mu-E} dE' \mathrm{Im}G^{\nu}_{-\sigma}(E') \mathrm{Im}\Gamma^{\nu}(E+E'), \qquad (26)$$

$$\mathrm{Re}\Gamma^{\nu}(E) = \frac{1/U^{\nu} + \mathrm{Re}D^{\nu}(E)}{[1/U^{\nu} + \mathrm{Re}D^{\nu}(E)]^2 + [\mathrm{Im}D^{\nu}(E)]^2}, \qquad (27)$$

$$\mathrm{Im}\Gamma^{\nu}(E) = -\frac{\mathrm{Im}D^{\nu}(E)}{[1/U^{\nu} + \mathrm{Re}D^{\nu}(E)]^2 + [\mathrm{Im}D^{\nu}(E)]^2}, \qquad (28)$$

with the abbreviations

$$\mathrm{Re}D^{\nu}(E) = -\frac{1}{2\pi}\int_{-\infty}^{\mu} dE'(\mathrm{Im}G_{\sigma}^{\nu}(E')\mathrm{Re}G_{-\sigma}^{\nu}(E-E') +$$

$$+ \mathrm{Im}G_{-\sigma}^{\nu}(E')\mathrm{Re}G_{\sigma}^{\nu}(E-E')) +$$

$$+ \frac{1}{2\pi}\int_{-\infty}^{E-\mu} dE'(\mathrm{Re}G_{\sigma}^{\nu}(E')\mathrm{Im}G_{-\sigma}^{\nu}(E-E') +$$

$$+ \mathrm{Re}G_{-\sigma}^{\nu}(E')\mathrm{Im}G_{\sigma}^{\nu}(E-E')), \qquad (29)$$

$$\mathrm{Im}D^{\nu}(E) = \frac{1}{\pi}\int_{\mu}^{E-\mu} dE'\mathrm{Im}G_{\sigma}^{\nu}(E')\mathrm{Im}G_{-\sigma}^{\nu}(E-E'), \quad (\nu = A,B). \qquad (30)$$

Here $\Sigma_{U\sigma}^{\nu}(E)$, $G_{\sigma}^{\nu}(E)$, $\Gamma^{\nu}(E)$ and $D^{\nu}(E)$ are now retarded functions; for simplicity, the subscripts "i|d" indicating the localization are dropped. D^{ν} represents the renormalization contribution to the bare vertex U^{ν}. The chemical potential μ is determined by the total electron number per site (see c)).

a) The CPA problem is expressed by three (complex) self-consistency conditions /13,14/

$$\langle \tau_{\ell\sigma}^{\nu}(z)\rangle = \left\langle \frac{a_{\ell\sigma}^{\nu}(z)}{1 - d_{\sigma}^{\nu}(z)} \right\rangle = 0, \quad (\ell = 0,1,2), \qquad (31)$$

where

$$a_{0\sigma}^{\nu} = (\delta_0^{\nu} + \Sigma_{U\sigma}^{\nu} - \sigma_{0\sigma}) + (\delta_1^{\nu} - \sigma_{1\sigma})^2 F_{2\sigma} + (\delta_0^{\nu} + \Sigma_{U\sigma}^{\nu} - \sigma_{0\sigma})\sigma_{2\sigma}F_{2\sigma}, \qquad (32)$$

$$a_{1\sigma}^{\nu} = (\delta_1^{\nu} - \sigma_{1\sigma}) - (\delta_1^{\nu} - \sigma_{1\sigma})^2 F_{1\sigma} - (\delta_0^{\nu} + \Sigma_{U\sigma}^{\nu} - \sigma_{0\sigma})\sigma_{2\sigma}F_{1\sigma}, \qquad (33)$$

$$a_{2\sigma}^{\nu} = -\sigma_{2\sigma} + (\delta_1^{\nu} - \sigma_{1\sigma})^2 F_{0\sigma} + (\delta_0^{\nu} + \Sigma_{U\sigma}^{\nu} - \sigma_{0\sigma})\sigma_{2\sigma}F_{0\sigma}, \qquad (34)$$

$$d_{\sigma}^{\nu} = (\delta_0^{\nu} + \Sigma_{U\sigma}^{\nu} - \sigma_{0\sigma})F_{0\sigma} + 2(\delta_1^{\nu} - \sigma_{1\sigma})F_{1\sigma} - \sigma_{2\sigma}F_{2\sigma} -$$

$$-[(\delta_1^{\nu} - \sigma_{1\sigma})^2 + (\delta_0^{\nu} + \Sigma_{U\sigma}^{\nu} - \sigma_{0\sigma})\sigma_{2\sigma}][F_{1\sigma}^2 - F_{0\sigma}F_{2\sigma}], (\nu = A,B). \qquad (35)$$

The parameters $[\delta_0^{\nu}, \delta_1^{\nu}]$ describing diagonal and off-diagonal randomness are equal to $[\epsilon^A - \epsilon^B, \frac{1}{2}(t^{AA} - t^{BB})]$ or $[0,0]$ according to whether an A or B atom occupies the i-th site, respectively. Note that the arbitrary index i was omitted. The scattering-matrix parts $\tau_{\ell\sigma}^{\nu}$ depend on z via $\Sigma_{U\sigma}^{\nu}$, $\sigma_{\ell\sigma}$, and $F_{\ell\sigma}$. Hereafter, we are working with only retarded functions provided that $\Sigma_{U\sigma}^{\nu}$ from a) is a retarded one.

c) The partially averaged Green function connecting a) and b) is (with dropping "i|d" in (23))

$$G_{\sigma}^{\nu}(z) = F_{0\sigma}(z) + F_{0\sigma}^2(z)\tau_{0\sigma}^{\nu}(z) + 2F_{0\sigma}(z)F_{1\sigma}(z)\tau_{1\sigma}^{\nu}(z) +$$

$$+ F_{1\sigma}^2(z)\tau_{2\sigma}^{\nu}(z), \quad (\nu = A,B). \qquad (36)$$

By inserting (19) and (21) into (24) one immediately gets the coherent Green functions

$$F_{\ell\sigma}(z) = \frac{1}{N}\sum_{\vec{k}} \frac{[s(\vec{k})]^{\ell}}{z - \epsilon^B - \sigma_{0\sigma}(z) - (t^{BB} + 2\sigma_{1\sigma}(z))s(\vec{k}) - \sigma_{2\sigma}(z)s^2(\vec{k})}, \quad (\ell = 0,1,2). \qquad (37)$$

The chemical potential μ obeys the relation

$$n = \sum_{\sigma} n_{\sigma} = -\frac{1}{\pi}\sum_{\sigma}\int_{-\infty}^{\mu} dE\, \mathrm{Im}F_{0\sigma}(E), \qquad (38)$$

where n is the average number of electrons per site. So far we have pointed out in a), b), and c) the closed set of completely self-consistent equations which must be solved numerically.

To complete the formalism one can introduce the coherent density of states (per site) of electrons with spin σ as

$$\rho_{\sigma}(E) = -\frac{1}{\pi}\mathrm{Im}F_{0\sigma}(E), \qquad (39)$$

and, analogously, the component densities of states associated with A and B atoms through

$$\rho_{\sigma}^{\nu}(E) = -\frac{1}{\pi}\mathrm{Im}G_{\sigma}^{\nu}(E), \quad (\nu = A,B). \qquad (40)$$

Accordingly, the average electron number with spin σ at A and B sites is

$$n_{\sigma}^{\nu} = \int_{-\infty}^{\mu} dE\,\rho_{\sigma}^{\nu}(E), \quad (\nu = A,B). \qquad (41)$$

By averaging (36) and combining with (39) to (41) we have

$$F_{0\sigma} = \langle G_{\sigma}^{\nu}\rangle = cG_{\sigma}^{A} + (1-c)G_{\sigma}^{B}, \qquad (42)$$

$$\rho_{\sigma}(E) = \langle\rho_{\sigma}^{\nu}(E)\rangle, \quad n_{\sigma} = \langle n_{\sigma}^{\nu}\rangle, \qquad (43)$$

where n_{σ} is the average number of electrons with spin σ per site defined in (38).

3. Numerical Analysis. Results and Discussion

To facilitate the calculations we choose a simplified input function associated with the band structure. The unperturbed density of states (per site per spin) of the pure B band (related to H_{Λ}^{B}) is assumed to have the semi-elliptic form

$$\rho_{\Delta}^{B}(E) = \frac{1}{N}\sum_{\vec{k}}\delta(E-\epsilon^{B}-t^{BB}\vec{s}(k)) = \begin{cases} \frac{1}{\pi}(1-E^2)^{1/2}, & |E| \le 1 \\ 0, & |E| > 1. \end{cases} \qquad (44)$$

Here the half-band width is set equal to unity (i.e., $t^{BB} = 1/6$ for the s.c. lattice) and the origin of the energy is chosen as $\epsilon^{B} = 0$. Using (44) and performing the $\vec{k}$-summations in (37) by the residue method, one directly obtains the $F_{\ell\sigma}$ as algebraic functions of $\sigma_{\ell\sigma}$ /17/.

The present approach involves six actual parameters c, Δ_0, Δ_1, U^A, U^B, n; here

$$\Delta_0 \equiv \delta_0^{A} = \epsilon^{A} - \epsilon^{B}, \quad \Delta_1 \equiv 12\delta_1^{A} = 6(t^{AA} - t^{BB}) \qquad (45)$$

describe the diagonal and off-diagonal randomness, respectively, resulting from the potential $V_{\Delta}^{(\nu)}$ in (1). In the numerical analysis we will consider only the nonmagnetic case defined by the solution-type

Fig. 2. (a) Electron densities of states ρ^ν and ρ, (b) real and imaginary parts of the self-energies Σ_U^ν and σ_0 on ν-sites (ν=A,B) and for the alloy, resp., with (c, Δ_0, Δ_1; U^A, U^B, n) = (0.25, 1.2, 0; 1.6, 0.8, 0.5). Split-off band case for the coherent ρ_Δ without electron-electron interaction.

$$\Sigma_U^\nu \equiv \Sigma_{U\sigma}^\nu = \Sigma_{U-\sigma}^\nu \ , \quad (\nu = A,B). \tag{46}$$

Accordingly, one redefines G_σ^ν, $\sigma_{\ell\sigma}$, $F_{\ell\sigma}$, $r_{\ell\sigma}^\nu$, ρ_σ, ρ_σ^ν by neglecting the spin indices in the following. Further we have $n/2 \equiv n_\sigma = n_{-\sigma}$ $n^\nu/2 \equiv n_\sigma^\nu = n_{-\sigma}^\nu$, and $n = \langle n^\nu \rangle$. For comparison the limit of zero Coulomb energy ($U^A = U^B = 0$) is pointed out, too (cf. also /17/).

The numerical procedure can be outlined as follows. To get initial values we start with virtual-crystal results for σ_ℓ at zero Coulomb energy; calculate successively F_ℓ from (37), μ through (38), G^ν via (36), n^ν from (40) and (41), and determine Hartree-Fock self-energies by $\Sigma_U^\nu = U^\nu n^\nu/2$. With this initial self-energies σ_ℓ, Σ_U^ν we solve the self-consistency problem (25) to (38) as a whole (unlike the two separated self-consistent chains in /13/) by an iteration method. In particular, we calculate via G^ν, μ, D^ν, Γ^ν, new Σ_U^ν values according to (36), (38), (29) and (30), (27) and (28), (25) and (26), respectively; and derive from the CPA conditions (31) new σ_ℓ values by using a modified iterative scheme /14/.

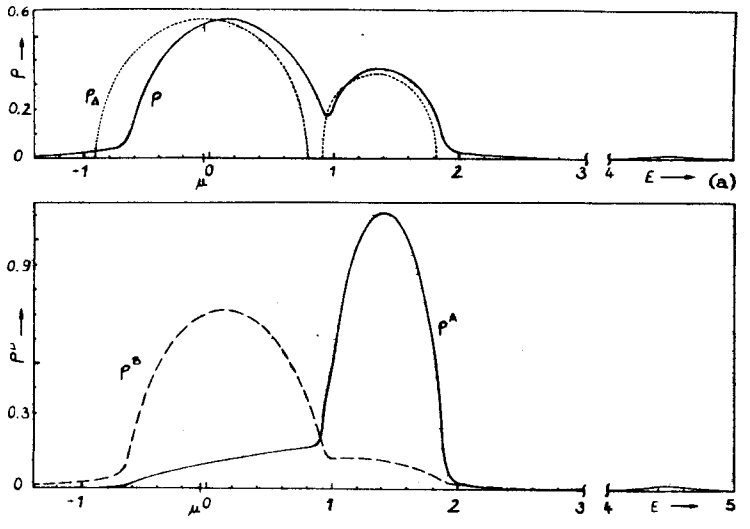

Fig. 2a

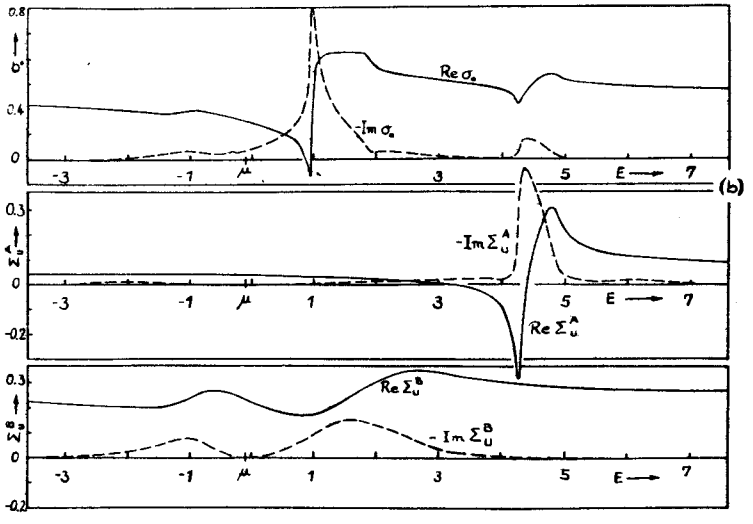

Fig. 2b

The whole procedure in repeated, and one gets, with alternate sub-iterations within the correlation and CPA sub-cycles, a good total convergence.

In Fig. 2 partial and total averages of one-particle densities of states and self-energies are plotted in the split ρ_Δ -band case without randomness in hopping integrals. At zero Coulomb energy, features of the coherent ρ_Λ were discussed /17/ in the more general case of two impurity-scattering mechanisms associated with Δ_0 and Δ_1. The gap in ρ_Λ (Fig. 2a) arising from strong diagonal disorder ($\Delta_0 > 1$) disappears by electron-electron correlations. The one-particle region defined by $\rho_\Lambda(E) \neq 0$ is augmented by a correlation region of ρ consisting of large tails and a small hump which can be ascribed to electron pair states on A sites as reflected by ρ^A. Such a type of partially averaged densities of states ρ^ν was also given in /12/. The continuous $\rho(E)$ spectrum (cf. also /13/, for pure systems /10/) differs strongly from the split-off picture obtained by using Hubbard's decoupling procedures /4,5/ (compare the splitting of arbitrarily filled bands in the crystals case /18/); even by including resonance broadening /6/ there are only weakly-damped correlation maxima with small tailing. Fig. 2b shows that the two-particle hump in ρ^A (ρ) is accompanied by precipitous changes of Σ_U^A (σ_0), especially there is a strong damping of one-particle states reflected by a peak of $\mathrm{Im}\Sigma_U^A$ ($\mathrm{Im}\sigma_0$). The correlation peak in σ_0 due to Σ_U^A is diminished by the interplay of correlations and disorder.

Characteristic results for one-particle and two-particle quantities are presented in Fig. 3 in the case of purely off-diagonal impurity scattering ($\Delta_0 = 0$) and random interaction strengths U^ν. The self-consistent sub-cycle for G^ν, Σ_U^ν, and Γ^ν provides damped two-particle humps in the component ρ^ν (Fig. 3a) caused, as discussed above, by peaks in the imaginary parts of the self-energies Σ_U^ν (Fig. 3b). Moreover, the effective two-particle vertices (or scattering amplitudes) $\Gamma^\nu(E)$ (Fig. 3c) depending on the sum of energies of the interacting electrons sharply change in the corresponding correlation regions. On the other hand, electron pairs whose energies lie in the main band are weakly scattered. The change of the sign of the retarded functions $\mathrm{Im}\Gamma^\nu(E)$ near $E=2\mu$ refers to an instability connected with an attractive effective interaction. The alloy averages ρ and σ_0 (contributing with σ_1, σ_2 to the coherent self-energy Σ, cf. /17/) in Fig. 3a can be explained as a weighted superposition of their partially averaged components. In the correlation region the results of the present method differ considerably from those of the incompletely self-consistent version /13/ as is shown by σ_0 in Fig. 3a. Note that the comparison was performed by using n^ν values of this calculation.

For the partially averaged quantities the quasi-particle conditions (for pure systems cf. /10/) $\mathrm{Im}\Sigma_U^\nu(\mu) = 0$, , $\mathrm{Im}\Sigma_U^\nu(E) \propto (E-\mu)^2$ near $E=\mu$ (local version of the Luttinger theorem /15/), $\partial \mathrm{Re}\Sigma_U^\nu(E)/\partial E|_\mu < 0$, and $\mathrm{Im}\Gamma^\nu(2\mu) = 0$ can be confirmed in Fig. 2 and Fig. 3. Obviously, additional impurity scattering

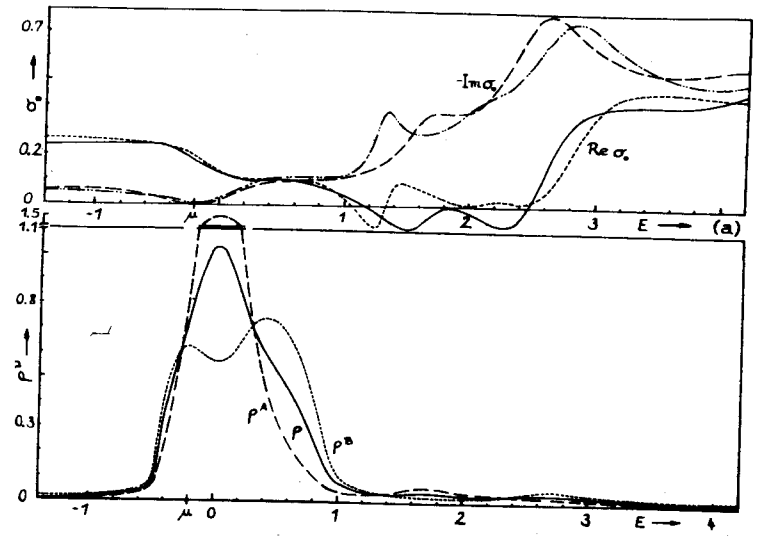

Fig. 3a

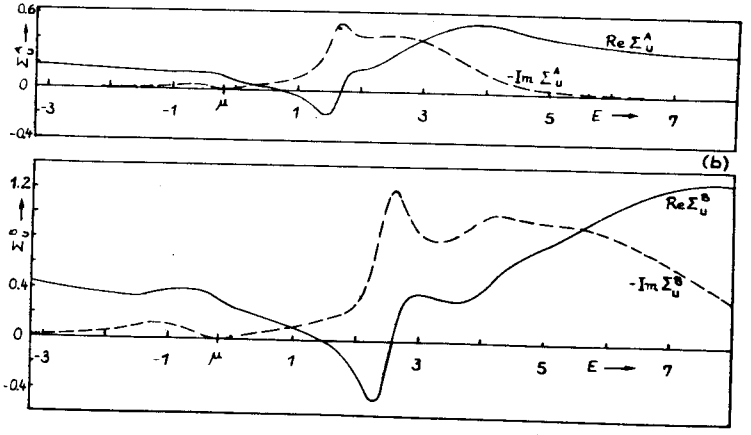

Fig. 3b

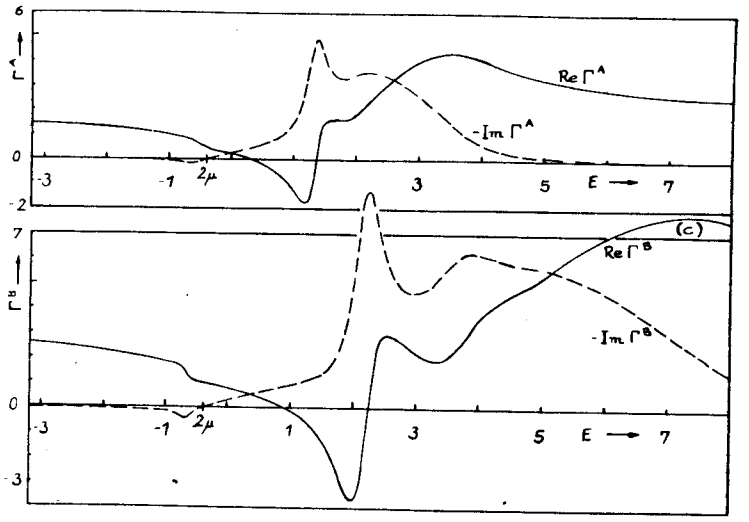

Fig. 3c

Fig. 3. (a) Component and alloy densities of states ρ^ν and ρ, resp., real (———) and imaginary (- - -) parts of the coherent self-energy σ_0 in comparison with $\mathrm{Re}\sigma_0$ (- - - -) and $\mathrm{Im}\sigma_0$ (- · - · - · -) obtained on the basis of /13/; real and imaginary parts of the (b) self-energies Σ_U^ν and (c) effective vertices Γ^ν at ν-sites ($\nu = A,B$) for the set (c, Δ_0, Δ_1; U^A, U^B, n) = (0.5, 0, -0.6; 2, 4, 0.3).

associated with random atomic levels leads to a finite lifetime of quasi-particles at the Fermi energy as reflected by $\mathrm{Im}\sigma_0(\mu) < 0$ in Fig. 2b, whereas random hopping integrals do not influence the local σ_0 in such a way (Fig. 3a). Asymptotic requirements as

$\mathrm{Re}\Sigma_U^\nu(\pm\infty) = U^\nu n^\nu/2$, $\mathrm{Re}\Gamma^\nu(\pm\infty) = U^\nu$,
$\mathrm{Im}\Sigma_U^\nu(\pm\infty) = 0$, etc., are also fulfilled.

The one-particle and correlation regions of the densities of states ρ^ν, ρ in Fig.4 are sensitively affected by varying the off-diagonal randonmess parameter Δ_1 particularly (here $\Delta_0 = 0$ as in Fig. 3). A typical numerical example for the gapless densities of states ρ^ν, ρ in a completely random Hubbard alloy is presented in Fig. 5. As is demonstrated by the total average ρ, dynamical correlations, i.e., all repeated binary interactions described by Γ^ν, work against the band splitting (deepening). Two small humps survive in the correlation region of ρ.

4. Conclusion

The horizontal ladder approximation [9] and the extended CPA [14] are unified into a completely self-consistent single-site theory for the random Hubbard model describing electronic properties of narrow-band alloys with diagonal and off-diagonal disorder. This dynamical theory avoids shortcomings of decoupling schemes as,e.g.,the violation of the Luttinger theorem.

By assuming an analytic form for the unperturbed density of states the numerical procedure is practicable even (unlike [10]) in the dilute carrier-concentration limit, e.g., for $n^A \approx 0.02$ in Fig. 5. Although the ladder approximation is more trustworthy at small n ($n \lesssim 1/3$) we have also given numerical examples beyond this value (Fig. 2); note that in the alloy case a criterion of

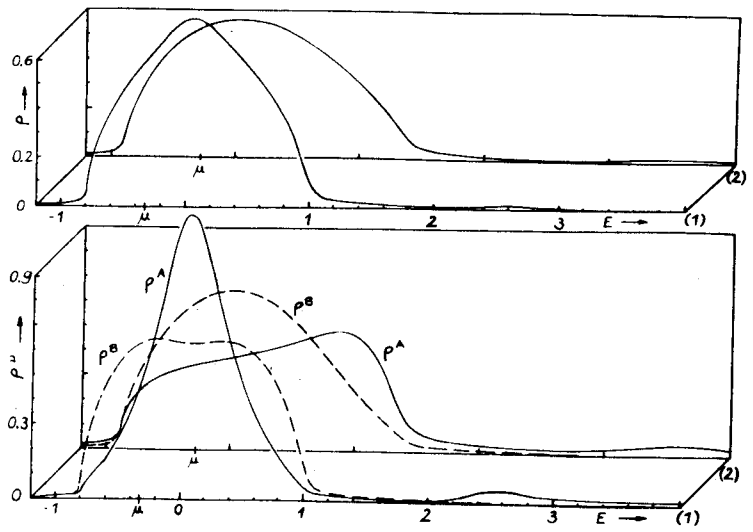

Fig. 4. Component and alloy densities of states ρ^ν ($\nu = A,B$) and ρ, resp., for (c, Δ_0, Δ_1; U^A, U^B, n) = (0.25, 0, -0.5; 3, 0.5, 0.4) and (0.3, 0, 0.5; 3.5, 0.5, 0.5) corresponding to the parameter sets (1) and (2), resp..

validity must be associated with the partial occupation numbers n^ν. In the present paper we have restricted numerically to nonmagnetic solutions by suitable choices of the parameters, especially U^ν and n.

Band gaps caused by strong impurity scattering in the one-particle region disappear by the Coulomb repulsion. Dynamical correlations described in terms of effective two-particle vertices provide continuous densities of one-particle states with large tails and small humps.

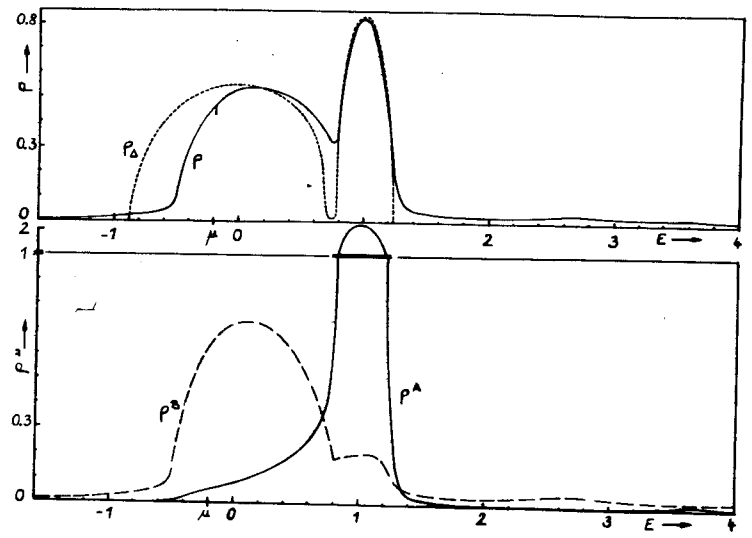

Fig. 5. Component and alloy densities of states ρ^ν ($\nu = A, B$) and ρ (ρ_Δ without electron-electron interaction), resp., in the case (c , Δ_0 , Δ_1 ; U^A, U^B, n) = (0.3, 0.9, -0.6; 1.5, 3.5, 0.25).

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