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Theory of Electronic Transport in Disordered Binary Alloys: Coherent-Potential Approximation*

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The coherent-potential approximation (CPA) for single-particle properties of electrons in a disordered alloy A_xB_{1-x} (Soven and others) is extended to complex admittances. The one-electron Kubo formula is used. The CPA is viewed as a single-site decoupling of the averaged multiple-scattering expansion. It properly gives the exact formulas in the limits of weak scattering (Edwards) and of dilute alloys (Langer). For any x and any random-potential strength, CPA satisfies a number of physical conditions, including energy and particle-number conservation. The CPA equations are exactly soluble for a single-band model with short-ranged random scatterers. The vertex corrections are related to the response of local densities to a given disturbance. For the electrical conductivity σ, they vanish. Variation of σ with the random-potential strength is studied numerically. A low-mobility region appears well before the band splits. In the split-band limit, CPA yields a reasonable finite σ in the host band, but it fails in the impurity band.

I. INTRODUCTION

Presently available theories of electronic transport in disordered alloys concern either the weak-scattering or the dilute-alloy limits, as represented by the works of Edwards[1] and Langer,[2] respectively. One important feature of these theories is that the equilibrium and transport properties obtained are mutually consistent, being treated on the same physical basis. Recently, the so-called coherent-potential approximation (CPA) was proposed by Soven[3] and Taylor,[4] and subsequently treated by various workers.[5–9] This theory is capable of dealing with single-particle (equilibrium) properties of elementary excitations (electrons, phonons, Frenkel excitons) in substitutionally disordered crystals A_xB_{1-x} for arbitrary x and for moderately different characteristics (potentials, masses, atomic levels) of A and B.

It is the purpose of the present paper to develop a theory of the linear response of electrons in the alloys, which should be parallel to and consistent with the single-particle CPA. The ranges of validity of this theory and of the single-particle CPA are expected to be equally broad. Although Ref. 1 was extended to deal with the third[10] and the fourth[11] orders in the scattering potential, the CPA approach to the linear response is the first to cover a really wide range of alloy parameters.

To make the whole task feasible, the commonly used restrictions are made: The alloy is assumed completely disordered, and the electrons are described by a one-electron Hamiltonian whose random part is composed of atomic contributions of two types, A and B.

The use of genuinely many-body techniques may be avoided within the one-electron approximation. Similarly to Refs. 1 and 2, we use the Kubo formula involving the single-particle density matrix.[12] Its configurational average reduces to averaging of a direct product of two one-electron resolvents $\langle GG\rangle$. In contrast, the equilibrium properties are simply determined by $\langle G\rangle$. The extension to the linear response consists, basically, in determination of the "vertex corrections" $\langle GG\rangle-\langle G\rangle\langle G\rangle$.

Formally speaking, this paper is characterized by constantly representing all quantities in operator (invariant) form. No specific basis is used until the very final, practical stages. This is in accord with the derivations[3,5] of the CPA, which are based on the multiple-scattering theory. In Ref. 3 and, especially, in Ref. 5, the CPA is treated as a single-site decoupling of the closed-form multiple-scattering equations[13,14] for the averaged resolvent $\langle G\rangle$. In the present paper, this approach is extended also to $\langle GG\rangle$.

The alloy potential is referred to the self-energy of an electron in the averaged alloy, and the difference is treated as a scattering potential. The total scattered wave is a sum of atomic contributions, each of which is a result of the scattering of an effective wave by the given atom. The effective wave contains the incident wave and all atomic contributions to the scattered wave, except that coming from the atom in question. Such an exclusion is characteristic of multiple-scattering theories, and motivates the Zubarev-type[15] single-site decoupling yielding the CPA: The atomic t-matrix and the effective

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wave are configurationally averaged independently of each other. Applied to $\langle G\rangle$, this procedure leads to the CPA condition for the electronic self-energy: All atomic t matrices must vanish on the average.[3–5] The application of the CPA to $\langle GG\rangle$ may be viewed in the following manner: Each G is associated with propagation of one independent particle. For each of the particles, the atomic t matrices and their effective waves are assumed to be statistically independent. However, this does not preclude statistical correlation in the motion of both particles.

The corresponding vertex corrections obey a coupled set of equations which replace in the CPA the exact averaging over all configurations. The multiple-scattering exclusions are vital for the theory, since they prevent an unphysical, immediately repeated scattering on the same site. However, they seem to bar an effective use of the Edwards-type diagrams.[1,2] Alternative diagrammatic techniques used by Leath[8] and Yonezawa[9] to obtain the single-particle CPA have the potential to make the exclusions, but are fairly sophisticated. All in all, the author believes that the method of diagram summation is most effective if the corresponding "renormalized coupling constant" is intuitively known. To his knowledge, this is not the case for the CPA. On the other hand, the notion of small fluctuations of the effective wave is at least well defined physically, if not fully justified. This suggests the decoupling technique as most natural and straightforward. The simplicity of the theory presented below seems to support this viewpoint.

An outline of the paper is now in order. The paper is divided into two major sections: Sec. II is devoted to a general discussion of the CPA and Sec. III to applications to a single-band model.

Section II: Under the above assumptions, the Kubo formula for complex admittances $\chi_{C_1C_2}$ is reduced to a form requiring only the configuration average $K=\langle GCG\rangle$, where C is a configuration-independent operator. This holds even for some configuration-dependent C_1, C_2 (e.g., total energy and energy current) (Sec. II A). To obtain the CP decoupling for K, two preparatory steps are made. The weak-scattering results[1] are rederived by the decoupling technique (Sec. II B 1), and the CPA for $\langle G\rangle$ is reviewed (Sec. II B 2).[3,5] Then, the equations for K in CPA are obtained as outlined above (Sec. II B 3).

These equations coincide, to linear terms in x, with the results of Ref. 2, and with Refs. 1, 10, and 11 to the third order in the scattering potential. The CPA is an interpolation scheme between the two limits, in agreement with the results[5,6] for $\langle G\rangle$ (Sec. II B 4). Several physical conditions on $\chi_{C_2C_1}$ (its behavior in the complex energy plane, conservation laws, and spatial symmetry) are expressed in terms of K. A kind of Ward's identity not only implies the energy and particle-number conservation, but also provides a compatibility criterion for K and $\langle G\rangle$ (Sec. II C 1). All the conditions are satisfied in the CPA. This indicates that the CPA is free of trivial inconsistencies. Most important is the Ward's identity, whose proof depends sensitively on the CPA condition for the self-energy as well as on the multiple-scattering exclusions in the vertex corrections (Sec. II C 2).

Section III deals with an application of the CPA to the specific case of a single-band model with short-range random atomic potentials. There are two model parameters, x and δ. The latter measures the strength of the random potential. The single-particle CPA for this model was studied in Refs. 5–7. These results are reviewed in Sec. III A. The short range of the atomic potentials allows an explicit solution of the CPA equations for K (Sec. III B 1). The vertex corrections measure the response of local densities to a given disturbance. The kinematic effect of the disturbance is separated out and a relation to the density-density response is obtained (Sec. III B 2). In the two-particle interpretation of K, the vertex corrections are equivalent to an effective interaction whose properties are discussed (Sec. III B 3).

For the electrical conductivity σ, the vertex corrections exactly vanish in the CPA, again because of the short range of the random potentials. A simple expression for σ results (Sec. III C 1). This result coincides with Ref. 11 to the order δ^3 and with the Boltzmann equation solution to δ^2. Vanishing of the vertex corrections and of the backward scattering in the collision term of the transport equation are physically related (Sec. III C 2). An extension of the Hubbard model[5,6] is used to obtain numerical results for σ with $x=0.1$ as δ is varied from 0 to ∞. As δ is increased, a low-mobility region is formed and eventually splits off as a minority-component sub-band. After that, the CPA seems to be reasonable only in the majority sub-band, where σ tends to a finite limit (Sec. III C 3).

II. CPA IN GENERAL

A. Reduction of the Kubo Formula for Electrons in Alloy

We shall consider the following model of a completely disordered binary substitutional alloy A_xB_{1-x}: In an ideal monatomic lattice with N sites in a large volume Ω, each side is occupied at random by an atom of type A or of type B, with respective probabilities x and $y=1-x$. There are c electrons per site. All interactions are neglected, so that the electrons are described by a one-electron Hamiltonian H, which is assumed to have the form

$$H=W+U=W+\sum_n U_n. \tag{1}$$

The operator W is the periodic part of H. The random part U is formed by single-site contributions U_n, which assume one of the two possible forms $U_n{}^A$, $U_n{}^B$ in correspondence with the kind of atom occupying site n. Operators W, $U_n{}^A$, and $U_n{}^B$ are assumed to be independent of both x and c. To a given concentration x, there are many equivalent distributions of atoms A and B among the sites. Only the averages over all these distributions (configurations) are macroscopically observable, and will be denoted by the brackets $\langle\cdots\rangle$.

For each configuration, the state of the electrons is specified by the single-particle density matrix ρ. At equilibrium,

$$\rho_0=f(H)\,, \tag{2}$$

where

$$f(E)=(1+e^{\beta(E-\mu)})^{-1}\,, \tag{3}$$

and μ, β, and c are related by the normalization condition

$$\mathrm{Tr}f(H)=cN\,. \tag{4}$$

The linear response of the electrons to a single-particle external disturbance $H'(t)$ can be described by a single-particle version of the Kubo formula, as used, e.g., by Lax.[12] The equation of motion for $\rho(t)$ is[16]

$$i(d/dt)\rho=[H+H',\,\rho]. \tag{5}$$

Without the loss of generality, the form of H' may be restricted to that of a harmonic disturbance turned on adiabatically:

$$H'(t)=e^{-i(\omega+i0)t}\mathfrak{F}C_1. \tag{6}$$

Here ω is real, $\mathfrak{F}$ is a c amplitude, and C_1 is time-independent. The initial condition is $\rho(-\infty)=f(H)$ in this case. The average value of a single-particle observable C_2 at time t is given by

$$\begin{aligned}\langle\mathrm{Tr}C_2\rho(t)\rangle=\langle\mathrm{Tr}C_2f(H)\rangle&\\+\chi_{C_2C_1}(\omega+i0)\mathfrak{F}e^{-i(\omega+i0)t}&+O(\mathfrak{F}^2)\,,\end{aligned} \tag{7}$$

where $\chi_{C_2C_1}$ is called the complex admittance, and equals

$$\chi_{C_2C_1}(z)=-i\int_0^\infty d\tau e^{iz\tau}\langle\mathrm{Tr}[e^{iH\tau}C_2e^{-iH\tau},\,C_1]f(H)\rangle,\qquad \mathrm{Im}z\geqslant0\,. \tag{8}$$

The configurational averaging in (7) and (8) applies to $f(H)$, $e^{iH\tau}$, and also to C_1, C_2. In the following, we restrict our considerations to operators C having the general form

$$C=\tfrac{1}{2}[\gamma(H)C'+C'\gamma(H)]\,, \tag{9}$$

where C' is configuration-independent. This class is broad enough to include important quantities like the components of total current $m^{-1}p^\alpha$ ($\alpha=1$, 2, 3), the total energy H, and the total energy flux components $w^\alpha=\frac{1}{2}m^{-1}(Hp^\alpha+p^\alpha H)$. For C_1, C_2 of the form (9), Eqs. (7) and (8) can be transformed to

$$\langle C_2f(H)\rangle=\int d\lambda f(\lambda)\gamma_2(\lambda)\,\mathrm{Tr}C_2{}'\langle\delta(\lambda-H)\rangle\,, \tag{10}$$

$$\begin{aligned}\chi_{C_2C_1}(z)=\frac{1}{4}\int d\lambda d\eta\frac{f(\lambda)-f(\eta)}{z-\lambda+\eta}&[\gamma_1(\eta)+\gamma_1(\lambda)]\\\times[\gamma_2(\eta)+\gamma_2(\lambda)]&I_{C_2{}'C_1{}'}(\lambda,\eta)\,,\end{aligned} \tag{11a}$$

$$I_{C_2{}'C_1{}'}(\lambda,\eta)=\mathrm{Tr}C_2{}'\langle\delta(\lambda-H)C_1{}'\delta(\eta-H)\rangle. \tag{11b}$$

Introducing the resolvent

$$G(z)=(z-H)^{-1}\,, \tag{12}$$

into (10) and (11) with the help of the identity

$$\delta(\lambda-H)=(2\pi i)^{-1}[G(\lambda-i0)-G(\lambda+i0)]\,, \tag{13}$$

we see that the quantities to be averaged directly are[1,2]

$$\bar{G}(z)=\langle G(z)\rangle\,, \tag{14}$$

$$K(z_1,C,z_2)=\langle G(z_1)CG(z_2)\rangle,\quad C\text{ config.-independent.} \tag{15}$$

These quantities enter (10) and (11a) through the relations

$$\langle\delta(\lambda-H)\rangle=(2\pi i)^{-1}[\bar{G}(\lambda^-)-\bar{G}(\lambda^+)] \tag{16}$$

and

$$\begin{aligned}I_{C_2{}'C_1{}'}(\lambda,\eta)=(4\pi^2)^{-1}\,\mathrm{Tr}C_2{}'[K(\lambda^+,C_1{}',\eta^-)+K(\lambda^-,C_1{}',\eta^+)&\\-K(\lambda^+,C_1{}',\eta^+)-K(\lambda^-,C_1{}',\eta^-)]&\,,\end{aligned} \tag{17}$$

where $\lambda^+=\lambda+i0$, etc.

This completes the reduction of the Kubo formula to the form convenient for CPA. In short, the difficult configuration averages in (7) and (8) were replaced by averages (14) and (15), yielding quantities $\bar{G}$ and K. The advantage of the latter is that they involve only the resolvent G, so that they have simple analytic properties, allow the perturbation expansions, etc.

The quantities $\bar{G}$ and K can be given a simple physical interpretation. First, $\bar{G}$ is the averaged resolvent of an electron in our alloy, so that it represents the Green's function of a single electron propagating through an effective medium with self-energy Σ given by the natural definition

$$\bar{G}(z)=[z-W-\Sigma(z)]^{-1}. \tag{18}$$

Second, K is a linear function of C, so that it is equivalently represented by a set of elements in any orthonormal basis:

$$K(z_1,C,z_2)=\sum_{\alpha,\beta,\gamma,\delta}|\alpha\rangle\langle G_{\alpha\beta}(z_1)G_{\gamma\delta}(z_2)\rangle C_{\beta\gamma}\langle\delta|\,. \tag{19}$$

Hence, K corresponds to the averaged direct product of two resolvents, i.e., to an effective problem of the averaged propagation of two particles, which are completely independent (or even not identical) for each configuration. However, they both respond to the same

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[16] We use the units in which $\hbar=1$.

random potential U associated with that configuration. On the average, this leads to a correlated motion of both particles. It is apparent that the operator K contains all two-particle correlations appearing in the correlation function (8). We shall refer to this "two-resolvent approach" occasionally.

B. CP Equations for $\bar{G}$ and K

The effect of the alloy Hamiltonian H can be best described by relating it to some auxiliary periodic Hamiltonian and observing the scattering corrections. An example of such decomposition of H into periodic and random scattering parts is the virtual crystal approach, where $H=(W+\langle U\rangle)+(U-\langle U\rangle)$. We shall use only the self-consistent approach, in which each configuration is related to the true effective medium, as defined in terms of $\bar{G}$. Using Eq. (18), we see that the Hamiltonian H should be decomposed as follows:

$$H=(W+\Sigma)+(U-\Sigma). \tag{20}$$

The self-energy Σ is not known at the beginning and must be determined in the course of averaging—hence the self-consistency label. To obtain the self-consistency conditions, we write the equations for G in terms of $\bar{G}$ and $U-\Sigma$, e.g.,

$$G=\bar{G}+\bar{G}(U-\Sigma)G=\bar{G}+G(U-\Sigma)\bar{G}. \tag{21}$$

Averaging these equations, we get the equations determining the self-consistent Σ:

$$\langle(U-\Sigma)G\rangle=0 \quad \text{or} \quad \langle G(U-\Sigma)\rangle=0. \tag{22}$$

It is more useful to define the related t matrix by

$$G=\bar{G}+\bar{G}T\bar{G}. \tag{23}$$

Again, T is a functional of Σ, and averaging of (23) yields the equation[5]

$$\langle T\rangle=0 \tag{24}$$

for the self-consistent Σ.

Introducing (23) into (15) and using (24), we obtain K in the form[17]

$$K=\bar{G}C\bar{G}+\bar{G}\langle T\bar{G}C\bar{G}T\rangle\bar{G}\equiv\bar{G}(C+\Gamma)\bar{G}. \tag{25}$$

The first term on the right side results from an independent averaging of both resolvents entering (15). The second term comes from the fact that both G's in (15) refer to the same configuration at a time. This gives rise to the vertex corrections Γ to the operator C. Returning to the discussion of Eq. (19), we may say that the vertex corrections are due to the correlation in motion of the two particles appearing in the two-resolvent approach.

Any approximation for determining K splits into two problems: (i) The approximate Σ and $\bar{G}$ must be found first; (ii) an approximation for Γ consistent with (i) must be developed. For the CPA, the first problem, which has an independent importance for equilibrium properties [Eq. (16)], has been already solved.[3–9] To answer the second question is the task of this part of the present paper.

1. Simple Example: Weak-Scattering Limit

Using the operator form (15) for K has some important advantages. The system has no preferred orthonormal basis in which the formalism simplifies. On the contrary, the multiple-scattering expansion is most transparent in the invariant form. At the same time, however, the resulting equations appear in a less familiar language. To remedy this difficulty, the well-known weak-scattering result of Edwards[1] will be obtained first. This will also provide an example of the power of the decoupling scheme used and, finally, will serve later for comparison with the CP equations.

In the weak-scattering limit, the potentials $U_n{}^A$, $U_n{}^B$ do not differ too much, and it is reasonable to expand all quantities in terms of $U-\langle U\rangle$, and to retain at most the second-order terms. The equation (24) for Σ then becomes

$$\Sigma=\langle U\rangle+\langle(U-\langle U\rangle)\bar{G}(U-\langle U\rangle)\rangle \tag{26}$$

or, after simple transformations using the equation

$$\langle U\rangle=\sum\langle U_n\rangle=\sum(xU_n{}^A+yU_n{}^B),$$

$$\Sigma=\sum_n\left[\langle U_n\rangle+xy(U_n{}^A-U_n{}^B)\bar{G}(U_n{}^A-U_n{}^B)\right]. \tag{27}$$

This is still an implicit equation for Σ, because of relation (18). If we dispense with the self-consistency and put $\Sigma=\langle U\rangle$ in $\bar{G}$, the second-order perturbation expression for Σ results,[1] with the typical "Nordheim"-concentration dependence[18] $x(1-x)$. More interesting is the decoupling for K. Using Eqs. (21), K is brought into the form

$$K=\bar{G}C\bar{G}+\bar{G}\langle(U-\Sigma)GCG(U-\Sigma)\rangle\bar{G}. \tag{28}$$

Keeping only terms of the order $(U-\langle U\rangle)^2$ or less allows us, first, to approximate Σ by $\langle U\rangle$ in the vertex corrections. Second, it also leads to an immediate decoupling in the vertex part, as the difference $GCG-K=GCG-\langle GCG\rangle$ can be neglected to the lowest order, so that the following closed equation for K is obtained:

$$\begin{aligned} K&=\bar{G}C\bar{G}+\bar{G}\sum_n\langle(U_n-\langle U_n\rangle)K(U_n-\langle U_n\rangle)\rangle\bar{G}\\ &=\bar{G}C\bar{G}+\bar{G}\sum_n xy(U_n{}^A-U_n{}^B)K(U_n{}^A-U_n{}^B)\bar{G}. \end{aligned} \tag{29}$$

It is easy to see that (27) and (29) are essentially identical with the results of Ref. 1. The hint contained

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[17] Wherever possible, the arguments z_1, z_2, C will be omitted. The rules for restoring them are simple, as the example of Eq. (25) shows whose explicit form is $K(z_1,C,z_2)=\bar{G}(z_1)[C+\Gamma(z_1,C,z_2)]\bar{G}(z_2)$.

[18] N. F. Mott and H. Jones, *The Theory of the Properties of Metals and Alloys* (Dover Publications, Inc., New York, 1958), Chap. VII.

in (29), as to the form of ladder equations in our approach, will be useful in Sec. II B 3.

2. *Multiple-Scattering Theory and CPA for Single-Particle Green's Function*

The next preparatory step is to review the form of the multiple-scattering theory used (following Lax,[13] see also Newton[14]) and to obtain the CP equation for the self-energy in the way used in Refs. 3 and 5. In order that the multiple-scattering expansion of G or T may be possible, we have to decompose the "perturbation" $U-\Sigma$ in (20) into a sum of single-site contributions. Since $U=\sum_n U_n$ by hypothesis, it remains to write Σ as a sum of periodically repeating atomic contributions:

$$\Sigma=\sum_n \Sigma_n. \tag{30}$$

This relation is connected with no additional assumptions, since Σ is periodic and there are infinitely many different decompositions (30). The quantity (30), with one of the Σ_n replaced by the true atomic potential U_n, describes the effect of one true atom (A or B) embedded in the effective medium, with self-energy Σ. The corresponding single-atom t matrix satisfies

$$T_n=(U_n-\Sigma_n)[1+\bar{G}T_n]. \tag{31}$$

In terms of these atomic t matrices, the full operator T is given by the standard series

$$T=\sum_n T_n+\sum\sum_{n\neq m} T_n\bar{G}T_m+\sum\sum\sum_{n\neq m\neq l} T_n\bar{G}T_m\bar{G}T_l+\cdots \tag{32}$$

with the characteristic exclusions which prevent the electron from scattering twice in sequence on the same site. There are two equivalent ways of replacing the series (32) by a closed set of equations: either

$$T=\sum_n Q_n, \tag{33}$$

$$Q_n=T_n(1+\bar{G}\sum_{m\neq n} Q_m) \tag{34}$$

or

$$T=\sum_n \tilde{Q}_n, \tag{35}$$

$$\tilde{Q}_n=(1+\sum_{n\neq m} \tilde{Q}_m\bar{G})T_n. \tag{36}$$

Because $T(z^*)=T^\dagger(z)$, the quantities Q, $\tilde{Q}$ are related by

$$\tilde{Q}_n(z^*)=Q_n{}^\dagger(z). \tag{37}$$

Equations (33) and (34) or (35) and (36) may be interpreted as follows: The total scattered wave is a sum of contributions coming from each atom. Each atomic contribution is given by the atomic t matrix applied on an effective wave. This effective wave consists of the incident wave and of the contributions to the scattered wave coming from all other sites.

All these quantities are configuration-dependent, and exact averaging of Eqs. (33)–(36) is no easier than, say, of Eq. (24). The CPA contains two ingredients: (i) The single-site approximation consists of the assumption that there exists a decomposition (30) for which the statistical correlation of T_n and of the corresponding effective wave is negligible. Equations (33) and (34) then average to

$$\langle T\rangle=\sum_m \langle Q_m\rangle, \tag{38}$$

$$\langle Q_m\rangle=\langle T_m\rangle(1+\bar{G}\sum_{n\neq m} \langle Q_n\rangle), \tag{39}$$

and similarly for Eqs. (35) and (36). (ii) The self-consistency condition (24) becomes in either case

$$\langle T_n\rangle=0, \tag{40}$$

the CP equation for the self-energy.

We obtain as many Eqs. (40) as there are sites, but they are equivalent owing to the periodicity of the averaged quantities. With obvious definitions, Eq. (40) reads

$$xT_n{}^A+yT_n{}^B=0 \tag{41}$$

or, still more explicitly,[3]

$$\Sigma_n=xU_n{}^A+yU_n{}^B-(U_n{}^A-\Sigma_n)\bar{G}(U_n{}^B-\Sigma_n). \tag{42}$$

3. *CP Approximation for K*

To extend the CPA to K, we introduce the atomic t matrices and their effective wave factors into the expression (25) for the vertex corrections Γ, doing it in a way that allows a decoupling similar to that made in Eq. (28) for the weak-scattering limit. Thus, we get

$$\Gamma=\sum_n\sum_m \langle Q_n\bar{G}C\bar{G}\tilde{Q}_m\rangle, \tag{43}$$

$$\langle Q_n\bar{G}C\bar{G}\tilde{Q}_m\rangle =\langle T_n(1+\bar{G}\sum_{p\neq n} Q_p)\bar{G}C\bar{G}(1+\sum_{s\neq m} \tilde{Q}_s\bar{G})T_m\rangle. \tag{44}$$

The CP decoupling consists, again, of neglecting the statistical correlation of the atomic t matrices and the effective wave factors. Therefore, (i) $\bar{G}$ is given by (18) with Σ defined by (40) and (ii) Eq. (44) is approximated by

$$\langle Q_n\bar{G}C\bar{G}\tilde{Q}_m\rangle =\langle T_n\langle(1+\bar{G}\sum_{p\neq n} Q_p)\bar{G}C\bar{G}(1+\sum_{s\neq m} \tilde{Q}_s\bar{G})\rangle T_m\rangle. \tag{45}$$

For $n\neq m$, the operators T_n, T_m are statistically independent and are averaged separately, each yielding zero, according to (40). Therefore, we may define quantities Γ_n by

$$\langle Q_n\bar{G}C\bar{G}\tilde{Q}_m\rangle=\Gamma_n\delta_{nm}. \tag{46}$$

This result may be used to simplify the internal average in (45), considering, naturally, only the case $n=m$:

$$\Gamma_n=\langle T_n\bar{G}(C+\sum_{p\neq n}\Gamma_p)\bar{G}T_n\rangle. \qquad (47)$$

The system of linear equations (47) for the unknowns Γ_n is closed and yields the vertex corrections in the CPA, since from (43) and (46) it follows that

$$\Gamma=\sum_n\Gamma_n. \qquad (48)$$

This relation, together with (25), allows us to give (47) the form

$$K=\bar{G}C\bar{G}+\bar{G}\sum_n\Gamma_n\bar{G}, \qquad (49)$$

$$\Gamma_n=\langle T_nKT_n\rangle-\langle T_n\bar{G}\Gamma_n\bar{G}T_n\rangle, \qquad (50)$$

useful, in particular, for comparison with other approximations. Equations (47) and (48) or (49) and (50) together with Eq. (40) represent the CPA for the quantity K and, by (11a) and (17), also for $\chi_{C_2C_1}$.

Equation (48) [or (49)] tells us that, in the CPA, the vertex corrections are a sum of single-site contributions. This is in agreement with the general single-site character of the CPA. The direct reason, as seen from (46), is that the contributions coming from different sites to both the scattered waves are regarded as statistically uncorrelated. The two-resolvent interpretation of K permits still another viewpoint: The two particles propagate independently through the effective medium unless they meet at the same site. In the latter event, they both feel the same atomic scattering potential $U_n-\Sigma_n$, and their motion becomes correlated.

The prominent feature of (47) [and of (50)] is the appearance of multiple-scattering exclusions. We shall see later that they are very important for the consistency of the CPA. Fortunately, the single-site approximation simplifies substantially the structure of (47) as compared to the exact relation (45). In fact, the structures of (47) and of (34) are analogous. This is particularly clear if (47) is solved formally:

$$\Gamma\ \sum_n\langle T_n\bar{G}C\bar{G}T_n\rangle +\sum_{n\neq m}\sum\langle T_n\bar{G}\langle T_m\bar{G}C\bar{G}T_m\rangle\bar{G}T_n\rangle+\cdots, \qquad (51)$$

and this series is compared with the exact series for T, Eq. (32). It is the averaging after each step in (51) which guarantees the single-site approximation. The role of the exclusions is best seen in the two-resolvent picture. They prevent an immediate return to the same site by both particles.

4. Limiting Cases: CPA as Interpolation Scheme

It was previously observed [5,6] that the CPA for the single-particle Green's function coincides with the results obtained by an expansion of the exact Σ in terms of the corresponding small parameters in two important limits: weak scattering ($U_n{}^A-U_n{}^B$ small) and dilute alloy (x or y small). Because these expansions are asymptotically exact, the CPA appears as an interpolation scheme between the two limits. As for the other possible limit, that of strong scattering, it is not well defined in general, but we shall discuss it for the special model of Sec. III.

Here, we shall extend the notion of the CPA as an interpolation scheme to the quantity K. The case of weak scattering will be considered first. As pointed out by Soven,[3,7] the CPA self-energy is exact up to the order $(U_n{}^A-U_n{}^B)^3$. To this order, the second right-hand term of (50) is formally negligible. Equation (50) then allows us to eliminate Γ_n from (49), which becomes a single equation for K. Expanding (31) in $U_n{}^A-U_n{}^B$ yields, finally,

$$\begin{aligned}K=\bar{G}C\bar{G}&+xy\bar{G}\sum_n(U_n{}^A-U_n{}^B)K(U_n{}^A-U_n{}^B)\bar{G}\\&+xy(x-y)\sum_n[\bar{G}(U_n{}^A-U_n{}^B)K(U_n{}^A-U_n{}^B)\\&\times\bar{G}(U_n{}^A-U_n{}^B)\bar{G}+\bar{G}(U_n{}^A-U_n{}^B)\\&\times\bar{G}(U_n{}^A-U_n{}^B)K(U_n{}^A-U_n{}^B)\bar{G}]\\&+O[(U^A-U^B)^4]. \qquad (52)\end{aligned}$$

The first line is identical with the weak-scattering equation (29), with the characteristic xy-concentration dependence. The rest of the right side represents the cubic corrections. Its concentration dependence is, of course, $xy(x-y)$. Not surprisingly, the cubic term is identical with the results of Verboven,[10] and the third-order[19] corrections of Moore.[11]

For the dilute alloy with the B atoms as the host, we have $x\ll 1$. With the use of (41), Eq. (50) is brought to the form indicating that the multiple-scattering correction may be neglected again:

$$\begin{aligned}\Gamma_n=xy^{-1}T_n{}^AKT_n{}^A-xy^{-1}T_n{}^A\bar{G}\Gamma_n\bar{G}T_n{}^A\\=xT_n{}^AKT_n{}^A+O(x^2). \qquad (53)\end{aligned}$$

Equation (49) becomes an equation for K,

$$K=\bar{G}C\bar{G}+x\sum_n T_n{}^AKT_n{}^A, \qquad (54)$$

which is essentially identical with the low-concentration results of, e.g., Langer.[2] Thus, the CPA for K is seen to be asymptotically exact for weak scattering or low concentration of one component. By this, the CPA is also established as an interpolation scheme for all concentrations and all scattering strengths. This is also supported by the evident fact that the CPA is symmetric with respect to A and B, i.e., the equations do not

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[19] The fourth-order terms treated in Ref. 11 include also the coherent scattering on the pairs of impurities. These effects can not be properly described within the CPA.

change under the transformation $x \rightleftarrows y$, $U_n{}^A \rightleftarrows U_n{}^B$ (compare the single-particle case of Ref. 5). However, such interpolation is not at all unique. In particular, the multiple-scattering subtraction in (50) was negligible in both limits, so that, as an interpolation, the equation $\Gamma_n = \langle T_n K T_n \rangle$ would be equally valid. Section II C is devoted to clarification of such uncertainties.

C. General Properties of CPA

No general quantitative criteria for the validity of the CPA seem to be available. But there are some qualitative properties of the observable quantities $\chi_{C_2C_1}$, which may be regarded as necessary conditions for the internal consistency of any approximation. In Sec. II C 1, several general features of complex admittances are listed and expressed in terms of $\bar{G}$ and K. Section II C 2 is devoted to the proof that $\bar{G}$ and K in the CPA render the relations for $\chi_{C_2C_1}$ obeyed for any concentration of alloy components and for any choice of the atomic potentials.

1. *Exact Properties of Complex Admittances*

The behavior of $\chi_{C_2C_1}$ in the complex frequency plane is discussed in any of the general references[20,21] or can be derived from (8) or (11a) and (11b) by inspection. The function $\chi_{C_2C_1}(z)$ is analytic in both complex half-planes and satisfies the crossing relation

$$\chi_{C_2C_1}(z) = \chi_{C_2C_1}{}^*(-z^*) . \qquad (55)$$

For $z \to \infty$, we have

$$\chi_{C_2C_1}(z) = z^{-1} \langle \mathrm{Tr}[C_2C_1] f(H) \rangle + O(z^{-2}) , \qquad (56)$$

so that the sum rule

$$\pm i \frac{1}{\pi} \int_{-\infty}^{\infty} \chi_{C_2C_1}(E \pm i0) dE = \langle \mathrm{Tr}[C_2, C_4] f(H) \rangle \qquad (57)$$

is satisfied. Finally, the upper and the lower half-planes are connected by

$$\chi_{C_2C_1}(z) = \chi_{C_1C_2}{}^*(z^*) . \qquad (58)$$

The configurational averaging restores the symmetry of the crystal lattice, so that for any transformation O from the crystal symmetry group, we have

$$\chi_{OC_2O^\dagger, OC_1O^\dagger} = \chi_{C_2C_1} . \qquad (59)$$

The particle number conservation is expressed by

$$\chi_{1C_1} = 0 . \qquad (60)$$

Energy is not dissipated in the linear approximation (e.g., the Joule heat is a quadratic effect), so that energy conservation implies

$$\chi_{HC_1} = 0 . \qquad (61)$$

Considering now Eqs. (11a) and (17), we see that the analyticity of χ does not depend on properties of K, and the following properties of K, defined by (15), are sufficient conditions for the validity of (55)–(61):

$$K(z_1, C, z_2) = K^\dagger(z_2{}^*, C, z_1{}^*) , \qquad (62)$$

$$\langle \mathrm{Tr}[C_2, C_1] f(H) \rangle = -\tfrac{1}{16}\pi^{-2} \int\int d\eta d\lambda [\gamma_1(\lambda) + \gamma_1(\eta)] \times [\gamma_2(\lambda) + \gamma_2(\eta)] I_{C_2'C_1'}(\lambda, \eta) , \qquad (63)$$

$$\mathrm{Tr} C_2 K(z_1, C_1, z_2) = \mathrm{Tr} C_1 K(z_2, C_2, z_1) , \qquad (64)$$

$$O K(z_1, C, z_2) O^\dagger = K(z_1, OCO^\dagger, z_2) , \qquad (65)$$

$$K(z_1, 1, z_2) = -(z_1 - z_2)^{-1} [\bar{G}(z_1) - \bar{G}(z_2)] . \qquad (66)$$

The operator arguments of K are, naturally, configuration-independent; the function I in (63) is given by (17). The logical relationship between (55)–(61) and (62)–(66) is as follows: (62) → (55), (63) → (56) and (57), (64) → (58), (65) → (59), (64) and (66) → (60) and (61).

Equation (63) merely expresses the left side in terms of K and, for approximate treatments, becomes the definition of $\mathrm{Tr}[C_1, C_2] f(H)$. In the special case of both C_1, C_2 configuration-independent, however, we also have the simpler relation (16) for obtaining this average from known $\bar{G}$. The equivalence of the two definitions is guaranteed by the relation

$$K(z_1, C, z_2) = z_1{}^{-1} C \bar{G}(z_2) + O(z_1{}^{-2}), \quad z_1 \to \infty \qquad (67)$$

between $\bar{G}$ and K. The validity of such a relation is important for any approximate treatment, since it indicates that the approximate $\bar{G}$ and K are mutually consistent.

Another relation of this character is Eq. (66). It may be called the Ward's identity, since it expresses the response K of the electrons to changes of the origin of energies,[22] by means of $\bar{G}$. Equivalently, (66) relates the vertex part Γ and the self-energy Σ:

$$\Gamma(z_1, 1, z_2) = -(z_1 - z_2)^{-1} [\Sigma(z_1) - \Sigma(z_2)] . \qquad (68)$$

This equality resembles closely the form of the Ward's identity common in the many-body theory (compare, e.g., Ref. 21, p. 268).

2. *Proof of Identities (62)–(68) in CPA*

Averages in the formal CPA solution for Γ, Eq. (51), can be carried out successively with the use of Eq. (41).

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[20] R. Kubo, J. Phys. Soc. Japan **12**, 570 (1957).

[21] P. Nozières, *Theory of Interacting Fermi Systems* (W. A. Benjamin, Inc., New York, 1964), p. 36ff.

[22] In a many-body treatment, this would correspond to the variations of the chemical potential.

The formal solution for K becomes

$$K=\bar{G}C\bar{G}+xy^{-1}\sum_{n}\bar{G}T_n{}^A\bar{G}C\bar{G}T_n{}^A\bar{G}$$
$$+(xy^{-1})^2\sum_{n\neq m}\sum\bar{G}T_n{}^A\bar{G}T_m{}^A\bar{G}C\bar{G}T_m{}^A\bar{G}T_n{}^A\bar{G}+\cdots. \tag{69}$$

Considering this expansion, term by term, shows immediately that the identities (62), (64), and (65) are satisfied by the approximate K. To verify (67), we observe first that $\bar{G}(z)\approx z^{-1}$ for $z\rightarrow\infty$. The "free" part of (49) $\bar{G}C\bar{G}$ has the asymptotic behavior $z_1{}^{-1}C\bar{G}(z_2)$. If we show that $\Gamma_n\rightarrow 0$ as $z_1\rightarrow\infty$, Eq. (67) will be proved. But $T_n(z)\rightarrow U_n-\langle U_n\rangle$ for $z\rightarrow\infty$, as follows from (31) and (42). Equation (47) then shows that $\Gamma_n=O(z_1{}^{-1})$ for $z_1\rightarrow\infty$. This completes the proof of (67).

It remains to prove the Ward's identity, which appears to be the most interesting of the discussed properties of K: It provides an important link between K and $\bar{G}$ and it implies particle-number and energy conservation. First of all, however, its validity depends more sensitively on the detailed structure of the CPA equations than was the case with the other identities. Hence, the Ward's identity represents important evidence of the internal consistency of the CPA.

To demonstrate this point, we shall give a more detailed proof considering the identity in the form (68). By (30) and (48), Eq. (68) is satisfied, if we put

$$\Gamma_n(z_1,1,z_2)=-(z_1-z_2)^{-1}[\Sigma_n(z_1)-\Sigma_n(z_2)]. \tag{70}$$

The validity of this choice may be verified by substituting Γ_n into the CPA equations (47), which should then become identities. The right side of (47) becomes

$$\Gamma_n=\langle T_n(z_1)\bar{G}\{1-\sum_{m\neq n}(z_1-z_2)^{-1}$$
$$\times[\Sigma_m(z_1)-\Sigma_m(z_2)]\}\bar{G}(z_2)T_n(z_2)\rangle$$
$$=-(z_1-z_2)^{-1}\langle T_n(z_1)\bar{G}(z_1)[U_n-\Sigma_n(z_2)]$$
$$-[U_n-\Sigma_n(z_1)]\bar{G}(z_2)T_n(z_2)\rangle. \tag{71}$$

In manipulations, Eqs. (18) and (31) were used, but the multiple-scattering exclusion $m\neq n$ was essential. Were there no exclusion, the result would be

$$-(z_1-z_2)^{-1}\langle T_n(z_1)[\bar{G}(z_1)-\bar{G}(z_2)]T_n(z_2)\rangle,$$

instead of (71). Continuing with (71), the self-consistency condition (40), i.e., $\langle T_n\rangle=0$, is used together with (31):

$$\Gamma_n=-(z_1-z_2)^{-1}\langle T_n(z_1)\bar{G}(z_1)[U_n-\Sigma_n(z_1)]$$
$$-[U_n-\Sigma_n(z_2)]\bar{G}(z_2)T_n(z_2)\rangle$$
$$=-(z_1-z_2)^{-1}[\Sigma_n(z_1)-\Sigma_n(z_2)]. \tag{72}$$

The left side equals the input to the right side of the original equation (47). This completes the proof of the Ward's identity (68). As a by-product, the "single-site Ward's identity" (70) was obtained. This single-site relation may be more convenient than the integral relation (68). It is only valid in the CPA, however.

III. SINGLE-BAND MODEL

A. Definition and Elementary Properties of the Model

In Sec. II of this paper, it was shown that for all systems having Hamiltonians of the general structure (1), the CPA can be extended to the calculation of the linear response to external fields. The single-particle self-energy is determined first by solving (40), then the quantity K is obtained as a solution of (49) and (50). Finally, (11a) and (17) are used to find the complex admittance $\chi_{C_2C_1}$. It is now desirable to consider at least one system for which this program is practical, to see the actual results. There is only one, particularly simple, single-band model[5–7] for which the single-particle properties in the CPA have been studied in any detail. We shall extend these studies to transport properties.

The Hamiltonian (1) is specialized to the single-band model[5–7] by assigning[23] a single Wannier orbital $|n\rangle$ to each site n, and assuming $|n\rangle$ to be independent of the kind of atom at site n. Assuming further that the random potential U is diagonal in the Wannier basis, (1) becomes

$$H=W+\sum U_n=\sum_{n\neq m}|n\rangle b_{nm}\langle m|+\sum_{n}|n\rangle\epsilon_n\langle n|. \tag{73}$$

The periodic part of H is diagonal in the Bloch basis:

$$\langle k|W|k'\rangle=\epsilon(k)\delta_{kk'}. \tag{74}$$

Here, k and k' are from the first Brillouin zone,

$$|k\rangle=N^{-1/2}\sum_{n}e^{i\mathbf{k}\cdot\mathbf{R}_n}|n\rangle, \tag{75}$$

and the label n stands for $\mathbf{R}_n=n_1\mathbf{e}_1+n_2\mathbf{e}_2+n_3\mathbf{e}_3$. All energies will be measured in units in which the half-bandwidth equals 1:

$$w=\tfrac{1}{2}[\max\epsilon(k)-\min\epsilon(k)]=1. \tag{76}$$

The random atomic contributions to H have the shortest possible range. An isolated U_n would represent a Koster-Slater impurity at site n. The "atomic levels" ϵ_n assume one of the two possible values ϵ^A or ϵ^B, with respective probabilities x and y. The origin of energies is chosen so that

$$\epsilon^A=-\epsilon^B=\tfrac{1}{2}\delta w=\tfrac{1}{2}\delta. \tag{77}$$

The dimensionless parameter δ measures the relative strength of the random and the periodic parts of H. The averaged properties of the system are specified by $\epsilon(k)$

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[23] The effects of the electron spin, neglected here, will be included simply by multiplying the resulting χ by two; compare Eq. (110).

and the two dimensionless parameters, x and δ; x varies between 0 and 1; δ may assume any real value.

The special case $\delta=0$ corresponds to the x-independent pure crystal with Hamiltonian W. All characteristics of this crystal will be regarded as known. We shall need the following quantities:

$$G^{(0)}(z)=(z-W)^{-1}=\sum_k |k\rangle[z-\epsilon(k)]^{-1}\langle k| , \qquad (78)$$

$$\mathfrak{F}_{n-m}(z)=\langle n|G^{(0)}(z)|m\rangle , \qquad (79)$$

$$F^{(0)}(z)=\mathfrak{F}_0(z)=\int_{-\infty}^{\infty} dE(z-E)^{-1}g^{(0)}(E) , \qquad (80)$$

$$g^{(0)}(E)=N^{-1}\,\mathrm{Tr}\delta(E-W)=\mp\mathrm{Im}F^{(0)}(E\pm i0) . \qquad (81)$$

Here, $g^{(0)}$ is the state density per atom.

The CPA for $\bar{G}$ is greatly simplified when the Hamiltonian has the form (73). From Eq. (42), it follows[5–7] that

$$\Sigma_n(z)=|n\rangle\langle n|\Sigma(z)|n\rangle\langle n| , \qquad (82)$$

so that the equation becomes a scalar one for a scalar unknown, denoted simply $\Sigma(z)$:

$$\Sigma(z)=\epsilon-(\epsilon^A-\Sigma)F(z)[\epsilon^B-\Sigma(z)] . \qquad (83)$$

Here we have

$$\epsilon=x\epsilon^A+y\epsilon^B=\tfrac{1}{2}(x-y)\delta , \qquad (84)$$

$$F(z)=\langle n|\bar{G}(z)|n\rangle . \qquad (85)$$

The short range of Σ_n is the most important qualitative result of the CPA as applied to (73). It has two joint causes: the short range of the atomic scattering potentials, and the single-site approximation, which gives Σ_n the range of the corresponding U_n. By (30), we have

$$\Sigma_{\mathrm{op}}=\Sigma|n\rangle\Sigma\langle n|=\Sigma 1 , \qquad (86)$$

where the operator unity refers to the single-band space. Therefore, we have

$$\begin{aligned}\bar{G}(z)&=(z-W-\Sigma_{\mathrm{op}})^{-1}\\ &=\{[z-\Sigma(z)]-W\}^{-1}=G^{(0)}[z-\Sigma(z)] , \end{aligned}\qquad (87)$$

$$F(z)=F^{(0)}[z-\Sigma(z)] . \qquad (88)$$

The latter equation eliminates F from (83) and shows that, in the CPA, a sufficient input for determination of Σ is the crystal density of states $g^{(0)}$ instead of the full knowledge of $\epsilon(k)$. Equation (83) is functional, however, and a numerical solution is generally necessary. Fortunately, it appears to be comparatively easy.

By analogy with (78) and (79), we have

$$\langle k|\bar{G}(z)|k'\rangle=\delta_{kk'}\mathcal{G}(k,z)=[z-\Sigma(z)-\epsilon(k)]^{-1} , \qquad (89)$$

$$F_{n-m}(z)=\langle n|\bar{G}(z)|m\rangle=\mathfrak{F}_{n-m}[z-\Sigma(z)] . \qquad (90)$$

Finally, from (31), (73), and (82), it follows that

$$T_n(z)=|n\rangle t_n(z)\langle n| , \qquad (91)$$

$$t_n(z)=[\epsilon_n-\Sigma(z)]\{1-[\epsilon_n-\Sigma(z)]F(z)\}^{-1} , \qquad (92)$$

and the density of states per atom is

$$g(E)=\mp\pi^{-1}\,\mathrm{Im}F(E\pm i0) . \qquad (93)$$

B. CP Approximation for K

1. General Solution

For definiteness, we shall use (49) and (50) as the CP equations for K. In contrast to Eq. (42) for Σ, the equations for K have a general solution for H of the form (73). Substituting (91) into (50) yields

$$\Gamma_n=|n\rangle\mathcal{L}\langle n|K|n\rangle\langle n| , \qquad (94)$$

$$\begin{aligned}\mathcal{L}&=\mathcal{L}(z_1,z_2)\\ &=\langle t_n(z_1)t_n(z_2)\rangle[1+F(z_1)\langle t_n(z_1)t_n(z_2)\rangle F(z_2)]^{-1} . \end{aligned}\qquad (95)$$

As indicated, $\mathcal{L}(z_1z_2)$ is universal for all C and is site-independent. The latter statement is easily demonstrated if the averages in (95) are carried out using (92). As a function of z_1 and z_2, $\mathcal{L}$ is analytic if neither variable assumes a real value, and

$$\mathcal{L}(z_1,z_2)=\mathcal{L}(z_2,z_1)=\mathcal{L}^*(z_1{}^*,z_2{}^*) . \qquad (96)$$

Substituting (94) into (49) eliminates the vertex corrections, and an equation for K is obtained:

$$K=\bar{G}C\bar{G}+\mathcal{L}\bar{G}\sum_n |n\rangle\langle n|K|n\rangle\langle n|\bar{G} . \qquad (97)$$

The diagonal elements of (97),

$$\begin{aligned}\langle m|K|m\rangle&=\langle m|\bar{G}C\bar{G}|m\rangle\\ &\quad+\mathcal{L}\sum_n [F_{m-n}(z_1)F_{n-m}(z_2)]\langle n|K|n\rangle , \end{aligned}\qquad (98)$$

represent a system of linear equations for the diagonal elements $\langle n|K|n\rangle$. Definition (90) was used to stress the fact that an element of the system's matrix depends only on the difference between the indices, $n-m$. Because of this circumstance, the system (98) is readily solved by Fourier transformation. Defining a_k and $\mathcal{A}_k$ by

$$a_k=\sum_m e^{-i\mathbf{k}\cdot\mathbf{R}_m}\langle m|\bar{G}C\bar{G}|m\rangle , \qquad (99)$$

$$\mathcal{A}_k=\sum_m e^{-i\mathbf{k}\cdot\mathbf{R}_m}F_mF_{-m} , \qquad (100)$$

we obtain the following solution of (98):

$$\langle m|K|m\rangle=N^{-1}\sum_k e^{i\mathbf{k}\cdot\mathbf{R}_m}a_k(1-\mathcal{L}\mathfrak{A}_k)^{-1} . \qquad (101)$$

Introducing (101) into the right side of the original equation (97), we get an explicit expression for the whole K, completing the solution of the CP equations (49) and (50).

Two comments on Eq. (97) are in order. The vertex corrections to C have the form $\Gamma=\sum_n|n\rangle\langle n|K|n\rangle\langle n|$. A slowly varying local potential $\phi(r)$ is represented in the single-band model by $\sum|n\rangle\phi(R_n)\langle n|$. It is seen that Γ behaves as an effective local potential added to C. We have made use of the fact that the diagonal elements $\langle n|K|n\rangle$ determine, uniquely, the whole K. For a given C, the operator K is equivalent to the set of all quantities $\mathrm{Tr}C'K$, which in turn determine all $I_{C'C}$ by (17) and, hence, all complex admittances $\chi_{C'C}$ by (11a). But $\langle n|K|n\rangle=\mathrm{Tr}(|n\rangle\langle n|K)$. This is of the form $\mathrm{Tr}C'K$, with $C'=|n\rangle\langle n|$ corresponding to the local density at site n. Thus, via Eq. (97), the whole family $\{\mathrm{Tr}C'K\}$, determining all possible responses to C, is completely specified by the subfamily $\{\mathrm{Tr}(|n\rangle\langle n|K)\}$ describing the reaction to C of the local densities at all sites.

2. Vertex Corrections in Terms of Density-Density Response

It was observed in the preceding subsection that the CPA for the model (73) is characterized by expressing the vertex corrections in terms of the response of local densities to the C in question. Here, we show how Γ for any C can be related to the response of local densities to one very special external disturbance, namely, that localized within the zeroth cell.

Using (64) and (97), we obtain

$$\begin{aligned}\langle n|K(z_1,C,z_2)|n\rangle&=\mathrm{Tr}CK(z_2,|n\rangle\langle n|,z_1)\\&=\mathrm{Tr}C[\bar{G}(z_2)|n\rangle\langle n|\bar{G}(z_1)+\mathfrak{L}(z_2,z_1)\bar{G}(z_2)\\&\quad\times\sum_m|m\rangle\langle m|K(z_2,|n\rangle\langle n|,z_1)|m\rangle\langle m|\bar{G}(z_1)].\end{aligned}\tag{102}$$

Inserting (102) into (94) and employing (96) and (64), we get

$$\begin{aligned}\Gamma_m(z_1,C,z_2)&=\mathfrak{L}(z_1,z_2)|m\rangle\sum_l\langle l|\bar{G}(z_1)C\bar{G}(z_2)|l\rangle\\&\quad\times[\delta_{lm}+\mathfrak{L}(z_1,z_2)\langle m|K(z_1,|l\rangle\langle l|,z_2)|m\rangle]\langle m|.\end{aligned}\tag{103}$$

Of all the elements $\langle m|K(z_1,|n\rangle\langle l|,z_2)|p\rangle$ of K [cf. (19)], only those with $m=p$, $n=l$ enter (103). They describe the response of the local density $|m\rangle\langle m|$ to a disturbance of the same form $|l\rangle\langle l|$. Their total defines, through (11a), the equivalent of the density-density correlation function for the single-band model. Hence, (103) shows the close relation between this function and the vertex corrections, again for the model (73) treated in the CPA.

The periodicity condition (65) leads to

$$\begin{aligned}&\langle m|K(z_1,|l\rangle\langle l|,z_2)|m\rangle\\&\quad=\langle m-l|K(z_1,|0\rangle\langle 0|,z_2)|m-l\rangle\equiv J_{m-l}(z_1,z_2).\end{aligned}\tag{104}$$

Introducing (104) into (103) and changing the summation variable, we obtain the final result

$$\begin{aligned}\Gamma_m(z_1,C,z_2)&=\mathfrak{L}|m\rangle\sum_l\langle m-l|\bar{G}(z_1)C\bar{G}(z_2)|m-l\rangle\\&\quad\times[\delta_{l,0}+\mathfrak{L}J_l(z_1,z_2)]\langle m|,\end{aligned}\tag{105}$$

expressing Γ_m through the single-indexed quantities J_l, which are related to the response of local densities to the disturbance $|0\rangle\langle 0|$ concentrated at the zeroth site. The convolution in (105) separates the influence of the kinematic properties of C from the dynamic characteristics of the system represented by J_l. Since the convolution should be equal to (101), a similar interpretation of this formal relation may be given. Indeed, rearranging (101) to

$$\langle m|K|m\rangle=\frac{1}{N}\sum_k e^{i\mathbf{k}\cdot\mathbf{R}_m}a_k\left(1+\mathfrak{L}\frac{\mathcal{A}_k}{1-\mathfrak{L}\mathcal{A}_k}\right),\tag{106}$$

one can easily verify that the right side is, term by term, the Fourier transform of the convolution in (105).

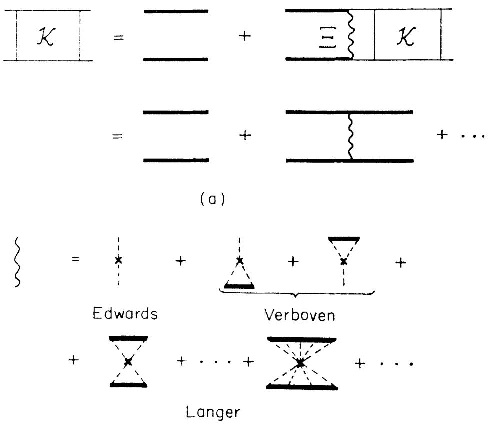

FIG. 1. (a) A diagrammatic representation of Eq. (108) for the quantity K. The momenta k_i are not indicated, for simplicity; the heavy lines correspond to the averaged single-particle Green's function $\mathcal{G}(k)\delta_{kk'}$. The equation is seen to have a ladder structure. (b) The CPA effective interaction Ξ as given by (95) and (109) cannot be conveniently represented by Edwards's diagrams. For δ or x small, however, Ξ is represented by a sum of the single-cross Edwards's diagrams: one, three, and all such diagrams are accounted for in Refs. 1, 10, and 2, respectively, as labelled by the authors' names.

3. Bloch Representation: Effective Interaction

The relation (19) allows K to be represented in the Bloch basis by the quantity

$$\mathcal{K}(k_1,k_2;\,k_3,k_4)=\langle\langle k_1|G(z_1)|k_3\rangle\langle k_4|G(z_2)|k_2\rangle\rangle.\tag{107}$$

The energy arguments z_1, z_2 are omitted for brevity. The CP equation (97) for K is equivalent to the equation

$$\begin{aligned}\mathcal{K}(k_1,k_2;\,k_3,k_4)&=\mathcal{G}(k_1)\mathcal{G}(k_2)\delta_{k_1k_3}\delta_{k_2k_4}\\&\quad+\mathcal{G}(k_1)\mathcal{G}(k_2)\sum_{k_5,k_6,B}\frac{1}{N}\mathfrak{L}\delta(k_1+k_5-k_2-k_6+B)\\&\quad\times\mathcal{K}(k_5,k_6;\,k_3,k_4).\end{aligned}\tag{108}$$

In (108), all k_i are from the first Brillouin zone, B are the reciprocal-lattice vectors, and $\delta(k\neq 0)=0$, $\delta(0)=1$.

Equations (107) and (108) are simply interpreted in two-particle terms. The quantity K describes the averaged propagation of two independent particles. Introducing

$$\Xi(k_1,k_2;\, k_3,k_4)=\sum_B \frac{1}{N}\,\mathcal{L}\delta(k_1-k_2+k_3-k_4+B)\,, \qquad (109)$$

we see that (108) has a ladder structure,[24] as represented in Fig. 1(a). It appears that after averaging, the two particles propagate, correlated by their mutual effective interaction Ξ. Equation (109) shows that this is a contact interaction, i.e., it acts only if both particles meet at the same site. This feature corresponds to the result (94) for Γ_n and can be understood as follows: As shown in Sec. II B 3, the effective interaction is a result of statistical correlation of the motion of both particles, and, in the CPA, only the correlation of particles being scattered both by the same atomic potential is accounted for. Because the atomic scattering potentials are short ranged in the present model, a short-range effective interaction results.

Equations (107) and (108) are formally close to the equations obtained in Refs. 1 and 2. There are two unessential differences. First, the other authors were concerned with the effect of randomly distributed impurities on a parabolic band. Therefore, no umklapp processes appeared in their Ξ. Second, in our model only U_n of short range are considered, hence Ξ also is short ranged (in the CPA as well as in the other approximations). The only real difference is in the function $\mathcal{L}$, which measures the strength of the effective interaction. The dependence of $\mathcal{L}$ on δ and x parallels the results of Sec. II B 4. For any x and δ, we have the CPA expression (23). The multiple-scattering exclusion in (50) causes the correction term in the denominator of (23). For x or δ small, this correction is also small, and $\mathcal{L}$ becomes $\langle t_n(z_1)t_n(z_2)\rangle$, which yields[25] $\mathcal{L}\approx xt^A(z_1)t^A(z_2)$ if x is small, and $\mathcal{L}\approx xy\delta^2$ if δ is small. The resulting equations (108) could have been obtained directly from (54) and (29), respectively. In the two limits, the effective interaction may be represented by Edward's diagrams, as shown in Fig. 1(b). These approximations for Ξ are identical with those used in Refs. 1 and 2, respectively. The cubic corrections of Verboven[10] are separated out. They correspond to the contribution $xy(x-y)\delta^3[F(z_1)+F(z_2)]$ to the quantity $\mathcal{L}$. The relation of the single-band results, as well as of the general results of Sec. II B, to the work of Edwards and Langer is now obvious. There is no simple way of describing (95) by Edwards's diagrams. However, there is a reasonable hope that the alternative diagrammatic techniques of Yonezawa[9] and of Leath,[8] which have already yielded the CPA for the single-particle self-energy, can be extended also to transport coefficients.

C. Example: Electrical Conductivity

Our study would not be complete if we did not consider the static electrical conductivity of model (73) in some detail. First, the dc conductivity is the basic transport coefficient of electrons in metals. Second, most of the previous theoretical work on transport in metals relates to the conductivity. Third, a deeper insight into both the CPA and the properties of model (73) is gained. The conductivity tensor σ is given by the well-known Kubo-Greenwood formula[1]

$$\sigma^{\alpha\beta}=\frac{2\pi e^2}{m^2\Omega}\int d\eta\left(-\frac{df}{d\eta}\right)\mathrm{Tr}\langle p^\alpha\delta(\eta-H)p^\beta\delta(\eta-H)\rangle\,. \qquad (110)$$

Here e and m denote the electron charge and mass, respectively, Ω is the crystal volume, Greek letters refer to the Cartesian coordinates, and the p^α are components of the linear momentum:

$$\langle k|p^\alpha|k'\rangle=m(\partial/\partial k^\alpha)\epsilon(k)\delta_{kk'}\equiv mv^\alpha(k)\delta_{kk'}\,. \qquad (111)$$

The two possible spin orientations are taken into account by an extra factor of 2. Equation (110) is but a special case of (11a). We can also write

$$\sigma^{\alpha\beta}=\frac{2\pi\theta^2}{m^2\Omega}\int d\eta\left(-\frac{df}{d\eta}\right)I_{p^\alpha p^\beta}(\eta,\eta)\,, \qquad (112)$$

with $I_{p^\alpha p^\beta}$ given by (17).

1. *Electrical Conductivity in CPA*

The first step necessary in order to determine $K(z_1,p^\alpha,z_2)$ in CPA is evaluation of the quantity

$$\langle l|\bar{G}(z_1)p^\alpha\bar{G}(z_2)|l\rangle =\frac{1}{N}\sum_k [z_1-\Sigma(z_1)-\epsilon(k)]^{-1}mv^\alpha(k)[z_2-\Sigma(z_2)-\epsilon(k)]^{-1}, \qquad (113)$$

where Eqs. (75), (89), and (111) were used. By time-reversal symmetry,[26]

$$\epsilon(k)=\epsilon(-k),\quad v^\alpha(k)=-v^\alpha(-k)\,, \qquad (114)$$

expression (113) vanishes identically. Looking at the Eqs. (99)–(101) or (105) for the vertex corrections, we see that $\Gamma_n=0$ and

$$K(z_1,p^\alpha,z_2)=\bar{G}(z_1)p^\alpha\bar{G}(z_2)\,. \qquad (115)$$

Equation (105) shows clearly that this result comes from the kinematic properties of p^α alone, and we do not even need to know the functions J_m, which may be

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[24] Some authors refer to (108) as to a Bethe-Salpeter equation. It should be pointed out that Eq. (108) corresponds both physically and formally to an electron-hole problem, whereas the above name seems to be commonly reserved for the two-electron case. See Ref. 21, pp. 239–247.

[25] The quantity t^A is obtained by putting $\epsilon_n=\epsilon^A$ in (92).

[26] H. Jones, *The Theory of Brillouin Zones and Electronic States in Crystals* (North-Holland Publishing Co., Amsterdam, 1962), p. 28.

essential in other cases. Equation (115) may also be linked with the interpretation of (97). Because no change of the local densities is expected in a homogeneous electric field, $\mathrm{Tr}|n\rangle\langle n|K=\langle n|K|n\rangle=0$, so that $\Gamma_n=0$, too. Because (97) is essentially dependent on both the CPA and the short range of the potentials U_n, the same is true about (115).[27] The simple result (115) can be used not only in the case of $\sigma^{\alpha\beta}$, but for any problem for which $C_1'=p^\alpha$ or even $C_2'=p^\alpha$, as follows from (11a) and (64). This includes, among others, the electrical and thermal flows caused by any external disturbance. With K given by (115), Eq. (112) becomes

$$\sigma^{\alpha\beta}=\frac{2e^2}{\pi\Omega}\int d\eta\left(-\frac{df}{d\eta}\right)\sum_k v^\alpha(k)v^\beta(k)[\mathrm{Im}\mathcal{G}(k,\eta^+)]^2. \quad (116)$$

The k independence of Σ in the CPA can be employed now. Introducing $\Omega_c=N^{-1}\Omega$,

$$\begin{aligned}\Lambda(E)&=\mathrm{Re}\Sigma(E\pm i0)-\epsilon,\\ \Delta(E)&=|\mathrm{Im}\Sigma(E\pm i0)|,\end{aligned} \quad (117)$$

(116) becomes

$$\sigma^{\alpha\beta}=\frac{2e^2}{\pi\Omega_c}\int d\eta\left(-\frac{df}{d\eta}\right)\times\int d\xi\left(\frac{\Delta(\eta)}{[\eta-\epsilon-\xi-\Lambda(\eta)]^2+\Delta^2(\eta)}\right)^2\times\frac{1}{N}\sum_k v^\alpha(k)v^\beta(k)\delta[\xi-\epsilon(k)]. \quad (118)$$

The three consecutive integrations involved represent three physical ingredients: the band structure of the pure substance, the effect of the random alloy potential, and the statistical distribution of electrons. Let us introduce a new function of complex energy,

$$\Phi^{\alpha\beta}(z)=\int d\xi(z-\xi)^{-1}(\pi N)^{-1}\sum_k v^\alpha(k)v^\beta(k)\delta[\xi-\epsilon(k)], \quad (119)$$

specified completely by the dispersion law $\epsilon(k)$. It is analytic in both half-planes and decreases as z^{-1} for $z\longrightarrow\infty$. Introducing $\Phi^{\alpha\beta}$ into (118) yields

$$\sigma^{\alpha\beta}=\frac{e^2}{\Omega_c}\int d\eta\left(-\frac{df}{d\eta}\right)\times\left[\Delta^{-1}\left(1-\Delta\frac{\partial}{\partial\Delta}\right)\mathrm{Im}\Phi^{\alpha\beta}(\eta-\epsilon-\Lambda-i\Delta)\right]_{\Lambda=\Lambda(\eta),\,\Delta=\Delta(\eta)}. \quad (120)$$

2. *Weak-Scattering Limit: Comparison with Boltzmann Equation*

In the weak-scattering limit, when δ is small, both Λ and Δ are proportional to δ^2 and roughly of the same magnitude. The CPA conductivity (120) becomes

$$\sigma^{\alpha\beta}=\frac{e^2}{\Omega_c}\int d\eta\left(-\frac{df}{d\eta}\right)\times[\Delta^{-1}\,\mathrm{Im}\Phi^{\alpha\beta}(\eta-\epsilon-\Lambda-i0)+O(\Delta)]_{\Lambda=\Lambda(\eta),\,\Delta=\Delta(\eta)} \quad (121)$$

or, still more crudely,

$$\sigma^{\alpha\beta}=\frac{e^2}{\Omega_c}\int d\eta\left(-\frac{df}{d\eta}\right)\times[\Delta^{-1}\,\mathrm{Im}\Phi^{\alpha\beta}(\eta-\epsilon-i0)+O(1)]_{\Delta=\Delta(\eta)}. \quad (122)$$

The leading term in $\sigma^{\alpha\beta}$ in the limit $\delta\longrightarrow 0$ is of the order Δ^{-1}, as is usual with transport coefficients. The approximation (121) is, therefore, seen to be exact to the order δ^3, as the relative order of $O(\Delta)$ is $\delta^2/\delta^{-2}=\delta^4$. An expression for σ equivalent to (121) was given by Moore.[11] In the approximation (122), only the lowest-order ($\sim\delta^{-2}$) term is kept, and this should be equivalent to Nordheim's result[18] obtained from the Boltzmann equation, consequently. The criterion for approximating (120) by (122) is

$$\Lambda(\eta)(\partial/\partial\eta)\,\mathrm{Im}\Phi^{\alpha\beta}(\eta-\epsilon-i0)\ll\mathrm{Im}\Phi^{\alpha\beta}(\eta-\epsilon-i0). \quad (123)$$

This is just a precise form of the London-Peierls criterion for the applicability of the transport equation[28] to the model (73). Two features are worth noting: First, the criterion is insensitive to the thermal state of the electrons (to the sharpness of the Fermi distribution[29]). Second, the renormalization of the virtual crystal levels Λ is involved, whereas the damping Δ would be important only in the order δ^4 [see Eq. (121)]. To compare (122) with the Boltzmann-equation solution,[30] we introduce the distribution functions $n_0(k)=f[\epsilon+\epsilon(k)]$ for the virtual crystal in equilibrium, and $n(k)$ for the steady state in a homogeneous electric field $\mathbf{E}$. The linearized transport equation for $n(k)$ is

$$\mathbf{v}(k)\cdot\mathbf{E}\left.\frac{df}{d\epsilon}\right|_{\epsilon=\epsilon(k)}=\sum_{k'}W(k,k')\times\{[n(k')-n_0(k')]-[n(k)-n_0(k')]\}, \quad (124)$$

where

$$\begin{aligned}W(k,k')=W(k',k)&=2\pi\delta[\epsilon(k)-\epsilon(k')]|\langle k|U-\langle U\rangle|k'\rangle|^2\\ &=2\pi xy\delta^2N^{-1}\delta[\epsilon(k)-\epsilon(k')]\end{aligned} \quad (125)$$

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[27] It should be remarked that the relation $\langle l|\bar{G}p^\alpha\bar{G}|l\rangle=0$ is exact for the considered band model and is not at all specific for the CPA. However, it has a very specific importance for the CPA vertex corrections, in full agreement with the qualitative argument just given.

[28] R. E. Peierls, *Quantum Theory of Solids* (Clarendon Press, Oxford, England, 1955), pp. 139–142.

[29] E. J. Moore, Ph.D. thesis, Harvard University, 1966 (unpublished).

[30] A. H. Wilson, *The Theory of Metals* (University Press, Cambridge, England, 1953), p. 266.

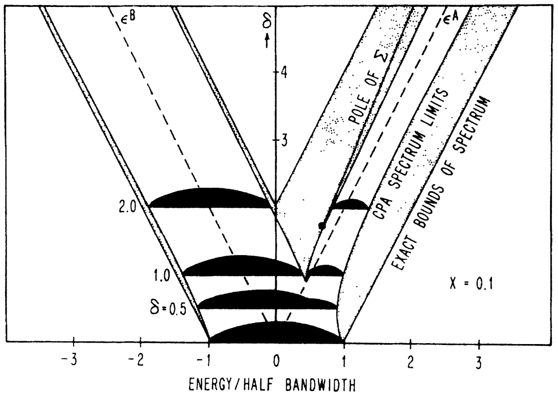

FIG. 2. Single-particle properties of the single-band model (73) for $x=0.1$ and $\delta \geq 0$ varied (Ref. 5). The unperturbed density of states $g^{(0)}$ is taken to have the form (129). The spectrum of (73) is exactly contained in the two strips of width 2, one parallel to ϵ^A and one to ϵ^B. The CPA limits of the spectrum are more restrictive. The area of allowed energies for which the CPA density of states vanishes is indicated by dots. The CPA band splits at $\delta \approx 0.93$. The black profiles depict the CPA averaged density of states per site for the values of δ: 0, 0.5, 1.0, and 2.0. The successive precipitation and separation of the minority sub-band is well observable. The pole in the CPA self-energy Σ appears first at $\delta \approx 1.67$ and follows the straight line $-\epsilon = -\frac{1}{2}(x-y)\delta$. Its role is to screen the two sub-bands for large δ.

is the lowest-order probability per unit time of the elastic scattering process $k \rightarrow k'$. The short range of U_n makes the matrix element in (125) k-independent. This, together with (114), causes the backward scattering term $\{\propto [n(k')-n_0(k')]\}$ to vanish. A current-relaxation time can be introduced:

$$\tau^{-1}(k)=2\pi xy\delta^2 \frac{1}{N}\sum_{k'} \delta[\epsilon(k)-\epsilon(k')], \qquad (126)$$

and the conductivity is

$$\sigma^{\alpha\beta}=\frac{2e^2}{\Omega_c}\sum_k \left(-\frac{df}{d\epsilon}\right)_{\epsilon(k)} \tau(k)v^\alpha(k)v^\beta(k)$$
$$=\frac{2e^2}{\Omega_c}\int d\eta\left(-\frac{df}{d\eta}\right)\tau(\eta)\ \mathrm{Im}\Phi^{\alpha\beta}(\eta-\epsilon-i0). \qquad (127)$$

This coincides with (122), if we identify

$$\tau^{-1}(k)=2\Delta[\epsilon+\epsilon(k)]=2\,|\mathrm{Im}\Sigma[\epsilon+\epsilon(k)]|\,. \qquad (128)$$

This identification is correct to the order δ^2, as a comparison of (126) with (83) shows: The current-relaxation time is equal to the single-particle relaxation time because the net backward scattering vanishes. This corresponds to the vanishing of vertex corrections in the CPA. It was shown in Ref. 1 that for parabolic bands and for weak scatterers of any range, the vertex corrections give rise to precisely the backward-scattering contribution to the relaxation time represented[18] by the cosine term in $\tau^{-1} \propto \int d\omega I(\nu)(1-\cos\nu)$. Here, ν is the polar angle, $I(\nu)$ is the corresponding differential cross section, and the integration extends over the sphere. If the scattering is isotropic, $I(\nu)=\text{const}$, the cosine integrates to give zero. In our case, a general band shape is considered, but the scatterers are short ranged and, hence, isotropic on the energy shell. This isotropy is the common physical reason for vanishing of both Γ in (115) and the backwards-scattering term in (124).

3. *Numerical Examples*

A few numerical examples are now in order. As seen from Eq. (120), $\sigma^{\alpha\beta}$ is determined by two functions of energy, $\Sigma(z)$ and $\Phi^{\alpha\beta}(z)$. The self-energy Σ is, by (83), expressed in terms of $g^{(0)}(E)$, x, and δ. The quantity $\Phi^{\alpha\beta}$ is specified by the function

$$\frac{1}{N}\sum_k v^\alpha(k)v^\beta(k)\delta[\xi-\epsilon(k)].$$

Thus, for calculation of $\sigma^{\alpha\beta}$, the knowledge of the detailed band structure is not really necessary and it is sufficient to know the two above functions of energy. We shall follow the approach of Refs. 5 and 6, in which $g^{(0)}$ was assumed to have a simple form, convenient for calculations, without specifying the corresponding $\epsilon(k)$. In correspondence with Refs. 5 and 6, we assume

$$g^{(0)}(E)=2\pi^{-1}(1-E^2)^{1/2}. \qquad (129)$$

The single-particle CPA then leads to simple equations for $\Sigma(z)$, $g(E)$, and other quantities. The results[5] for $x=0.1$ and $\delta>0$ ($\epsilon^A>\epsilon^B$, i.e., the host levels are lower than the impurity ones) are plotted in Fig. 2. The concentration 0.1 is chosen because it is beyond the low-concentration region but, at the same time, small enough to ensure an "impurity" and a "host" character to the A and B atoms, respectively. A detailed discussion of the results may be found in Ref. 5. The main features can be characterized as follows: (1) For all δ, the region of nonvanishing density of states is within the limits required by the localization theorem.[5] (2) For small δ, the density of states is symmetric and shifts as a rigid band (virtual-crystal limit). (3) For moderate δ, a distortion due to the minority A atoms appears at the top of the band. (4) The increasing distortion eventually results in the band's splitting into two sub-bands with relative weights 0.9 and 0.1. These two sub-bands may be shown to have an increasingly B and A character, respectively ("split-band limit").

The dependence of the density on δ is paralleled by that of the self-energy. For δ small, we have

$$\mathrm{Im}\Sigma(E\pm i0)=\mp\pi xy\delta^2 g^{(0)}(E-\epsilon)$$

in agreement with the Golden Rule. For moderate δ, the "impurity region" is characterized by a much higher damping, measured by $\mathrm{Im}\Sigma$, than is found in the host part of the band. For δ large, saturation occurs, and $\mathrm{Im}\Sigma$ does not increase beyond a certain level. This can be related to the appearance of a pole in Σ, which exhausts most of the sum rules[5] governing ImΣ. The two sub-bands behave markedly differently, the average levels of the damping being in the ratio of $(x/y)^{3/2} \approx 0.03$.

To obtain the conductivity, we have to make an additional assumption about the functions $\Phi^{\alpha\beta}$. We assume a cubic crystal, so that $\Phi^{\alpha\beta}=0$ for $\alpha \neq \beta$, and for the diagonal elements $\Phi^{\alpha\alpha}$ we assume

$$\sum_k v^\alpha v^\alpha \delta[E-\epsilon(k)] \propto (1-E^2)^{3/2}. \qquad (130)$$

It is easy to see that this function behaves properly at the band edges. Within the band, it has no critical points. However, this is less crucial in (130) than in (129), because in (130) the critical points induce singularities of the form $(E-E_0)^{+3/2}$, whereas in (129) the branching points are of the form $(E-E_0)^{+1/2}$. For the intended qualitative discussion, function (130) seems not to worsen the physical meaning of the model considered, which is limited basically by (129).[31]

The results for $\sigma^{11}=\sigma^{22}=\sigma^{33}\equiv\sigma$ are shown in Fig. 3 as a function of the fraction of the band occupied by the electrons. For simplicity, we put $T=0$ in (120). In the virtual-crystal limit ($\delta=0.005$), the plot of σ is symmetric, in agreement with the symmetry of the pure-crystal band. The conductivity vanishes for the band both empty and occupied, of course.

For the intermediate case, $\delta=0.5$, we observe first the reduction in the magnitude of σ as compared to the preceding case, which is of the order $(0.005/0.5)^2$ and is due primarily to the increase in ImΣ in (120). We see that in this sense, even for $\delta=0.5$, the "Nordheim rule" $\sigma \propto xy\delta^2$ is valid. However, the formation of the impurity part of the band leads to a pronounced asymmetry in the plot of σ, which can be understood as follows: For small occupation numbers, the Fermi level falls in the host part of the band, where the carriers move mostly between the B atoms and have a higher mobility, therefore. For the occupation numbers close to unity, practically all carriers are energetically in the impurity region and their mobility is reduced. Again, ImΣ causes the dominant effect, although the distortion in $\Phi[E_F-\Sigma(E_F^-)]$ also contributes appreciably. It is interesting to observe the sharp boundary between the high-mobility and the low-mobility regions.

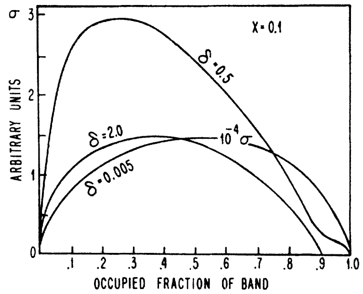

FIG. 3. The CPA static electrical conductivity σ at 0°K for a model (73) specified further by the cubic symmetry of the lattice and by $g^{(0)}$ and Φ given by (129), and (130), (119). The conductivity is given by (120) and is plotted versus the fraction of the band occupied by the electrons for $\delta=0.005$, 0.5, and 2.0. The absolute values of σ have no direct meaning for this artificial model. The ratio of the electron linewidth to the bandwidth is of the order 10^{-5} for $\delta=0.005$, 10^{-2}, and 10^{-1} in the host and the impurity parts of the band for $\delta=0.5$, and 10^{-2}, and 1 for $\delta=2.0$.

The split-band case is represented by $\delta=2.0$. First of all, the average σ appears to be of the same order as for $\delta=0.5$. This is because of exhaustion of the sum rules by the pole in Σ, and shows that in this region the Nordheim rule is even qualitatively invalid. Function ImΦ plays an important role in this case, since it causes $\sigma \rightarrow 0$ when the occupation number approaches 0.9. In the impurity region, σ is smaller by two orders of magnitude than it is in the host sub-band, as indicated. No enlarged plot of this region is shown, since the region can not be reliably treated in the CPA, because the clustering corrections are too important.[7] In the host sub-band, however, the results seem to be reasonable. For $\delta \rightarrow \infty$, the magnitude of σ does not change appreciably; the plot of σ merely becomes symmetric in the interval (0, 0.9): In the spilt-band limit, the A and the B sub-bands are entirely independent, so that $\delta \rightarrow \infty$ and $\delta \rightarrow -\infty$ must yield identical results.

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[31] There exist meaningful dispersion laws $\epsilon(k)$ yielding $g^{(0)}$, arbitrarily close to (129), as shown in Ref. 5, Appendix D. Detailed CPA calculations of σ and other transport coefficients for $\epsilon(k)$ corresponding to a single tight-binding band in a simple cubic lattice are reported by K. Liebermann, B. Velický, and H. Ehrenreich, Bull. Am. Phys. Soc. **14**, 320 (1968). These results support the conclusion that Φ is rather insensitive to the appearance of critical points.

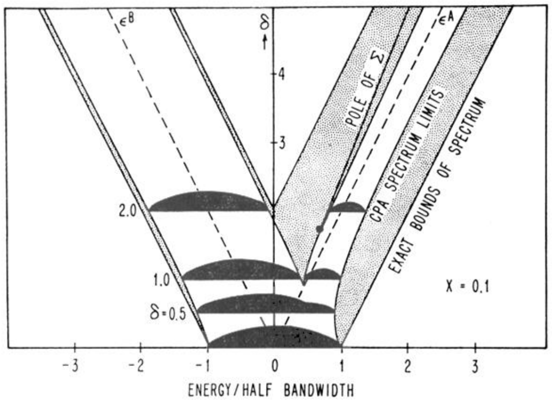

FIG. 2. Single-particle properties of the single-band model (73) for $x=0.1$ and $\delta\geq 0$ varied (Ref. 5). The unperturbed density of states $g^{(0)}$ is taken to have the form (129). The spectrum of (73) is exactly contained in the two strips of width 2, one parallel to ϵ^A and one to ϵ^B. The CPA limits of the spectrum are more restrictive. The area of allowed energies for which the CPA density of states vanishes is indicated by dots. The CPA band splits at $\delta\approx 0.93$. The black profiles depict the CPA averaged density of states per site for the values of δ: 0, 0.5, 1.0, and 2.0. The successive precipitation and separation of the minority sub-band is well observable. The pole in the CPA self-energy Σ appears first at $\delta\approx 1.67$ and follows the straight line $-\epsilon=-\frac{1}{2}(x-y)\delta$. Its role is to screen the two sub-bands for large δ.