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Theory of electronic transport in random alloys: Korringa-Kohn-Rostoker coherent-potential approximation

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The Korringa-Kohn-Rostoker coherent-potential approximation is a powerful and versatile tool for calculating the single-particle properties of disordered alloys. Here this technique is extended to transport properties. The formalism is based on the one-electron Kubo formula. It yields correct results in the limits of weak scattering or low concentration, i.e., the solution to the Boltzmann equation including vertex corrections. Transport coefficients can also be easily evaluated in the strong-scattering, high-concentration regime where the Boltzmann equation is not valid. The structure of the formalism is displayed by applying it to a one-dimensional muffin-tin model alloy.

I. INTRODUCTION

The Korringa-Kohn-Rostoker coherent-potential approximation (KKR-CPA) has been used to calculate the one-electron properties of many alloy systems.[1] Although it is not an exact theory, it accounts remarkably well for many properties of real alloys. It works especially well when it is made charge self-consistent.[2]

Recently, the KKR-CPA has been used to calculate the transport properties of alloys.[3–5] Although the calculations of Refs. 3—5 showed remarkable agreement with experiment, they suffered from two important defects. They assumed the existence of well-defined energy bands in the alloy, and they neglected the vertex corrections which give the "scattering-in" term of the Boltzmann equation. It was shown in Ref. 4 that these approximations are valid for the palladium-rich alloys of the $\mathrm{Ag}_x\mathrm{Pd}_{1-x}$ system which was the subject of that paper. In general, however, the two approximations significantly restrict the systems for which the KKR-CPA can be expected to yield accurate transport properties. Specifically, the neglect of vertex corrections leads to significant errors whenever there is appreciable *s-p* or *p-d* scattering, and the assumption of well-defined energy bands precludes the application of the theory to very strongly scattering systems in which the mean free path is on the order of a lattice spacing.

These limitations on the KKR-CPA are removed in this paper. The formal development presented here closely follows the work of Velický,[6,7] who developed a CPA theory for transport which he applied to a model alloy system with a two-level tight-binding Hamiltonian. The present development differs from that of Velický, however, because his formalism uses an invariant set of basis functions which are independent of the type of atom on a particular site. The use of this basis greatly simplifies the evaluation of the transport coefficients, but it causes severe difficulties when one attempts to apply the theory to real systems. If, for example, a tight-binding Hamiltonian is used, it is necessary in applying Velický's theory to assume that the wave functions are the same on every site regardless of the type of atom occupying the site.

Although the derviation of the present theory is more tedious than that of Velický, the resultant equations are only slightly more complicated and are quite tractable numerically. The accuracy and limitations of the present theory can best be ascertained by comparing the results of first-principles calculations which use the theory with experiment. That is not done here, but calculations are presented for a one-dimensional muffin-tin model alloy in order to illustrate the structure of the theory.

II. KUBO FORMULA FOR A MUFFIN-TIN HAMILTONIAN

Consider a system of noninteracting electrons moving in the presence of a random potential. The evaluation of most transport coefficients for such a system can, fairly generally, be reduced to the evaluation of an expression of the form[6–8]

$$C = \mathrm{Tr}\,\langle O_1 G O_2 G \rangle \ , \tag{1}$$

where C represents the transport coefficient, G is a single-particle Green function (which depends upon the details of the random potential), O_1 and O_2 are operators (which are independent of the potential), and the angle brackets indicate an average over the possible configurations of the potential.

The zero-temperature dc conductivity, for example, may be obtained from an expression of the form of Eq. (1). A commonly used expression for the conductivity is[9]

$$\sigma_{\mu\nu}(\varepsilon) = \frac{\pi\hbar}{N\Omega}\left\langle \sum_{\alpha,\alpha'} \langle \alpha | j_\mu | \alpha' \rangle \langle \alpha' | j_\nu | \alpha \rangle \times \delta(\varepsilon - \varepsilon_\alpha)\delta(\varepsilon - \varepsilon_{\alpha'}) \right\rangle \ , \tag{2}$$

where j_μ is the current operator,

$$j_\mu = -i\hbar \frac{e}{m} \frac{\partial}{\partial r_\mu} \ , \tag{3}$$

Ω is the volume per atom, and N is the number of atoms. The quantum states $|\alpha\rangle$ in Eq. (2) represent the exact eigenfunctions of a particular configuration of the random potential, and the large angle brackets indicate an average over configurations. By use of the identity

$$\sum_{\alpha} |\alpha\rangle\langle\alpha|\delta(\varepsilon-\varepsilon_\alpha) = -\frac{1}{\pi}\lim_{\eta\to 0}\operatorname{Im}G(\varepsilon+i\eta)$$

$$= -\frac{1}{2\pi i}\lim_{\eta\to 0}[G(\varepsilon+i\eta)-G(\varepsilon-i\eta)] , \tag{4}$$

Eq. (2) may be written in the same form as Eq. (1),

$$\sigma_{\mu\nu}(\varepsilon) = \tfrac{1}{4}\lim_{\eta\to 0}[\tilde{\sigma}_{\mu\nu}(\varepsilon+i\eta,\varepsilon+i\eta)+\tilde{\sigma}_{\mu\nu}(\varepsilon-i\eta,\varepsilon-i\eta)-\tilde{\sigma}_{\mu\nu}(\varepsilon+i\eta,\varepsilon-i\eta)-\tilde{\sigma}_{\mu\nu}(\varepsilon-i\eta,\varepsilon+i\eta)] , \tag{5}$$

$$\tilde{\sigma}_{\mu\nu}(z_1,z_2) = -\frac{\hbar}{\pi N\Omega}\operatorname{Tr}\langle j_\mu G(z_1) j_\nu G(z_2)\rangle . \tag{6}$$

The configurational average in Eq. (6) extends over the possible configurations of the one-electron Hamiltonian. In this paper that Hamiltonian will be assumed to have the form

$$H = -\frac{\hbar^2}{2m}\nabla^2 + \sum_n v_n(\mathbf{r}-\mathbf{R}_n) . \tag{7}$$

The atomic positions $\mathbf{R}_n$ will be taken as fixed and forming a regular lattice ($\mathbf{R}_n = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$, n_i integers). The potentials $v_n(\mathbf{r})$ are allowed to vary from site to site. For simplicity it will be assumed that the potential on a site may be one of only two types [$v_n(\mathbf{r}) = v_A(\mathbf{r})$ or $v_n(\mathbf{r}) = v_B(\mathbf{r})$]. Allowing more types of potentials would not cause serious difficulties. It *is* essential for the applicability of the CPA, however, that the potentials on different sites be statistically independent.

In the following it will also be assumed that the potentials $v_n(\mathbf{r})$ are spherically symmetric and that they do not overlap. The requirement of spherical symmetry is not essential[10]—it merely simplifies the formulas somewhat. On the other hand, the requirement that the potentials do not overlap, or more generally that their bounding spheres do not overlap, is necessary for the rigorous application of multiple-scattering theory.[11]

The Green function for electron propagation in a potential of the type assumed here can be written as[10]

$$G(\mathbf{r},\mathbf{r}';z) = \frac{2m}{\hbar^2}\sum_{L,L'}\tau_{LL'}^{mn}(z)Z_L^m(\mathbf{r}_m,z)Z_{L'}^n(\mathbf{r}'_n,z) - \delta_{mn}\left[\frac{2m}{\hbar^2}\right]\left[\Theta(r'_m - r_m)\sum_L Z_L^m(\mathbf{r}_m,z)S_L^m(\mathbf{r}'_m,z) + \Theta(r_m - r'_m)\sum_L Z_L^m(\mathbf{r}'_m,z)S_L^m(\mathbf{r}_m,z)\right] , \tag{8}$$

where $\tau_{LL'}^{mn}(z)$ is the scattering path operator[12] for propagation between sites m and n, $Z_L^m(\mathbf{r},z)$ is a wave function in the cell surrounding site m which is regular at the origin, and $S_L^m(\mathbf{r}_m,z)$ is a wave function in the cell surrounding site m which is generally irregular at the origin. The arguments of the wave functions in Eq. (8) are defined relative to the center of the nearest atom, i.e., $\mathbf{r}_m = \mathbf{r} - \mathbf{R}_m$ (where $\mathbf{R}_m$ is the center of atom m) if $\mathbf{r}$ is closest to $\mathbf{R}_m$.

The scattering path operator is given by[10]

$$\tau_{LL'}^{mn}(z) = [M^{-1}]_{LL'}^{mn} , \tag{9}$$

$$M_{LL'}^{mn} = [t_L^n(z)]^{-1}\delta_{mn}\delta_{LL'} - g_{LL'}^{mn}(z) , \tag{10}$$

$$g_{LL'}^{mn}(z) = -4\pi i^{l-l'}\kappa\sum_{L''} i^{-l''}C(L,L',L'')h_{l''}^{+}(\kappa R_{mn})Y_{L''}(\hat{R}_{mn}) , \tag{11}$$

$$C(L,L',L'') = \int d\hat{\mathbf{r}}\, Y_L(\hat{r})Y_{L'}(\hat{r})Y_{L''}(\hat{r}) . \tag{12}$$

In Eqs. (9)—(12) the index L stands for both the orbital angular momentum index (l) and the azimuthal index, and $\kappa = (2mz/\hbar^2)^{1/2}$. In Eq. (10), $t_L^n(z)$, which may be written as $t_l^n(z)$ because it is independent of the azimuthal index, is the t matrix for the scattering of a partial wave of orbital angular momentum l off the spherical potential at site n, and, in Eq. (11), h_l^+ is a spherical Hankel function.

The wave functions satisfy the Schrödinger equation for a single potential,

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + v_n(r) - z\right]\times\left\{\begin{matrix} Z_L^n(\mathbf{r},z) \\ S_L^n(\mathbf{r},z)\end{matrix}\right\} = 0 . \tag{13}$$

For values of r greater than r_n^{mt}, the range of $v_n(r)$, they may be expressed in terms of spherical Bessel functions (j_l and n_l), (real) spherical harmonics (Y_L), and phase shifts (η_L^n),

$$Z_L^n(\mathbf{r},z) = -\kappa[j_l(\kappa r)\cot\eta_l^n(z) - n_l(\kappa r)]Y_L(\hat{r}) , \tag{14}$$

$$S_L^n(\mathbf{r},z) = j_l(\kappa r)Y_L(\hat{r}) . \tag{15}$$

The second term of Eq. (8) may be excluded when calculating the conductivity because, as noted in Ref. 10, it is real when calculated for a real potential and for real energy. Hence the conductivity can be determined from

$$\tilde{\sigma}_{\mu\nu}(z_1,z_2)=-\frac{\hbar}{\pi N\Omega}\int d^3r\int d^3r'\left\langle\left[-i\hbar\frac{e}{m}\frac{\partial}{\partial r_\mu}\right]G'(\mathbf{r},\mathbf{r}';z_1)\left[-i\hbar\frac{e}{m}\frac{\partial}{\partial r'_\nu}\right]G'(\mathbf{r}',\mathbf{r};z_2)\right\rangle , \tag{16}$$

where

$$G'(\mathbf{r},\mathbf{r}';z)=\frac{2m}{\hbar^2}\sum_{L,L'}Z_L^m(\mathbf{r}_m,z)Z_{L'}^n(\mathbf{r}'_n,z)\tau_{LL'}^{mn}(z) . \tag{17}$$

Substitution of Eq. (17) into Eq. (16) yields

$$\tilde{\sigma}_{\mu\nu}(z_1,z_2)=-\frac{4m^2}{\pi N\Omega\hbar^3}\sum_{m,n}\sum_{L_1,L_2,L_3,L_4}\langle J_{L_4L_1}^{m\mu}(z_2,z_1)\tau_{L_1L_2}^{mn}(z_1)J_{L_2L_3}^{n\nu}(z_1,z_2)\tau_{L_3L_4}^{nm}(z_2)\rangle , \tag{18}$$

with

$$J_{LL'}^{m\mu}(z,z')=-\frac{ie\hbar}{m}\int_{\text{cell } m}d^3r_m\,Z_L^m(\mathbf{r}_m,z)\frac{\partial}{\partial r_\mu}Z_{L'}^m(\mathbf{r}_m,z') . \tag{19}$$

Equations (5) and (18), which are the primary result of this section, are formally similar to Eqs. (17) and (19) of Ref. 6, with the scattering path operators τ^{mn} in the present formalism playing the role of Velický's Green functions. There are important differences in physical content, of course. There is also an important formal difference. In Velický's formalism the operator matrix elements are configuration independent. Here, because the wave functions vary according to type of atom on a site, the matrix elements (19), as well as the τ^{mn}'s, are configuration dependent.

III. KORRINGA-KOHN-ROSTOKER COHERENT-POTENTIAL APPROXIMATION FOR THE CONDUCTIVITY

Equations (5), (18), and (19) could, in principle, and perhaps even in practice, be evaluated for a large but finite system, and for a sufficiently large ensemble to calculate the conductivity. That approach will not be attempted here, however; instead, the ensemble average will be performed approximately analytically.

When the average implied by Eq. (18) is performed, care must be taken to distinguish the terms for which $m=n$, for in this case J^m and J^n must (obviously) be the same. If, on the other hand, m is not equal to n, then J^m and J^n are statistically independent. Consequently, it is necessary to treat the term with $m=n$ separately be writing

$$\tilde{\sigma}_{\mu\nu}(z_1,z_2)=\tilde{\sigma}^0_{\mu\nu}(z_1,z_2)+\tilde{\sigma}^1_{\mu\nu}(z_1,z_2) , \tag{20}$$

$$\tilde{\sigma}^0_{\mu\nu}(z_1,z_2)=\frac{-4m^2}{\pi\hbar^3\Omega}\sum_{L_1,L_2,L_3,L_4}\langle J_{L_4L_1}^{0\mu}(z_2,z_1)\tau_{L_1L_2}^{00}(z_1)J_{L_2L_3}^{0\nu}(z_1,z_2)\tau_{L_3L_4}^{00}(z_2)\rangle , \tag{21}$$

$$\tilde{\sigma}^1_{\mu\nu}(z_1,z_2)=\frac{-4m^2}{\pi\hbar^3\Omega}\sum_{n\,(\neq 0)}\sum_{L_1,L_2,L_3,L_4}\langle J_{L_4L_1}^{0\mu}(z_2,z_1)\tau_{L_1L_2}^{0n}(z_1)J_{L_2L_3}^{n\nu}(z_1,z_2)\tau_{L_3L_4}^{n0}(z_2)\rangle . \tag{22}$$

In writing Eqs. (21) and (22) use was made of the translational invariance of the averaged system.

In order to evaluate the ensemble averages of Eqs. (21) and (22), it is helpful to express the scattering path operator (SPO) τ as the SPO in the CPA, τ^c, plus corrections:

$$\tau=\tau^c+\tau^cT\tau^c . \tag{23}$$

The SPO in the KKR-CPA is that for a periodic lattice with a coherent scatterer (with t matrix t^c) on every site. Consequently, it is given by Eqs. (9)—(12), with $t_L^n(z)=t_L^c(z)$ for all n. When the system is periodic, Eqs. (9)—(12) are best evaluated by Fourier transform,

$$\tau_{LL'}^{cmn}(z)=\Omega_z^{-1}\int_{\text{BZ}}d^3q[M(\mathbf{q},z)]_{LL'}^{-1}e^{i\mathbf{q}\cdot(\mathbf{R}_n-\mathbf{R}_m)} , \tag{24}$$

$$M_{LL'}(\mathbf{q},z)=[t_L^c(z)]^{-1}\delta_{LL'}-g'_{LL'}(\mathbf{q},z) , \tag{25}$$

$$g'_{LL'}(\mathbf{q},z)=\sum_{\substack{m\neq n\\ m,n}}g_{LL'}^{mn}(z)e^{i\mathbf{q}\cdot(\mathbf{R}_n-\mathbf{R}_m)} . \tag{26}$$

The integral in Eq. (24) extends over the Brillouin zone of volume Ω_z.

In order to obtain the correction term $\tau^cT\tau^c$ in Eq. (23), it is necessary to compare τ and τ^c. For a particular configuration of atoms, τ^{-1} can be obtained from Eqs. (9) and (10) whence (omitting the L and L' indices)

$$[\tau^{-1}]_{mn}=(t^m)^{-1}\delta_{mn}-g^{mn} , \tag{27}$$

whereas $(\tau^c)^{-1}$ is

$$[(\tau^c)^{-1}]_{mn}=(t^c)^{-1}\delta_{mn}-g^{mn} . \tag{28}$$

Thus,

$$[\tau^{-1}]_{mn}=[(\tau^c)^{-1}-\Delta m]_{mn} , \tag{29}$$

where Δm is a diagonal matrix with random elements equal to

$$\Delta m^n=[(t^c)^{-1}-(t^n)^{-1}] . \tag{30}$$

In the following it may be helpful for the reader who is familiar with the CPA for a tight-binding Hamiltonian to think in terms of the following *formal* analogy: $\tau\leftrightarrows G$, $\tau^c\leftrightarrows G^c$, and $\Delta m^n=\sigma^c-\varepsilon^n$, where G is the Green function for a tight-binding Hamiltonian with diagonal disorder only; $G=[E-H]^{-1}$,

$$H=\sum_n \varepsilon^n |n\rangle\langle n| + \sum_{m,n} W_{mn} |m\rangle\langle n| ,$$

and G^c is the CPA Green function, $G^c=[\varepsilon-H^c]^{-1}$,

$$H^c=\sum_n \sigma^c |n\rangle\langle n| + \sum_{m,n} W_{mn} |m\rangle\langle n| .$$

The analogy is, of course, only formal, and τ is not a Green function; its inverse is not a linear function of energy and the multiple-scattering formalism, at least in the opinion of the author, is a more powerful and versatile tool for treating physical systems than the tight-binding approximation with a species-independent basis.

By use of Eq. (29), Eq. (23) can be written as

$$T^{mn}=\Delta m^m \delta_{mn} + \Delta m^m \tau^{cmn} \Delta m^n + \sum_p \Delta m^m \tau^{cmp} \Delta m^p \tau^{cpn} + \cdots . \tag{31}$$

Repeated successive scatterings on the same site can be summed in the usual way,

$$T^{mn}=x^m \delta_{mn} + \sum_{p\,(\neq m)} x^m \tau^{cmp} T^{pn} , \tag{32}$$

or

$$T^{mn}=x^n \delta_{mn} + \sum_{p\,(\neq n)} T^{mp} \tau^{cpn} x^n , \tag{33}$$

where

$$x^n=[1-\Delta m^n \tau^{cnn}]^{-1} \Delta m^n . \tag{34}$$

Note that x^n in the present formalism plays the role of the single-site t matrix in the tight-binding formalism.

The coherent-potential approximation for the single-particle propagator consists of neglecting certain correlations in Eq. (32). Thus, in the CPA,

$$\langle T^{mn}\rangle_{\text{CPA}}=\langle x^m\rangle \delta_{mn} + \sum_{p\,(\neq m)} \langle x^m\rangle \tau^{cmp} \langle T^{pn}\rangle_{\text{CPA}} . \tag{35}$$

Given this decoupling, t^c can be chosen such that

$$\langle x^m\rangle = 0 , \tag{36}$$

with the result that $\langle T\rangle_{\text{CPA}}=0$ and $\langle \tau\rangle_{\text{CPA}}=\tau^c$. Equation (36) is shown to be equivalent to the usual expressions for the KKR-CPA self-consistency condition in Appendix A. It is important to note that terms in Eq. (32) such as

$$\langle x^m \tau^{cmn} x^n \tau^{cnm} x^m \tau^{cmn} x^n \rangle ,$$

which involve repeated scatterings back and forth between a pair of sites, are neglected in the CPA because they are not made to vanish by Eq. (36). Terms of this type will also be neglected in extending the CPA to the conductivity.

Returning to the evaluation of Eqs. (21) and (22), it is helpful to define the response functions K and L which contain only one current operator. Our strategy will be to seek a decoupling which yields a closed set of equations for these response functions. Thus,

$$\tilde{\sigma}^0_{\mu\nu}(z_1,z_2)=\frac{-4m^2}{\pi\hbar^3\Omega} \sum_\alpha c^\alpha \sum_{L_1,L_4} K^{0\alpha}_\nu(z_1,z_2;L_1,L_4) J^{\alpha\mu}_{L_4L_1}(z_2,z_1) , \tag{37}$$

$$\tilde{\sigma}^1_{\mu\nu}(z_1,z_2)=\frac{-4m^2}{\pi\hbar^3\Omega} \sum_{n\,(\neq 0)} \sum_{\alpha,\beta} \sum_{L_1,L_4} c^\alpha c^\beta L^{0\alpha,n\beta}_\nu(z_1,z_2;L_1,L_4) J^{\alpha\mu}_{L_4L_1}(z_2,z_1) , \tag{38}$$

$$K^{0\alpha}_\nu(z_1,z_2;L_1,L_4)=\sum_{L_2,L_3} \langle \tau^{00}_{L_1L_2}(z_1) J^{\alpha\nu}_{L_2L_3}(z_1,z_2) \tau^{00}_{L_3L_4}(z_2)\rangle_{0=\alpha} , \tag{39}$$

$$L^{0\alpha,n\beta}_\nu(z_1,z_2;L_1,L_4)=\sum_{L_2,L_3} \langle \tau^{0\eta}_{L_1L_2}(z_1) J^{\beta\nu}_{L_2L_3}(z_1,z_2) \tau^{n0}_{L_3L_4}(z_2)\rangle_{0=\alpha,\,n=\beta} . \tag{40}$$

Equations (37)—(40) need some explanation. Equations (37) and (39) are equivalent to Eq. (21). Equation (37) recognizes that the matrix element $J^{0\mu}_{LL'}$ of Eq. (21) must be either the matrix element for an A atom (with probability c^A) or a B atom (with probability c^B). The subscript $0=\alpha$ on the ensemble average of Eq. (39) means that this average is restricted such that the atom at site 0 must be of type α. The notation for the current matrix elements has been changed slightly between Eqs. (21) and (37). In Eq. (37), $J^{\alpha\mu}_{LL'}$ is the matrix element for an atom of type α, i.e., $J^{\alpha\mu}_{LL'}=(J^{n\mu}_{LL'})_{n=\alpha}$. This is sensible because $J^{n\mu}_{LL'}$ depends on n only because it depends on the *type* of atom sitting on site n.

Equations (38) and (40) are equivalent to Eq. (22), and the average in Eq. (40) is restricted so that atoms of types α and β are on site 0 and n, respectively. Restricted averages of this type were considered by Riedinger and Nauciel-Bloch[13] in a different context. Their results were helpful in the present derivation, but they differ from those presented here because certain terms involving repeated scatterings between pairs of atoms were retained in their work.

In approximately evaluating Eqs. (39) and (40), it is useful to use operators Q^k and $\tilde{Q}^k$, which are defined in terms of the total scattering operator T of Eqs. (23), (32), and (33),

$$Q^k=\sum_l T^{kl}=x^k \left[1+\sum_{m\,(\neq k)} \tau^{ckm} Q^m\right] , \tag{41}$$

$$\tilde{Q}^l=\sum_k T^{kl}=\left[1+\sum_{m\,(\neq l)} \tilde{Q}^m \tau^{cml}\right] x^l . \tag{42}$$

Note that Q^k and $\tilde{Q}^l$ should be understood as operators, i.e.,

$$(Q^k\tau^c)_{kn}=\sum_l T^{kl}\tau^{cln} .$$

The fundamental approximation of the CPA can also be expressed as

$$\langle x^k\tau^{ckl}Q^l\rangle=0,\quad k\neq l \tag{43}$$

or

$$\langle \widetilde{Q}^{\,l}\tau^{clk}x^k\rangle=0,\quad k\neq l\ . \tag{44}$$

These approximations will be used over and over in deriving a closed set of equations for Eqs. (39) and (40).

Equation (39) may be written by use of Eqs. (41) and (43) as

$$\begin{aligned}K^{0\alpha}=\tau^{c00}J^\alpha\tau^{c00}&+\sum_k\langle(\tau^cQ^k\tau^c)_{00}J^\alpha\tau^{c00}\rangle_{0=\alpha}\\&+\sum_l\langle\tau^{c00}J^\alpha(\tau^c\widetilde{Q}^{\,l}\tau^c)_{00}\rangle_{0=\alpha}\\&+\sum_{k,l}\langle(\tau^cQ^k\tau^c)_{00}J^\alpha(\tau^c\widetilde{Q}^{\,l}\tau^c)_{00}\rangle_{0=\alpha}\ .\end{aligned} \tag{45}$$

Equation (45) is still exact within the muffin-tin approximation. We now proceed to apply the CPA. The second and third terms on the right-hand side (rhs) of Eq. (45) are easily evaluated since $\langle Q^k\rangle_{0=\alpha}=0$ if $k\neq 0$ in the CPA. Furthermore,

$$\langle Q^0\rangle_{0=\alpha}=\left\langle x^0\left[1+\sum_{k\,(\neq 0)}\tau^{c0k}Q^k\right]\right\rangle_{0=\alpha}=x^\alpha\ . \tag{46}$$

Thus Eq. (45) may be written as

$$\begin{aligned}K^{0\alpha}=\tau^{c00}J^\alpha\tau^{c00}&+\tau^{c00}x^\alpha\tau^{c00}J^\alpha\tau^{c00}\\&+\tau^{c00}J^\alpha\tau^{c00}x^\alpha\tau^{c00}+X\ ,\end{aligned} \tag{47}$$

where X, the last term on the rhs of Eq. (45) or (47), can be written as the sum of four terms:

$$\begin{aligned}X=\langle\tau^{c00}Q^0\tau^{c00}J^\alpha\tau^{c00}\widetilde{Q}^{\,0}\tau^{c00}\rangle_{0=\alpha}&\\+\sum_{k\,(\neq 0)}\langle(\tau^cQ^k\tau^c)_{00}J^\alpha\tau^{c00}\widetilde{Q}^{\,0}\tau^{c00}\rangle_{0=\alpha}&\\+\sum_{k\,(\neq 0)}\langle\tau^{c00}Q^0\tau^{c00}J^\alpha(\tau^c\widetilde{Q}^{\,k}\tau^c)_{00}\rangle_{0=\alpha}&\\+\sum_{k\,(\neq 0)}\langle(\tau^cQ^k\tau^c)_{00}J^\alpha(\tau^c\widetilde{Q}^{\,k}\tau^c)_{00}\rangle_{0=\alpha}&\ .\end{aligned} \tag{48}$$

In the final sum of Eq. (48), terms involving $\langle Q^k\widetilde{Q}^{\,l}\rangle$ $(k\neq 0,\ l\neq 0)$ vanish in the CPA [see Eqs. (35) and (36)].

Let us define a quantity $\gamma_k^{0\alpha}$ (which will play the role of a vertex function) by

$$\gamma_k^{0\alpha}=\langle(Q^k\tau^c)_{k0}J^\alpha(\tau^c\widetilde{Q}^{\,k})_{0k}\rangle_{0=\alpha}\ . \tag{49}$$

Using Eq. (49), the last term of Eq. (48) may be written as $\sum_{k\,(\neq 0)}(\tau^c\gamma_k^{0\alpha}\tau^c)_{00}$. By substituting for Q^0 using Eq. (41) in the second term of Eq. (48), by substituting for $\widetilde{Q}^{\,0}$ using Eq. (42) in the third term of Eq. (48), and by use of Eqs. (41) and (42) in the first term, we obtain

$$\begin{aligned}K^{0\alpha}=\tau^{c00}J^\alpha\tau^{c00}+\tau^{c00}x^\alpha\tau^{c00}J^\alpha\tau^{c00}+\tau^{c00}J^\alpha\tau^{c00}x^\alpha\tau^{c00}+\tau^{c00}x^\alpha\tau^{c00}J^\alpha\tau^{c00}x^\alpha\tau^{c00}+\sum_{k\,(\neq 0)}\tau^{c00}x^\alpha(\tau^c\gamma_k^{0\alpha}\tau^c)_{00}x^\alpha\tau^{c00}&\\+\sum_{k\,(\neq 0)}(\tau^c\gamma_k^{0\alpha}\tau^c)_{00}x^\alpha\tau^{c00}+\sum_{k\,(\neq 0)}\tau^{c00}x^\alpha(\tau^c\gamma_k^{0\alpha}\tau^c)_{00}+\sum_{k\,(\neq 0)}(\tau^c\gamma_k^{0\alpha}\tau^c)_{00}\ .&\end{aligned} \tag{50}$$

Equation (50) can be simplified by defining an operator D^α,

$$D^\alpha=1+\tau^{c00}x^\alpha=(1-\tau^{c00}\Delta m)^{-1}\ , \tag{51}$$

$$\widetilde{D}^{\,\alpha}=1+x^\alpha\tau^{c00}=(1-\Delta m\,\tau^{c00})^{-1}\ , \tag{52}$$

which has the property of converting a site-diagonal SPO for a periodic system into the SPO for a system with an impurity,

$$\tau^{c00,(\alpha)}=D^\alpha\tau^{c00}=\tau^{c00}\widetilde{D}^{\,\alpha}\ . \tag{53}$$

Here, $\tau^{c00,(\alpha)}$ is the SPO for a system with an atom of type α at the origin and coherent scatterers on all other sites. Use of Eqs. (51) and (52) to simplify Eq. (50) yields

$$K^{0\alpha}=D^\alpha\widetilde{K}^{\,0\alpha}\widetilde{D}^{\,\alpha}\ , \tag{54}$$

$$\widetilde{K}^{\,0\alpha}=\tau^{c00}J^\alpha\tau^{c00}+\sum_{k\,(\neq 0)}\tau^{c0k}\gamma_\kappa^{0\alpha}\tau^{ck0}\ . \tag{55}$$

The evaluation of $L^{0\alpha,n\beta}$, Eq. (40), proceeds similarly to that of $K^{0\alpha}$, but it is even more tedious because of the additional restriction on the ensemble average. The details of the evaluation are given in Appendix B. The result is

$$L^{0\alpha,n\beta}=D^\alpha\widetilde{L}^{\,0n\beta(\alpha)}\widetilde{D}^{\,\alpha}\ , \tag{56}$$

$$\widetilde{L}^{\,0n\beta(\alpha)}=\tau^{c0n}\widetilde{J}^{\,\beta}\tau^{cn0}+\sum_{k\,(\neq 0,n)}\tau^{c0k}\gamma_k^{n\beta(\alpha)}\tau^{ck0}\ , \tag{57}$$

$$\widetilde{J}^{\,\beta}=\widetilde{D}^{\,\beta}J^\beta D^\beta\ , \tag{58}$$

$$\gamma_k^{n\beta(\alpha)}=\langle(Q^k\tau^c)_{kn}\widetilde{J}^{\,\beta}(\tau^c\widetilde{Q}^{\,k})_{nk}\rangle_{0=\alpha,\,n=\beta}\ . \tag{59}$$

Equations (49) and (54)—(59) are the primary results of this section. These equations determine the conductivity through Eqs. (37) and (38). There remains the problem of solving for the vertex functions $\gamma_k^{0\alpha}$, Eq. (49), and $\gamma_k^{n\beta(\alpha)}$, Eq. (59). In the next section these vertex functions will be written in terms of the response functions $\widetilde{K}$ thereby providing a closed set of equations for the conductivity.

IV. VERTEX FUNCTIONS, RESPONSE FUNCTIONS, AND CONDUCTIVITY

Equations (49) and (59) represent a ladderlike approximation for the vertex functions $\gamma_k^{0\alpha}$ and $\gamma_k^{n\beta(\alpha)}$, respectively. The second vertex function is slightly different from the first because two atoms are specified in its definition

($0=\alpha$, $n=\beta$), whereas only one ($0=\alpha$) is specified in the definition of $\gamma_k^{0\alpha}$. Since neither k nor n may equal 0 in Eq. (59), it should cause only a very small error to neglect the dependence of $\gamma_k^{n\beta(\alpha)}$ on α. Thus in the following it will be assumed that

$$\gamma_k^{n\beta(\alpha)}=\gamma_k^{n\beta}=\langle (Q^k\tau^c)_{kn}J^\beta(\tau^c\widetilde{Q}^k)_{nk}\rangle_{n=\beta} . \tag{60}$$

Approximation equation (60) also simplifies Eq. (57) by removing an implicit dependence on α, and thus $\widetilde{L}^{0n\beta(\alpha)}\rightarrow\widetilde{L}^{0n\beta}$.

The vertex function, Eq. (60), can be expanded using Eqs. (41) and (42). Neglecting repeated scattering between pairs of sites one obtains

$$\begin{aligned}\gamma_k^{n\beta}={}&\langle x^k\tau^{ckn}J^\beta\tau^{cnk}x^k\rangle_{n=\beta}+\langle x^k\tau^{ckn}x^\beta\tau^{cnn}J^\beta\tau^{cnk}x^k\rangle_{n=\beta}+\langle x^k\tau^{ckn}J^\beta\tau^{cnn}x^\beta\tau^{cnk}x^k\rangle_{n=\beta}\\&+\langle x^k\tau^{ckn}x^\beta\tau^{cnn}J^\beta\tau^{cnn}x^\beta\tau^{cnk}x^k\rangle_{n=\beta}+\sum_{l\,(\neq k,n)}\langle x^k\tau^{ckl}(Q^l\tau^c)_{ln}J^\beta(\tau^c\widetilde{Q}^l)_{nl}\tau^{clk}x^k\rangle_{n=\beta} .\end{aligned} \tag{61}$$

Use of Eqs. (51), (52), (58), and (60) yields a closed equation for the vertex function,

$$\gamma_k^{n\beta}=\langle x^k\tau^{ckn}\widetilde{J}^\beta\tau^{cnk}x^k\rangle+\sum_{l\,(\neq k,n)}\langle x^k\tau^{ckl}\gamma_l^{n\beta}\tau^{clk}x^k\rangle_{n=\beta} . \tag{62}$$

Comparison of Eqs. (62) and (57) allows the vertex function $\gamma_k^{n\beta}$ to be written in terms of the response function $\widetilde{L}^{kn\beta}$,

$$\gamma_k^{n\beta}=\sum_\alpha c^\alpha x^\alpha\widetilde{L}^{kn\beta}x^\alpha . \tag{63}$$

Equation (63) can be used to derive closed expressions for the conductivity response functions.

We now have a closed set of equations for the conductivity of a random alloy in the KKR-CPA approximation. They consist of Eqs. (5), (20), (37), and (38), the latter two of which may be written as

$$\widetilde{\sigma}^0_{\mu\nu}(z_1,z_2)=-\frac{4m^2}{\pi\hbar^3\Omega}\sum_\alpha\sum_{L_1,L_4}c^\alpha\widetilde{J}^{\alpha\mu}_{L_4L_1}(z_2,z_1)\widetilde{K}^{0\alpha}_\nu(z_1,z_2;L_1,L_4) \tag{37$'$}$$

and

$$\widetilde{\sigma}^1_{\mu\nu}(z_1,z_2)=-\frac{4m^2}{\pi\hbar^3\Omega}\sum_{n\,(\neq 0)}\sum_{\alpha,\beta}\sum_{L_1,L_4}c^\alpha c^\beta\widetilde{J}^{\alpha\mu}_{L_4L_1}(z_2,z_1)\widetilde{L}^{0n\beta}_\nu(z_1,z_2;L_1,L_4) . \tag{38$'$}$$

The matrix elements $\widetilde{J}$ are defined by Eqs. (58) and (19), and the response functions are given by

$$\begin{aligned}\widetilde{K}^{0\alpha}_\nu(z_1,z_2;L_1,L_4)={}&\sum_{L_2,L_3}\tau^{c00}_{L_1L_2}(z_1)J^{\alpha\nu}_{L_2L_3}(z_1,z_2)\tau^{c00}_{L_3L_4}(z_2)\\&+\sum_{k\,(\neq 0)}\sum_{L_2,L_3}\sum_{L_2',L_3'}\tau^{c0k}_{L_1L_2}\widetilde{L}^{k0\alpha}_\nu(z_1,z_2;L_2'L_3')w(z_1z_2;L_2L_2';L_3L_3')\tau^{ck0}_{L_3L_4}(z_2) ,\end{aligned} \tag{64}$$

$$\begin{aligned}\widetilde{L}^{0n\beta}_\nu(z_1,z_2;L_1,L_4)={}&\sum_{L_2,L_3}\tau^{c0n}_{L_1L_2}(z_1)\widetilde{J}^{\beta\nu}_{L_2L_3}(z_1,z_2)\tau^{cn0}_{L_3L_4}(z_2)\\&+\sum_{k\,(\neq 0,n)}\sum_{L_2,L_3}\sum_{L_2',L_3'}\tau^{c0k}_{L_1L_2}(z_1)\widetilde{L}^{kn\beta}_\nu(z_1,z_2;L_2'L_3')w(z_1z_2;L_2L_2';L_3L_3')\tau^{ck0}_{L_3L_4} .\end{aligned} \tag{65}$$

The effective "interaction" which appears in Eqs. (64) and (65) is

$$w(z_1,z_2;L_1,L_1';L_2,L_2')=\sum_\alpha c^\alpha x^\alpha_{L_1L_1'}(z_1)x^\alpha_{L_2L_2'}(z_2) . \tag{66}$$

The remaining quantities appearing in these equations, $x^\alpha_{LL'}$ and $\tau^{cmn}_{LL'}$ are given by Eqs. (34) and (24)–(26), respectively.

V. SOLUTION OF THE TRANSPORT EQUATION

There remains only the problem of solving Eq. (65) to determine the response function $\widetilde{L}^{0n\beta}_\nu$. Fortunately, the solution is surprisingly simple. Let us begin by defining a function $\chi^{0n}(z_1,z_2;K_1,K_2)$,

$$\chi^{0n}(z_1,z_2;K_1,K_2)=\begin{cases}\tau^{c0n}_{L_1L_2}(z_1)\tau^{cn0}_{L_3L_4}(z_2), & n\neq 0\\ 0, & n=0\end{cases} \tag{67}$$

where K_1 stands for the pair of indices (L_1,L_4), and K_2 stands for the pair (L_2,L_3).

Consider Eq. (65) and the function $\widetilde{L}^{0n\beta}_\nu$. Since Eq. (65) is only valid for $n\neq 0$, and since the $k=n$ term is omitted in the second terms on the rhs of Eq. (65), we can define

$$\widetilde{L}^{nn\beta}_\nu=0 . \tag{68}$$

Using Eqs. (67) and (68) and the new notation in which a single index K_i represents a pair of indices $(L_i,L_{i'})$, we have, for Eq. (65) (omitting nonessential indices and variables),

$$\tilde{L}^{0n}(K_1)=\sum_{K_2}\chi^{0n}(K_1,K_2)\tilde{J}(K_2)+\sum_{k}\sum_{K_2}\sum_{K_3}\chi^{0k}(K_1,K_2)w(K_2,K_3)\tilde{L}^{kn}(K_3)\ . \tag{69}$$

Equation (69) can be solved by defining Fourier transforms,

$$\chi_{K_1K_2}(q)=\sum_{n}\chi^{0n}(K_1,K_2)e^{i\mathbf{q}\cdot\mathbf{R}_n}\ , \tag{70}$$

$$\tilde{L}_K(q)=\sum_{n}\tilde{L}^{0n}(K)e^{i\mathbf{q}\cdot\mathbf{R}_n}\ . \tag{71}$$

Using Eqs. (70) and (71), Eq. (69) becomes

$$\tilde{L}(q)=\chi(q)\tilde{J}+\chi(q)w\tilde{L}(q)\ , \tag{72}$$

which has a solution

$$\tilde{L}(q)=[1-\chi(q)w]^{-1}\chi(q)\tilde{J}\ . \tag{73}$$

In fact, only the $q=0$ limit of Eq. (73) is needed in σ^1, since, from Eq. (38′), we have

$$\tilde{\sigma}^{1}_{\mu\nu}=\frac{-4m^2}{\pi\hbar^3\Omega}\sum_{\alpha,\beta}c^{\alpha}c^{\beta}\sum_{K,K'}\tilde{J}^{\alpha\mu}_{K}\{[1-\chi(0)w]^{-1}\chi(0)\}_{KK'}\tilde{J}^{\beta\nu}_{K'}\ . \tag{74}$$

The second term on the rhs of Eq. (64) vanishes since it is proportional to

$$\int d^3q\,\chi(q)w\tilde{L}(q)=\int d^3q[\tilde{L}(q)-\chi(q)\tilde{J}]\ . \tag{75}$$

But both terms on the rhs of Eq. (75) are zero owing to Eqs. (68) and (67), respectively. Thus, in addition to Eq. (74), the conductivity is determined by

$$\tilde{\sigma}^{0}_{\mu\nu}(z_1,z_2)=\frac{-4m^2}{\pi\hbar^3\Omega}\sum_{\alpha}\sum_{L_1,L_2,L_3,L_4}c^{\alpha}\tilde{J}^{\alpha\mu}_{L_4L_1}(z_2,z_1)\tau^{c00}_{L_1L_2}(z_1)J^{\alpha\nu}_{L_2L_3}(z_1,z_2)\tau^{c00}_{L_3L_4}(z_2)\ . \tag{76}$$

VI. DERIVATION OF THE BOLTZMANN EQUATION

In this section it will be shown that Eqs. (74) and (76) have the same solution as the semiclassical Boltzmann equation if the electronic energy bands in the alloy are well defined. For simplicity of exposition, the case in which "vertex corrections" are neglected will be considered first. Vertex corrections are neglected by replacing the matrix $[1-\chi(0)w]^{-1}$ in Eq. (74) with the unit matrix. The conductivity $\tilde{\sigma}^{\text{NVC}}$, including the contributions from Eq. (76), as well as Eq. (74), is then

$$\tilde{\sigma}^{\text{NVC}}_{\mu\nu}(z_1,z_2)=\frac{-4m^2}{\pi\hbar^3\Omega}\sum_{\alpha,\beta}\sum_{\substack{L_1L_1'\\L_2,L_2'}}c^{\alpha}c^{\beta}\tilde{J}^{\alpha\mu}_{L_1L_1'}(z_2,z_1)\left[\frac{1}{\Omega_z}\int_{\text{BZ}}d^3q[M(\mathbf{q},z_1)]^{-1}_{L_1'L_2}[M(\mathbf{q},z_2)]^{-1}_{L_2'L_1}\tilde{J}^{\beta\nu}_{L_2L_2'}(z_1,z_2)\right.$$
$$\left.+\tau^{c00}_{L_1'L_2}(z_1)\tau^{c00}_{L_2'L_1}(z_2)[J^{\alpha\nu}_{L_2L_2'}(z_1,z_2)-\tilde{J}^{\beta\nu}_{L_2L_2'}(z_1,z_2)]\right]\ , \tag{77}$$

where Eq. (24) was used to represent $\sum_n\tau^{c0n}\tau^{cn0}$ as a Brillouin-zone integral.

The second term of Eq. (77) will be negligible compared to the first when the mean free path is long, because the Brillouin-zone integral in the first term contains singular contributions (to be discussed below) which make it much larger than the product of the diagonal scattering path operators in the second term. In addition, the difference $J^{\alpha\nu}-\tilde{J}^{\beta\nu}$ vanishes in the limit of a periodic system. We can also simplify Eq. (77) further by defining

$$\bar{J}^{\mu}_{LL'}(z_1,z_2)=\sum_{\alpha}c^{\alpha}\tilde{J}^{\alpha\mu}_{LL'}(z_1,z_2)\ , \tag{78}$$

so that $\tilde{\sigma}^{\text{NVC}}_{\mu\nu}(z_1,z_2)$ becomes

$$\tilde{\sigma}^{\text{NVC}}_{\mu\nu}(z_1,z_2)=\frac{-4m^2}{\pi\hbar^3\Omega}\sum_{\substack{L_1,L_1'\\L_2,L_2'}}\bar{J}^{\mu}_{L_1L_1'}(z_2,z_1)\bar{J}^{\nu}_{L_2L_2'}(z_1,z_2)\frac{1}{\Omega_z}\int_{\text{BZ}}d^3q[M(\mathbf{q},z_1)]^{-1}_{L_1'L_2}[M(\mathbf{q},z_2)]^{-1}_{L_2'L_1}\ . \tag{79}$$

The integrand of the Brillouin-zone integral will have singularities for those values of $\mathbf{q}$ for which the determinant of the matrix $M(\mathbf{q},z)$ vanishes. Because of the disorder, these singularities will occur for complex values of $\mathbf{q}$. The assumption that the bands are well defined, however, is equivalent to the assumption that the singularities occur *near* the real axis. Suppose a singularity for energy z is at $\mathbf{q}_0(z)$; then, for $\mathbf{q}\approx\mathbf{q}_0$, we can write[14]

$$[M(\mathbf{q},z)]^{-1}_{LL'}=\frac{\hbar^2}{2m}i^{l-l'}\frac{C^{c}_{L}(\mathbf{q}_0,z)C^{c}_{L'}(q_0,z)}{z-\varepsilon_{\mathbf{q}}}\ , \tag{80}$$

where $C_L^c(\mathbf{q}_0,z)$ is a coherent-wave-function coefficient satisfying

$$\sum_{L'} M_{LL'}(\mathbf{q}_0,z)i^{l'}C_{L'}^c(q_0,z)=0 \ , \tag{81}$$

$$\sum_{L} i^{-l}C_L^c(\mathbf{q}_0,z)M_{LL'}(\mathbf{q}_0,z)=0 \ . \tag{82}$$

The "coherent wave function" and its use in calculating matrix elements is described in Appendix C.

The denominator in Eq. (80) vanishes when the band energy ε_q is equal to z. By assumption, this occurs at wave vector $\mathbf{q}_0$. Thus Eq. (80) may be written (for $\mathbf{q}\approx\mathbf{q}_0$) as

$$[M(\mathbf{q},z)]_{LL'}^{-1}=\frac{\hbar^2 C_L^c(q_0,z)C_{L'}^c(q_0,z)i^{l-l'}}{-2m(\nabla_q\varepsilon_q)_{q_0(z)}\cdot[\mathbf{q}-\mathbf{q}_0(z)]} \ . \tag{83}$$

The singular contributions to the Brillouin-zone integral, Eq. (79), will be of the form

$$I=\int dq\frac{1}{[q-q_0(z_1)]}\,\frac{1}{[q-q_0(z_2)]} \ . \tag{84}$$

When $z_1=z_2$ $(=\varepsilon\pm i\eta)$, the integral, Eq. (84), will be negligibly small compared to the case in which $z_2=z_1^*$, for then $q_0(z_2)=q_0^*(z_1)$, and Eq. (84) can be approximated by

$$I=\int dq\frac{1}{(q-q_0^1)^2+\gamma_q^2}=\frac{\pi}{\gamma_q} \ , \tag{85}$$

where $\gamma_q=|\operatorname{Im}[q_0 z_1)]|$ is essentially the inverse of the mean free path, and $q_0^1=\operatorname{Re}[q_0(z_1)]$.

In Appendix C it is argued that the alloy group velocity $\mathbf{v}_q=\hbar^{-1}\nabla_q\varepsilon_q$ is given by

$$ev_{q_0}^{\mu}=\sum_{L,L'} C_L^c(q_0,\varepsilon)C_{L'}^c(q_0,\varepsilon)\bar{J}_{LL'}^{\mu}(\varepsilon,\varepsilon)i^{l'-l} \ . \tag{86}$$

Using Eqs. (80), (85), and (86) in Eq. (79), we have

$$\tilde{\sigma}_{\mu\nu}^{\mathrm{NVC}}(\varepsilon\pm i\eta,\varepsilon\mp i\eta)=-\frac{\hbar e^2}{(2\pi)^3}\int d\hat{\mathbf{q}}\frac{q_0^2}{[\hat{\mathbf{q}}\cdot(\nabla_q\varepsilon_q)_{q_0}]^2} \times\frac{v_{q_0}^{\mu}v_{q_0}^{\nu}}{\gamma_{q_0}} \ . \tag{87}$$

Equation (87) can be put in a more familiar form by recognizing that the factor $\hbar/[\gamma_{q_0}(\hat{\mathbf{q}}\cdot\nabla_q\varepsilon_q)_{q_0}]$ is a lifetime,

$$\hbar/[\gamma_{q_0}(\hat{\mathbf{q}}\cdot\nabla_q\varepsilon_q)_{q_0}]=2\tau_q^B \ . \tag{88}$$

It is actually twice the Boltzmann lifetime because γ_{q_0} describes an *amplitude* decay which is only one-half as fast as the *density* decay which appears in the Boltzmann equation. The factor $\hat{\mathbf{q}}\cdot\nabla_q\varepsilon_q$ converts a width in q along direction $\hat{\mathbf{q}}$ into a width in energy. The final result for the conductivity neglecting vertex corrections and assuming well-defined energy bands is

$$\begin{aligned}\sigma_{\mu\nu}^{\mathrm{NVC}}(\varepsilon)&=-\tfrac{1}{4}[\tilde{\sigma}_{\mu\nu}^{\mathrm{NVC}}(\varepsilon+i\eta,\varepsilon-i\eta)\\&\qquad+\tilde{\sigma}_{\mu\nu}^{\mathrm{NVC}}(\varepsilon-i\eta,\varepsilon+i\eta)]\\&=\frac{e^2}{(2\pi)^3}\int_{\varepsilon}\frac{dS_q}{\hbar v_q}v_q^{\mu}v_q^{\nu}\tau_q^B \ ,\end{aligned} \tag{89}$$

where the integral is over the alloy Fermi surface. This is the Boltzmann-type formula[15] (neglecting vertex corrections and excluding a factor of 2 for spin) which was used to calculate the conductivity in Refs. 3–5.

In order to show that when the bands are well defined Eqs. (74) and (76) yield the same solution as the Boltzmann equation (including vertex corrections), we first write the Boltzmann equation and solve it. For an electric field in the ν direction it is[16]

$$eEv_q^{\nu}\frac{\partial f}{\partial\varepsilon_q}=\sum_{q'}P_{qq'}(g_q^{\nu}-g_{q'}^{\nu}) \ , \tag{90}$$

where f is the Fermi function, $P_{qq'}$ is the probability for an electron to scatter between states q and q', and g_q^{ν} is the "deviation" function which describes the departure of the electron distribution from the Fermi function. If Eq. (90) is solved for g_q^{ν}, then the conductivity (per spin) may be obtained from

$$\sigma_{\mu\nu}=-e\sum_{q}v_q^{\mu}g_q^{\nu}E^{-1} \ . \tag{91}$$

Since $P_{qq'}$ is the probability for an electron to scatter between states q and q', the total scattering rate, or inverse lifetime for an electron in state q, is

$$(\tau_q^B)^{-1}=\sum_{q'}P_{qq'} \ . \tag{92}$$

Use of Eq. (92) in Eq. (90) yields

$$-eEv_q^{\nu}\frac{\partial f}{\partial\varepsilon_q}\tau_q^B=g_q^{\nu}-\tau_q^B\sum_{q'}P_{qq'}g_{q'}^{\nu} \ , \tag{93}$$

which may be solved for g_q^{ν},

$$g_q^{\nu}=-\sum_{q'}[1-\tau^B P]_{qq'}^{-1}eEv_{q'}^{\nu}\frac{\partial f}{\partial\varepsilon_{q'}}\tau_{q'}^B \ . \tag{94}$$

From Eqs. (91) and (94), the Boltzmann conductivity at zero temperature including vertex corrections is

$$\sigma_{\mu\nu}(\varepsilon_F)=e^2\sum_{q,q'}v_q^{\mu}[1-\tau^B P]_{qq'}^{-1}v_{q'}^{\nu}\tau_{q'}^B\delta(\varepsilon_F-\varepsilon_{q'}) \ . \tag{95}$$

If the matrix $[1-\tau^B P]_{qq'}^{-1}$ in Eq. (95) is replaced by $\delta_{qq'}$, Eq. (89) is recovered. This result may also be obtained by neglecting the "scattering-in" term of Eq. (90), the second term on the rhs. From the structures of Eqs. (95) and (74), it seems reasonable to speculate that the two expansions

$$-\tilde{\sigma}_{\mu\nu}(\varepsilon+i\eta,\varepsilon-i\eta)=-\tilde{\sigma}_{\mu\nu}(z,z^*)=\frac{4m^2}{\pi\Omega\hbar^3}\mathrm{Tr}\{\bar{J}^{\mu}(z^*,z)[\chi(0)+\chi(0)w\chi(0)+\chi(0)w\chi(0)w\chi(0)+\cdots]\bar{J}^{\nu}(z,z^*)\} \tag{96}$$

and

$$\sigma_{\mu\nu}(\varepsilon)=e^2\sum_{q,q'} v_q^\mu[\tau_q^B\delta_{qq'}+\tau_q^B P_{qq'}\tau_{q'}^B+\cdots]v_q^\nu\delta(\varepsilon-\varepsilon_q) \tag{97}$$

might be equal term by term in the limit of well-defined bands. This is, in fact, the case. The equality of the first terms was demonstrated by Eq. (89). The equality of the second terms can also be shown straightforwardly. The second term of Eq. (96) is approximately

$$\begin{aligned}\frac{+4m^2}{\pi\Omega\hbar^3}\sum_{L_1,L_1'}\sum_{L_2,L_2'}\sum_{L_3,L_3'}\sum_{L_4,L_4'}&\bar{J}^{\mu}_{L_1L_1'}(z^*,z)\bar{J}^{\nu}_{L_4L_4'}(z^*,z)\\ &\times\frac{1}{\Omega_z}\int d\hat{\mathbf{q}}\frac{q_0^2}{[\hat{\mathbf{q}}\cdot(\nabla_q\varepsilon_q)_{q_0}]^2}\frac{\pi}{\gamma_{q_0}}i^{l_1'-l_2}C_{L_1'}(q_0,z)C_{L_2}(q_0,z)C_{L_2'}(q_0,z^*)C_{L_1}(q_0,z^*)i^{l_2'-l_1}\\ &\times\sum_\alpha c^\alpha x^\alpha_{L_2L_3'}(z)x^\alpha_{L_2'L_3}(z^*)\\ &\times\frac{1}{\Omega_z}\int d\hat{\mathbf{q}}'\frac{q_0'^2}{[\hat{\mathbf{q}}'\cdot(\nabla_{q'}\varepsilon_{q'})_{q_0'}]^2}\frac{\pi}{\gamma_{q_0'}}i^{l_3'-l_4}C_{L_3'}(q_0',z)C_{L_4}(q_0',z)C_{L_4'}(q_0',z^*)C_{L_3}(q_0',z^*)i^{l_4'-l_3}\ ,\end{aligned} \tag{98}$$

which, using Eqs. (86) and (88), can be written as

$$\frac{\hbar\pi^4}{(2\pi)^3\Omega_z}\int\frac{dS_q}{\hbar v_q}\int\frac{dS_{q'}}{\hbar v_q'}\tau_q^B\tau_{q'}^B v_q^\mu v_{q'}^\nu\sum_\alpha c^\alpha|T^\alpha_{qq'}|^2\ , \tag{99}$$

where $T^\alpha_{qq'}(z)=[T^\alpha_{qq'}(z^*)]^*$ is

$$T^\alpha_{qq'}(z)=\sum_{L,L'}C_L(q,z)C_{L'}(q',z)x^\alpha_{LL'}(z)i^{l'-l}\ . \tag{100}$$

Equation (99) is equivalent to the second term of Eq. (97) if $P_{qq'}$ is related to the transition probability in Eqs. (99) and (100) through

$$P_{qq'}=\frac{2\pi}{\hbar}\sum_\alpha c^\alpha|T^\alpha_{qq'}|^2\delta(\varepsilon_q-\varepsilon_{q'})\ . \tag{101}$$

Using Eqs. (100) and (101) it is straightforward to demonstrate the equivalence of the higher-order terms in the expansions of Eqs. (95) and (74).

In this section it has not only been shown that Eq. (74) reduces to a Boltzmann-like equation, but an explicit result has been obtained for the scattering probability, Eqs. (100) and (101). In the limit of low concentration these equations reduce to the accepted results for impurity scattering within the muffin-tin formalism.[17–20]

In order to show that Eqs. (100) and (101) are also correct for arbitrary concentration but weak scattering, it is convenient to use the average cotangent approximation to determine the reference energy bands. Thus

$$m_L^c=\bar{m}_L+\delta m_L\ , \tag{102}$$

where

$$\bar{m}_L=c^A m_L^A+c^B m_L^B\ . \tag{103}$$

From the CPA equation (A4) we obtain (to lowest nonvanishing order in m^A-m^B)

$$\delta m=-c^Ac^B(m^A-m^B)\tau^{00}[\bar{m}](m^A-m^B)\ , \tag{104}$$

where $\tau^{00}[\bar{m}]$ is τ^{00} for a periodic system with a t matrix on each site equal to $\bar{m}^{-1}$. The scattering probability in this approximation is

$$\begin{aligned}P_{qq'}=\frac{2\pi}{\hbar}\sum_{L,L'}&C_L(q)C_{L'}(q)C_L(q')C_{L'}(q')c^Ac^B(m_L^A-m_L^B)\\ &\times(m_{L'}^A-m_{L'}^B)\delta(\varepsilon_q-\varepsilon_{q'})\ ,\end{aligned} \tag{105}$$

which may be written as[21]

$$P_{qq'}=\frac{2\pi}{\hbar}\sum_\alpha c^\alpha(\Delta v^\alpha_{qq'})^2\delta(\varepsilon_q-\varepsilon_{q'})\ , \tag{106}$$

$$\Delta V^\alpha_{qq'}=\int d^3r\,\Psi_q^*(r)\left[v^\alpha-\sum_\alpha c^\alpha v^\alpha\right]\Psi_{q'}(r)\ . \tag{107}$$

Equations (106) and (107) are simply the "Fermi golden rule" and are valid if $v^A(\mathbf{r})-v^B(\mathbf{r})$, the difference between the atomic potentials, is sufficiently small, so Eqs. (100) and (101) are correct in that limit.

As a final demonstration of the reasonableness of Eqs. (100) and (101), we note that the Boltzmann lifetime calculated from Eq. (101) using Eq. (92) should be consistent with the position in the complex energy plane of the pole which determines the alloy energy band. Thus if $\mathbf{q}$ is real, the equation

$$\det[M(\mathbf{q},z_c)]=0 \tag{108}$$

will determine $z_c(\mathbf{q})$, the complex energy band. The imaginary part of $z_c(\mathbf{q})$ should be related to the Boltzmann lifetime through

$$2\,\mathrm{Im}[z_c(q)]\approx\hbar/\tau_q^B\ . \tag{109}$$

It is shown in Appendix D that Eq. (109) is valid through terms of order three in m^A-m^B.

VII. A ONE-DIMENSIONAL EXAMPLE

In one dimension the electronic states of a disordered system are localized and an exact evaluation of the conductivity [Eq. (2)] should yield zero. The theory described in this paper does not include the quantum-interference effects[22] necessary to properly treat localized states. I suspect, in fact, that Eqs. (74) and (76) will always yield a nonzero conductivity if the CPA density of states is nonzero in the vicinity of the Fermi energy. It is instructive, nevertheless, to treat a one-dimensional example before proceeding with three-dimensional calculations. The objective of this exercise is not an understanding of physical one-dimensional systems, but rather a better understanding of Eqs. (74) and (76).

Fortunately, there is a one-dimensional version of the KKR-CPA (Ref. 23) that preserves the structure of the three-dimensional version. In one dimension, however, all of the quantities that enter Eqs. (74) and (76) can be expressed analytically in terms of the scattering properties t^A and t^B of the alloy potentials and of the scattering properties t^c of the coherent potential. The CPA must still be solved numerically to determine t^c, but that task can be reduced to finding the zeros of a fourth-order polynomial.

We begin with a one-dimensional Hamiltonian,

$$-\left[\frac{\hbar^2}{2m}\right]\frac{d^2}{dx^2}+\sum_n v_n(x-na)\ , \tag{110}$$

in which the potentials $v_n(x)$ are symmetric and may be of either type A (with probability c^A) or of type B (with probability c^B). The first step in solving for the conductivity is to determine the scattering properties of $v^A(|x|)$ and $v^B(|x|)$. Just as in three dimensions, we use a partial-wave basis. The single-potential Schrödinger equation,

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+v^\alpha(r)-\varepsilon\right]Z_l^\alpha(x,\varepsilon)=0\ , \tag{111}$$

has regular solutions $Z_l^\alpha(x,\varepsilon)$ which can be expressed in terms of "one-dimensional spherical waves,"

$$Z_l^\alpha(x,\varepsilon)=R_l^\alpha(r,\varepsilon)Y_l(\hat{x})\ , \tag{112}$$

which for values of r greater than r_{MT}, the muffin-tin radius, may be written as

$$R_l^\alpha(r,\varepsilon)=-\kappa^{-1}[j_l(\kappa r)\cot\eta_l^\alpha(\varepsilon)-n_l^\alpha(\kappa r)] \qquad (r=|x|>r_{\mathrm{MT}})\ , \tag{113}$$

$$\kappa=(2m\varepsilon/\hbar^2)^{1/2}\ . \tag{114}$$

In one dimension the "spherical harmonics" are given by

$$Y_0(\hat{x})=1/\sqrt{2}\ , \tag{115}$$

$$Y_1(\hat{x})=\frac{1}{\sqrt{2}}\frac{x}{r}=\frac{1}{\sqrt{2}}\mathrm{sgn}(x)\ , \tag{116}$$

and the one-dimensional "spherical Bessel functions" are sines and cosines,

$$j_l(\rho)=\cos(\rho-l\pi/2)\ , \tag{117}$$

$$n_l(\rho)=\sin(\rho-l\pi/2)\ . \tag{118}$$

The phase shifts obtained in Eq. (113) define the scattering properties of the individual potentials,

$$m_l^\alpha(\varepsilon)=(t_l^\alpha)^{-1}=-\kappa^{-1}(\cot\eta_l^\alpha-i)\ . \tag{119}$$

Once the scattering properties of the individual potentials have been obtained, the next step is to solve the CPA equations,

$$m_l^c=c^A m_l^A+c^B m_l^B+(m_l^c-m_l^A)\tau_l^{c00}(m_l^c-m_l^B)\ , \tag{120}$$

to determine m_l^c. This is easier in one dimension than in three because there is an analytic expression for τ_l^{c00} in one dimension given by Eqs. (3.3)—(3.7) of Ref. 23.

The above steps are necessary in a KKR-CPA calculation for the single-particle properties. The additional steps necessary to obtain the conductivity are the calculation of D_l^α [Eqs. (51) and (52)], $J_{ll'}^\alpha$ [Eq. (19)], and $\chi(0)$ [Eq. (70)]. The first of these is trivial since the KKR-CPA equation (120) can be easily manipulated to yield

$$D_l^{A\,(B)}=\frac{[m_l^c-m_l^{B\,(A)}]}{[\overline{m}_l-m_l^{B\,(A)}]}\ , \tag{121}$$

$$\overline{m}_l=c^A m_l^A+c^B m_l^B\ . \tag{122}$$

The current matrix elements will probably have to be determined numerically in three dimensions, but in one dimension they can be determined analytically. The one-dimensional version of Eq. (19) is

$$J_{ll'}^\alpha(z_1,z_2)=\frac{-ie\hbar}{m}\int_0^{a/2}dr\,R_l^\alpha(r,z_1)\frac{d}{dr}R_{l'}^\alpha(r,z_2)\ . \tag{123}$$

Since

$$m_l^\alpha(z^*)=[m_l^\alpha(z)]^*\ , \tag{124}$$

it follows that

$$\lim_{\eta\to 0}R_l^\alpha(r,\varepsilon\pm i\eta)=(\pm 1)^l R_l^\alpha(r,\varepsilon)\ , \tag{125}$$

so that if $z_1=\varepsilon+i\eta$ and $z_2=\varepsilon-i\eta$, we have

$$\lim_{\eta\to 0}J_{01}^\alpha(z_1,z_2)=\lim_{\eta\to 0}J_{01}^\alpha(z_2,z_2)\ , \tag{126}$$

$$\lim_{\eta\to 0}J_{10}^\alpha(z_1,z_2)=\lim_{\eta\to 0}J_{10}^\alpha(z_1,z_1)\ . \tag{127}$$

The equal energy matrix elements can be obtained very simply since

$$J_{01}^\alpha(z,z)+J_{10}^\alpha(z,z)=\frac{-ie\hbar}{m}R_0^\alpha(a/2,z)R_1^\alpha(a/2,z) \tag{128}$$

and

$$J_{01}^\alpha(z,z)-J_{10}^\alpha(z,z)=\int_0^{a/2}W(z,x)dx\ , \tag{129}$$

where $W(z,x)$ is independent of x, as may be shown by use of Eq. (111). Thus,

$$J_{01}^\alpha(z,z)-J_{10}^\alpha(z,z)=\frac{ie\hbar}{m}\frac{a}{2}\kappa^{-1}(1+\cot\eta_0^\alpha\cot\eta_1^\alpha)\ . \tag{130}$$

The calculation of $\chi(0)$ can also be performed analytically. From Eqs. (67) and (70), we have

$$\chi_{K_1K_2}(q=0,z_1,z_2)=\sum_{n\,(\neq 0)}\tau_{l_1l_2}^{c0n}(z_1)\tau_{l_3l_4}^{cn0}(z_2)\ , \qquad K_1=\{l_4,l_1\},\ \ K_2=\{l_2,l_3\}\ . \tag{131}$$

Equation (131) contains $\tau_{ll'}^{c0n}$, which may be evaluated by a slight extension of the techniques used in obtaining Eqs. (3.7a) and (3.7b) of Ref. 23. We have

$$\tau^{c0n}_{ll}=\frac{-\kappa\cot\eta^c_{l'}}{1+\cot\eta^c_0\cot\eta^c_1}\frac{\cos\theta_c-f_{l'}}{i\sin\theta_c}e^{i|n|\theta_c}, \tag{132}$$

$$\tau^{c0n}_{ll'}=\frac{(-1)^{l'}\kappa}{1+\cot\eta^c_0\cot\eta^c_1}e^{i|n|\theta_c}sgn(n),\quad l\neq l' \tag{133}$$

$$\cos\theta_c=\frac{\cos(\kappa a+\eta^c_0+\eta^c_1)}{\cos(\eta^c_0-\eta^c_1)}, \tag{134}$$

$$f_l=\cos(\kappa a)-\tan\eta^c_l\sin(\kappa a). \tag{135}$$

The angle θ_c is the complex value of qa at which the KKR matrix (for the CPA scattering amplitude) is singular. Thus, $\theta_c(z)$ defines the (complex) CPA energy bands. Twice the imaginary part of θ_c is the inverse of the mean free path in units of the lattice constant

Using Eqs. (132) and (133) in Eq. (131), we obtain

$$\chi(K_1,K_2;z_1,z_2)=\frac{(2m/\hbar^2)(z_1z_2)^{1/2}(i\cot\bar{\theta}_c-1)\Psi(K_1,K_2;z_1,z_2)}{[1+\cot\eta^c_0(z_1)\cot\eta^c_1(z_1)][1+\cot\eta^c_0(z_2)\cot\eta^c_1(z_2)]}, \tag{136}$$

where

$$\bar{\theta}_c=\tfrac{1}{2}[\theta_c(z_1)+\theta_c(z_2)], \tag{137}$$

and $\Psi(K_1,K_2;z_1,z_2)$ is given by Table I. Note that all combinations of l_1,l_2, l_3, and l_4 are not needed because of the selection rule on the current matrix element,

$$J^{\alpha}_{ll'}(z_1,z_2)=0,\quad l\neq l'\pm 1. \tag{138}$$

The scattering operator w [Eq. (66)], which determines the vertex corrections, can be obtained from the results of Eqs. (119) and (120),

$$\Delta m^{\alpha}_l(z)=m^c_l(z)-m^{\alpha}_l(z), \tag{30'}$$

$$x^{\alpha}_l(z)=\frac{\Delta m^{\alpha}_l(z)}{1-\Delta m^{\alpha}_l(z)\tau^{c00}_l(z)}, \tag{34'}$$

$$w(z_1,z_2;l,l')=\sum_{\alpha}c^{\alpha}x^{\alpha}_l(z_1)x^{\alpha}_{l'}(z_2). \tag{66'}$$

Finally, the conductivity can be obtained from Eqs. (76), (74), (20), and (5). Equation (74), for example, becomes

$$\tilde{\sigma}^1(z_1,z_2)=-\frac{4m^2}{\pi\hbar^3\Omega}\sum_{K_1,K_2}\bar{J}_{K_1}(z_2,z_1)A_{K_1K_2}(z_1,z_2)\times\bar{J}_{K_2}(z_1,z_2), \tag{139}$$

$$A^{-1}_{K_1K_2}(z_1,z_2)=\delta_{K_1K_2}-\chi_{K_1K_2}(z_1,z_2)w_{K_2}(z_1,z_2). \tag{140}$$

The results of calculations for model one-dimensional systems are shown in Figs. 2—4. Figure 1 depicts the model alloy potential which consists of square wells of depth $0.1E_0$ (A) and $0.2E_0$ (B), where $E_0=(h/a)^2/(2m)$. The wells are $0.7a$ in diameter and are arranged in a random sequence along the line.

Figure 2 shows the dispersion relations for systems consisting of pure A, pure B, and A-B alloys. The alloy concentrations are $c^A=0.25$ [panel (a)], 0.50 [panel (b)], and 0.75 [panel (c)]. Since the CPA equations are most naturally solved for fixed real energies, it was convenient to determine the dispersion relation or the (complex) momentum as a function of real energy. Thus $q_c(\varepsilon)$ was determined such that $\det[M(q_c,\varepsilon)]=0$ for fixed, real ε. The real part of q_c is shown by the curves labeled C in Fig. 2. The imaginary part of q_c is indicated by the error bars, the length of which (from bottom to top) is twice $\mathrm{Im}(q_c)$.

Figure 3 shows the conductivity calculated using Eqs. (139) and (76) (solid line) and also by omitting the vertex corrections (dashed lines). The vertex corrections are omitted by replacing $A_{K_1K_2}$ [Eq. (140)] by the unit matrix. The conductivity is shown as $\ln(\sigma/\sigma_0)$, where $\sigma_0=e^2a/\pi\hbar$. This is the conductivity one would obtain from the Boltzmann equation neglecting vertex corrections if the mean free path were equal to the lattice spacing. All three alloys show relatively small vertex corrections in the low-energy band and quite large vertex corrections in the higher-energy band. The vertex corrections are small in the lower-energy band because the states there have mainly $l=0$ character. In the higher-energy band the states have both $l=0$ and $l=1$ character. The large increase in the conductivity due to vertex corrections is caused by a near vanishing of the backward scattering amplitude.

TABLE I. The function $\Psi(K_1,K_2;z_1,z_2)$ which determines the kernel $\chi_{K_1K_2}(0)$ through Eq. (136). $g_l(z)=\cot[\eta^c_l(z)][\cos\theta_c(z)-f_l(z)]/i\sin[\theta_c(z)]$.

K_1	K_2	l_1	l_2	l_3	l_4	$\Psi(K_1,K_2;z_1,z_2)$
1	1	1	0	1	0	-1
1	2	1	1	0	0	$g_0(z_1)g_1(z_2)$
2	1	0	0	1	1	$g_0(z_2)g_1(z_1)$
2	2	0	1	0	1	-1

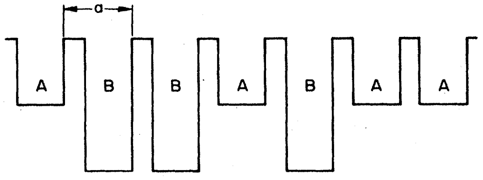

FIG. 1. One-dimensional muffin-tin alloy potential. In this example the muffin-tin potentials are square wells with depths of 0.1 (A) and 0.2 (B) in units of $E_0=(\hbar^2/2m)(2\hbar/a)$, where a is the lattice constant. The width of both wells is $0.7a$.

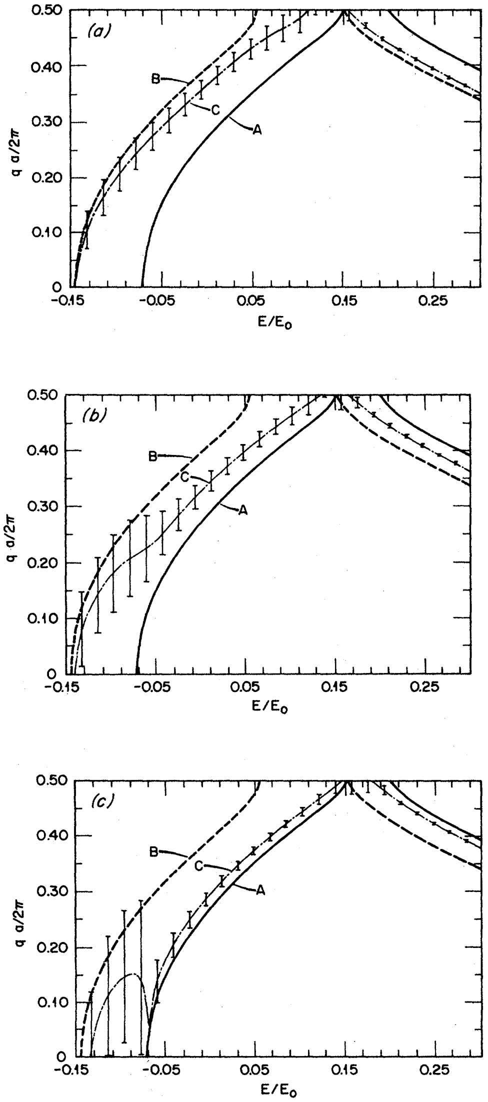

FIG. 2. Alloy dispersion relations for three concentrations: (a) $c^A=0.25$, (b) $c^A=0.50$, and (c) $c^A=0.75$. The solid (dashed) curves represent the dispersion relation for a system of pure A (B), and the curves labeled C represent the alloy dispersion relation in the CPA. The "error bars" indicate the width of the alloy energy bands.

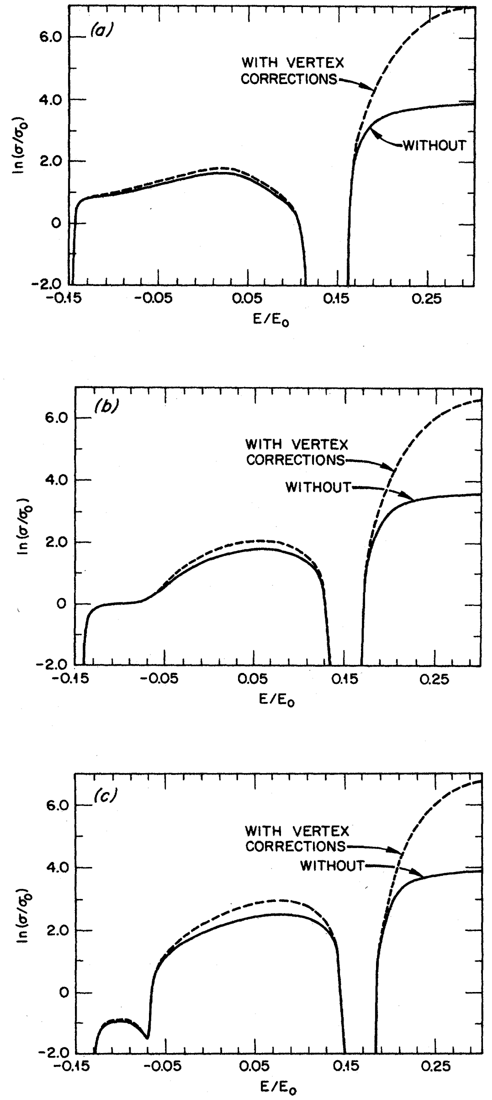

FIG. 3. CPA conductivity for three concentrations: (a) $c^A=0.25$, (b) $c^A=0.50$, and (c) $c^A=0.75$, without (solid line) and with (dashed line) vertex corrections.

Figure 4 compares the conductivity calculated using the CPA formalism of this paper with that of its Boltzmann-equation limit derived in Sec. VI. The Boltzmann equation is a remarkably good approximation to the full theory. It fails, however, near band edges and when the mean free path is less than a lattice spacing. Clearly, the pole approximation [Eq. (85)] cannot be expected to be valid when $\gamma_q \gtrsim 1/a$ or when q_c is within γ_q of a zone boundary.

VIII. DISCUSSION

The ability of the theory presented in this paper to describe the properties of disordered alloys can best be determined by applying it to real systems. Such calcula-

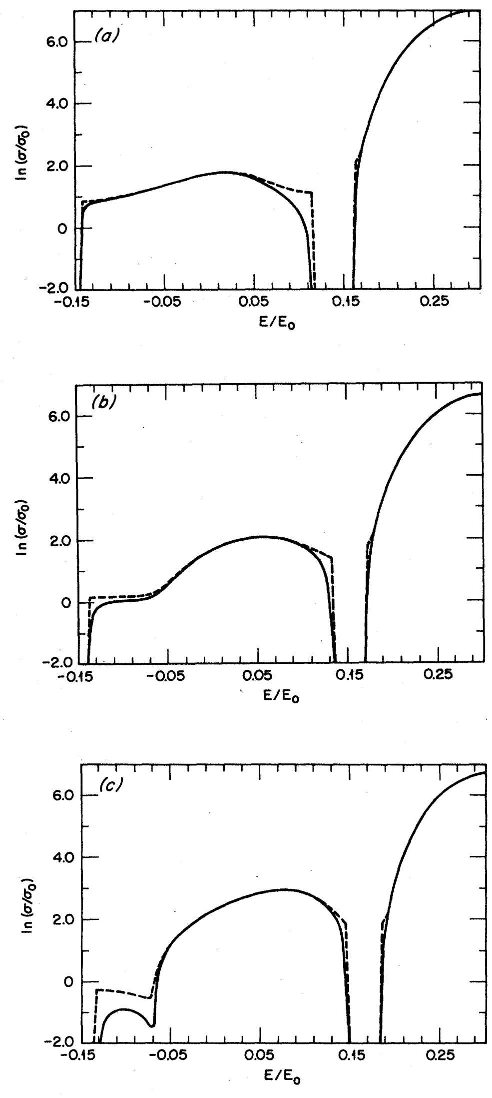

FIG. 4. Comparison of CPA conductivity with vertex corrections (solid line) with the Boltzmann-equation limit for the same concentrations as in Figs. 2 and 3.

tions are certainly feasible, and would seem to add only minor additional complications to current KKR-CPA calculations. Since the present theory reduces, in the limit of fairly long mean free path, to that used in Refs. 3—5 to successfully calculate the electrical resistivity of Ag-Pd alloys, there is good reason to believe that it will work well in that limit.

An extremely interesting question is whether or not the theory presented here will also work well in the limit of very short mean free path. Can it, for example, explain the empirical observation that metallic resistivities seldom exceed about 200 $\mu\Omega$ cm?[24–27] This phenomenon is sometimes called "resistivity saturation" and is thought to occur when the electronic mean free path approaches a lattice spacing. It is sometimes "explained" by the observation that a wave with a mean free path shorter than its wavelength is difficult to contemplate.

A mechanism which may explain resistivity saturation is contained within the present theory. All systems known to me that exhibit this effect have several narrow bands in the vicinity of the Fermi energy. When the disorder is small and the bands are well defined, each band can be treated using Eqs. (83)—(85). In this regime each band that crosses the Fermi energy gives a separate contribution to the conductivity [Eq. (89)]. As the disorder is increased, however, the width in q of the bands will increase until they overlap. Then, in addition to intraband contributions to the conductivity, such as Eq. (85), there will be interband contributions.[25] These additional contributions are omitted in deriving the Boltzmann equation.

It is possible to make a simple rough estimate of the resistivity in the saturation limit, i.e., when the energy bands are "completely smeared out" by disorder. In this limit I expect that Eq. (79) can be approximated by

$$\sigma \simeq \frac{2\hbar\langle v^2\rangle\pi}{3\Omega_a\Omega_z}\int d^3q\, A^2(q,\varepsilon)\,, \tag{141}$$

where $\langle v^2\rangle$ is a mean-square band velocity and $A(q,\varepsilon)$ is the Bloch spectral density. The Bloch spectral density is related to the density of states through

$$N(\varepsilon)=\frac{1}{\Omega_z}\int d^3q\, A(q,\varepsilon)\,. \tag{142}$$

I speculate that, in the saturation regime, $A(q,\varepsilon)$ is approximately constant over the Brillouin zone, so that the saturation conductivity is approximately

$$\sigma \simeq \frac{2e^2\hbar\langle v^2\rangle\pi^2}{3\pi\Omega_a}N^2(\varepsilon_F)\,. \tag{143}$$

Reasonable guesses for $\langle v^2\rangle$ and $N(\varepsilon_F)$ for a d-band metal are

$$\hbar^2\langle v^2\rangle \simeq (aW/4\pi)^2 \tag{144}$$

and

$$N(\varepsilon_F)\simeq 5/W\,, \tag{145}$$

where W is the width of the d-band complex. Thus, Eq. (143) becomes

$$\sigma \simeq \frac{e^2a^2}{\pi\hbar\Omega_a} \simeq e^2/\hbar a\,, \tag{146}$$

which corresponds to a resistivity of approximately 150 $\mu\Omega$ cm. This estimate is clearly very rough, but it does appear to be consistent with observed values of the saturation resistivity.

A definitive test of the theory in the saturation regime will probably require its extension, so that resistance in the simultaneous presence of alloy and thermal disorder can be calculated. Fortunately, it appears to be relatively easy to generalize the theory to treat disorder due to the displacement of the atoms off of their lattice sites.[28] A displaced atom in an otherwise periodic lattice can be treated as a special kind of nonspherical impurity. Within the rigid-muffin-tin approximation it is quite easy to express the t matrix for the displaced atom (viewed as a nonspherical impurity atom sitting on the original lattice site) in terms of the t matrix of the undisplaced atom. At temperatures sufficiently high that the atoms can be viewed as vibrating independently ($T > \Theta_D$), one can apply the CPA [Eq. (36)]. Each possible value of the displacement in this version of the CPA is analogous to a different species in the alloy version of the CPA. Such an extension of the KKR-CPA will be presented later.[29]

The most significant limitation of a theory of transport based on a single-site theory such as the CPA is that it is applicable only to random alloys. The potential at a particular site is assumed to be statistically independent of the potentials at all of the other sites. In reality, all physical alloy systems show some degree of short-range order. It is not yet clear how serious this limitation is for physically interesting alloy systems, but some systems (e.g., fcc Ni-Mo) have a lower resistivity in the cold-worked state than in the annealed state.[30] Presumably this effect is caused by the presence of short-range order in the annealed state.

Additional limitations of the present theory are that it does not include the effects that lead to Anderson localization[31] or to "disorder-enhanced electron-electron scattering."[22] These effects are often dominant in one- and two-dimensional systems, but I believe that they are not often important in three-dimensional systems with metallic bonding. The validity of this belief will be tested as detailed calculations on physical systems become available.

A final comment concerns the relation between this work and a recent paper by Schwartz,[32] who has also obtained an expression for transport coefficients in a muffin-tin alloy model within the CPA. Unfortunately, it is difficult to compare the two formalisms. Schwartz's formalism requires an "off-energy-shell" scattering amplitude, i.e., $t_L^n(q,q',z)$, in place of $t_L^n(z)$, which enters Eq. (9). In addition, Schwartz's work involves integrals over all of $\mathbf{q}$ space rather than only over the first Brillouin zone.

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APPENDIX A

The assertion that Eq. (36) is equivalent to the more usual self-consistency equations for the KKR-CPA is demonstrated in this appendix. Equation (36) may be written as

$$\sum_\alpha c^\alpha x^\alpha = 0 \ , \tag{A1}$$

which [using Eq. (51)] is equivalent to

$$\sum_\alpha c^\alpha D^\alpha = \sum_\alpha c^\alpha = 1 \ . \tag{A2}$$

This is a form of the KKR-CPA equations used by Faulkner and Stocks.[10] Multiplication of Eq. (A2) by τ^{c00} and reference to Eq. (53) yields a more common version of the KKR-CPA equations,[1]

$$\sum_\alpha c^\alpha \tau^{c00(\alpha)} = \tau^{c00} \ . \tag{A3}$$

An even more common form is obtained by multiplying Eq. (A2) on the left-hand side by $1-\tau^{c00}\Delta m^A$, on the right-hand side by $1-\tau^{c00}\Delta m^B$. The result can be simplified to[1]

$$m^c = c^A m^A + c^B m^B + (m^c - m^A)\tau^{c00}(m^c - m^B) \ , \tag{A4}$$

where $m^c = (t^c)^{-1}$ and $m^\alpha = (t^\alpha)^{-1}$.

APPENDIX B

Our objective is an accurate and useful evaluation of Eq. (40) within the context of the CPA. Use of Eqs. (23), (41), and (42) in Eq. (40) yields

$$L^{0\alpha,n\beta} = \tau^{c0n} J^\beta \tau^{cn0} + \sum_k \langle (\tau^c Q^k \tau^c)_{0n} \rangle_{\alpha\beta} J^\beta \tau^{cn0} + \sum_k \tau^{c0n} J^\beta \langle (\tau^c \tilde{Q}^k \tau^c)_{n0} \rangle_{\alpha\beta} + \sum_{k,l} \langle (\tau^c Q^k \tau^c)_{0n} J^\beta (\tau^c \tilde{Q}^k \tau^c)_{n0} \rangle_{\alpha\beta} \ . \tag{B1}$$

Here the notation $\langle \ \rangle_{\alpha\beta}$ means that the atom at site 0 is of type α, and the atom at site n, is of type β. This equation is still exact within the muffin-tin approximation.

Denote the four terms on the rhs of Eq. (B1) by T_1, T_2, T_3, and T_4, respectively. The second and third terms, T_2 and T_3, can be evaluated easily. Neglecting terms involving repeated scattering between sites 0 and n, we obtain

$$T_2 = \tau^{c00} x^\alpha \tau^{c0n} J^\beta \tau^{cn0} + D^\alpha \tau^{c0n} x^\beta \tau^{cnn} J^\beta \tau^{cn0} \ , \tag{B2}$$

$$T_3 = \tau^{c0n} J^\beta \tau^{c0n} x^\alpha \tau^{c00} = \tau^{c0n} J^\beta \tau^{cnn} x^\beta \tau^{cn0} \tilde{D}^\alpha \ . \tag{B3}$$

The evaluation of the final term of Eq. (B1), T_4, requires more work. It is helpful to write T_4 as

$$T_4 = \left[\sum_{\substack{k\ (\neq 0,n), \\ l\ (\neq 0,n)}} + \sum_{\substack{k=0,n; \\ l\ (\neq 0,n)}} + \sum_{\substack{k\ (\neq 0,n); \\ l=0,n}} + \sum_{\substack{k=0,n; \\ l=0,n}} \right] \langle (\tau^c Q^k \tau^c)_{0n} J^\beta (\tau^c \tilde{Q}^l \tau_c)_{n0} \rangle_{\alpha\beta} \ . \tag{B4}$$

Denote the four terms on the rhs of Eq. (B4) by T_{41}, T_{42}, T_{43}, and T_{44}, respectively. The terms in T_{41} vanish unless $k=l$, and thus

$$T_{41}=\sum_{k\,(\neq 0,n)}(\tau^c\gamma_k^{n\beta(\alpha)}\tau^c)_{00}\;, \tag{B5}$$

where

$$\gamma_k^{n\beta(\alpha)}=\langle (Q^k\tau^c)_{kn}J^\beta(\tau^c\widetilde{Q}^{\,k})_{nk}\rangle_{\alpha\beta}\;. \tag{B6}$$

The second and third terms of Eq. (B4), T_{42} and T_{43}, may be written as

$$T_{42}=\tau^{c\,00}x^\alpha\sum_{k\,(\neq 0,n)}(\tau^c\gamma_k^{n\beta(\alpha)}\tau^c)_{00}+\tau^{c\,0n}x^\beta\sum_{k\,(\neq 0,n)}(\tau^c\gamma_k^{n\beta(\alpha)}\tau^c)_{n0}\;, \tag{B7}$$

$$T_{43}=\sum_{k\,(\neq 0,n)}(\tau^c\gamma_k^{n\beta(\alpha)}\tau^c)_{00}x^\alpha\tau^{c\,00}+\sum_{k\,(\neq 0,n)}(\tau^c\gamma_k^{n\beta(\alpha)}\tau^c)_{0n}x^\beta\tau^{cn0}\;. \tag{B8}$$

The second terms on the rhs of Eqs. (B7) and (B8) will be neglected in the following because they contain repeated scatterings between sites k and n.

The fourth term on the rhs of Eq. (B4) is the most tedious to evaluate. It is helpful to write it as the sum of four terms,

$$\begin{aligned}T_{44}=&\langle(\tau^cQ^0\tau^c)_{0n}J^\beta(\tau^c\widetilde{Q}^{\,0}\tau^c)_{n0}\rangle_{\alpha\beta}+\langle(\tau^cQ^0\tau^c)_{0n}J^\beta(\tau^c\widetilde{Q}^{\,n}\tau^c)_{n0}\rangle_{\alpha\beta}+\langle(\tau^cQ^n\tau^c)_{0n}J^\beta(\tau^c\widetilde{Q}^{\,0}\tau^c)_{n0}\rangle_{\alpha\beta}\\&+\langle(\tau^cQ^n\tau^c)_{0n}J^\beta(\tau^c\widetilde{Q}^{\,n}\tau^c)_{n0}\rangle_{\alpha\beta}\;.\end{aligned} \tag{B9}$$

Denoting the four terms on the rhs of Eq. (B9) by T_{441}, T_{442}, T_{443}, and T_{444}, respectively, we have

$$\begin{aligned}T_{441}=&\tau^{c\,00}x^\alpha\tau^{c\,0n}J^\beta\tau^{cn0}x^\alpha\tau^{c\,00}+\tau^{c\,00}x^\alpha\tau^{c\,0n}x^\beta\tau^{cnn}J^\beta\tau^{cn0}x^\alpha\tau^{c\,00}+\tau^{c\,00}x^\alpha\tau^{c\,0n}J^\beta\tau^{cnn}x^\beta\tau^{cn0}x^\alpha\tau^{c\,00}\\&+\tau^{c\,00}x^\alpha\sum_{k\,(\neq 0,n)}(\tau^c\gamma_k^{n\beta(\alpha)}\tau^c)_{00}x^\alpha\tau^{c\,00}+\tau^{c\,00}x^\alpha\tau^{c\,0n}x^\beta\tau^{cnn}J^\beta\tau^{cnn}x^\beta\tau^{cn0}x^\alpha\tau^{c\,00}\;,\end{aligned} \tag{B10}$$

$$T_{442}=\tau^{c\,00}x^\alpha\tau^{c\,0n}J^\beta\tau^{cnn}x^\beta\tau^{cn0}+\tau^{c\,00}x^\alpha\tau^{c\,0n}x^\beta\tau^{cnn}J^\beta\tau^{cnn}x^\beta\tau^{cn0}\;, \tag{B11}$$

$$T_{443}=\tau^{c\,0n}x^\beta\tau^{cnn}J^\beta\tau^{cn0}x^\alpha\tau^{c\,00}+\tau^{c\,0n}x^\beta\tau^{cnn}J^\beta\tau^{cnn}x^\beta\tau^{cn0}x^\alpha\tau^{c\,00}\;, \tag{B12}$$

$$T_{444}=\tau^{c\,0n}x^\beta\tau^{cnn}J^\beta\tau^{cnn}x^\beta\tau^{cn0}\;. \tag{B13}$$

The result which we seek is given by the sum

$$T_1+T_2+T_3+T_{41}+T_{42}+T_{43}+T_{441}+T_{442}+T_{443}+T_{444}\;.$$

This can be simplified substantially. Let

$$\underline{\tau}_J=\tau^{c\,0n}J^\beta\tau^{cn0}\;, \tag{B14}$$

$$\underline{\tau}_{xJ}=\tau^{c\,0n}x^\beta\tau^{cnn}J^\beta\tau^{cn0}\;, \tag{B15}$$

$$\underline{\tau}_{Jx}=\tau^{c\,0n}J^\beta\tau^{cnn}x^\beta\tau^{cn0}\;, \tag{B16}$$

$$\underline{\tau}_{xJTx}=\tau^{c\,0n}x^\beta\tau^{cnn}J^\beta T^{cnn}x^\beta\tau^{cn0}\;, \tag{B17}$$

$$\underline{\tau}_\gamma=\sum_{k\,(\neq 0,n)}(\tau^c\gamma_k^{n\beta(\alpha)}\tau^c)_{00}\;. \tag{B18}$$

Then,

$$T_1=\underline{\tau}_J\;, \tag{B19}$$

$$T_2=\tau^{c\,00}x^\alpha\underline{\tau}_J+D^\alpha\underline{\tau}_{xJ}\;, \tag{B20}$$

$$T_3=\underline{\tau}_Jx^\alpha\tau^{c\,00}+\underline{\tau}_{Jx}\widetilde{D}^{\,\alpha}\;, \tag{B21}$$

$$T_{41}=\underline{\tau}_\gamma\;, \tag{B22}$$

$$T_{42}=\tau^{c\,00}x^\alpha\underline{\tau}_\gamma\;, \tag{B23}$$

$$T_{43}=\underline{\tau}_\gamma x^\alpha\tau^{c\,00}\;, \tag{B24}$$

$$T_{441}=\tau^{c\,00}x^\alpha(\underline{\tau}_J+\underline{\tau}_{xJ}+\underline{\tau}_{Jx}+\underline{\tau}_{xJTx}+\underline{\tau}_\gamma)X^\alpha\tau^{c\,00}\;, \tag{B25}$$

$$T_{442}=\tau^{c\,00}x^\alpha\underline{\tau}_{Jx}+\tau^{c\,00}x^\alpha\underline{\tau}_{xJTx}\;, \tag{B26}$$

$$T_{443}=\underline{\tau}_{xJ}x^\alpha\tau^{c\,00}+\underline{\tau}_{xJTx}\tau^{c\,00}x^\alpha\;, \tag{B27}$$

$$T_{444}=\underline{\tau}_{xJTx}\;. \tag{B28}$$

Use of Eqs. (51) and (52) in Eqs. (B19)—(B28) yields

$$L^{0\alpha,n\beta}=D^\alpha(\underline{\tau}_J+\underline{\tau}_{xJ}+\underline{\tau}_{Jx}+\underline{\tau}_{xJTx}+\underline{\tau}_\gamma)\widetilde{D}^{\,\alpha}\;, \tag{B29}$$

and use of Eqs. (51) and (52) in Eqs. (B14)—(B17) yields

$$\underline{\tau}_J+\underline{\tau}_{xJ}+\underline{\tau}_{Jx}+\underline{\tau}_{xJTx}=\tau^{c\,0n}\widetilde{D}^{\,\beta}J^\beta D^\beta\tau^{cn0}\;. \tag{B30}$$

Equations (56) and (57) are obtained from using Eq. (B30) in Eq. (B29).

APPENDIX C

The KKR-CPA equations reduce to those of the KKR method of band theory when the disorder is reduced sufficiently either by reducing the concentration of the impurity species or by reducing the difference between the scattering properties of the constituents. In order to make contact with the Boltzmann equation in the regime in which there is some disorder, but where the energy bands are still well defined, it is helpful to know the form of the Bloch function corresponding to these bands.

For a pure-A system the Bloch function is

$$\Psi_{\mathbf{q}}^A(\mathbf{r}_m,z)=\sum_L i^le^{i\mathbf{q}\cdot\mathbf{R}_m}C_L^A(\mathbf{q},z)Z_L^A(\mathbf{r}_m,z)\;, \tag{C1}$$

where

$$\sum_{L'}[m_L^A\delta_{LL'}-g'_{LL'}(\mathbf{q},z)]i^{l'}C_{L'}^A(\mathbf{q},z)=0\;. \tag{C2}$$

In order to determine the proper generalization of Eqs. (C1) and (C2) for CPA energy bands, we examine the alloy Green function, which [omitting the singular term in Eq. (8)] may be written

$$G(\mathbf{r},\mathbf{r}';z)=\sum_{L,L'}\tau^{mn}_{LL'}(z)Z^m_L(\mathbf{r}_m,z)Z^n_{L'}(\mathbf{r}'_n,z)\ , \qquad \text{(C3)}$$

where $\mathbf{r}$ is in cell m and $\mathbf{r}'$ is in cell n. Performing a CPA-like average in which the species on sites m and n are held fixed yields[10]

$$\langle G(\mathbf{r},\mathbf{r}';z)\rangle_{mn}=\sum_{L,L'}[D^m\tau^{cmn}\widetilde{D}^{\,n}]_{LL'}Z^m_L(\mathbf{r}_m,z)Z^n_{L'}(\mathbf{r}'_n,z)\ . \qquad \text{(C4)}$$

However, τ^{cmn} can be written as an integral over the Brillouin zone, Eq. (24), which allows us to obtain an expression for $G_q(\mathbf{r},\mathbf{r}';z)$,

$$G_q(\mathbf{r},\mathbf{r}';z)=\sum_{L,L'}\sum_{L_1,L_2}[M(q,z)]^{-1}_{L_1L_2}e^{iq\cdot(\mathbf{R}_n-\mathbf{R}_m)}D^m_{LL_1}(z)Z^m_L(r_m,z)\widetilde{D}^{\,n}_{L_2L'}(z)Z^n_{L'}(r'_n,z)\ . \qquad \text{(C5)}$$

Using the pole approximation Eq. (80) in Eq. (C5) yields

$$G_q(\mathbf{r},\mathbf{r}';z)\simeq\sum_{L,L'}\sum_{L_1,L_2}i^{\,l_1-l_2}\frac{C^c_{L_1}(\mathbf{q}_0,z)C^c_{L_2}(\mathbf{q}_0,z)}{z-\varepsilon_q}e^{i\mathbf{q}_0\cdot(\mathbf{R}_n-\mathbf{R}_m)}Z^m_L(\mathbf{r}_m,z)D^m_{LL_1}(z)\widetilde{D}^{\,n}_{L_2L'}(z)Z^n_{L'}(r'_n,z)\ . \qquad \text{(C6)}$$

Comparison of Eq. (C6) with the usual expression for the Green's function,

$$G_{\mathbf{q}}(\mathbf{r},\mathbf{r}';z)=\frac{\Psi_{\mathbf{q}_0}(\mathbf{r})\widetilde{\Psi}_{\mathbf{q}_0}(\mathbf{r}')}{z-\varepsilon_{\mathbf{q}}}\ , \qquad \text{(C7)}$$

yields an expression for the Bloch function,

$$\Psi^c_{\mathbf{q}}(\mathbf{r})=\sum_{m,L,L_1}C^c_{L_1}(q)i^{\,l_1}e^{-i\mathbf{q}\cdot\mathbf{R}_m}[\xi^A_m Z^A_L(\mathbf{r},z)D^A_{LL_1}(z)+\xi^B_m Z^B_L(\mathbf{r},z)D^B_{LL_1}(z)]\ , \qquad \text{(C8)}$$

$$\widetilde{\Psi}^{\,c}_{\mathbf{q}}(\mathbf{r})=\sum_{n,L',L_2}C^c_{L_2}(q)i^{\,-l_2}e^{i\mathbf{q}\cdot\mathbf{R}_n}[\xi^A_n\widetilde{D}^{\,A}_{L_2L'}(z)Z^A_{L'}(\mathbf{r},z)+\xi^B_n\widetilde{D}^{\,B}_{L_2L'}(z)Z^B_{L'}(\mathbf{r},z)]\ , \qquad \text{(C9)}$$

where ξ^A_m is 1 or 0, depending on whether site m is or is not occupied by an atom of type A.

In the low-concentration limit, Eq. (C8) gives the correct wave function within the cell containing the impurity and within cells not influenced by the impurity. It is also consistent with the results of Faulkner and Stocks[10] for the Bloch spectral density within the KKR-CPA.

Equations (C8) and (C9) allow us to calculate the group velocity of an alloy energy band in the KKR-CPA. This quantity may be defined as

$$\mathbf{v}_q=\hbar^{-1}\nabla_q\varepsilon_q\ , \qquad \text{(C10)}$$

where ε_q is a (generally complex) root of

$$\det[M_{LL'}(\mathbf{q},\varepsilon_q)]=0\ . \qquad \text{(C11)}$$

Using

$$v^{\mu}_{\mathbf{q}}=\frac{-i\hbar}{m}\int d^3r\,\widetilde{\Psi}^{\,c}_{\mathbf{q}}(\mathbf{r})\frac{\partial}{\partial r_\mu}\Psi^c_{\mathbf{q}}(\mathbf{r}) \qquad \text{(C12)}$$

yields Eq. (86).

APPENDIX D

In this section it is shown that the Boltzmann lifetime calculated from Eqs. (92) and (101) is consistent with the width in energy of the KKR-CPA alloy energy bands. For simplicity, only systems with sufficient symmetry that $\tau^{c00}_{LL'}$ is diagonal in the angular momentum indices will be considered. Cubic systems satisfy this requirement for $l\leq 2$. This restriction also insures that x^α is diagonal and that D^α and $\widetilde{D}^{\,\alpha}$ are equal and diagonal.

According to Eqs. (101) and (92), the Boltzmann lifetime is given by

$$\frac{\hbar}{\tau^B_q}=2\pi\sum_{\alpha,q'}c^\alpha\,|\,T^\alpha_{qq'}\,|^2\delta(\varepsilon_q-\varepsilon_{q'})\ . \qquad \text{(D1)}$$

Performing the sum on q' yields

$$\frac{\hbar}{\tau^B_q}=-2\sum_\alpha c^\alpha\sum_L x^\alpha_L(z)x^\alpha_L(z^*)C_L(q,z)\times C_L(q,z^*)\mathrm{Im}[\tau^c_L(\varepsilon_q)]\ . \qquad \text{(D2)}$$

In order to obtain x^α in Eq. (D2), we must obtain an approximate solution to the KKR-CPA equations of Appendix A. It is convenient to use the "average cotangent approximation" as a reference. Thus we substitute

$$m^c=c^Am^A+c^Bm^B+\delta m$$

into Eq. (A4) and solve for δm through terms of third order in m^A-m^B. The result is

$$\delta m=-c^Ac^B(m^A-m^B)^2\tau^{00}[\overline{m}]\times\{1+(c^A-c^B)(m^A-m^B)\tau^{00}[\overline{m}]\}\ , \qquad \text{(D3)}$$

where $\tau^{00}[\bar{m}]$ is the site-diagonal scattering path operator calculated with a scattering amplitude of $\bar{t}$ on every site where

$$\bar{t}^{-1}=\bar{m}=c^A m^A+c^B m^B \;. \tag{D4}$$

Since $\bar{m}$ is the average cotangent approximation, it corresponds to a real potential on every site. Using Eq. (D3), $\Delta m^A=m^c-m^A$ is to second order given by

$$\Delta m^A=c^B(m^B-m^A)[1+c^A(m^A-m^B)]\tau^{00}[\bar{m}]+\cdots \;, \tag{D5}$$

and similarly for Δm^B. Using Eqs. (D5) and (34), x^A can be obtained to second order in m^A-m^B,

$$x^A=c^B(m^B-m^A)\{1+(c^B-c^A)(m^B-m^A)\tau^{00}[\bar{m}]\} \;, \tag{D6}$$

and similarly for x^B. Thus, to third order in m^A-m^B, we have

$$\sum_\alpha c^\alpha x^\alpha (x^\alpha)^* = c^A c^B (m^A-m^B)^2\{1+(c^A-c^B)(m^A-m^B)(\tau[\bar{m}]+\tau^*[\bar{m}])\} \;, \tag{D7}$$

which may be used in Eq. (D2) to obtain the Boltzmann lifetime to third order in m^A-m^B,

$$\frac{\hbar}{\tau_q^B}=-2c^A c^B \sum_L (m_L^A-m_L^B)^2\{1+(c^A-c^B)(m_L^A-m_L^B)(\tau_L[\bar{m}]+\tau_L^*[\bar{m}])\}\mathrm{Im}(\tau_L[\bar{m}]) \;. \tag{D8}$$

Equation (D8) will be compared with an approximate expression for $\mathrm{Im} z_q$, the imaginary part of that energy which, for given q, satisfies

$$\det[M(q,z_q)]=0 \;. \tag{D9}$$

We consider the determinant of the KKR matrix M at fixed q as a function of the inverse of the scattering amplitude m and the energy z. The pole in M^{-1} which gives the KKR-CPA alloy energy band is the solution z_c of

$$\det[M(m_c,z_c)]=0 \;. \tag{D10}$$

If the inverse of the scattering amplitude is $\bar{m}$ rather than m^c, a pole at (real) energy $\bar{z}$ will be obtained. We write

$$\det[M(\bar{m},\bar{z})]=0 \;. \tag{D11}$$

Assuming that $\delta m=m^c-\bar{m}$ is not too large, we have

$$\sum_L \left[\frac{\partial \det[M(m_L,z)]}{\partial m_L}\right]_{\bar{m}\bar{z}} \delta_{m_L} + \left[\frac{\partial \det[M(m_L,z)]}{\partial z}\right]_{\bar{m}\bar{z}} (z_c-\bar{z})=0 \;, \tag{D12}$$

or

$$z_c-\bar{z}=-\sum_L \left[\frac{\partial \det[M(m_L,z)]}{\partial m_L}\right]_{\bar{m}\bar{z}} \times \left[\frac{\partial \det[M(m_L,z)]}{\partial z}\right]_{\bar{m}\bar{z}}^{-1} \delta m_L \;. \tag{D13}$$

However, according to Ref. 14,

$$\left[\frac{\partial \det[(M(m_L,z)]}{\partial m_L}\right]_{\bar{m}\bar{z}} = \left[-\frac{\partial \det[M(m_L,z)]}{\partial z}\right]_{\bar{m}\bar{z}} \times C_L(q,\bar{z})C_L(q,\bar{z}) \;, \tag{D14}$$

and using δm from Eq. (D3), we obtain, to third order in m^A-m^B,

$$2\,\mathrm{Im} z=\hbar/\tau_q^B \;. \tag{D15}$$

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