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Hall effect in concentrated alloys*

A. K. Bhattacharya,[†] M. Brauwers,[‡] and F. Brouers
Institut de Physique, Université de Liège, Sart Tilman, 4000 Liège, Belgium

S. K. Joshi
Department of Physics, University of Roorkee, India

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Coherent-potential approximation has been used to derive an expression for the Hall coefficient in the two s-d hybridized band model of Brouers and Vedyayev which has been used to describe the conductivity of disordered alloys of noble and transition metals. We investigate the effect of hybridization and d disorder on the alloy Hall coefficient, and this allows us to generalize and improve the discussion already presented by Levin *et al.* in a one-band picture.

I. INTRODUCTION

The coherent-potential approximation (CPA) has been extensively used to provide a description of equilibrium properties of elementary excitations in disordered alloys. The theory of transport properties of disordered alloys has not yet received as much attention as the study of the density of states. A theory of electronic transport in substitutionally disordered binary alloys was developed by Velicky.[1] In that paper, an expression for the static electrical conductivity of a single-band model with short-ranged random scatterers was developed in the spirit of single-particle CPA. Brouers and Vedyayev[2] (hereafter referred to as BV) extended the CPA theory to the calculation of the static conductivity of a two s-d band model introduced by Levin and Ehrenreich.[3] The BV model contains some of the features of noble and transition-metal alloys and includes the effect of s-d hybridization and the width of the d levels due to d-d hopping. This model was found to account for the Matterhorn-type behavior of the residual resistivity of transition–noble-metal alloys. This conductivity theory was later developed to deal with ferromagnetic alloys and can provide an explanation of the anisotropy of the residual resistivity in some of them.[4] Moreover qualitative information has been obtained for the frequency dependence of the optical relaxation time in gold-silver alloys[5] and for the temperature dependence of the static resistivity in transition–noble-metal alloys.[6]

Other alloys transport properties such as Hall effect and thermoelectric power have been discussed in the one-band model by Levin, Velicky, and Ehrenreich[7] (thereafter referred to as LVE). In that paper, no attempt was made to relate the theory to experimental data. One of the reasons is that even in pure transition metals, it is very difficult to interpret Hall-effect and thermoelectric power measurements and to relate them to single and precise physical information. These transport properties involve electrons of different characters s and d with very different effective mass and scattering and depend strongly on the anisotropy of the Fermi surface. Moreover the type of electrons involved in the transport process depends on the strength of the magnetic field. At very small field, the Hall effect depends mainly on the number of the most mobile electrons, the contribution of the less mobile ones increasing with the field and therefore Hall effect gives only indirect information on the conduction band.

However, with the development of the theory of alloys, one could hope to be able to explain the variation of the Hall coefficient with concentration. A good summary of the experimental situation can be found in the book by Hurd.[8] To go in this direction, one cannot use the LVE model because of the presence of both s and d electrons interacting via an hybridization, the d electrons being more affected than the s ones by the configurational disorder. The present paper uses the BV model to the calculation and discussion of the weak-field Hall coefficient. Although this theoretical formalism is more realistic, we do not make any attempt to apply it to any particular system. This is because of the following limitations:

(i) The model used here should be applied to nonmagnetic noble and transition-metal alloys (i.e., the components of which are Au, Ag, Cu, Pt, Pd) at very low temperature. In Table I, we have summarized cases where the Hall coefficient has been measured for a wide range of concentrations at relatively low temperature. Although the completely disordered phases of these alloys exhibit a Matterhorn-type concentration dependence for the residual resistivity, the experimental curves given in the references in Table I do not allow to establish such a regular feature for the Hall coefficient. As an example, in Au-Ag and Ag-Pd, the concentration dependence of the Hall coefficient is quite different.

TABLE I. Experimental curves for the concentration dependence of the Hall coefficient in various alloys.

Alloy	Temperature (°K)	Authors
Au–Ag	90–800	Köster *et al.* (Ref. 9)
	6–300	Barnard *et al.* (Ref. 10)
Au–Cu	10–300	Barnard *et al.* (Ref. 10)
	4.2	Caton *et al.* (Ref. 11)
Ag–Pd	80–800	Köster *et al.* (Ref. 9)
	80–400	Ricker and Pflüger (Ref. 12)
	4.2	Greig and Livesey (Ref. 13)
Au–Pd	300	Kim and Flanagan (Ref. 14)
Cu–Pd	300	Kim and Flanagan (Ref. 14)
Pd–Pt	300	Köster *et al.* (Ref. 15)
	4.2	Greig and Livesey (Ref. 13)

(ii) In order to make our model tractable we have been forced to make a number of assumptions. These are: the use of a single-site approximation, tight-binding bands, s-d hybridization constant throughout the Brillouin zone, virtual-crystal approximation for the s bands and the s-d hybridization, off-diagonal disorder neglected and finally, the same shape for s and d dispersion curves.

(iii) To make our calculations amenable to numerical computations, we have made supplementary assumptions discussed in Sec. VI. Two different approximations have been investigated: Hubbard semielliptic density of states for the pure metal and Velicky-type approximation to describe the energy dependence of the velocity and, second, the use of the simple-cubic tight-binding dispersion curve. These approximations allow us to avoid integrations over the Brillouin zone.

The purpose of the present paper is to give a complete formulation of the Hall coefficient in the framework of the approximations (ii) given above. Some of them can be avoided in a reasonably simple way: the virtual-crystal approximations for the s and s-d disorder are replaced by self-consistent solutions in the model introduced by Gelatt *et al.*[16]; effect of d-off-diagonal disorder can also be taken into account for transport properties in the two s-d band model.[17] However a complete theory would use the detailed band structure of the pure metal density of states and an exact representation for the velocity function in the Brillouin zone.

The present work is thus a first step in understanding the Hall effect; the model used is more realistic than that of LVE and allows to rediscuss their conclusion, the sign of the Hall coefficient being now related to the quantity $\epsilon_F - \mathrm{Re}\Sigma_s$, where ϵ_F is the Fermi level and Σ_s an effective s self-energy including the effect of the d disorder.

On the other hand, the present formalism could be applied to investigate the Hall effect in liquid transition metals and alloys (as this has been done for the static conductivity[18]) where many interesting and unexplained features have been observed.[19] Other possibilities to apply the present formalism are, at first, the Hall effect in heavily doped semiconductors at very low temperature (which has been considered in a one-band picture by Matsubara and Kaneyoshi[20]) and, second, the Hall effect in the Hubbard model (already considered in a one-band picture by Malwah and Bené[21]).

We finally give an outline of the paper, insisting on the new formal results.

In Sec. II, we establish the two s-d band model alloy Hamiltonian in presence of a magnetic field, using a procedure similar to that of Malwah and Bené[21] in the calculation of the Hall coefficient for the Hubbard model.

In Sec. III, we give the Kubo formalism for the configuration average of the transverse conductivity σ_{xy} and, in the two following sections, we evaluate in the CPA the configuration average for the Green's function and for the other quantities related to two- and three-particle Green's functions and needed in the evaluation of σ_{xy}.

In Sec. V, we give an expression for σ_{xy} which generalizes that obtained by LVE in the one-band picture. We have moreover retained the off-diagonal components of the inverse effective-mass tensor, which were neglected in LVE. In the case of an isotropic band structure, we show that our formulation generalizes that obtained by Matsubara and Kaneyoshi[20] for the Hall coefficient of an impurity-band model.

In Sec. VI, we give a numerical illustration showing, within the assumptions (iii) presented above, the behavior of the transport properties as functions of the band filling.

Finally, in the **Appendix**, we give an analytical expression for the longitudinal conductivity σ_{xx} obtained from residues calculations in the case of Velicky-type approximation for the velocity function. This reduces considerably the computation time in the evaluation of σ_{xx} and also to relate σ_{xx} to the alloy s density of states and the effective s self-energy, that gives a direct qualitative understanding of the dependence of σ_{xx} with the band filling. Such a relation has been obtained by Chen *et al.*[22] in the one-band model using a more complicated procedure.

II. TWO s-d BAND ALLOY HAMILTONIAN IN PRESENCE OF MAGNETIC FIELD

We want to calculate the configurationally averaged Hall coefficient of a completely random binary alloy A_xB_{1-x} whose Hamiltonian has the form

$$\mathcal{H}_0 = \sum_{m\neq n} t^s_{mn} a^\dagger_{sm} a_{sn} + \sum_n \epsilon^s_n a^\dagger_{sn} a_{sn}$$

$$+\sum_{m\neq n} t^{d}_{mn} a^{\dagger}_{dm} a_{dn} + \sum_{n} \epsilon^{d}_{n} a^{\dagger}_{dn} a_{dn}$$

$$+\sum_{n} \gamma(\epsilon^{d}_{n})\,(a^{\dagger}_{sn} a_{dn} + a^{\dagger}_{dn} a_{sn}) \;, \qquad (1)$$

where $a^{\dagger}_{sm}$ $(a^{\dagger}_{dm})$ and a_{sm} (a_{dm}) are, respectively, the creation and annihilation operators for an s (d) electron at the site m, and we have

$$t^{s(d)}_{mn} = N^{-1} \sum_{\vec{k}} \epsilon_{s(d)}(\vec{k})\, e^{i\vec{k}\cdot(\vec{R}_m - \vec{R}_n)} \;. \qquad (2)$$

The lattice is assumed to be monoatomic with N sites in a large volume Ω. Each site n is occupied at random by an atom of type A or B with respective probabilities x and $1-x$. The crystal is supposed to have an s band and we assume the d band to be made up of five independent subbands. The function $\epsilon_{s(d)}(\vec{k})$ gives the dispersion relation of s (d) electrons. Its interaction with the Brillouin-zone boundary determines the width $2w_s$ $(2w_d)$ of the unhybridized s (d) bands. The unhybridized d band can be calculated as in a nearest neighbor tight-binding model and will have the general form

$$\epsilon_d(\vec{k}) = w_d\, s(\vec{k}) \;, \qquad (3)$$

with

$$-1 \leqslant s(\vec{k}) \leqslant 1 \;, \quad \vec{k} \in \mathrm{BZ} \;.$$

The first two terms of the model Hamiltonian describe the s electrons, the third and fourth terms represent the d electrons, and the last term represents the s-d hybridization. The unhybridized s band and the hybridization constant are treated in the virtual-crystal approximation, whereas the d bands whose potentials are not expected to be weak are treated self-consistently in the CPA. The hybridization parameter in the alloy, for simplicity assumed to be $\vec{k}$ independent, is given by

$$\gamma = x\gamma(\epsilon^{d}_{A}) + (1-x)\,\gamma(\epsilon^{d}_{B}) \;, \qquad (4)$$

where ϵ^{d}_{A} and ϵ^{d}_{B} are the random d energy levels corresponding to A and B type of atoms, respectively.

For arriving at the form of the Hamiltonian in the presence of a magnetic field we assume that the only effect of the magnetic field is to change the kinetic energies of s and d electrons given respectively by the first and third term in Eq. (1).

The Hamiltonian of a free particle in a magnetic field is given by

$$\mathcal{H}_M = (1/2m)[\vec{p} - (e/c)\vec{A}]^2 \;, \qquad (5)$$

where $\vec{A}$ is the vector potential. We have omitted the Zeeman term since our interest is to calculate the Hall coefficient of a nonmagnetic alloy. The kinetic energy of an electron in the absence of a magnetic field has already been included in the expression for $\mathcal{H}_0$.

Proceeding in a manner similar to that given in Malwah and Bené,[21] we have

$$\mathcal{H}_M = (eH/4c)[(V_x Y + Y V_x) - (V_y X + X V_y)] \;, \qquad (6)$$

where V stands for the velocity operator and H for the magnetic field directed along the z direction.

The position operator in the Wannier basis is defined[2]

$$\vec{R}^{\mathrm{op}} = \sum_{n} (\vec{R}_n |ns\rangle\langle ns| + \vec{R}_n |nd\rangle\langle nd|) \;. \qquad (7)$$

In (7) we have tacitly assumed that the position operator is diagonal in the $\{|ns\rangle, |nd\rangle\}$ basis. Strictly speaking this is true only in the case of a free atom where the matrix elements of $\vec{R}^{\mathrm{op}}$ between s and d states vanish in accordance with optical selection rules. However in order that our formalism does not become too unwieldy we assume that in the alloy the position operator is given by (7) so that

$$\langle n\alpha | \vec{R}^{\mathrm{op}} | m\beta \rangle = \vec{R}_n \delta_{nm} \delta_{\alpha\beta} \;. \qquad (8)$$

Furthermore we assume that the velocity operator is diagonal in the band indices so that

$$\langle n\alpha | V^{\mathrm{op}}_{x,y} | m\beta \rangle = V^{mn}_{x,y} \delta_{\alpha\beta} \;. \qquad (9)$$

Since the velocity operator in the presence of a magnetic field is given by

$$\vec{V}^{\mathrm{op}} = (-i/\hbar)\,[\vec{R}^{\mathrm{op}}, \mathcal{H}] \;, \qquad (10)$$

where

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_M \;, \qquad (11)$$

we now write $\mathcal{H}_M$ in the form

$$\mathcal{H}_M = \sum_{mn\alpha} h^{\alpha}_{mn} a^{\dagger}_{\alpha m} a_{\alpha n} \;, \qquad (12)$$

where $\alpha(\equiv s, d)$ denotes the band index and h^{α}_{mn} is given by

$$h^{\alpha}_{mn} = (eH/4c)[(Y_m + Y_n)(V^{mn}_x)_{\alpha\alpha} - (X_m + X_n)(V^{mn}_y)_{\alpha\alpha}] \;. \qquad (13)$$

In (13), $(V^{mn}_{x,y})_{\alpha\alpha}$ stands for $\langle m\alpha | V^{\mathrm{op}}_{x,y} | n\alpha \rangle$. From (10), one gets after some straightforward algebra

$$V^{\mathrm{op}}_x = \left(-\frac{i}{\hbar}\right)\Bigg(\sum_{mn\alpha} (X_m - X_n)\, t^{\alpha}_{mn} a^{\dagger}_{\alpha m} a_{\alpha n} + \frac{eH}{4c} \sum_{mn\alpha} \{[(Y_m + Y_n)(V^{mn}_x)_{\alpha\alpha} - (X_m + X_n)(V^{mn}_y)_{\alpha\alpha}] \times (X_m - X_n)\}\, a^{\dagger}_{\alpha m} a_{\alpha n}\Bigg) \;. \qquad (14)$$

In the weak-field limit, we can write

$$(V^{mn}_x)_{\alpha\alpha} = (-i/\hbar)\, t^{\alpha}_{mn}(X_m - X_n)(1 - Q_{mn}) \qquad (15)$$

$$(V^{mn}_y)_{\alpha\alpha} = (-i/\hbar)\, t^{\alpha}_{mn}(Y_m - Y_n)(1 - Q_{mn}) \;, \qquad (16)$$

where

$$Q_{mn}=(ieH/4\hbar c)[(X_m-X_n)(Y_m+Y_n)-(Y_m-Y_n)(X_m+X_n)] \ . \tag{17}$$

Substituting the expressions for V_x^{mn} and V_y^{mn} into (13) we get to first order in the magnetic field

$$h_{mn}^{\alpha}=(-ieH/4\hbar c)\,t_{mn}^{\alpha}[(Y_m+Y_n)(X_m-X_n)-(X_m+X_n)(Y_m-Y_n)] \ . \tag{18}$$

III. KUBO FORMULA FOR HALL COEFFICIENT

In the weak-field regime the Hall coefficient is defined[8]

$$\begin{aligned}R_H&=[\sigma_{xy}(H)-\sigma_{yx}(-H)]/2\sigma_{xx}^2H\\&=\sigma_{xy}^a(H)/\sigma_{xx}^2H \ .\end{aligned} \tag{19}$$

Here σ_{xx} is the longitudinal component of the electrical conductivity in zero magnetic field and has been already obtained by Brouers and Vedyayev for the two s-d band model; $\sigma_{xy}^a(H)$ designates the antisymmetric part of the transverse component of the electrical conductivity. For finding R_H our task reduces to deriving an expression for $\sigma_{xy}^a(H)$.

Starting with the linear response theory of Kubo,[23] one gets the following expression for the magnetic-field-dependent conductivity:

$$\langle\sigma_{ij}(H)\rangle=-\frac{i\hbar}{\Omega}\,\mathcal{P}\int\int d\eta\,d\omega\,\omega^{-2}[\rho(\eta)-\rho(\eta+\omega)]\times\mathrm{Tr}J_i^{\mathrm{op}}\langle\delta(\eta+\omega-\mathcal{H})\,J_j^{\mathrm{op}}\,\delta(\eta-\mathcal{H})\rangle \ , \tag{20}$$

where the symbol $\langle\cdots\rangle$ indicates a configurational averaging; the suffixes i and j stand for the cartesian coordinates x and y, and J_i^{op} designates the current operator in the i direction; $\rho(\eta)$ is the Fermi function

$$\rho(\eta)=\{\exp[\beta(\eta-\epsilon_F)]+1\}^{-1} \ , \tag{21}$$

with ϵ_F as the Fermi energy and $\beta=(k_BT)^{-1}$.

We now introduce the magnetic-field-dependent and field-independent Green's functions, respectively, by

$$G_H(z)=(z-\mathcal{H})^{-1} \ , \tag{22}$$

$$G(z)=(z-\mathcal{H}_0)^{-1} \ . \tag{23}$$

To first order in the applied magnetic field

$$G_H(z)=G(z)+G(z)\mathcal{H}_MG(z) \ . \tag{24}$$

Using (24) and the well-known representation for δ function, namely

$$\delta(\eta-\mathcal{H})=(1/2i\pi)[G_H(\eta^+)-G_H(\eta^-)] \ , \quad \eta^{\pm}=\eta\pm i0 \ , \tag{25}$$

we can write

$$\begin{aligned}\langle\sigma_{xy}(H)\rangle=\frac{i\hbar}{4\pi^2\Omega}\,\mathcal{P}\int\int d\eta\,d\omega\,\omega^{-2}[\rho(\eta)-\rho(\eta+\omega)]\,\mathrm{Tr}J_x^{\mathrm{op}}\langle[G(\eta^++\omega)+G(\eta^++\omega)\mathcal{H}_MG(\eta^++\omega)-G(\eta^-+\omega)\\-G(\eta^-+\omega)\mathcal{H}_MG(\eta^-+\omega)]J_y^{\mathrm{op}}[G(\eta^+)+G(\eta^+)\mathcal{H}_MG(\eta^+)-G(\eta^-)-G(\eta^-)\mathcal{H}_MG(\eta^-)]\rangle \ .\end{aligned} \tag{26}$$

It is now convenient to decompose the current operator into two parts: one independent of and the other proportional to the magnetic field

$$J_x^{\mathrm{op}}=eV_x^{\mathrm{op}}=J_x^A+J_x^B \ , \tag{27}$$

with

$$J_x^A=-\frac{ie}{\hbar}\sum_{mn\alpha}t_{mn}^{\alpha}(X_m-X_n)\,a_{\alpha m}^{\dagger}a_{\alpha n} \ , \tag{28}$$

$$J_x^B=-\frac{e^2H}{4\hbar^2c}\sum_{mn\alpha}t_{mn}^{\alpha}(X_m-X_n)[(X_m-X_n)(Y_m+Y_n)-(Y_m-Y_n)(X_m+X_n)]\,a_{\alpha m}^{\dagger}a_{\alpha n} \ . \tag{29}$$

We also introduce a new variable defined by

$$Z_{\lambda_i}=\eta+is\lambda_i \ ,$$

where $\lambda_i=\pm1$ and s is an infinitesimally small positive number. Using Eqs. (27)–(29) and retaining only terms linear in H we have from (26)

$$\begin{aligned}\langle\sigma_{xy}^a(H)\rangle=\frac{i\hbar}{4\pi^2\Omega}\mathcal{P}\int\int d\eta\,d\omega\,\omega^{-2}[\rho(\eta)-\rho(\eta+\omega)]\sum_{\lambda_i,\lambda_j=\pm1}(-1)^{(\lambda_i-\lambda_j)/2}\,[A(J_x^B,Z_{\lambda_i}+\omega;J_y^A,Z_{\lambda_j})\\+A(J_x^A,Z_{\lambda_i}+\omega;J_y^B,Z_{\lambda_j})+B(J_x^A,Z_{\lambda_i}+\omega;J_y^A,Z_{\lambda_j};\mathcal{H}_M,Z_{\lambda_j})+C(J_x^A,Z_{\lambda_i}+\omega;\mathcal{H}_M,Z_{\lambda_i}+\omega;J_y^A,Z_{\lambda_j})] \ ,\end{aligned} \tag{30}$$

where we define A, B, and C by

$$A(O_1,z_1;O_2,z_2)=\mathrm{Tr}O_1\langle G(z_1)O_2G(z_2)\rangle \ ,$$

$$B(O_1,z_1;O_2,z_2,\mathcal{H}_M,z_3)=\mathrm{Tr}O_1\langle G(z_1)O_2G(z_2)\mathcal{H}_MG(z_3)\rangle \ ,$$

$$C(O_1,z_1;\mathcal{H}_M,z_2;O_2,z_3)=\mathrm{Tr}O_1\langle G(z_1)\mathcal{H}_MG(z_2)O_2G(z_3)\rangle \ . \tag{31}$$

The important task now is to perform the configurational averaging of products of two and three

Green's functions as given in Eq. (31). For this we need a knowledge of $\langle G\rangle \equiv \overline{G}$. The averaged Green's function for the two s-d band model has already been evaluated in CPA by BV. We summarize these results in Sec. IV.

IV. CPA FOR G IN TWO-BAND MODEL

Since in our present case the only random term in the Hamiltonian is the one involving random d levels we can define a self-energy in the space of d states as

$$\sum_{\vec{k}} \Sigma_d(z) \,|\, kd\rangle \langle kd \,|$$

and write the averaged Green's function as a 2×2 matrix in the $\{|ks\rangle, |kd\rangle\}$ representation:

$$\overline{G}(\vec{k}, z) = \begin{pmatrix} z - \Delta - \epsilon_s(\vec{k}) & -\gamma \\ -\gamma & z - \Sigma_d - \epsilon_d(\vec{k}) \end{pmatrix}^{-1} . \tag{32}$$

We have assumed that in the pure crystal the center of the unhybridized d band is located at the energy origin while the center of the s band is located at Δ.

From (32) we have

$$\begin{aligned} \overline{G}_{ss}(\vec{k}, z) &= \{z - \Delta - \epsilon_s(\vec{k}) - \gamma^2[z - \Sigma_d - \epsilon_d(\vec{k})]^{-1}\}^{-1} , \\ \overline{G}_{dd}(\vec{k}, z) &= \{z - \Sigma_d - \epsilon_d(\vec{k}) - \gamma^2[z - \Delta - \epsilon_s(\vec{k})]^{-1}\}^{-1} , \\ \overline{G}_{sd}(\vec{k}, z) &= \overline{G}_{ds}(\vec{k}, z) = \gamma\{[z - \Delta - \epsilon_s(\vec{k})] \\ &\qquad \times [z - \Sigma_d - \epsilon_d(\vec{k})] - \gamma^2\}^{-1} . \end{aligned} \tag{33}$$

In the two s-d band model, the CPA self-consistency condition is[2]

$$\Sigma_d(z) = \overline{\epsilon}_d - (\epsilon_A^d - \Sigma_d) F_{dd}(z, \Sigma_d)\, (\epsilon_B^d - \Sigma_d) , \tag{34}$$

where

$$\overline{\epsilon}_d = x\epsilon_A^d + (1 - x)\epsilon_B^d \tag{35}$$

and

$$F_{dd}(z, \Sigma_d) = N^{-1}\, \mathrm{Tr}_d \overline{G}(z) = N^{-1} \sum_{\vec{k}} \langle kd \,|\, \overline{G} \,|\, kd\rangle . \tag{36}$$

To derive an expression for F_{dd} which will be easily amenable to numerical computations we make the following approximations. First we assume that in the pure metal the unhybridized s and d bands have the same shape but differ in location and width so that we can write

$$\epsilon_d(\vec{k}) = \xi\epsilon_s(\vec{k}) , \quad \xi < 1 .$$

We also fix the energy origin such that $\epsilon_A^d = \frac{1}{2}\delta$ and $\epsilon_B^d = -\frac{1}{2}\delta$, the parameter δ being a measure of the strength of the scattering potential.

With these assumptions we can write

$$F_{dd}(z, \Sigma_d) = \Omega_c (2\pi)^{-3} \int_{\mathrm{BZ}} d^3k \times \int_{-\infty}^{\infty} \frac{\delta(\epsilon - \epsilon_s(\vec{k}))}{z - \Sigma_d - \xi\epsilon - \gamma^2(z - \Delta - \epsilon)^{-1}}\, d\epsilon , \tag{37}$$

where Ω_c is the volume of the unit cell. In terms of the Hilbert transform of the density of states of the pure crystal s band, namely,

$$F_{0s}(z) = \int_{-\infty}^{\infty} g_{0s}(\epsilon)\, (z - \epsilon)^{-1}\, d\epsilon ,$$

we get the following expression for F_{dd}:

$$\begin{aligned} F_{dd}(z, \Sigma_d) &= [\xi(E_- - E_+)]^{-1} \\ &\quad \times [(z - \Delta - E_+) F_{0s}(E_+) \\ &\quad - (z - \Delta - E_-) F_{0s}(E_-)] , \end{aligned} \tag{38}$$

with

$$E_\pm = \frac{1}{2}\left\{ z - \Delta + \frac{z - \Sigma_d}{\xi} \pm \left[\left(z - \Delta - \frac{z - \Sigma_d}{\xi}\right)^2 + \frac{4\gamma^2}{\xi}\right]\right\} . \tag{39}$$

The function

$$F_{ss}(z, \Sigma_d) = N^{-1} \sum_{\vec{k}} \langle ks \,|\, \overline{G}(z) \,|\, ks\rangle$$

can also be expressed in terms of $F_{0s}(z)$ as

$$\begin{aligned} F_{ss}(z, \Sigma_d) &= (E_- - E_+)^{-1}\left[\left(\frac{z - \Sigma_d}{\xi} - E_+\right) F_{0s}(E_+) \right. \\ &\quad \left. - \left(\frac{z - \Sigma_d}{\xi} - E_-\right) F_{0s}(E_-)\right] . \end{aligned} \tag{40}$$

V. EVALUATION OF A, B, AND C IN CPA

In this section we discuss the procedure for evaluating the quantities A, B, and C defined by Eq. (31). A is related to a two-particle Green's function and describes the averaged propagation of two particles. B and C are related to three-particle Green's functions.

Velicky[1] was the first to apply the CPA to the calculation of the electrical conductivity of disordered binary alloys in a one-band model. In this context he derived the important result that in CPA the vertex correction defined as $\langle GG\rangle - \langle G\rangle\langle G\rangle$ vanishes. This result has been shown to follow as a consequence of the single-site approximation in usual CPA and the short-range nature of the scattering potential. By establishing a contact with the Boltzman transport equation, Velicky pointed out that the vanishing of the vertex correction and of the back scattering in the collision term of the transport equation are physically related.

Generalizing Velicky's arguments, BV have concluded that as in the one-band model and for the same underlying physical reasons, the vertex correction for the product of two Green's functions vanishes in the two s-d band model also.

The work of Velicky has been extended by LVE for calculating Hall coefficient and thermoelectric power of a one-band alloy model. In the calculation of Hall coefficient from the Kubo formalism one invariably encounters the averaging of a direct product of three Green's functions. A straightforward extension of the algebraic approach used by Velicky for averaging the products of two Green's functions becomes unwieldy in this case. LVE have however devised a simple diagrammatic procedure for finding vertex corrections for a product of three Green's functions. It is quite easy to generalize the arguments used by LVE to our present model and verify that as in the one-band model, the vertex corrections for B and C also vanish.

Using the arguments outlined above we have

$$\begin{aligned} &A(O_1, z_1; O_2, z_2) = \mathrm{Tr}\, O_1 \overline{G}(z_1) O_2 \overline{G}(z_2) \ , \\ &B(O_1, z_1; O_2, z_2; \mathcal{H}_M, z_3) \\ &\quad = \mathrm{Tr}\, O_1 \overline{G}(z_1) O_2 \overline{G}(z_2) \mathcal{H}_M \overline{G}(z_3) \ , \\ &C(O_1, z_1; \mathcal{H}_M, z_2; O_2, z_3) \\ &\quad = \mathrm{Tr}\, O_1 \overline{G}(z_1) \mathcal{H}_M \overline{G}(z_2) O_2 \overline{G}(z_3) \ . \end{aligned} \tag{41}$$

Turning back to Eq. (30) we see that for finding $\langle \sigma^a_{xy}(H) \rangle$ we have to evaluate to following traces:

$$\begin{aligned} \Lambda^1 &= \mathrm{Tr}\, J^B_x \overline{G}(z_1) J^A_y \overline{G}(z_2) \ , \\ \Lambda^2 &= \mathrm{Tr}\, J^A_x \overline{G}(z_1) J^B_y \overline{G}(z_2) \ , \\ \Lambda^3 &= \mathrm{Tr}\, J^A_x \overline{G}(z_1) J^A_y \overline{G}(z_2) \mathcal{H}_M \overline{G}(z_3) \ , \\ \Lambda^4 &= \mathrm{Tr}\, J^A_x \overline{G}(z_1) \mathcal{H}_M \overline{G}(z_2) J^A_y \overline{G}(z_3) \ . \end{aligned} \tag{42}$$

We evaluate these traces in the $\{|ns\rangle, |nd\rangle\}$ basis. In this representation the Green's function and the current operators are given by 2×2 matrices. We have therefore

$$\Lambda^1 = \sum_{\alpha, \beta} \Lambda^1_{\alpha\beta} \ ,$$

where

$$\Lambda^1_{\alpha\beta} = \sum_{lmnp} (J^B_{x_{lm}})_{\alpha\alpha} \overline{G}_{\alpha\beta}(m, n; z_1) \times (J^A_{y_{np}})_{\beta\beta} \overline{G}_{\alpha\beta}(p, l; z_2) \ . \tag{43}$$

Using Eqs. (28) and (29) for J^A and J^B, $\Lambda^1_{\alpha\beta}$ can be expressed in the form

$$\begin{aligned} \Lambda^1_{\alpha\beta} = \left(\frac{ie^3 H}{4\hbar^3 c}\right) \Bigg(\sum_{\substack{lmnp \\ \alpha}} \big[& t^\alpha_{lm} (X_l - X_m)^2 Y_m \overline{G}_{\alpha\beta}(m, n; z_1) t^\beta_{np} (Y_n - Y_p) \overline{G}_{\alpha\beta}(p, l; z_2) + t^\alpha_{lm} (X_l - X_m)^2 \overline{G}_{\alpha\beta}(m, n; z_1) t^\beta_{np} (Y_n - Y_p) Y_l \\ & \times \overline{G}_{\alpha\beta}(p, l; z_2) - t^\alpha_{lm} (X_l - X_m)(Y_l - Y_m) X_m \overline{G}_{\alpha\beta}(m, n; z_1) t^\beta_{np} (Y_n - Y_p) \overline{G}_{\alpha\beta}(p, l; z_2) - t^\alpha_{lm} (X_l - X_m)(Y_l - Y_m) \\ & \times \overline{G}_{\alpha\beta}(m, n; z_1) t^\beta_{np} (Y_n - Y_p) X_l \overline{G}_{\alpha\beta}(p, l; z_2) \big] \Bigg) \ . \end{aligned} \tag{44}$$

For expressing $\Lambda^1_{\alpha\beta}$ in the k representation we use the following identities[21] which are easy to verify:

$$\begin{aligned} &(X_m - X_n) t^\alpha_{mn} = \frac{i}{N} \sum_{\vec{k}} [\nabla_{k_x} \epsilon_\alpha(\vec{k})]\, e^{i\vec{k}\cdot(\vec{R}_m - \vec{R}_n)} \ , \\ &(X_m - X_n)^2 t^\alpha_{mn} = -\frac{1}{N} \sum_{\vec{k}} [\nabla^2_{k_x} \epsilon_\alpha(\vec{k})]\, e^{i\vec{k}\cdot(\vec{R}_m - \vec{R}_n)} \ , \\ &(X_m - X_n)(Y_m - Y_n) t^\alpha_{mn} = (Y_m - Y_n)(X_m - X_n) t^\alpha_{mn} = -\frac{1}{N} \sum_{\vec{k}} [\nabla_{k_x} \nabla_{k_y} \epsilon_\alpha(\vec{k})]\, e^{i\vec{k}\cdot(\vec{R}_m - \vec{R}_n)} \ . \end{aligned} \tag{45}$$

We consider only one term in (44), say the first, and express it in the $\vec{k}$ representation. The corresponding expressions for the other terms can then be written down by analogy. Using (45) we have after some straightforward algebra

$$\sum_{lmnp} t^\alpha_{lm} (X_l - X_m)^2 Y_m \overline{G}_{\alpha\beta}(m, n; z_1) t^\beta_{np} (Y_n - Y_p) \overline{G}_{\alpha\beta}(p, l; z_2) = -\sum_{\vec{k}} \frac{\partial^2 \epsilon_\alpha(\vec{k})}{\partial k_x^2} \frac{\partial \epsilon_\beta(\vec{k})}{\partial k_y} \frac{\partial \overline{G}_{\alpha\beta}(\vec{k}; z_1)}{\partial k_y} \overline{G}_{\alpha\beta}(\vec{k}; z_2) \ . \tag{46}$$

Simplifying the other terms in (44) in a similar manner we have finally

$$\Lambda^1_{\alpha\beta} = \left(-\frac{ie^3 \hbar H}{4c}\right) \sum_{\vec{k}} [M^{-1}_{xy\alpha}(\vec{k}) v^{\alpha\alpha}_x(\vec{k}) v^{\beta\beta}_y(\vec{k}) - M^{-1}_{xx\alpha}(\vec{k}) v^{\alpha\alpha}_y(\vec{k}) v^{\beta\beta}_y(\vec{k})]\, \lambda_{\alpha\beta}(\vec{k}; z_1, z_2) \ , \tag{47}$$

where

$$\lambda_{\alpha\beta}(\vec{k}; z_1, z_2) = \overline{G}_{\alpha\beta}(\vec{k}; z_1) \frac{\partial \overline{G}_{\alpha\beta}(\vec{k}; z_2)}{\partial \epsilon_\alpha(\vec{k})} - \frac{\partial \overline{G}_{\alpha\beta}(\vec{k}; z_1)}{\partial \epsilon_\alpha(\vec{k})} \overline{G}_{\alpha\beta}(\vec{k}; z_2) \ ,$$

and we have defined the effective-mass tensor and the velocity function, respectively, by

$$M^{-1}_{ij\alpha}(\vec{k})=\frac{1}{\hbar^2}\frac{\partial^2\epsilon_\alpha(\vec{k})}{\partial k_i\,\partial k_j}\,,\quad v_i^{\alpha\alpha}(\vec{k})=\frac{1}{\hbar}\frac{\partial\epsilon_\alpha(\vec{k})}{\partial k_i}\,.$$

Using the fact that trace operation is invariant under a cyclic permutation and interchanging the indices x and y in (47), it is easy to see that

$$\Lambda^2_{\alpha\beta}=\Lambda^1_{\beta\alpha}\,. \tag{48}$$

Following the method used for simplifying the form of $\Lambda^1_{\alpha\beta}$, it is easily verified that $\Lambda^3_{\alpha\beta}=\Lambda^4_{\alpha\beta}=0$.

Substituting the expressions for Λ^1 and Λ^2 in (30) we have

$$\langle\sigma^a_{xy}(H)\rangle=\frac{\hbar^2e^3H}{8\pi^2c\Omega}\,\mathcal{P}\int\int d\eta\,d\omega\,\omega^{-2}[\rho(\eta)-\rho(\eta+\omega)]\sum_{\lambda_i,\lambda_j=\pm1}(-1)^{(\lambda_i-\lambda_j)/2}\sum_{\substack{\vec{k}\\ \alpha\beta}}c_{\alpha\beta}\,[M^{-1}_{xy\alpha}(\vec{k})v_x^{\alpha\alpha}(\vec{k})v_y^{\beta\beta}(\vec{k})$$
$$-M^{-1}_{xx\alpha}(\vec{k})v_y^{\alpha\alpha}(\vec{k})v_y^{\beta\beta}(\vec{k})]\,\lambda_{\alpha\beta}(\vec{k};Z_{\lambda_i}+\omega,Z_{\lambda_j})\,, \tag{49}$$

where $C_{ss}=2$, $C_{sd}=C_{ds}=\sqrt{20}$ and $C_{dd}=10$. Performing first the summation over the indices λ_i and λ_j and then integrating over ω, we have

$$\langle\sigma^a_{xy}(H)\rangle=\left(\frac{\hbar^2e^3H}{\pi^2c\Omega}\right)\int d\eta\left(-\frac{d\rho(\eta)}{d\eta}\right)\sum_{\substack{\vec{k}\\ \alpha\beta}}c_{\alpha\beta}\,[M^{-1}_{xy\alpha}(\vec{k})v_x^{\alpha\alpha}(\vec{k})v_y^{\beta\beta}(\vec{k})-M^{-1}_{xx\alpha}(\vec{k})v_y^{\alpha\alpha}(\vec{k})v_y^{\beta\beta}(\vec{k})]\,\Gamma_{\alpha\beta}(\vec{k};\eta)\,\frac{\partial R_{\alpha\beta}(\vec{k};\eta)}{\partial\epsilon_\alpha(\vec{k})}\,, \tag{50}$$

where $\Gamma_{\alpha\beta}(\vec{k};z)=\mathrm{Im}\,\overline{G}_{\alpha\beta}(\vec{k};z)$ and $R_{\alpha\beta}(\vec{k};z)=\mathrm{Re}\,\overline{G}_{\alpha\beta}(\vec{k};z)$. Since we are interested in the region of very low temperature we can approximate $d\rho(\eta)/d\eta$ by $-\delta(\eta-\epsilon_F)$ and write

$$\langle\sigma^a_{xy}(H)\rangle=\frac{\hbar^2e^3H}{\pi^2c\Omega}\sum_{\substack{\vec{k}\\ \alpha\beta}}c_{\alpha\beta}\,[M^{-1}_{xy\alpha}(\vec{k})v_x^{\alpha\alpha}(\vec{k})v_y^{\beta\beta}(\vec{k})-M^{-1}_{xx\alpha}(\vec{k})v_y^{\alpha\alpha}(\vec{k})v_y^{\beta\beta}(\vec{k})]\,\Gamma_{\alpha\beta}(\vec{k};\epsilon_F)\,\frac{\partial R_{\alpha\beta}(\vec{k};\epsilon_F)}{\partial\epsilon_\alpha(\vec{k})}\,. \tag{51}$$

The only other quantity that we need for finding the Hall coefficient as given by (19) is the longitudinal component of the conductivity in the absence of the magnetic field. This has already been calculated by BV, and is given in the form

$$\langle\sigma_{xx}\rangle=\frac{2e^2\hbar}{\pi\Omega}\sum_{\substack{\vec{k}\\ \alpha\beta}}c_{\alpha\beta}v_x^{\alpha\alpha}(\vec{k})v_x^{\beta\beta}(\vec{k})[\Gamma_{\alpha\beta}(\vec{k};\epsilon_F)]^2\,. \tag{52}$$

The one-band analog of our expression for $\sigma^a_{xy}(H)$ reduces to the expressions obtained by LVE and Fukuyama.[24] LVE have assumed $M^{-1}_{xy}=0$ in their calculation. We have however retained the off-diagonal components of the effective mass tensor in our formulation.

If we assume an isotropic band structure so that $\epsilon(\vec{k})=\epsilon(|\vec{k}|)$, our Eq. (51) reduces to

$$\langle\sigma^a_{xy}(H)\rangle=\left(-\frac{\hbar^4e^3H}{3\pi^2c\Omega}\right)\sum_{\substack{\vec{k}\\ \alpha\beta}}c_{\alpha\beta}\,[v^{\alpha\alpha}(\vec{k})]^2\,\frac{v^{\beta\beta}(\vec{k})}{k}\,\Gamma_{\alpha\beta}(\vec{k};\epsilon_F)\,\frac{\partial R_{\alpha\beta}(\vec{k};\epsilon_F)}{\partial\epsilon_\alpha(\vec{k})}\,,$$

which is a generalization of the result obtained by Matsubara and Kaneyoshi[20] for the Hall coefficient of an impurity band model.

VI. NUMERICAL RESULTS AND DISCUSSION

We make the following two different types of approximation in our numerical work: (a) Hubbard semielliptic density of states and a Velicky-type approximation[1] for the velocity function so as to simplify the evaluation of the summation over $\vec{k}$ vectors implied in Eq. (51). (b) For the case $\xi=0$ we use a simple-cubic tight-binding band structure as in LVE. (a) and (b) represent two extreme ways of incorporating the effect of band structure in our calculation without going through a Draconian integration over the Brillouin zone. In principle there is no difficulty in assuming a more realistic band structure. But in view of the limitations of our model such a detailed numerical calculation does not seem to be worthwhile.

In both of our approximations we assume that the off-diagonal components of the effective-mass tensor are zero. This is certainly true of a simple-cubic tight-binding band structure and compatible with approximation (a).

To proceed with approximation (a) we assume that the density of states (per site) of the unhybridized s band is given by the Hubbard semielliptic form, i.e.,

$$g_{0s}(\epsilon)=N^{-1}\sum_{\vec{k}}\delta(\epsilon-\epsilon_s(\vec{k}))$$
$$\sim\begin{cases}(2/\pi)(1-\epsilon^2)^{1/2} & \text{for } |\epsilon|\leq1\,,\\ 0 & \text{elsewhere}\,,\end{cases} \tag{53}$$

where ϵ designates the energy in units of the half s bandwidth. The alloy density of states at the Fermi level is then given by

$$g(\epsilon_F)=g_s(\epsilon_F)+g_d(\epsilon_F) \;, \tag{54}$$

where

$$\begin{aligned} g_s(\epsilon_F)&=-(2/\pi)\,\mathrm{Im}F_{ss}(\epsilon_F+i0,\Sigma_d) \;, \\ g_d(\epsilon_F)&=-(10/\pi)\,\mathrm{Im}F_{dd}(\epsilon_F+i0,\Sigma_d) \;, \end{aligned} \tag{55}$$

and the Fermi level ϵ_F is determined from the relation

$$\int_{-\infty}^{\epsilon_F} g(\epsilon)\,d\epsilon = xn_A+(1-x)n_B \;, \tag{56}$$

n_A and n_B being the number of electrons per atom for pure A and B metals.

For computing the longitudinal electrical conductivity we adopt Velicky's approximation[1] for the velocity function, namely,

$$N^{-1}\sum_{\vec{k}}[v^{ss}(\vec{k})]^2\,\delta(\epsilon-\epsilon_s(\vec{k}))\sim\frac{2v_m^2}{\pi}(1-\epsilon^2)^{3/2} \;, \tag{57}$$

where $v^{ss}(\vec{k})=\hbar^{-1}|\nabla_k\epsilon_s(\vec{k})|$ and v_m is the maximum velocity in the band. Equation (57) produces the correct behavior at the band edges. Using (57) the longitudinal electrical conductivity is given by

$$\sigma_{xx}(\epsilon_F)=\sigma_{xx}^{ss}(\epsilon_F)+2\sigma_{xx}^{sd}(\epsilon_F)+\sigma_{xx}^{dd}(\epsilon_F) \;, \tag{58}$$

where

$$\sigma_{xx}^{\alpha\beta}(\epsilon_F)=\sigma_0 q_{\alpha\beta}\int_{-1}^{1}d\epsilon\,(1-\epsilon^2)^{3/2}[\Gamma_{\alpha\beta}(\epsilon;\epsilon_F)]^2 \;, \tag{59}$$

with

$$\sigma_0=\frac{4v_m^2e^2\hbar}{3\pi^2\Omega_c}\;,\qquad q_{ss}=2\;,$$

$$q_{sd}=\sqrt{20}\,\xi\;,\qquad q_{dd}=10\xi^2\;.$$

$\Gamma_{\alpha\beta}(\epsilon;\epsilon_F)$ in (59) has the same analytic form as $\Gamma_{\alpha\beta}(\vec{k};\epsilon_F)$ with $\epsilon_s(\vec{k})$ replaced by ϵ.

Using residue calculus it is possible to obtain from (59) algebraic expressions for $\sigma_{xx}^{\alpha\beta}(\epsilon_F)$. We thus need not perform the numerical quadratures which because of the sharp variation of the integrands are difficult to evaluate accurately. We relegate to the Appendix the derivation of these results. Somewhat similar results have been obtained earlier by Chen *et al.*[22] by following an analysis more involved than that of ours.

For calculating the transverse electrical conductivity we start with Eq. (51) and assume $M_{xy}^{-1}=0$. We thus need to evaluate

$$\sum_{\substack{\vec{k}\\ \alpha\beta}}\frac{\partial^2\epsilon_\alpha(\vec{k})}{\partial k_x^2}\,\frac{\partial\epsilon_\alpha(\vec{k})}{\partial k_y}\,\frac{\partial\epsilon_\beta(\vec{k})}{\partial k_y}\,\Gamma_{\alpha\beta}(\vec{k};\epsilon_F)\,\frac{\partial R_{\alpha\beta}(\vec{k};\epsilon_F)}{\partial\epsilon_\alpha(\vec{k})}\;.$$

Changing the $\vec{k}$ summation to an integral and integrating by parts, it is easy to see that the above expression reduces to

$$-\frac{1}{9}\sum_{\substack{\vec{k}\\ \alpha\beta}}\chi_{\alpha\beta}[v^{ss}(\vec{k})]^4\,\frac{\partial}{\partial\epsilon_s(\vec{k})}\left(\Gamma_{\alpha\beta}(\vec{k};\epsilon_F)\,\frac{\partial R_{\alpha\beta}(\vec{k};\epsilon_F)}{\partial\epsilon_s(\vec{k})}\right)\,, \tag{60}$$

where

$$\chi_{ss}=1\;,\qquad\chi_{sd}=\chi_{ds}=\xi\;,\qquad\chi_{dd}=\xi^2\;.$$

At a natural generalization of (57) we assume following Fukuyama[24]

$$N^{-1}\sum_{\vec{k}}[v^{ss}(\vec{k})]^4\,\delta(\epsilon-\epsilon_s(\vec{k}))\sim\frac{2v_m^4}{\pi}(1-\epsilon^2)^{5/2}\;. \tag{61}$$

Expressions similar to (59) can now be deduced for the magnetic-field-dependent transverse conductivity

$$\sigma_{xy}(\epsilon_F)=\sigma_{xy}^{ss}(\epsilon_F)+2\sigma_{xy}^{sd}(\epsilon_F)+\sigma_{xy}^{dd}(\epsilon_F)\;,$$

where

$$\sigma_{xy}^{\alpha\beta}(\epsilon_F)=\sigma_H q_{\alpha\beta}\int_{-1}^{1}d\epsilon\,(1-\epsilon^2)^{5/2}\,\mathfrak{F}_{\alpha\beta}(\epsilon;\epsilon_F)\;, \tag{62}$$

with

$$\begin{aligned}\mathfrak{F}_{\alpha\beta}(\epsilon;\epsilon_F)=&\frac{\partial^2R_{\alpha\beta}(\epsilon;\epsilon_F)}{\partial\epsilon^2}\,\Gamma_{\alpha\beta}(\epsilon;\epsilon_F)\\ &+\frac{\partial R_{\alpha\beta}(\epsilon;\epsilon_F)}{\partial\epsilon}\,\frac{\partial\Gamma_{\alpha\beta}(\epsilon;\epsilon_F)}{\partial\epsilon}\end{aligned}$$

and

$$\sigma_H=-2v_m^4\hbar^2e^3H/9\pi^3c\Omega_c\;.$$

For the purpose of numerical illustration we assign the following values to the alloy parameters: $\delta=2.8\,\mathrm{eV}$, $\gamma=1\,\mathrm{eV}$, $\xi=0.2$, $w_s=7\,\mathrm{eV}$, the position of the common s band being such that its bottom is 4.4 eV lower than the zero of energies situated midway between ϵ_A^d and ϵ_B^d. Figure 1 shows the alloy density of states g, the longitudinal electrical conductivity σ_{xx}, the transverse conductivity σ_{xy}, and the Hall coefficient R_H as functions of band filling (or the Fermi energy) for an equiconcentrated alloy.

The band-filling dependence of σ_{xx} has already been investigated by BV; using the result got in the Appendix for $\xi=0$, it is easy to understand qualitatively this behavior. Indeed, σ_{xx} is proportional to the alloy s density of states which presents a minimum for energies corresponding to the centers of the d bands and to the inverse of the effective s damping $|\Sigma_{2s}|$ which presents a maximum for energies corresponding to the centers of the d bands and which is vanishing outside the d bands. The behavior of σ_{xy} presents more important variations and its change in sign determines that of R_H which is negative at the bottom of the s band and positive at the top. This behavior is similar to that observed by LVE in a one-band picture (i.e., R_H negative at the bottom of the band and positive at the top) where the electrons of that band are directly affected by the disorder. Here, the disorder affects directly the d electrons and the s electrons are indirectly affected through the s-d hybridization. However the general behavior observed in the one-band picture is reproduced for the s band. Coming now to our second approximation we put $\xi = 0$ and assume that $\epsilon_s(\vec{k})$ has a simple-cubic tight-binding form

$$\epsilon_s(\mathrm{k}) = -\tfrac{1}{3} w_s (\cos ak_x + \cos ak_y + \cos ak_z) \ .$$

In the case $\xi = 0$, the two s-d band model of BV reduces to that of Levin and Ehrenreich[3] where the d bands are approximated by d levels. Such a model provides a good description for noble-metal alloys as well as transition–noble-metal alloys when the Fermi level is not lying inside the d bands (Brouers *et al.*[5]). For $\xi = 0$, the s–d and d–d components of the conductivity vanish, and we have

$$\sigma_{xx}(\epsilon_F) = \sigma_{xx}^{ss}(\epsilon_F) \ , \quad \sigma_{xy}(\epsilon_F) = \sigma_{xy}^{ss}(\epsilon_F) \ .$$

The expressions for σ_{xx}^{ss} and σ_{xy}^{ss} are the same as in the one-band model of LVE except for the fact that we have to replace the one-band CPA Green's function by $\bar{G}_{ss}(\epsilon;\epsilon_F)$, where

$$\bar{G}_{ss}(\epsilon;\epsilon_F) = (\epsilon_F - \Sigma_s - \epsilon)^{-1} \ ,$$

with

$$\Sigma_s = \Delta + \gamma^2/(\epsilon_F - \Sigma_d) \ .$$

Following LVE, one can then obtain the Fermi energy dependence of the two conductivities from the following expressions:

$$\sigma_{xx}(\epsilon_F) \propto \int_0^\infty dt \cos(\epsilon_F - \mathrm{Re}\Sigma_s)t[J_0(t) + J_2(t)]J_0^2(t) \ ,$$

$$\sigma_{xy}(\epsilon_F) \propto -\int_0^\infty dt \sin(\epsilon_F - \mathrm{Re}\Sigma_s)t[J_0(t) + J_2(t)]J_0(t)J_1(t).$$

In Fig. 2, we plot σ_{xx}, σ_{xy}, R_H, and $\epsilon_F - \mathrm{Re}\Sigma_s$ as a function of band filling, giving the following values to the alloy parameters: $x = 0.5$, $\delta = 2.8$ eV, $\gamma = 2$ eV, $w_s = 7$ eV, $\xi = 0.2$ (to avoid any unphysical gap in the alloy density of states), the position of the s band being such that its bottom is 4.4 eV lower than the zero of energies. Versus the band filling, the alloy s density of states and σ_{xx} have the same behaviors. The Hall coefficient presents the same qualitative behavior as previously (negative at the bottom of the s band and positive at the top); as pointed out by Fukuyama[24] in a one-band picture, this shows that the Velicky-type approximation for the velocity function is consistent with the assumption of a simple-cubic tight-binding band structure. On the other hand, as pointed out by LVE in the one-band picture, the sign of R_H is the same as that of the quantity $\epsilon_F - \mathrm{Re}\Sigma$ which is the only parameter appearing in the ex-

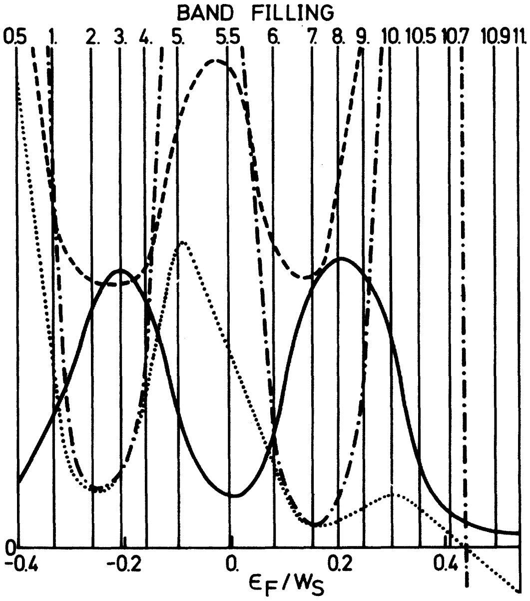

FIG. 1. Alloy density of states (solid line), longitudinal electrical conductivity (dashed line), transverse electrical conductivity (dash-dot line) with opposite sign, Hall coefficient (dotted line) with opposite sign, as functions of the band filling (number of electrons) and of the Fermi energy in units of the half s bandwidth w_s. The vertical scale is given in arbitrary units; the alloy parameters are defined in the text. Velicky's approximation has been used for the velocity function.

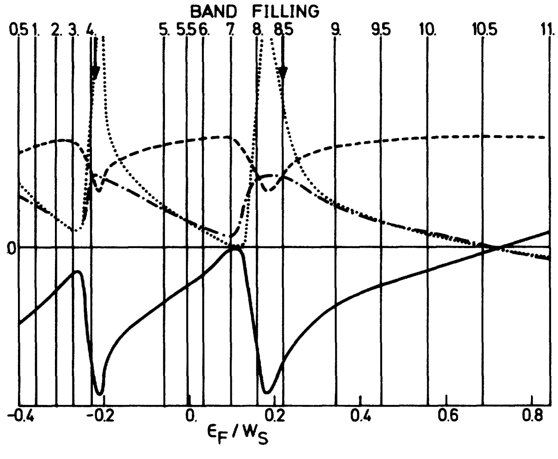

FIG. 2. Longitudinal electrical conductivity (dashed line), transverse electrical conductivity (dash-dot line) with opposite sign, Hall coefficient (dotted line) with opposite sign, the quantity $\epsilon_F - \mathrm{Re}\Sigma_s$ (solid line), as functions of the band filling (number of electrons) and of the Fermi energy in units of the half s bandwidth w_s. The vertical scale is given in arbitrary units; the alloy parameters are defined in the text. The arrows give the position of the two d levels and the velocity function is derived from a simple-cubic tight-binding band structure.

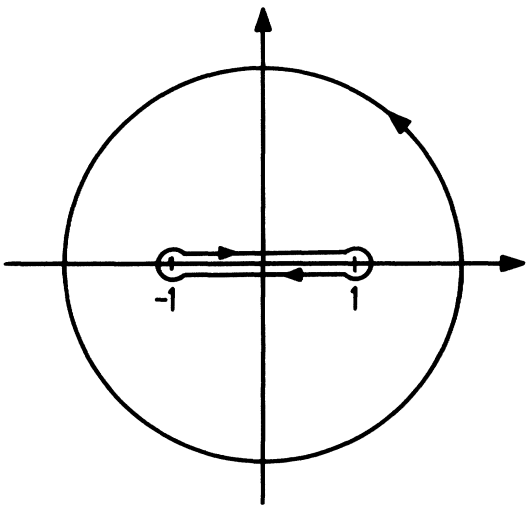

FIG. 3. Contour used for residues calculations of the Appendix.

pression of R_H, Σ being the self-energy corresponding to the band which is directly affected by the disorder. In our model, the sign of R_H is the same as that of $\epsilon_F - \mathrm{Re}\Sigma_s$, where Σ_s is the effective *s* self-energy which contains the effect of the *d* disorder and the *s*-*d* hybridization.

We do not investigate the concentration dependence of R_H; indeed in contrast with σ_{xx} for which a simple relation can be found with the alloy density of states (Appendix), the physical parameters of the model, because of the approximations made as we already pointed out in the Introduction, do not seem to be still enough relevant to make in the present state of the theory any convincing comparison with experiments.

In the future, we believe that efforts should be made first in the calculation of transport properties of dilute alloys using a detailed band picture for the density of states and the velocity function. Then, when such a problem will be under control, one could go back to the concentrated alloy problem taking account of some formal results discussed in the present paper.

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APPENDIX

Combining (58) and (59) we have

$$\sigma_{xx}(\epsilon_F) = \frac{\sigma_0 \Sigma_2^2}{\xi^4} \int_{-1}^{1} d\epsilon\, (1-\epsilon^2)^{3/2}\, [\gamma^2 + \sqrt{5}\, \xi(\epsilon_F - \Delta - \epsilon)^2]^2 \Big/ \prod_{j=1}^{4} (\epsilon - v_j)^2 \ , \tag{A1}$$

where the v_j's are the four complex roots of the quartic equation

$$[(\epsilon_F - \Delta - \epsilon)(\epsilon_F - \Sigma_1 - \xi\epsilon) - \gamma^2]^2 + \Sigma_2^2 (\epsilon_F - \Delta - \epsilon)^2 = 0 \ , \tag{A2}$$

and we have put

$$\Sigma_d = \Sigma_1 + i\Sigma_2 \ .$$

For performing the integral in (A1) we use the contour shown in Fig. 3.

In terms of the residues at the double poles v_j, we get

$$\sigma_{xx}(\epsilon_F) = \pi \frac{\sigma_0 \Sigma_2^2}{\xi^4} \left[5\,\xi^2 - \sum_{i=1}^{4} \mathrm{Res}\left((z^2-1)^{3/2} [\gamma^2 + \sqrt{5}\, \xi(\epsilon_F - \Delta - z)^2]^2 \Big/ \prod_{j=1}^{4} (z - v_j)^2 \right)_{z=v_i} \right] \ ,$$

more explicitly

$$\sigma_{xx}(\epsilon_F) = \pi \frac{\sigma_0 \Sigma_2^2}{\xi^4} \left\{ 5\,\xi^2 + \sum_{i=1}^{4} \left[\left((v_i^2-1)^{3/2} [\gamma^2 + \sqrt{5}\, \xi(\epsilon_F - \Delta - v_i)^2]^2 \Big/ {\prod_{j=1}^{4}}' (v_i - v_j)^2 \right) \times \left(\frac{3v_i}{1-v_i^2} - \frac{4\sqrt{5}\, \xi(v_i - \epsilon_F + \Delta)}{\gamma^2 + \sqrt{5}\, \xi(\epsilon_F - \Delta - v_i)^2} + {\sum_{j=1}^{4}}' \frac{2}{v_i - v_j} \right) \right] \right\} \ , \tag{A3}$$

where the prime indicates that $i \neq j$.

Using a similar procedure we can express the *s* and *d* densities of states in terms of the v_j's as follows:

$$g_s(\epsilon_F) = \frac{4}{\pi} \frac{\gamma^2 \Delta}{\xi^2} \sum_{i=1}^{4} (v_i^2 - 1)^{1/2} \Big/ {\prod_{j=1}^{4}}' (v_i - v_j) \ , \tag{A4}$$

$$g_d(\epsilon_F) = \frac{20}{\pi} \frac{\Delta}{\xi^2} \sum_{i=1}^{4} (v_i^2 - 1)^{1/2} (\epsilon_F - \Delta - v_i)^2 \Big/ {\prod_{j=1}^{4}}' (v_i - v_j) \ . \tag{A5}$$

In general it is quite a formidable task to eliminate the v_j's by combining Eqs. (A3)–(A5). However for $\xi = 0$ one can derive a very simple expression for $\sigma_{xx}(\epsilon_F)$ solely in terms of the s density of states. Putting $\Sigma_s = \Sigma_{1s} + i\Sigma_{2s}$, we have

$$\sigma_{xx}(\epsilon_F, \xi = 0) = 2\sigma_0 \Sigma_{2s}^2 \int_{-1}^{1} d\epsilon \, \frac{(1-\epsilon^2)^{3/2}}{(\epsilon - w_1)^2 (\epsilon - w_2)^2} \, , \tag{A6}$$

where $w_1 = \epsilon_F - \Sigma_{1s} + i\Sigma_{2s}$ and $w_2 = \epsilon_F - \Sigma_{1s} - i\Sigma_{2s}$ are the two complex roots of the quadratic equation

$$(\epsilon_F - \Sigma_{1s} - \epsilon)^2 + \Sigma_{2s}^2 = 0 \, .$$

Using the same contour as previously we have

$$\sigma_{xx}(\epsilon_F, \xi = 0) = 2\sigma_0 \pi \Sigma_{2s}^2 \left[1 + \frac{(w_1^2 - 1)^{1/2}}{(w_1 - w_2)^2} \left(\frac{2(w_1^2 - 1)}{w_1 - w_2} - 3w_1 \right) + \frac{(w_2^2 - 1)^{1/2}}{(w_2 - w_1)^2} \left(\frac{2(w_2^2 - 1)}{w_2 - w_1} - 3w_2 \right) \right] \, . \tag{A7}$$

The corresponding s density of states at the Fermi level is given by

$$g_s(\epsilon_F, \xi = 0) = \frac{4\Sigma_{1s}}{\pi} \left(\frac{(w_1^2 - 1)^{1/2}}{w_1 - w_2} + \frac{(w_2^2 - 1)^{1/2}}{w_2 - w_1} - 1 \right) \, . \tag{A8}$$

Eliminating w_1 and w_2 from (A7) and (A8), we get

$$\sigma_{xx}(\epsilon_F, \xi = 0) = \sigma_0 \, \frac{\pi^4}{16} \left(\frac{g_s^3(\epsilon_F, \xi = 0)}{4 | \Sigma_{2s} |} + \frac{3}{\pi} g_s^2(\epsilon_F, \xi = 0) \right) \, . \tag{A9}$$

This expression is similar to the one derived for the one-band model by Chen *et al.*[22] by using a somewhat more complicated procedure. Relation (A9) provides a direct qualitative understanding of the behavior of σ_{xx} as function of the Fermi energy (see Fig. 1).

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[†] On leave of absence from the Department of Physics, University of Roorkee, India.

[‡] Aspirant du Fonds National Belge de la Recherche Scientifique.

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