

## Transport properties of one-dimensional, disordered two-band systems

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**Abstract.** We have studied the transport properties of disordered one-dimensional two-band systems. The model includes a narrow *d* band hybridised with an *s* band. The Landauer formula was used in the case of a very narrow *d* band or in the case of short chains. The results were compared with the localisation length of the wavefunctions calculated by the transfer matrix method, which allows the use of very long chains, and an excellent agreement was obtained.

### 1. Introduction

We are interested in the study of the transport properties of disordered transition metal systems. It is with this aim that we make a first approximation to them by proposing a very simple disordered *s*–*d* model, with a narrow *d* band embedded in an *s* band and hybridised as in transition metals. The model is a tight-binding one-dimensional one.

The first theoretical works on these materials assumed that *d* electrons did not contribute to the conductivity of these systems because they were too localised (Ziman 1961, Mott 1972). However, ten Bosch and Benemann (1975) took them into account in the study of three-dimensional liquid metals and concluded that their contribution is important. This is because the scattering due to disorder mostly affects the conductivity of *s* electrons and makes it of the same order as that of the more localised and less affected *d* electrons. They used linear response theory and considered the *s* electrons free. Aoki (1981) performed calculations of localisation for small two-dimensional tight-binding systems and also concluded that *d* electrons and hybridisation are important.

In our case we use the Landauer formula for the resistance (Landauer 1970) of some simplified models and the transfer matrix method (MacKinnon and Kramer 1983) to calculate the localisation of the wavefunctions. Both results agree very well qualitatively and show the importance of the *d* contribution to the transport properties and the relative effects of disorder and hybridisation.

The effect of hybridisation is to produce an effective *d* band with an increasing maximum in the resistance with increasing hybridisation.

**2. Model**

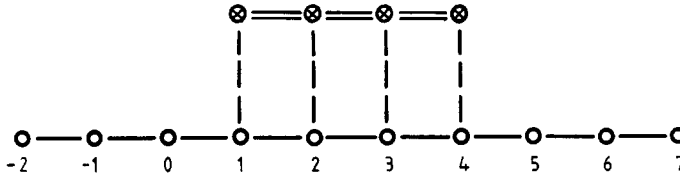
We have used for this calculation a disordered one-dimensional first-neighbour tight-binding Hamiltonian, with two orbitals per site. Both orbitals were assumed to be of *s* type, as a first approximation, and hybridisation was considered only between orbitals on the same site. To remind us of transition metals we have named  $|ns\rangle$  the orbitals with a wider band and  $|nd\rangle$  the ones with a smaller bandwidth. Therefore,

$$H = \sum_n (\epsilon_n^s |ns\rangle\langle ns| + \epsilon_n^d |nd\rangle\langle nd| + t^s |ns\rangle\langle n + 1, s| + t^s |n + 1, s\rangle\langle ns| + t^d |nd\rangle\langle n + 1, d| + t^d |n + 1, d\rangle\langle nd| + h |ns\rangle\langle nd| + h |nd\rangle\langle ns|) \tag{1}$$

where the  $\epsilon_n$  indicate the self-energies corresponding to the  $n$ th atom,  $t$  the corresponding integrals between first neighbours and  $h$  the hybridisation. Disorder was introduced mainly in the diagonal elements  $\epsilon_n$ , and with a uniform distribution of width  $W$ .

To study the resistance of a finite system of  $N$  sites we have embedded it in an ordered chain of only one orbital per site. Therefore the following conditions had to be fulfilled:  $\epsilon_n^s = \epsilon$ ,  $\epsilon_n^d = 0$ ,  $t^d = 0$  and  $h = 0$  for  $n < 1$  and  $n > N$ .

In what follows we take  $\epsilon = 0$  and  $t^s = 1$  as our energy scale. Figure 1 shows these interactions for  $N = 4$  schematically.



**Figure 1.** Schematic representation of an  $N = 4$  disordered two-band model embedded in a perfect linear chain. ---,  $h$ ; —,  $t^s$ ; ===,  $t^d$ ;  $\circ$ ,  $\epsilon^s$ ;  $\otimes$ ,  $\epsilon^d$ .

If the wavefunctions are written as:

$$\psi = \sum_n (a_n |ns\rangle + b_n |nd\rangle) \tag{2}$$

the tight-binding Hamiltonian leads to the recurrence relations

$$\begin{aligned} \epsilon_n^s a_n + t^s(a_{n+1} + a_{n-1}) + hb_n &= Ea_n \\ \epsilon_n^d b_n + t^d(b_{n+1} + b_{n-1}) + ha_n &= Eb_n \end{aligned} \tag{3}$$

which are equivalent, in matrix notation, to

$$\begin{pmatrix} a_{n+1} \\ a_n \\ b_{n+1} \\ b_n \end{pmatrix} = \begin{bmatrix} (E - \epsilon_n^s)/t^s & -1 & -h/t^s & 0 \\ 1 & 0 & 0 & 0 \\ -h/t^d & 0 & (E - \epsilon_n^d)/t^d & -1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{pmatrix} a_n \\ a_{n-1} \\ b_n \\ b_{n-1} \end{pmatrix}. \tag{4}$$

The Landauer formula (Landauer 1970) for the dimensionless resistance is  $\rho = R/T$  where  $R$  and  $T$  are the total reflection and transmission coefficients of the disordered region.  $\rho$  is related to  $P_N$ , the  $2 \times 2$  transfer matrix leading

$$\text{from vector } \begin{pmatrix} a_0 \\ a_{-1} \end{pmatrix} \text{ to vector } \begin{pmatrix} a_{N+2} \\ a_{N+1} \end{pmatrix}.$$

Its calculation involves the product of  $(N - 2) 4 \times 4$  matrices such as that of equation (4) and taking care of the boundary conditions. Once  $P_N$  is known, the dimensionless resistance is easily obtained with the expression given by Stone *et al* (1981):

$$\rho = \frac{1}{(4 - E^2)} [(P_N^{11})^2 + (P_N^{12})^2 + (P_N^{21})^2 + (P_N^{22})^2 + E(P_1^{11} - P_N^{22})(P_N^{12} - P_N^{21}) - E^2 P_N^{12} P_N^{21} - 2]. \quad (5)$$

In fact, the dimensionless resistance of the system we study is always different from zero for all values of  $E$ , even in the absence of disorder. The reason for this is that the d orbitals exist only in one region of the whole chain. Anyway, the residual resistivity is very small for all values of  $E$  and can be therefore disregarded.

### 3. Calculation of the resistance with the Landauer formula

Numerical calculations of the matrix  $P_N$  for chains of different lengths, hybridisations and degrees of disorder were attempted. For each set of parameters an ensemble average had to be performed among different realisations of the disordered chain. The appropriate quantity to be averaged for each energy  $E$  is  $\ln(1 + \rho)$  (Abrahams *et al* 1979).

However, for energies that are not well inside the d band the product of  $4 \times 4$  matrices blows up. This problem is not new for it also appeared in the calculation of the resistance for finite two-dimensional disordered systems (Anderek 1984).

Because of the difficulty mentioned above we studied some possible simpler cases:

#### 3.1. Very narrow d band, $t^d = 0$

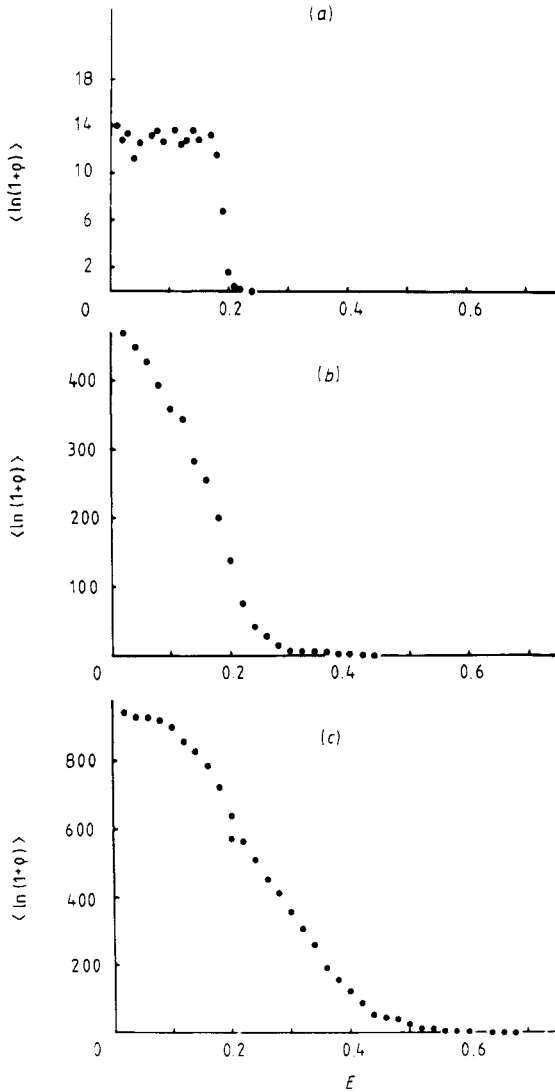
In this case equations (4) give  $b_n = ha_n/(E - \epsilon_n^d)$  and therefore

$$[E - \epsilon_n^s - h^2/(E - \epsilon_n^d)] a_n = a_{n+1} + a_{n-1}. \quad (6)$$

This equation corresponds to a single chain with only one orbital per site but having an energy dependent diagonal element,

$$\bar{\epsilon}_n^s = \epsilon_n^s + h^2/(E - \epsilon_n^d). \quad (7)$$

Numerical calculations for this case are shown in figure 2, averaged over 70 chains for  $N = 200$ ,  $W^d = 0.4$  and  $W^s = 0$ . Due to the fact that the s band is ordered, if the hybridisation is small the resistance is appreciable only for energies inside the d range of disorder. When the hybridisation is increased its effect is equivalent to a larger disorder, according to equation (7), and a finite resistance is seen for  $E > 0.2$ . For



**Figure 2.**  $\langle \ln(1 + \rho) \rangle$  calculated by means of the Landauer formula for the cases  $t_s = 1$ ,  $t_d = 0$ ,  $W_s = 0$ ,  $W_d = 0.4$  and (a)  $h = 0.1$ ; (b),  $h = 0.5$ ; (c),  $h = 1$ . In each of the examples the average was made over 70 samples of 200 atoms.

example, figure 2 shows  $h = 0.1$ ,  $0.5$  and  $1.0$ . The effect of the hybridisation is that the  $d$  states participate in the resistance for a wider range of energies than that given by  $\epsilon^d$ .

The effect of introducing disorder in the  $s$  band also is seen mostly at the largest energies, where the resistance increases due to the localisation of states at the band limits. We have also introduced off-diagonal disorder in some cases but it produced no qualitative differences.

Chains of different lengths follow the well known scaling law (Abrahams *et al* 1979)  $\langle \ln(1 + \rho) \rangle \propto N$  for  $E = 0$  and values of  $N > 50$ .

3.2. Direct diagonalisation of short chains  $N \sim 50$

The embedded group of  $N$  sites was diagonalised separately and a new basis set for the complete Hamiltonian was defined using the eigen-functions obtained,  $|\nu\rangle$

$$\begin{aligned} |\nu\rangle &= |ns\rangle & \nu < 1 \\ |\nu\rangle &= \sum_{n=1}^N (\alpha_n^\nu |ns\rangle + \beta_n^\nu |nd\rangle) & 1 \leq \nu \leq 2N \\ |\nu\rangle &= |n + N, s\rangle & \nu > 2N. \end{aligned} \tag{8}$$

In this basis the complete Hamiltonian has a diagonal part of  $2N \times 2N$  and the only new elements are those of the surrounding part, the interaction or boundary terms:

$$\begin{aligned} \langle 0|H|\nu\rangle &= \alpha_1^\nu \\ \langle 2N + 1|H|\nu\rangle &= \alpha_{2N}^\nu \quad 1 \leq \nu \leq 2N. \end{aligned} \tag{9}$$

This example corresponds to a simple chain with one impurity having  $2N$  levels. Some simple algebra leads to the expression for the transfer matrix  $P_N$  relating

$$\begin{pmatrix} a_{2N+2} \\ a_{2N+1} \end{pmatrix} \text{ to } \begin{pmatrix} a_0 \\ a_{-1} \end{pmatrix}$$

$$P_N = \begin{bmatrix} \frac{(E - G_{11})(E - G_{NN})}{G_{1N}} - G_{1N} & \frac{-(E - G_{NN})}{G_{1N}} \\ \frac{(E - G_{11})}{G_{1N}} & -\frac{1}{G_{1N}} \end{bmatrix} \tag{10}$$

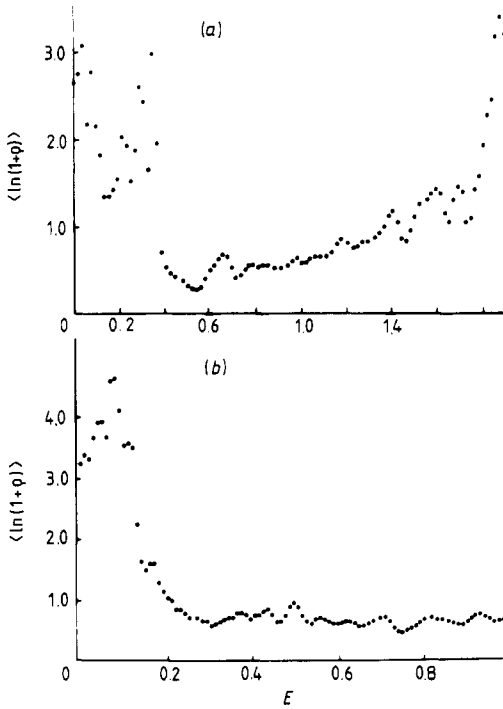
where

$$G_{ij} = \sum_{\nu=1}^{2N} \alpha_i^\nu \alpha_j^\nu / (E - E_\nu) \quad \text{for } E \neq E_\nu$$

This expression was evaluated giving  $E$  a small imaginary part and averaged over different samples. There is a considerable noise in the results for small hybridisation in the region of energies where the d electrons are important. Figure 3 shows the results obtained for 40 chains with  $N = 50$ ,  $W^d = 0.2$ ,  $W^s = 0.8$ ,  $t^d = 0.25$  and  $h = 0.5$  and  $0.9$ . The interesting difference with the previous case,  $t^d = 0$ , is that the maximum of the curve is not at  $E = 0$  but possibly at the edge of the effective d band. We define the effective d band as the energy region comprised between the inner two peaks of the density of states of the ordered system. These two peaks are present for  $h < 2 (t^d t^s)^{1/2}$ . For larger values of the hybridisation the density of states has two bands separated by a gap and we can speak no more of an effective d band.

4. Localisation of the wavefunctions

A magnitude directly related to the transport properties of the system, for large  $N$ , is the localisation length of the wavefunctions. The case of two orbitals per site is, for these calculations, similar to that of two coupled chains. Pichard (1984) has generalised the



**Figure 3.**  $\langle \ln(1 + \rho) \rangle$  calculated by means of the Landauer formula for  $t_s = 1, t_d = 0.25, W_s = 0.8, W_d = 0.2$  and (a)  $h = 0.5$ ; (b)  $h = 0.9$ .

Landauer formula for a system of  $\alpha$  coupled chains and found for large disorder that the conductance is given by

$$G(N) \sim 2 \sum_{\alpha} \exp[-2N/\xi_{\alpha}(N)] \tag{11}$$

where  $\xi_{\alpha}(N)$  are the localisation lengths in each channel (Pichard 1984). If all  $\xi_{\alpha} \ll N$ , they are the inverses of the  $\alpha$  positive Lyapunov exponents of the system,  $\gamma_{\alpha}(N)$ .

The smallest Lyapunov coefficient will dominate the summation for large  $N$  so that

$$G(N) \sim 2 \exp[-2N\gamma_1(N)]. \tag{12}$$

In the limit, the following relation is exact:

$$\lim_{N \rightarrow \infty} (1/N) \ln \rho(N) = 2\gamma_1. \tag{13}$$

The calculation of  $\gamma_1$  involves the product of transfer matrices  $T_i$  of the type of equation (4), which presents numerical difficulties. However, Osledec's theorem proves that the limit matrix

$$\Lambda = \lim_{N \rightarrow \infty} (M_N M_N^{\dagger})^{1/2N} \tag{14}$$

where  $M_N = \prod_i T_i$ , exists and its eigenvalues  $\lambda_i$  and eigenvectors should be well determined (Osledec 1968). The Lyapunov coefficients are  $\gamma_i = \log \lambda_i$ .

To overcome the divergencies in the matrix product Kramer and MacKinnon suggested a renormalisation procedure from which one can extract the growth rate of the

eigenvectors (MacKinnon *et al* 1983). It consists in orthogonalising each column of the product,  $\mathbf{B}_i$ , to the previous ones:

$$\begin{aligned} \mathbf{B}'_i{}^{(n)} &= \mathbf{B}_i{}^{(n)} - \sum_{j<i} (\mathbf{B}'_j{}^{(n)} \cdot \mathbf{B}_i{}^{(n)}) \mathbf{B}'_j{}^{(n)} / b_i{}^{(n)} \\ b_i{}^{(n)} &= |\mathbf{B}_i{}^{(n)} - \sum_{j<i} (\mathbf{B}'_j{}^{(n)} \cdot \mathbf{B}_i{}^{(n)}) \mathbf{B}'_j{}^{(n)}| \end{aligned} \quad (15)$$

at every step of the calculation ( $n$ ) or whenever one element of the matrix product at that step is larger than a certain prefixed constant. In that case the first column converges to the eigenvector corresponding to the largest eigenvalue, the second to the second largest and so on. For large  $N$ , we have

$$\gamma_1^N = c_1^N / N \quad c_1^N = \ln b_1^N + c_1^{N-1} \quad c_0 = 0. \quad (16)$$

This calculation could be done for chains as large as 60 000 sites, and gives the limiting value of  $\gamma_1(E)$  with significant accuracy. The results are shown in figure 4 together with the corresponding density of states histogram obtained with the negative eigenvalue counting method (Dean 1972).

The effect of increasing hybridisation is that the peak in  $\gamma_1(E)$  increases and moves towards the centre of the band. Comparison with figure 3 shows very similar results for large hybridisation and is more difficult for smaller hybridisation due to the large fluctuations. The numerical value of  $1/N \langle \log(1 + \rho) \rangle$  should be compared with the calculated  $2\gamma_1$ . Figure 4 also shows that the peak in  $\gamma_1(E)$  is at the position of the limit of the effective d band, by comparing it with the density of states. To confirm this result, the participation ratio of s orbitals in the eigenvectors was calculated for one matrix of  $N = 100$ . In that case the parameters were  $W^s = 0.8$ ,  $W^d = 0.2$ ,  $h = 0.9$  and the direct diagonalisation of the  $200 \times 200$  matrix gave the results shown in figure 5. The wavefunction plotted was one of the more localised for that particular example and corresponds to the eigenvalue  $E = 0.03244$ . The contribution of d orbitals was certainly much larger than that of s orbitals. If  $E > 0.1$  the s contribution increased abruptly but for  $E < 0.1$  it remained almost constant.

## 5. Conclusions

We have studied the transport properties and the localisation of the wavefunctions of a disordered two-band one-dimensional system. The results can be summarised as follows.

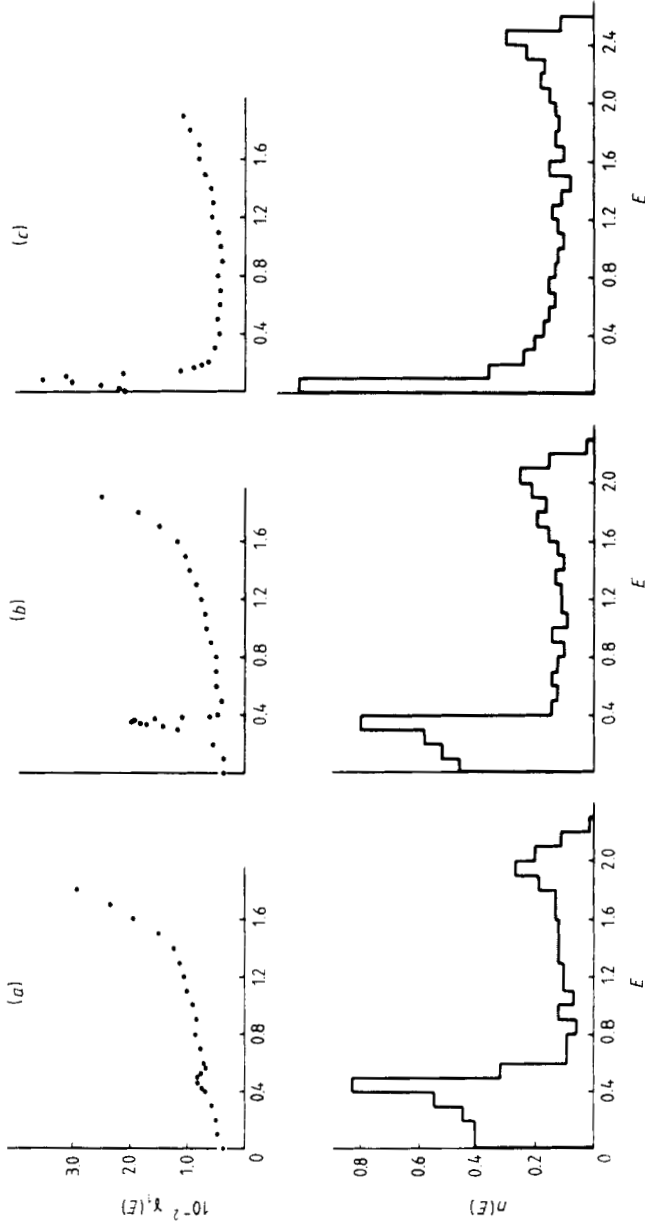
(i) In the narrow d band limit ( $t^d \ll W^d$ ) the conduction is due only to the s electrons. However, the resistance is very sensitive to the Fermi level,  $E_F$ . It shows a maximum for  $E_F = 0$ , i.e. the centre of gravity of the distribution of d levels. For  $E_F > W^d$  the transport properties are dominated by the disorder in the s orbitals.

(ii) For  $t^d > W^d$  the resistance shows a relative minimum for  $E_F = 0$ , and a pronounced maximum near the edge of the effective d band.

(iii) Our calculation shows that the coefficient  $\gamma_1(E)$  describes correctly the resistance as a function of  $E_F$  (position of the Fermi level). An excellent agreement has been obtained for  $\gamma_1(E)$  and  $\langle \ln(1 + \rho(E)) \rangle$  calculated by direct diagonalisation of the chain.

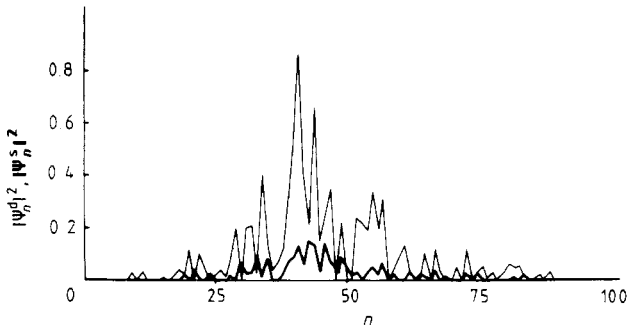
(iv) The relative maximum in  $\gamma_1(E)$  (or the resistance) coincides with a maximum in the density of states and moves towards the origin as the hybridisation  $h$  increases.

(v) The analysis of the wavefunctions shows that the participation ratio of the d orbitals is much larger than that of the s ones for  $E_F$  near the centre of the band. For



**Figure 4.**  $\gamma_1(E)$  and  $n(E)$  for the example  $t_s = 1, t_d = 0.25, W_s = 0.8, W_d = 0.2$  and (a),  $h = 0.1$ ; (b),  $h = 0.5$ ; (c),  $h = 0.9$ .  $\gamma_1(E)$  was calculated using chains of 60 000 atoms.  $n(E)$  was obtained by taking an average over five samples of 100 atoms each.





**Figure 5.** Squares of the coefficients of the tight-binding wavefunction for one sample of the case  $t_s = 1$ ,  $t_d = 0.25$ ,  $W_s = 0.8$ ,  $W_d = 0.2$  and  $h = 0.9$  plotted against the site in the chain. The coefficients plotted correspond to the eigen-energy  $E = 0.03244$  and were obtained by direct diagonalisation of a  $200 \times 200$  matrix. The heavy line corresponds to the s orbitals and the light one to the d orbitals.

energies,  $E_F$ , near the maximum of the density of states the d participation ratio decreases abruptly. These allows us to conclude that:

(vi) When the Fermi level is inside the effective d band, conduction is small and due mostly to the d electrons. When the Fermi level is outside the d band the conduction increases and is due mostly to the s electrons.

(vii) In all the cases studied here the centre of gravity of both bands were taken equal to zero. We expect the same effects if the d band is shifted.

(viii) Our results agree qualitatively with those obtained by ten Bosch and Benemann for three-dimensional systems (ten Bosch and Benemann 1975). They also obtained a relative minimum and a maximum in the resistivity when  $E_F$  is at the centre and the edge of the d band respectively. In our case the maximum is more pronounced probably due to the one-dimensionality of the system.

## Acknowledgment

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