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**THEORETICAL MODEL OF THE DENSITY OF STATES
OF RANDOM BINARY ALLOYS**

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ABSTRACT

A theoretical formulation of the density of states for random binary alloys is examined based on a mean field treatment. The present model includes both diagonal and off-diagonal disorder and also short-range order. Extensive results are reported for various concentrations and compared to other calculations.

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I- INTRODUCTION

During the last decades improved experimental techniques have allowed extensive reports on alkali-metal based random binary alloys [1-7]. Since their attracting structures considerable attention has been devoted to the study of their electronic states (metal-insulator transition, conductivity, ...). Usually theories involving an effective medium treatment, such Coherent Potential Approximation (CPA) techniques [8-10] which although satisfactory for describing many features of random alloys has a number of shortcomings. Probably the most significant is its inability to account for local atomic configuration and its inability to describe the localization properties induced by disorder.

Therefore the need to go beyond the single-site CPA has been felt from long time [9,10]. Indeed the effects of random clustering are expected to be significant but the incorporation of off-diagonal disorder inherent in any realistic model and short-range order due chemical clustering tendencies implies the extension of the single-site CPA.

In this context, various approaches have been put forward to generalize the CPA in incorporating both off-diagonal and short-range order [11, 12]. Calculations based on these suggestions suffer from main drawbacks: the "correct" formulations are often intractable and simplified approximations lead to unphysical averaged Green function.

It is the purpose of this paper via a new formalism recently proposed by one of us [13] using the tight-binding approach of Bethe lattice method to study the electronic density of states (DOS) of substitutional random alloys in the dilute limit, i.e. very low concentrations. We extend this formalism to all concentrations and improve it in using an appropriate distribution of the self-energy in one-cluster atom approximation. This method includes effects of local correlations between neighbours atoms by introducing a short-range order (SRO) parameter. Extensive results of DOS are discussed in comparison with other calculations.

II- FORMALISM OF DOS

a/ Model 1

We consider a random substitutional binary alloys $A_x B_{1-x}$ formed

of two types of atoms A and B and where x denotes the concentration. The electronic properties may be obtained from the Anderson [14] one-electron one-band tight-binding Hamiltonian :

$$H = \sum_i \epsilon_i |i\rangle\langle i| + \sum_{j \neq i} V_{ij} |i\rangle\langle j| \quad (1)$$

the sites (i) forming a periodic lattice. Here $|i\rangle$ describes the atomic orbital on site i and the disorder is usually introduced by assuming that the sites energies (ϵ_i) and the hopping matrix elements (V_{ij}) are random variables given by the following joint probability distributions :

$$P_A(\epsilon_i, V_{Aj}) = x \delta(\epsilon_i - \epsilon_A) \delta(|V_{Aj}| - V_{AA}) + (1-x) \delta(\epsilon_i - \epsilon_B) \delta(|V_{Aj}| - V_{AB}) \quad (2)$$

$$P_B(\epsilon_i, V_{Aj}) = x \delta(\epsilon_i - \epsilon_A) \delta(|V_{Aj}| - V_{BA}) + (1-x) \delta(\epsilon_i - \epsilon_B) \delta(|V_{Aj}| - V_{BB}) \quad (3)$$

We shall be interested in determining the alloy density of states which may be written in terms of the components of the partial densities of states $n_A(E)$ and $n_B(E)$ as follow :

$$n(E) = x n_A(E) + (1-x) n_B(E) \quad (4)$$

where the quantities $n_A(E)$ and $n_B(E)$ are given by :

$$n_A(E) = \pm \frac{1}{\pi} \text{Im} \langle G_{AA}(E \mp i\epsilon) \rangle = \pm \frac{1}{\pi} \text{Im} \langle \langle i_A | (E \mp i\epsilon - H)^{-1} | i_A \rangle \rangle \quad (5-a)$$

$$n_B(E) = \pm \frac{1}{\pi} \text{Im} \langle G_{BB}(E \mp i\epsilon) \rangle = \pm \frac{1}{\pi} \text{Im} \langle \langle i_B | (E \mp i\epsilon - H)^{-1} | i_B \rangle \rangle \quad (5-b)$$

Here G_{ii} stands for the site diagonal matrix elements of the one - particle Green function in the tight-binding basis. $G_{ii}(z)$ may be expanded in the form :

$$G_{ii}(z) = g_{ii}^{(0)}(z) + g_{ii}^{(1)}(z) \sum_{j \neq i} V_{ij} G_{jj}(z) \quad (6)$$

with :

$$g_{ii}^{(0)}(z) = \langle i | \left[z - \sum_i \epsilon_i |i\rangle\langle i| \right]^{-1} | i \rangle = (z - \epsilon_i)^{-1} \quad (7)$$

and

$$G_{ij}(z) = \langle i | (z-H)^{-1} | j \rangle = g_{ii}^{(0)}(z) \delta_{ij} + g_{ii}^{(1)}(z) \sum_{k \neq i} V_{ik} G_{kj}(z) \quad (8)$$

Interacting eq. (4) and using eqs. (5) and (6) enables one to rewrite $G_{ii}(z)$ in the following way :

$$G_{ii}(z) = \left[z - \epsilon_i - S_i(z) \right]^{-1} \quad (9)$$

Here $S_i(z)$ denotes the self-energy associated to the state $|i\rangle$ and its renormalized perturbation series is given by :

$$S_i(z) = \sum_{j \neq i} V_{ij} \left[z - \epsilon_j - S_j^{(i)}(z) \right]^{-1} V_{ji} + \sum_{j \neq i} \sum_{k \neq i} V_{ik} \left[z - \epsilon_k - S_k^{(i,j)}(z) \right]^{-1} V_{kj} \left[z - \epsilon_j - S_j^{(i)}(z) \right]^{-1} V_{ji} + \dots \quad (10)$$

$S_j^{(i)}$ standing for the self-energy of state $|j\rangle$ for a path in which the lattice site i has been removed and is defined similarly to $S_i(z)$. The density of states is related to the average site diagonal Green function of the binary alloy :

$$G_{ii} = x G_{ii}^A + (1-x) G_{ii}^B \quad (11)$$

with

$$G_{ii}^{A/B} = \left[z - \epsilon_{A/B} - S_{A/B}(z) \right]^{-1} \quad (12)$$

denoting the partial Green function associated to either an A atom or B atom occupies the lattice i .

In the present description of random binary alloy AB_{1-x} the random atomic levels take one of the 2 possible values $\epsilon_A = -w$ and $\epsilon_B = w$ if an atom of type A or B respectively occupies the lattice site i . The hopping integrals V_{ij} can take three values $V_{AA}, V_{AB} = V_{BA}$ and V_{BB} depending on the nature of the atom occupying the lattice sites i and j .

Because of the computational complexities which occur in studies involving the properties of realistic disorder systems, workers

use a Bethe lattice to approximate the underlying structure of the material under consideration. The usual justification is the assertion that since the impurity modes are localized, hence only the local environment is significant. Since the Bethe lattice preserves the constellation of nearest neighbour atoms, it may be used as a description of the structural basis. Random Bethe alloys [15], and the study of the electronic structure of semiconductors by means of the Bethe lattice has a long tradition and the application have been shown powerful [15,16].

Taking advantage of the particular topology of the Bethe lattice, namely the absence of closed loops, the self-energy reduces to :

$$S_A = \frac{Z_{AA} V_{AA}^2}{E - \epsilon_A - S_A^A} + \frac{Z_{AB} V_{AB}^2}{E - \epsilon_B - S_B^A} \quad (13)$$

$$S_B = \frac{Z_{BA} V_{BA}^2}{E - \epsilon_A - S_A^B} + \frac{Z_{BB} V_{BB}^2}{E - \epsilon_B - S_B^B} \quad (14)$$

where Z_{ij} is the number of j atoms surrounding and i atom and the set $\{S_i^{(j)}\}$ is defined by :

$$S_A^A = \frac{Z_{AA}^A V_{AA}^2}{E - \epsilon_A - S_A^A} + \frac{Z_{AB}^A V_{AB}^2}{E - \epsilon_B - S_B^A} \quad (15)$$

$$S_A^B = \frac{Z_{AA}^B V_{AA}^2}{E - \epsilon_A - S_A^B} + \frac{Z_{AB}^B V_{AB}^2}{E - \epsilon_B - S_B^B} \quad (16)$$

$$S_B^A = \frac{Z_{BA}^A V_{BA}^2}{E - \epsilon_A - S_A^A} + \frac{Z_{BB}^A V_{BB}^2}{E - \epsilon_B - S_B^A} \quad (17)$$

$$S_B^B = \frac{Z_{BA}^B V_{BA}^2}{E - \epsilon_A - S_A^B} + \frac{Z_{BB}^B V_{BB}^2}{E - \epsilon_B - S_B^B} \quad (18)$$

where $Z_{AB}^{A(B)}$ describes the average number of B-atoms descendants of an A-atom that has a B (A) parent along the Bethe lattice paths. The quantities Z_{ij} and $Z_{ij}^{(j)}$ may be substituted by their average value, i.e. :

$$Z_{ij} \equiv \langle Z_{ij} \rangle = p_{ij} Z \quad (19)$$

$$Z_{ij}^{(j)} \equiv \langle Z_{ij}^{(j)} \rangle = p_{ij} (Z-1) = p_{ij} K \quad (20)$$

where Z is the coordination number and K the connectivity constant.

At this stage we have to introduce approximations in order to handle these general equations. Therefore we consider the situation where $S_A^A = S_A^B$ and $S_B^A = S_B^B$. The set of equations (X - Y) may be treated self-consistently. The probabilistic definitions of the site energies ϵ_i and the matrix elements V_{ij} (eqs. 2 and 3) implies that the self-energies are also defined by probability density distributions. In the present treatment we consider a self-consistent approximation as usual :

$$P_{\Sigma}(S_i) = \int \dots \int \delta \left(S_i - \sum_{j \neq i} \frac{|V_{ij}|^2}{E - \epsilon_j - S_j(z)} \right) \times \\ \times \prod_{j \neq i} P_j(\epsilon_j, V_{ij}, S_j) d\epsilon_j d|V_{ij}| dS_j \quad (21)$$

where the self-energies at a given site are statistically independent random variables. From the particular topology of the Bethe lattice, S_j is independent of the variables ϵ_j and V_{ij} and thus :

$$P_{A/B}(\epsilon_j, V_{ij}, S_j^C) = P_{A/B}(\epsilon_j, V_{ij}) P_{\Sigma}(S_j) \quad (22)$$

we get the following expressions of the Fourier transforms $\tilde{P}_{\Sigma_A}(t)$ and $\tilde{P}_{\Sigma_B}(t)$:

$$\tilde{P}_{\Sigma_A}(t) = \left[x \int_{-\infty}^{+\infty} dS_A P_{\Sigma}(S_A) \exp \left[- \frac{it V_{AA}^2}{E - \epsilon_A - S_A} \right] + \right. \\ \left. + (1-x) \int_{-\infty}^{+\infty} dS_B P_{\Sigma}(S_B) \exp \left[- \frac{it V_{AB}^2}{E - \epsilon_B - S_B} \right] \right]^Z \quad (23)$$

$$\tilde{P}_{\Sigma_B}(t) = \left[x \int_{-\infty}^{+\infty} dS_A P_{\Sigma}(S_A) \exp \left[- \frac{it V_{AB}^2}{E - \epsilon_A - S_A} \right] + \right. \\ \left. + (1-x) \int_{-\infty}^{+\infty} dS_B P_{\Sigma}(S_B) \exp \left[- \frac{it V_{BB}^2}{E - \epsilon_B - S_B} \right] \right]^Z \quad (24)$$

At this stage we have not been able to make any use of these equa -

tions and so we are looking for solutions less general. In the following treatment we make use of a mean field approximation, i.e. we consider that the probability distributions $P_A(S_A)$ and $P_B(S_B)$ are strongly peaked around their mean values $\langle S_A \rangle$ and $\langle S_B \rangle$ to be determined. Using the integral definition of delta function :

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{itx} dt \quad (25)$$

and expanding equations (7) and (8) yields :

$$P_A(S_A) = x^Z \delta(S_A - S_A^{(0)}) + z(1-x) x^{Z-1} \delta(S_A - S_A^{(1)}) + \dots \\ \dots + x z(1-x)^{Z-1} \delta(S_A - S_A^{(Z-1)}) + (1-x)^Z \delta(S_A - S_A^{(Z)}) \quad (26)$$

$$P_B(S_B) = x^Z \delta(S_B - S_B^{(0)}) + z(1-x) x^{Z-1} \delta(S_B - S_B^{(1)}) + \dots \\ \dots + x z(1-x)^{Z-1} \delta(S_B - S_B^{(Z-1)}) + (1-x)^Z \delta(S_B - S_B^{(Z)}) \quad (27)$$

where :

$$\left. \begin{aligned} S_{A/B}^{(0)} &= \frac{Z V_{AA/BB}^2}{E - \epsilon_{A/B} - \langle S_{A/B} \rangle} \\ S_{A/B}^{(1)} &= \frac{(Z-1) V_{AB/BB}^2}{E - \epsilon_{A/B} - \langle S_{A/B} \rangle} + \frac{V_{AB}^2}{E - \epsilon_{B/A} - \langle S_{A/B} \rangle} \\ &\vdots \\ S_{A/B}^{(Z)} &= \frac{Z V_{AB}^2}{E - \epsilon_{B/A} - \langle S_{B/A} \rangle} \end{aligned} \right\} \quad (28)$$

where the mean values $\langle S_A \rangle$ and $\langle S_B \rangle$ are the solutions of the equations (15 - 18).

At this stage, we are now in a position to investigate the density of states of disordered system on a Bethe lattice. The partial densities of states are related to the average diagonal Green's function of the binary alloy by using the self-energy probability distributions given by eqs. (26) and (27) :

$$n_{A/B} = \pm \int_{-\infty}^{\infty} dS_{A/B} P_{\pm}(S_{A/B}) \text{Im } G_{AA/BB} \quad (29)$$

with :

$$G_{AA/BB} = \frac{1}{E - \epsilon_{A/B} - S_{A/B}} \quad (30)$$

describing the partial Green's function associated to either an A-atom or B-atom. The partial DOS may be expanded as :

$$n_A(E) = \frac{1}{\pi} \text{Im} \left\{ \frac{x^Z}{E - \epsilon_A - S_A^{(0)}} + \frac{z x^{Z-1} (1-x)}{E - \epsilon_A - S_A^{(1)}} + \dots + \frac{z x (1-x)^{Z-1}}{E - \epsilon_A - S_A^{(Z-1)}} + \frac{(1-x)^Z}{E - \epsilon_A - S_A^{(Z)}} \right\} \quad (31)$$

$$n_B(E) = \frac{1}{\pi} \text{Im} \left\{ \frac{(1-x)^Z}{E - \epsilon_B - S_B^{(0)}} + \frac{z x (1-x)^{Z-1}}{E - \epsilon_B - S_B^{(1)}} + \dots + \frac{z x^{Z-1} (1-x)}{E - \epsilon_B - S_B^{(Z-1)}} + \frac{x^Z}{E - \epsilon_B - S_B^{(Z)}} \right\} \quad (32)$$

where the quantities $S_{A/B}^{(i)}$ ($i=0, \dots, z$) are the expressions defined by eq.(28).

b/ Short-Range Order parameter 1

The striking difference between amorphous and crystalline materials provides a strong demonstration of the primacy of the short-range order (SRO) in determining the basic nature of their properties. In particular the change with chemical composition in the electronic properties has been attributed to the establishment of a well defined BRD, for instance alkali-metals doped with gold and silver or amorphous transition metal alloys can be checked experimentally by diffraction measurements [2,3,6].

From a theoretical point of view, including BRD in disordered alloys remains a challenge [17-21]. The most used theory describing electronic properties of disordered alloys is the Coherent-Potential Approximation (CPA) [8,9,15]. Despite of its many appreciated properties, the CPA approach fails in handling parameters such as BRD. Going beyond these limitations, several theories have been put

forward [19-21], at the cost of some computational efforts. We propose here an extension of the previous section including SRO by an analytic method.

Towards this end the description of SRO, or equivalently the lack of randomness in the number of like or unlike nearest neighbours around a given atom, may be parametrized by new variables, namely the short range order parameter σ and the probability p_{ij} of a j-atom being next to a i-atom. σ and p_{ij} are chosen to be related similarly to Brouers et al. [18], i.e. :

$$p_{AA} = x + (1-x)\sigma \quad ; \quad p_{BA} = x(1-\sigma) \quad (33)$$

$$p_{BB} = (1-x) + x\sigma \quad ; \quad p_{AB} = (1-x)(1-\sigma) \quad (34)$$

The range of possible values of σ is :

$$-\frac{x}{1-x} \leq \sigma \leq 1 \quad \text{for } x \leq \frac{1}{2} \quad (35)$$

$$-\frac{1-x}{x} \leq \sigma \leq 1 \quad \text{for } x \geq \frac{1}{2} \quad (36)$$

The negative values correspond to ordering, $\sigma = 0$ to complete disorder and positive values to segregation. Under this scheme, the probability distribution for site energies transforms as :

$$p_A(\epsilon_i, V_{ij}) = p_{AA} \delta(\epsilon_i - \epsilon_A) \delta(V_{Aj} - V_{AA}) + p_{AB} \delta(\epsilon_i - \epsilon_B) \delta(V_{Aj} - V_{AB}) \quad (37)$$

$$p_B(\epsilon_i, V_{ij}) = p_{BA} \delta(\epsilon_i - \epsilon_A) \delta(V_{Bj} - V_{BA}) + p_{BB} \delta(\epsilon_i - \epsilon_B) \delta(V_{Bj} - V_{BB}) \quad (38)$$

and the equations for self-energies as :

$$S_A = \frac{K p_{AA} V_{AA}^2}{E - \epsilon_A - S_A} + \frac{K p_{AB} V_{AB}^2}{E - \epsilon_B - S_B} \quad (39)$$

$$S_B = \frac{K p_{BA} V_{BA}^2}{E - \epsilon_A - S_A} + \frac{K p_{BB} V_{BB}^2}{E - \epsilon_B - S_B} \quad (40)$$

Using the same mean field treatment as previously yields for the partial density of states :

$$n_A(E) = \frac{1}{\pi} \text{Im} \left\{ \frac{p_{AA}^Z}{E - \epsilon_A - S_A^{(0)}} + \frac{z p_{AA}^{Z-1} p_{AB}}{E - \epsilon_A - S_A^{(1)}} + \dots + \frac{z p_{AA}^{Z-1} p_{AB}^{Z-1}}{E - \epsilon_A - S_A^{(Z-1)}} + \frac{p_{AB}^Z}{E - \epsilon_A - S_A^{(Z)}} \right\} \quad (41)$$

$$n_B(E) = \frac{1}{\pi} \text{Im} \left\{ \frac{p_{BB}^Z}{E - \epsilon_B - S_B^{(0)}} + \frac{z p_{BA} p_{BB}^{Z-1}}{E - \epsilon_B - S_B^{(1)}} + \dots + \frac{z p_{BA}^{Z-1} p_{BB}^{Z-1}}{E - \epsilon_B - S_B^{(Z-1)}} + \frac{p_{BA}^Z}{E - \epsilon_B - S_B^{(Z)}} \right\} \quad (42)$$

where the set $(S_{A/B}^{(i)}, i = 0, \dots, z)$ appearing in the denominator has been calculated in taking into account the parameter σ via eqs. (15 - 18) and (28).

III- RESULTS AND DISCUSSION

In this section, we have reported our results for the density of states (DOS) of Bethe lattice for both cases diagonal and off-diagonal disorder, the latter parametrized by $V_{ij} = \zeta_i V \zeta_j$ where ζ_i is equal to ζ_A or ζ_B depending on the occupation of site i . Here the constant V is taken as our unit of energy. We have restricted ourselves without loss of generality to $Z = 4$ in order to compare our data with other theories.

a/ Random systems ($\sigma=0$) 1

a-1/ Diagonal disorder 1

Fig.1 shows with diagonal disorder only. We have examined the case $\epsilon_A = -\epsilon_B = 1.7$ for the concentrations $x = 0.01$ and $x = 0.1$. For the above parameters the bandwidth of ordered lattice is $4\sqrt{3}$. It is particularly observed that the curves for $n(E)$ exhibit some interesting features as well as the evolution of the structures as function of the concentration. Mainly the CPA calculations

(see Fig.1-b) fail in reproducing these structures and the discrepancies are more effective in the regime of low-concentration. It is well established that CPA approach provides a poor description of the minority band although it has some bearing for the majority band [9].

a-2/ Off-diagonal disorder :

We have considered a binary alloy with a purely off-diagonal disorder. We have focussed our attention to the case $\epsilon_A = \epsilon_B = 0$ and $\zeta_A = 0.8$ and $\zeta_B = 1.1$. The alloy DOS $n(E)$ for $x = 0.3$ is shown in Fig. 2 where we also show results for the partial components $n_A(E)$ (broken curve) and $n_B(E)$ (chain curve). The DOS presents a perfect symmetry around $E = 0$. As expected the DOS on A sites is concentrated around the origine while the states on the B sites are spread out into the centre of band. It should be noted a rather perfect similarity from the renormalization-group approaches of d'Albuquerque et al. [22].

b/ Short-Range Order :

We introduce here the SRO parameter described previously to determine the DOS for different values of the band energy parameter, concentration and SRO parameter in random, ordered and segregation regimes.

Fig.3 shows the DOS for $x = 0.4$, $\epsilon_A = -\epsilon_B = -2$ in random binary alloys, i.e. $\sigma = 0$ (full curve) and in partially ordered alloy, $\sigma = -0.4$ (broken curve). The main feature observed is an increase of the gap with increasing σ and furthermore the structures revealed in the DOS become more pronounced and appear located at the same energies, namely $E \approx -3$ and $E \approx 3$. Such results are in agreement with conclusions reached from other models calculations [19].

Fig.4 describes the DOS for random binary alloys $\sigma = 0$ (full curve) and completely ordered binary alloys $\sigma = -1/3$, (broken curve), for a concentration $x = 0.25$ while Fig.5 shows partial-A DOS of binary alloys for different values of the SRO parameter corresponding to segregation, $\sigma = 0.2$ (full curve), random $\sigma = 0$ (broken curve) and partially ordered $\sigma = 0.5$ (chain curve). Monte-Carlo simulations based on the tight-binding method for the Bethe cluster model using a large N-clusters [18] are efficient in producing more structures in

the DOS mainly due to the large N-atoms cluster limit. However the effect of Short-Range Order parameter on the DOS is similar to their calculations in one-atom cluster case and mainly we obtain a DOS more structured.

Finally, we have also examined the segregation case in Fig.6 for diagonal disorder with $\epsilon_A = -\epsilon_B = -1$ and $x = 0.5$. A Monte-Carlo calculation based on a virtual cristal approximation has been recently proposed [21] for 5, 9, 13 and 17-atoms cluster. By the present model we reproduce their two first peaks at $E = 1$ and $E = -1$ correctly while in their approach they have to go beyond 9-atoms cluster to obtain a similar result.

IV- CONCLUSION

We have presented a new formulation of cluster Bethe lattice method to calculate the density of electronic states of a random substitutional binary alloys. Extensive results have been compared to other calculations. This method yields more structures than other ones for a one or small N-atoms cluster. To improve our model we have to include N-cluster atoms and distributions of real and imaginary self-energies which is the subject of a forthcoming paper.

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FIGURE CAPTIONS

- FIG. 1 Density of states for diagonal disorder ($V=1$) in the case $\epsilon_A = -\epsilon_B = -1.7$ and $x = 0.01$ (full curve), $x = 0.1$ (broken curve). a/ Present method, b/ CPA method.
- FIG. 2 Density of states for non-diagonal disorder ($V_{AA} = 0.64$, $V_{AB} = 0.88$ and $V_{BB} = 1.21$) ; $\epsilon_A = \epsilon_B = 0$ and $x = 0.3$. Total DOS (full curve), partial-A DOS (broken curve) and partial-B DOS (chain curve).
- FIG. 3 Density of states for $\epsilon_A = -\epsilon_B = -2$, $x = 0.4$ and a diagonal disorder $V = 1$. Random $\sigma = 0$ (full curve) and partially ordered $\sigma = -0.4$ (broken curve).
- FIG. 4 Total DOS for $x = 0.25$ and $\epsilon_A = -\epsilon_B = -2.5$ in diagonal disorder ($V = 1$). Random case $\sigma = 0$ (full curve) and completely ordered case $\sigma = -1/3$ (broken curve).
- FIG. 5 Partial -A DOS for diagonal disorder ($V = 1$) and for $x = 0.2$, $\sigma = 0.2$ (full curve), $x = 0.4$, $\sigma = 0$ (broken curve) and $x = 0.6$, $\sigma = -0.5$ (chain curve).
- FIG. 6 Total density of states for diagonal ($V = 1$) and segregation case ($\sigma = -1$) and for $x = 0.5$ and $\epsilon_A = -\epsilon_B = -1$.

FIGURE 1a

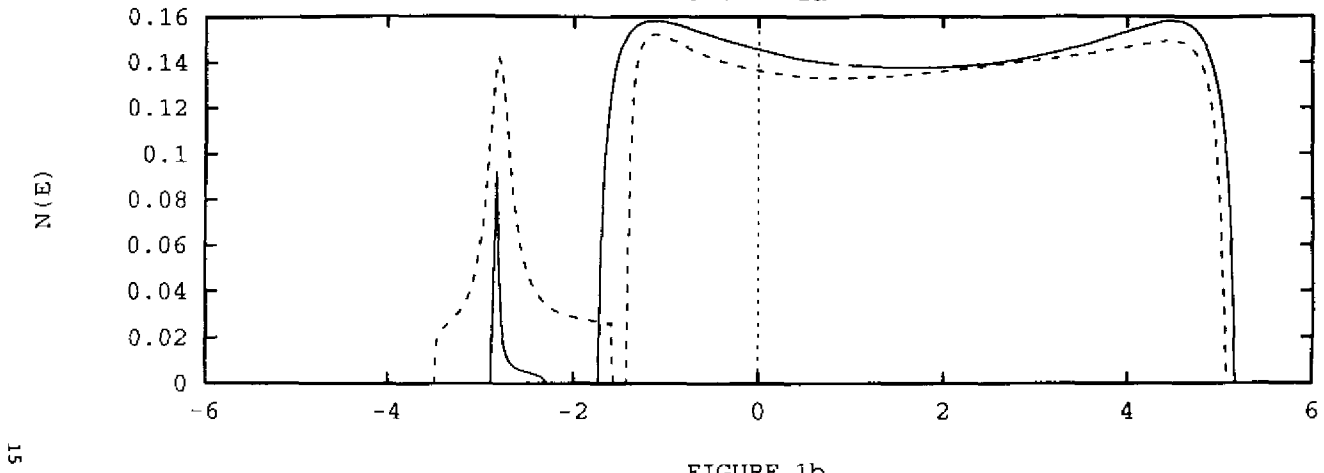


FIGURE 1b

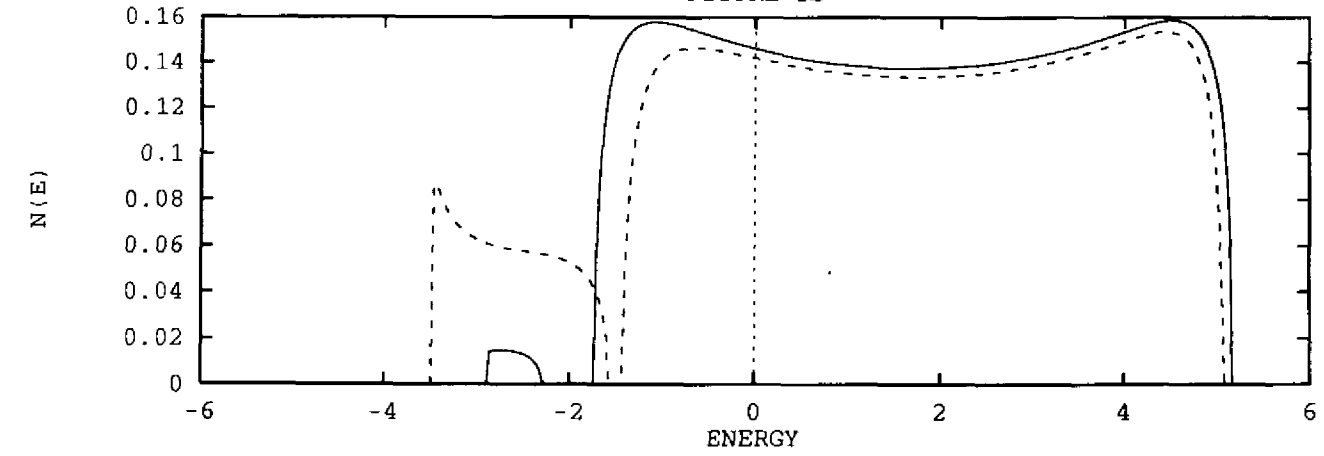


FIGURE 2

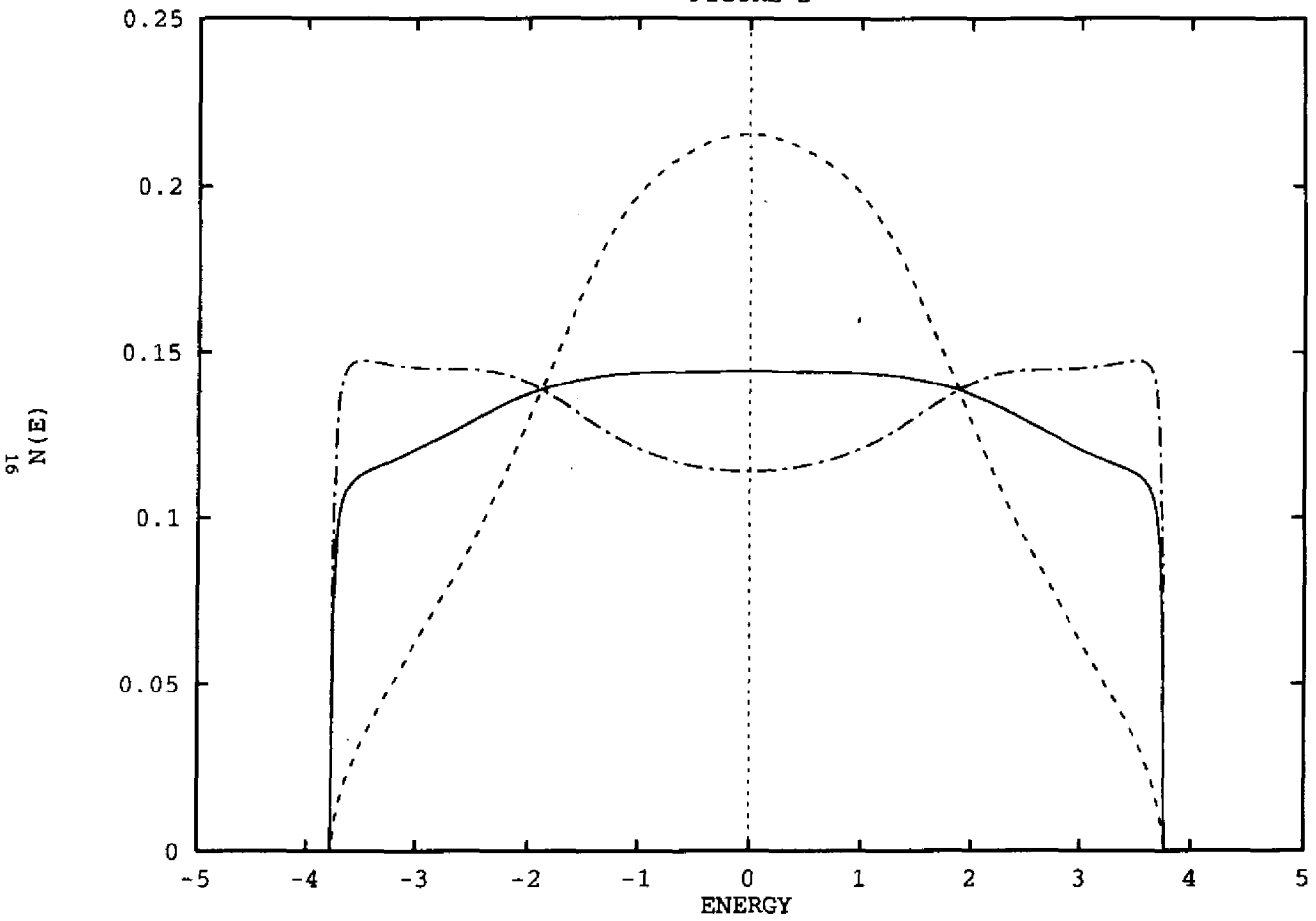


FIGURE 3

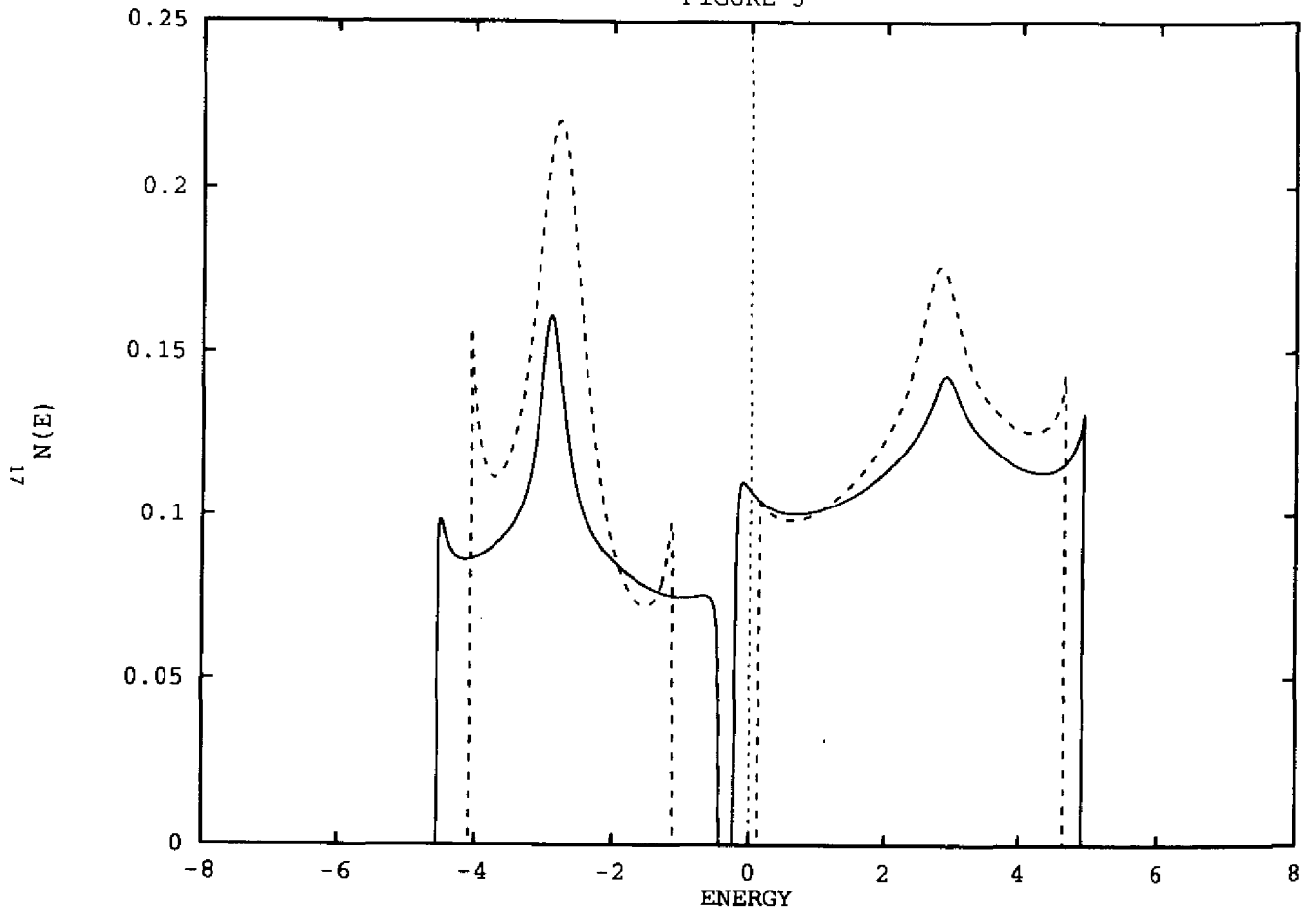


FIGURE 4

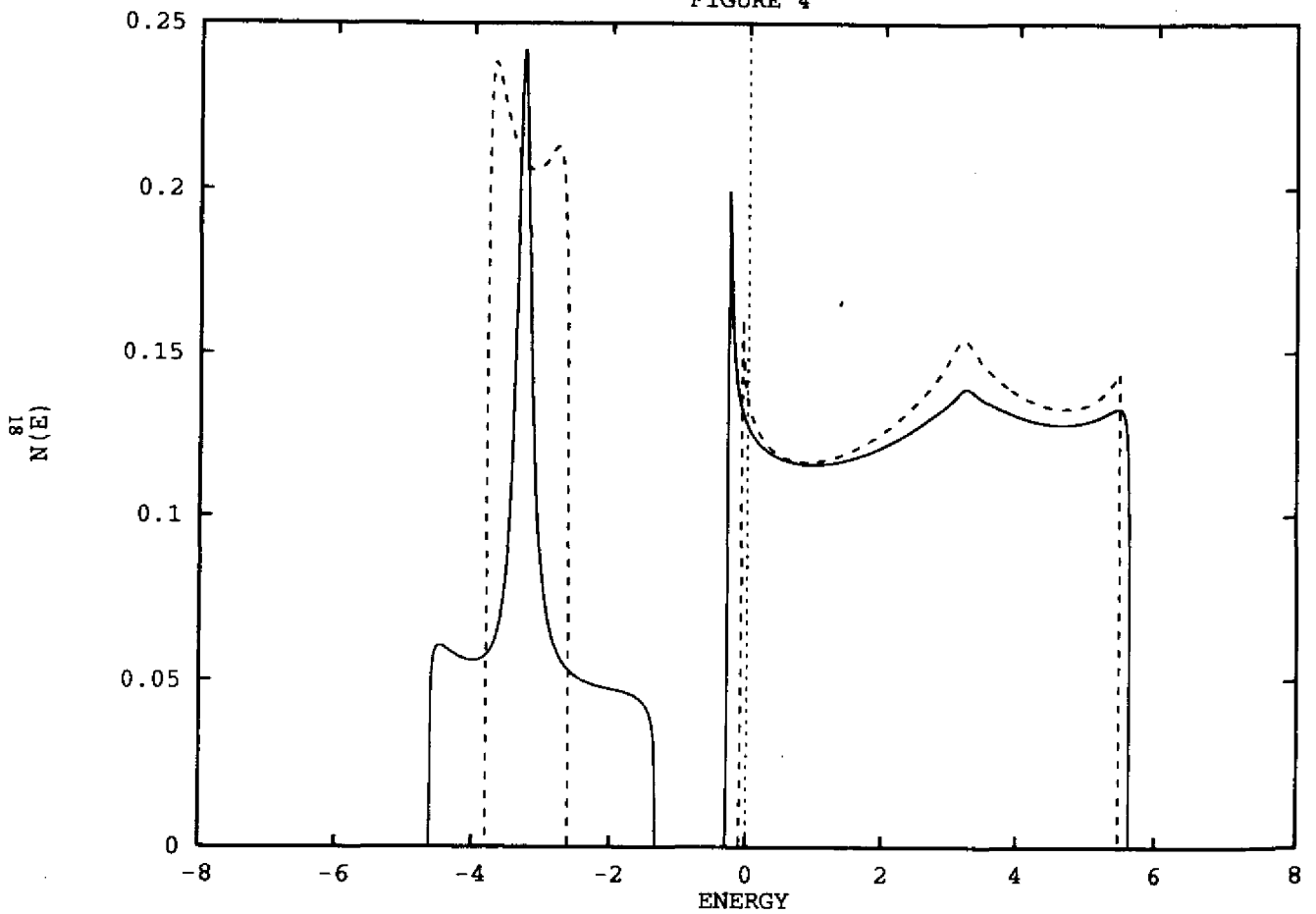


FIGURE 5

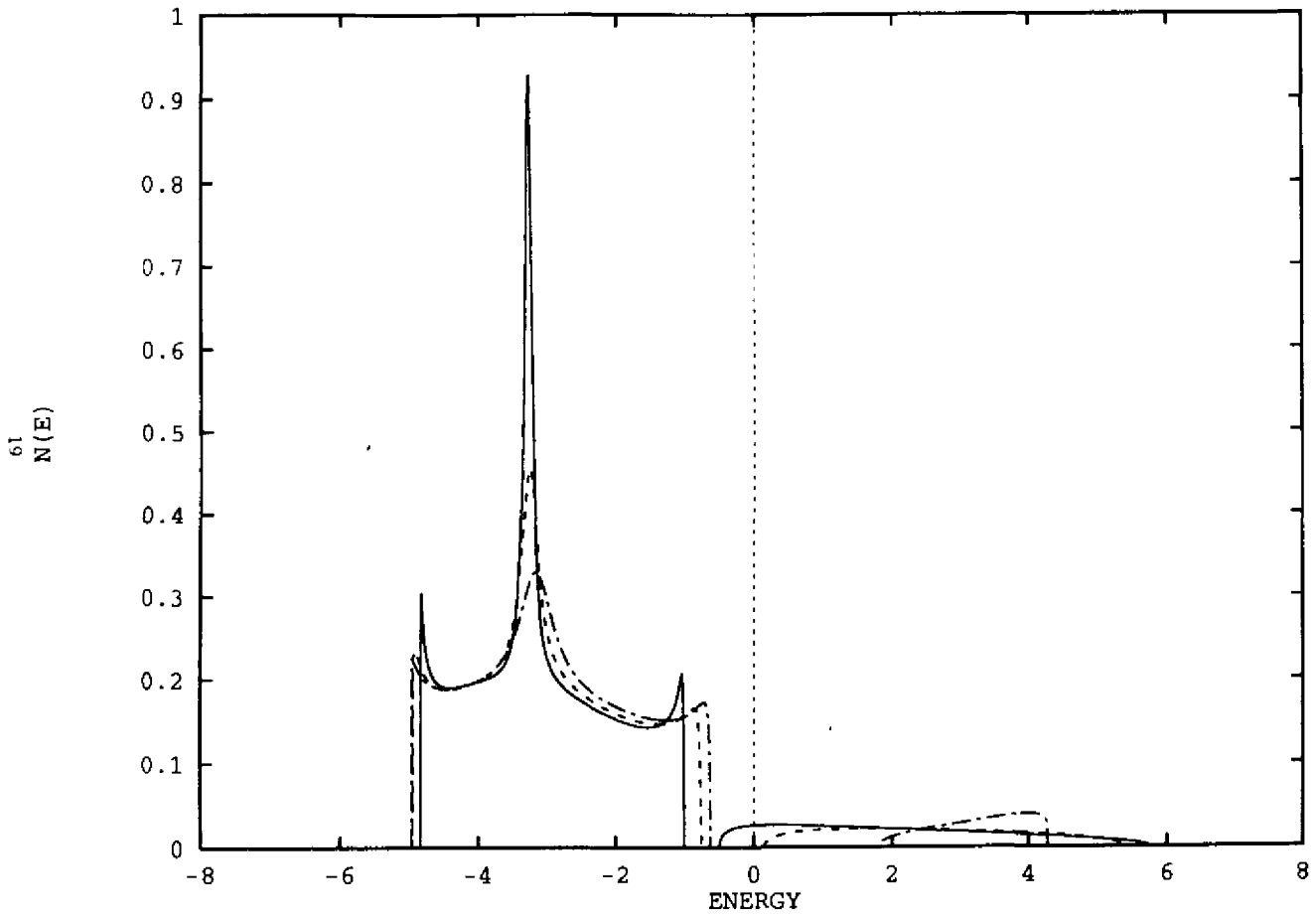


FIGURE 6

