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LETTER TO THE EDITOR

A simple algorithm for the calculation of moments of the density of states in a one-dimensional random binary alloy

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Abstract. A simple practical procedure is described for the calculation of moments of the density of states of 1D random binary systems obeying tight-binding-type Hamiltonians. Short-order correlation effects are included. The procedure allows, in principle, the calculation of moments up to an arbitrary order. Explicit results for the 13 first moments are presented.

In the last few years many applications of the tight-binding approximation in the moment method problem have been made with regard to the study of the electronic structure of crystals and alloys (Gaspard and Cyrot-Lackmann 1973, Wheeler *et al* 1974, Corcoran and Langhoff 1977, Lopez *et al* 1974). This method is an important tool in the study of the local density of states, and provides a powerful procedure for the estimation of integrals of the density of states. This is especially important in problems with substitutional disorder where no information other than the Hamiltonian and the geometrical structure is available (Yndurain and Yndurain 1975, Trías *et al* 1979).

In this work an algorithm is described for the calculation of the moments of the density of state of a one-dimensional binary random alloy with short-order correlations. This method allows the computation of the moments up to any order. However, computer numerical accuracy limitations may arise in actual practice.

We consider a one-dimensional alloy characterised by the Hamiltonian

$$\mathcal{H} = \sum_i |i\rangle \varepsilon_i \langle i| + \sum_{ij} |i\rangle T \langle j| \tag{1}$$

where $\varepsilon_i = \varepsilon_A$ or ε_B in a proportion given by $x = N_B/(N_A + N_B)$, the second sum is over nearest-neighbour positions only and T is independent of the indices i and j.

It is well known that the nth moment of the density of states is given by

$$\mu_n = N^{-1} \sum_s \sum_{\lambda_1, \lambda_2, \ldots} \langle s|\mathcal{H}|\lambda_1\rangle\langle\lambda_1|\mathcal{H}|\lambda_2\rangle \ldots \langle\lambda_m|\mathcal{H}|s\rangle. \tag{2}$$

Any given term in this summation can be related to a one-dimensional walk or path, which starts at the lattice site s, goes through a number of neighbouring lattice sites and returns to s. At this point we can think of a graph, which in this case is precisely defined by the extreme vertices of the path. This graph can be travelled in many different ways

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(i.e. walks), each one corresponding to different terms in (2). Now the factor $\langle\lambda|\mathscr{H}|\lambda'\rangle$ takes the value ε_λ if $\lambda=\lambda'$ or T if $\lambda\neq\lambda'$. In the former case we have a 'stop' at lattice site λ and in the latter case we have a 'step' from λ to λ'.

In a given configuration, a path with q steps will produce a factor T^q, and each of the remaining n-g stops gives rise to two possible factors, ε_A or ε_B. Hence we may write

$$\mu_n = N^{-1}\sum_s\sum_p \varepsilon_A^{t(p)}\varepsilon_B^{n-q(p)-t(p)}T^{q(p)} \tag{3}$$

where Σ_p denotes a summation over all possible paths p compatible with the value of n. The value of q depends on the path p and $t(p)$ is the number of stops at atoms of type A on a given path.

In order to proceed further we classify the paths according to the graph g travelled by the path p. Then we have to compute the number of paths, with q and t fixed, in a given graph g. This number will be denoted by $C_s(g,t)$ and will implicitly depend also on n, q and the number of A and B atoms encountered in the path p. However, since we are concerned with random alloys only, we have to take an equal weight average over all possible configurations and use the number

$$N^{-1}\left\langle\sum_s C_s(g,t)\right\rangle = C(g,t,x)$$

instead. Therefore we may write

$$\mu_n = \sum_{g,q,t} C(g,t,x)\varepsilon_A^t\varepsilon_B^{n-q-t}T^q. \tag{4}$$

The problem has thus been reduced to finding the numbers $C(g,t,x)$. From now on we set $\varepsilon_A=0$; hence only those terms for which $t=0$ remain in (4). μ_n with $\varepsilon_A\neq 0$ can be easily obtained from the moments with $\varepsilon_A=0$. Now consider a given graph. The vertex s at the origin will be denoted by the number 0 and the remaining vertices by integer numbers. The maximum value of this integer is $M_1\geqslant 0$ and the minimum value $M_2<0$. Thus the pair (M_1,M_2) defines the graph uniquely. This graph has $L=M_1-M_2+1$ vertices and $L-1$ branches.

For a walk of q steps, each vertex of the graph is in general visited more than once. The number of times a path passes through a vertex j is called the number of stations l_j in this vertex. A given path defines the set $\{l_j\}$ in a graph in a unique way, but the reciprocal statement is not true and we have to know the number of possible paths in a graph for fixed $\{l_j\}$. This number is denoted by $W(\{l_j\})$ and its calculation is performed below.

Let $C(g,x)=C(g,t=0,x)$. The contribution of graph g to μ_n corresponds to a path in which $n-q$ stops occur at atoms of type B. If all these stops occur at the same vertex a factor x appears in $C(g,x)$, since this is the probability of finding a B-type atom at an arbitrary lattice site in a random binary alloy. By the same token, if all stops occur at two different vertices only, a factor x^2 appears and so on. Therefore $C(g,x)$ has the form

$$C(g,x) = W_g\delta_{n,q} + \sum_{k'=1}^{K} C_g^{(k')}x^{k'} \tag{5}$$

where $W_g=\Sigma\, W(\{l_j\})$ and K is the smallest integer of the pair $(L,n-q)$.

We now turn to the calculation of $C_g^{(1)}$. Consider a given vertex j of graph g; the contribution of this vertex is equal to the number of ways in which we can place $n-q$

stops in l_j different places, that is

$$\frac{(n-q+l_j-1)!}{(n-q)!(l_j-1)!},$$

and hence

$$C_g^{(1)} = \sum_{\{l_j\}} \sum_{j=1}^{L} W(\{l_j\}) \frac{(n-q+l_j-1)!}{(n-q)!(l_j-1)!}. \tag{6}$$

$C_g^{(2)}$ can be computed in a similar way by computing the number of ways we can place $n-q$ stops in $l_{j1}+l_{j2}$ places and subtracting the cases where all stops are made at only one of the two vertices. Therefore

$$C_g^{(2)} = \sum_{\{l_j\}} \sum_{m=1}^{\binom{L}{2}} W(\{l_j\}) \frac{(n-q+\Omega_m^{(2)}-1)!}{(n-q)!(\Omega_m^{(2)}-1)!} - (L-1)C_g^{(1)}. \tag{7}$$

These expressions can be easily generalised for any k':

$$C_g^{(k')} = \sum_{\{l_j\}} \sum_{m=1}^{\binom{L}{k'}} W(\{l_j\}) \frac{(n-q+\Omega_m^{(k')}-q)!}{(n-1)!(\Omega_m^{(k')}-1)!} - \sum_{\lambda=1}^{k'-1} \binom{L-k'+\lambda}{\lambda} C_g^{(k'-\lambda)} \tag{8}$$

where $\Omega_m^{(k')}$ is the mth member of the set of numbers

$$\{l_{j1}+l_{j2}+\ldots+l_{jk'}\}, \qquad ji = 1, 2, \ldots, L.$$

If short-order correlations are taken into account, the second powers of x appearing in equation (5) have to be replaced by xP_{ij} where P_{ij} is the probability of finding an atom B at site j if an atom B is at site i. Then $C_g^{(2)}x^2$ has to be replaced by

$$\sum_{\{l_m\}} \times \sum_{ij} (\beta_{ij} - \alpha_i - \alpha_j) P_{ij} W(\{l_m\}) \tag{9}$$

where

$$\alpha_i = \frac{(n-q+l_i-1)!}{(n-q)!(l_i-1)!} \qquad \text{and} \qquad \beta_{ij} = \frac{(n-q+l_i+l_j-1)!}{(n-q)!(l_i+l_j-1)!}.$$

Higher-order terms are replaced by similar expressions, i.e.

$$x^3 C_g^{(3)} \to x \sum_{\{l_p\}} \sum_{ijk} (\gamma_{ijk} - \beta_{ij} - \beta_{ik} - \beta_{jk} + \alpha_i + \alpha_j + \alpha_k) P_{ijk} W(\{l_p\}) \tag{10}$$

$$x^4 C_g^{(4)} \to x \sum_{\{l_p\}} \sum_{ijkm} (\delta_{ijkm} - \gamma_{ijk} - \gamma_{imk} - \gamma_{mjk} - \gamma_{ijm} + \beta_{ij} + \beta_{ik} + \beta_{im} + \beta_{jk} + \beta_{jm} + \beta_{km} - \alpha_i - \alpha_j - \alpha_k - \alpha_m) P_{ijkm} W(\{l_p\}), \tag{11}$$

respectively, where

$$\gamma_{ijk} = \frac{(n-q+l_i+l_j+l_k-1)!}{(n-q)!(l_i+l_j+l_k-1)!} \qquad \text{and} \qquad \delta_{ijkm} = \frac{(n-q+l_i+l_j+l_k+l_m-1)!}{(n-q)!(l_i+l_j+l_k+l_m-1)!}.$$

By an obvious generalisation of these expressions we may write higher-order terms.

The multiple-site correlation probabilities can be approximated by a sum of products of two-site correlation probabilities for instance, P_{ijk} is replaced by $\frac{1}{3}(P_{ij}P_{ik} + P_{ji}P_{jk} + P_{ki}P_{kj})$.

Now we consider the problem of determining $W(\{l_j\})$, i.e. the number of paths in a given graph g defined by the numbers (M_1, M_2), for which the number of stations at each vertex, i.e. the set $\{l_j\}$, is known. In order to proceed, we suppose that the number of steps between states 0 and 1 is known. We call this number s_1 and, as will be seen later, it is wholly determined by the set $\{l_j\}$. Initially, we have no other step in the whole graph. The initial number of stations at vertex 0 is denoted by Z_0 and at vertex 1 by Z_1. Notice that $s_1 = 2Z_1$ and $Z_0 = Z_1 + 1$. In order to form one path in the graph we proceed as follows: we take one station at vertex 1, then split this station into two stations and insert $2e$ steps between these two stations and vertex 2 (see figure 1). In this way we add e stations at vertex 2 and e stations at vertex 1. We then treat the remaining stations at vertex 1 in a similar way and find $l_1 = Z_1 + Z_2$. The same procedure can be used to reach vertices 3, 4, etc, up to vertex N, and we find the set of equations

$$l_j = Z_j + Z_{j+1}, \qquad j = 1, \ldots, M_1 - 1; \qquad l_{M_1} = Z_{M_1}. \tag{12}$$

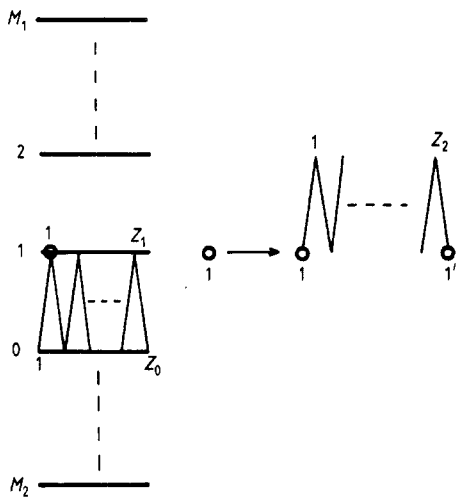

Figure 1. Illustration of the insertion technique used to find the value of $W(\{l_j\})$. See the text for details.

By proceeding in the same way 'downwards' up to vertex M, we find

$$l_j = Z_j + Z_{j-1}, \qquad j = 0, -1, -2, \ldots, M_2 + 1; \qquad l_{M_2} = Z_{M_2}. \tag{13}$$

The solution of (9) and (10) is

$$\begin{aligned} Z_j &= \sum_{q=0}^{M_1 - j} (-1)^q l_{j+q} \qquad \text{for } j > 0, \\ &= \sum_{q=0}^{j - M_2} (-1)^q l_{j-q} \qquad \text{for } j \leqslant 0. \end{aligned} \tag{14}$$

One can easily show that the set $\{l_j\}$ satisfies the following constraints:

$$\sum_{j=M_2}^{M_1} l_j = q + 1, \qquad \sum_{j=M_2}^{M_1} (-1)^{j-1} l_j = 1. \tag{15}$$

In the procedure described above we may insert Z_{i+1} stations in the Z_i original stations in

$$(Z_i + Z_{i+1} - 1)!/Z_i!(Z_{i+1} - 1)!$$

different ways, from which we may obtain

$$W(\{l_j\}) = [Z_0!(Z_0 - 1)!/(2Z_0 - 1)!] \prod_{j=M_2}^{M_1} (Z_j + Z_{j+1} - 1)!/[Z_{j+1}!(Z_j - 1)!]. \tag{16}$$

Table 1.

$$\mu_0 = 1 \qquad \mu_1 = xG \qquad \mu_2 = 2T^2 + xG^2 \qquad \mu_3 = 6xGT^2 + xG^3$$

$$\mu_4 = 6T^4 + 4[2 + P(1)]xG^2T^2 + xG^4 \qquad \mu_5 = 30xGT^4 + 10[1 + P(1)]xG^3T^2 + xG^5$$

$$\mu_6 = 20T^6 + [30 + 42P(1) + 18P(2)]xG^2T^4 + 6[2 + 3P(1)]xG^4T^2 + xG^6$$

$$\mu_7 = 140xGT^6 + \{70 + 112P(1) + 14P(2) + \tfrac{14}{3}[P(1)P(1) + 2P(1)P(2)]\}xG^3T^4 + 14[1 + 2P(1)]xG^5T^2 + xG^7$$

$$\begin{aligned}\mu_8 = {} & 70T^8 + [256 + 232P(1) + 64P(2) + 8P(3)]xG^2T^6 + \{96 + 244P(1) + 24P(2) \\ & + \tfrac{56}{3}[P(1)P(1) + 2P(1)P(2)]\}xG^4T^4 + 8[2 + 5P(1)]xG^6T^2 + xG^8\end{aligned}$$

$$\begin{aligned}\mu_9 = {} & 630xGT^8 + [420 + 846(1) + 180P(2) + 18P(3) + 60P(1)P(1) + 132P(1)P(2) \\ & + 12P(1)P(3) + 12P(2)P(3)]xG^3T^6 \\ & + \{126 + 450P(1) + 36P(2) + \tfrac{144}{3}[P(1)P(1) + 2P(1)P(2)]\}xG^5T^4 \\ & + 18[1 + 3P(1)]xG^7T^2 + xG^9\end{aligned}$$

$$\begin{aligned}\mu_{10} = {} & 252T^{10} + [1280 + 1300P(1) + 460P(2) + 100P(3) + 10P(4)]xG^2T^8 + \{640 + 2130P(1) \\ & + 360P(2) + 30P(3) \\ & + \tfrac{20}{3}[43P(1)P(1) + 93P(1)P(2) + 7P(1)P(3) + 7P(2)P(3)] \\ & + 20P(1)P(1)P(2) + 20P(1)P(2)P(3)\}xG^4T^6 \\ & + [160 + 750P(1) + 50P(2) + 100P(1)P(1) \\ & + 200P(1)P(2)]xG^6T^4 + [20 + 70P(1)]xG^8T^2 + xG^{10}\end{aligned}$$

$$\begin{aligned}\mu_{11} = {} & 2772xGT^{10} + 22\{105 + 244P(1) + 68P(2) + 12P(3) + P(4) + \tfrac{1}{3}[68P(1)P(1) + 160P(1)P(2) + 26P(1)P(3) \\ & + 2P(1)P(4) + P(2)P(2) + 24P(2)P(3) + 2P(2)P(4) + 2P(3)P(4)]\}xG^3T^8 + 22\{42 + 204P(1) \\ & + 28P(2) + 2P(3) \\ & + \tfrac{1}{3}[118P(1)P(1) + 252P(1)P(2) + 16P(1)P(3) + 16P(2)P(3)] + 5P(1)P(1)P(2) \\ & + 5P(1)P(2)P(3)\}xG^5T^6 \\ & + 22\{9 + 53P(1) + 3P(2) + \tfrac{25}{3}[P(1)P(1) + 2P(1)P(2)]\}xG^7T^4 \\ & + 22[1 + 4P(1)]xG^9T^2 + xG^{11}\end{aligned}$$

$$\begin{aligned}\mu_{12} = {} & 924T^{12} + [6144 + 6744P(1) + 2784P(2) + 804P(3) + 144P(4) + 12P(5)]xG^2T^{10} \\ & + [3840 + 15180P(1) + 3390P(2) + 504P(3) + 36P(4) + 2744P(1)P(1) \\ & + 6280P(1)P(2) + 848P(1)P(3) + 56P(1)P(4) + 28P(2)P(2) + 792P(2)P(3) + 56P(2)P(4) \\ & + 56P(3)P(4) + 348P(1)P(1)P(2) + 372P(1)P(2)P(3) + 24P(1)P(2)P(4) + 24P(1)P(1)P(3) \\ & + 24P(1)P(2)P(2) + 24P(2)P(3)P(4) + 24P(1)P(3)P(4)]xG^4T^8 \\ & + [1280 + 8464P(1) + 960P(2) + 60P(3) + 2088P(1)P(1) + 4416P(1)P(2) \\ & + 240P(1)P(3) + 240P(2)P(3) + 366P(1)P(1)P(2) + 366P(1)P(2)P(3)]xG^6T^6 \\ & + [240 + 1722P(1) + 84P(2) + 308P(1) + 616P(1)P(2)]xG^8T^4 + [24 + 108P(1)]xG^{10}T^2 + xG^{12}\end{aligned}$$

A simple practical procedure to obtain the set $\{l_j\}$ in a given graph (M_1, M_2) is as follows. Start with a path with a minimum number of steps, $q_{\min}$. The possible sets $\{l_j\}$ are very simple in this instance, e.g. $l_{M_1} = 1$, $l_{M_2} = 1$, $l_0 = 3$, $l_j = 2$, $j \neq 0$, M_1, M_2. Take one of these sets and add unity to a pair of adjacent vertices, i.e. $l_i \to l_i + 1$, $l_j \to l_j + 1$, where i, j are nearest neighbours. This will ensure that the set $\{l_j\}$ satisfies the constraint (15). All sets $\{l_j\}$ for $q = q_{\min}$ will be eventually obtained in this manner. By repeating the same procedure we may continue up to any value of q.

Finally we present, in table 1, the first 13 moments calculated by this method, where we have written $P(k)$ for the probability of finding an atom type B at site $m \pm k$, if at site m an atom type B is found. The value of $P(k)$ for $k > 1$ is related to $P(1)$, through the formula (J Rössler 1979, unpublished)

$$1 - Q(k)/y = (1 - Q(1)/k)^k \tag{17}$$

where $y = 1 - x$, $Q(k) = 1 - P(k)$, $Q(1) = 1 - P(1)$. The diagonal element ε_B is denoted by G.

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