

Approximate formulae for the density of states of disordered linear chains

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Abstract. Any disordered linear chain may be conceived as consisting of connected finite ordered subchains of different lengths. We show that the integrated as well as differential density of electron states of any disordered chain may approximately be written as an average over the densities of states of the subchains. The accuracy of the approximate density of states is given by $1/\bar{n}$, where \bar{n} is the average length of the subchains. Numerical results show that the approximation is very good for \bar{n} about 10 or 20 and the main features of the density of states are reproduced even for $\bar{n} = 5$ or 3.

1. Introduction

Any disordered linear chain may be conceived as consisting of connected finite ordered subchains of different lengths. The larger the average length \bar{n} of the subchains, the more significant is the contribution of the subchains to the resulting density of states of the whole chain. For very large \bar{n} , all the main features of the density of states have to be determined by the properties of the subchains and there is a good chance of describing approximately the density of states of a disordered chain in terms of the densities of states of the subchains. For small \bar{n} , the interaction of the subchains becomes significant and the density of states of a disordered chain is a complex function of the properties of the subchains, their interaction and the concrete character of disorder. In such a case, description of the density of states of a disordered chain in terms of the densities of states of the subchains may be only a rough approximation.

The aim of this paper is to find, in the above-formulated sense, an approximate formula for the density of electron states of a disordered chain in terms of known densities of states of the subchains. This is done in sections 2–4 for the integrated as well as the differential density of states. Numerical results for general, diagonal and off-diagonal disorder are given in section 5. It appears that the approximate formulae give

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very good results for \bar{n} about 10 or 20 and the main features of the density of states are reproduced even for $\bar{n} = 5$ or 3.

2. Approximate formula for the integrated density of states

If we assume for simplicity the nearest-neighbour interaction and denote the diagonal matrix elements of the electron Hamiltonian H as ϵ and the off-diagonal elements as V the Hamiltonian discussed in this paper has the form

$$H_{ij} = \begin{cases} \epsilon_m & \left\{ \begin{array}{l} i \text{ from the } m\text{th subchain} \\ \text{the nearest neighbours } i \text{ and } j \text{ from the } m\text{th subchain} \\ \text{the nearest-neighbour interaction between the } m\text{th and } \\ n\text{th subchains} \end{array} \right. \\ V_m & \\ V_{mn} & \\ 0 & \left. \begin{array}{l} \text{otherwise.} \end{array} \right. \end{cases} \quad \text{for} \quad (1)$$

In order to express the integrated density of states of a disordered chain in terms of those of the subchains we use the negative eigenvalue theorem. This theorem which appears in different forms in different fields of physics [1-11] allows us to calculate the number of eigenvalues of a real symmetric matrix \mathbf{H} less than a given energy E . This number is an unnormalized integrated density of states denoted as $I(E)$ henceforth. The normalized integrated density of states, i.e. the relative number of eigenvalues less than E , will be denoted as $\bar{I}(E)$.

In this paper the following formulation of the negative eigenvalue theorem [1, 7, 8] is used:

$$I(E) = \sum_i \Theta(-X_i) \quad (2)$$

where $\Theta(x) = 1$ for $x \geq 0$ and $\Theta(x) = 0$ otherwise, the real numbers X_i are (1, 1) elements of the matrices \mathbf{U}_i :

$$\mathbf{U}_1 = \mathbf{H} - E \quad (3)$$

$$\mathbf{U}_i = \mathbf{Z}_{i-1} - \mathbf{Y}_{i-1}\mathbf{Y}_{i-1}^+/\mathbf{X}_{i-1}, \quad i = 2, \dots, n \quad (4)$$

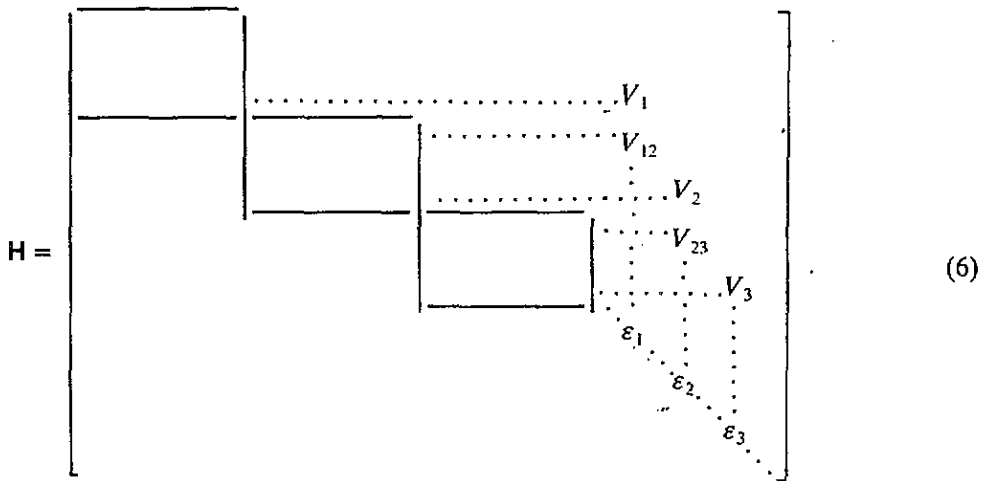
and the matrices \mathbf{U}_i are partitioned as follows:

$$\mathbf{U}_i = \left[\begin{array}{c|c} \mathbf{X}_i & \mathbf{Y}_i^+ \\ \hline \mathbf{Y}_i & \mathbf{Z}_i \end{array} \right] \quad (5)$$

The cross denotes the Hermitian conjugation.

To express the density $I(E)$ of states of a disordered linear chain in terms of those of the subchains we introduce the following numbering of atoms. First we number, say from left to right, all atoms in the subchains except for the last atom in any subchain. In the second step we number the remaining atoms at the ends of the subchains. The Hamiltonian then has the structure shown in equation (6). Only the upper triangle of the Hamiltonian H is shown. The blocks correspond to the tridiagonal Hamiltonian for the subchains with the last atoms removed. The diagonal matrix elements $\epsilon_1, \epsilon_2, \epsilon_3, \dots$

correspond to the last atoms in the subchains. The interaction of these atoms with the last and first atom in the corresponding blocks is also shown.



Now we apply the negative-eigenvalue theorem to the matrix $\mathbf{H} - E$. It is obvious from equations (2)–(5) that when applying the theorem to the upper left part of $\mathbf{H} - E$ containing blocks shown in equation (6) we get the sum of the integrated densities of states of the non-interacting subchains with the last atoms removed. Their interaction is taken into account in the next step when the numbers X_i corresponding to the matrix elements $\epsilon_1, \epsilon_2, \epsilon_3, \dots$ shown in equation (6) are calculated. We get as a result

$$I(E) = \sum_{n=1}^{\infty} \sum_{\epsilon} \sum_V N_{n+1,\epsilon,V} I_{n,\epsilon,V}(E) + \sum_i \Theta(-X_i). \tag{7}$$

Here, the summation runs over the length of the subchains $n = 1, 2, 3, \dots$ and the values of the diagonal and off-diagonal elements ϵ and V , respectively. $N_{n,\epsilon,V}$ is the number of the subchains for given n, ϵ and V and $I_{n,\epsilon,V}$ is the integrated density of states of the isolated ordered subchain with n atoms and the matrix elements ϵ and V . The last term in equation (7) is the correction to the previous sum representing the effect of the removed atoms and the interaction of the subchains. It takes into account also one-atom ‘subchains’ which are not included in the first sum. This term is in general complicated; however, it must be less than or equal to the number of the atoms removed from the subchains:

$$0 \leq \sum_i \Theta(-X_i) \leq \sum_{n=1}^{\infty} \sum_{\epsilon} \sum_V 1. \tag{8}$$

Now, dividing equation (7) by the total number of atoms given by

$$N = \sum_{n=1}^{\infty} \sum_{\epsilon} \sum_V n \tag{9}$$

we get the following expression for the normalized integrated density of states:

$$\bar{I}(E) = \frac{1}{N} I(E) = \sum_{n=1}^{\infty} \sum_{\epsilon} \sum_V \frac{N_{n+1,\epsilon,V}}{N} n \bar{I}_{n,\epsilon,V}(E) + \frac{1}{N} \sum_i \Theta(-X_i). \tag{10}$$

Introducing the average length of the subchains given by

$$\bar{n} = N/N_s \tag{11}$$

where N_s is the number of the subchains and the probability

$$p_{n,\varepsilon,V} = N_{n,\varepsilon,V}/N_s \quad (12)$$

of finding the subchain with given n , ε and V , we can rewrite equation (10) in the form

$$\bar{I}(E) = \frac{1}{\bar{n}} \sum_{n=1}^{\infty} n \sum_{\varepsilon} \sum_V p_{n+1,\varepsilon,V} \bar{I}_{n,\varepsilon,V}(E) + \frac{1}{N} \sum_i \Theta(-X_i). \quad (13)$$

The first sum in equation (13) is not normalized as it goes to $(\bar{n} - 1)/\bar{n}$ for $E \rightarrow \infty$. Normalizing it to unity and taking into account the relation

$$0 \leq \frac{1}{N} \sum_i \Theta(-X_i) \leq \frac{1}{\bar{n}} \quad (14)$$

we get the upper bound to the difference between the exact and approximate integrated density of states:

$$\left| \bar{I}(E) - \frac{1}{\bar{n} - 1} \sum_{n=1}^{\infty} n \sum_{\varepsilon} \sum_V p_{n+1,\varepsilon,V} \bar{I}_{n,\varepsilon,V}(E) \right| \leq \frac{1}{\bar{n}}. \quad (15)$$

This is the result that we mentioned in the introduction. The exact density \bar{I} of states is approximated by the sum of the densities $\bar{I}_{n,\varepsilon,V}$ of states of the ordered finite linear subchains. The accuracy of the approximate expression is given by $1/\bar{n}$.

We note that the assumption of the nearest-neighbour interaction in the Hamiltonian (1) is not essential. Assuming for example the second-nearest-neighbour interaction we could select an elementary unit consisting of two atoms. The interaction of the elementary units would be then the nearest-neighbour interaction and \bar{n} would denote the average number of elementary units.

The approximate density of states in equation (15) corresponds to the removed last atoms in the subchains. It is possible, however, to find a better approximation. It is obvious that it is not necessary to remove these atoms. To get non-interacting subchains, it is sufficient to put $V_{mn} = 0$. The corresponding approximate density of states reads

$$\bar{I}_{\text{app}}(E) = \frac{1}{\bar{n}} \sum_{n=1}^{\infty} n \sum_{\varepsilon} \sum_V p_{n,\varepsilon,V} \bar{I}_{n,\varepsilon,V}(E). \quad (16)$$

It is not, however, possible to derive an estimate of the accuracy of this approximate density of states directly. We obtain first

$$\frac{1}{\bar{n}} \sum_{n,\varepsilon,V} n p_{n,\varepsilon,V} \bar{I}_{n,\varepsilon,V} = \frac{1}{\bar{n}} \sum_{n,\varepsilon,V} n p_{n+1,\varepsilon,V} \bar{I}_{n,\varepsilon,V} + \frac{1}{\bar{n}} \sum_{n,\varepsilon,V} n (p_{n,\varepsilon,V} - p_{n+1,\varepsilon,V}) \bar{I}_{n,\varepsilon,V}. \quad (17)$$

Then, using equations (13), (14) and (17) the lower and upper bounds to the difference $\bar{I}(E) - \bar{I}_{\text{app}}(E)$ may be derived:

$$\begin{aligned} \frac{-1}{\bar{n}} \sum_n^{>0} n \left(\sum_{\varepsilon,V} p_{n,\varepsilon,V} - \sum_{\varepsilon,V} p_{n+1,\varepsilon,V} \right) &\leq \bar{I}(E) - \bar{I}_{\text{app}}(E) \\ &\leq \frac{1}{\bar{n}} - \frac{1}{\bar{n}} \sum_n^{<0} n \left(\sum_{\varepsilon,V} p_{n,\varepsilon,V} - \sum_{\varepsilon,V} p_{n+1,\varepsilon,V} \right). \end{aligned} \quad (18)$$

Here, >0 and <0 denote the summation over positive and negative terms

$(\sum_{\epsilon, V} p_{n, \epsilon, V} - \sum_{\epsilon, V} p_{n+1, \epsilon, V})$, respectively. In a special case $\sum_{\epsilon, V} p_{n, \epsilon, V} \geq \sum_{\epsilon, V} p_{n+1, \epsilon, V}$ we have the simple result

$$|\bar{I}(E) - \bar{I}_{app}(E)| \leq 1/\bar{n}. \tag{19}$$

This includes the case $p_{n, \epsilon, V} = p_{n+1, \epsilon, V}$, $n = 1, \dots, n_{max} - 1$ investigated in section 5.

As the approximate density of states (16) corresponds to smaller changes in the Hamiltonian (1) than that in equation (15) and usually gives better results, the rest of the paper is devoted to the discussion of the approximation based on equation (16).

3. Approximate integrated density of states

The integrated density $\bar{I}_{n, \epsilon, V}$ of states appearing in equation (16) is the integrated density of states of the ordered linear chain with n atoms, the diagonal matrix element of the Hamiltonian ϵ and the off-diagonal element V . The corresponding system of difference equations has the form

$$\begin{aligned} \epsilon c_1 + V c_2 &= E c_1 \\ V c_{i-1} + \epsilon c_i + V c_{i+1} &= E c_i \quad i = 2, \dots, n-1 \\ V c_{n-1} + \epsilon c_n &= E c_n \end{aligned} \tag{20}$$

where c_i are the components of the eigenfunction. The solution of this system of equations is well known [12]. The energies in which we are interested here equal

$$E_i = \epsilon + 2V \cos[i\pi/(n+1)] \quad i = 1, \dots, n \tag{21}$$

so that $\bar{I}_{n, \epsilon, V}$ is

$$\bar{I}_{n, \epsilon, V}(E) = \frac{1}{n} \sum_{i=1}^n \Theta(E - \epsilon - 2|V|c_{in}) \tag{22}$$

where

$$c_{in} = \cos[i\pi/(n+1)]. \tag{23}$$

For simplicity let us assume now the separation of the probabilities $p_{n, \epsilon, V}$ in the space of variables n , ϵ and V

$$p_{n, \epsilon, V} = p_n p_{\epsilon, V}. \tag{24}$$

The approximate density $\bar{I}(E)$ of states (equation (16)) then becomes

$$\bar{I}_{app}(E) = \frac{1}{\bar{n}} \sum_{n=1}^{\infty} n p_n \sum_{\epsilon} \sum_V p_{\epsilon, V} \bar{I}_{n, \epsilon, V}(E). \tag{25}$$

For a continuous distribution of ϵ and V we get

$$\bar{I}_{app}(E) = \frac{1}{\bar{n}} \sum_{n=1}^{\infty} p_n \sum_{i=1}^n \int_{\epsilon + 2|V|c_{in} < E} p_{\epsilon, V} d\epsilon dV \tag{26}$$

where the region of the integration is shown. This simple expression is an interesting result giving the relation of the approximate integrated density of states and the integrated density of states in the space of ϵ - and V -distributions.

Assuming diagonal disorder only, $p_{\epsilon, V} = p_{\epsilon}$, we get

$$\int_{\epsilon + 2|V|c_{in} < E} p_{\epsilon, V} d\epsilon dV = \int_{-\infty}^{E - 2|V|c_{in}} p_{\epsilon} d\epsilon \tag{27}$$

where the relation to the integrated density of states in ϵ -space is clearly seen.

For the off-diagonal disorder $p_{\epsilon, V} = p_V$ a similar result can be derived.

Especially simple are the above formulae for the uniform distribution of the probabilities in ϵ - or V -space. For the uniform distribution in ϵ -space given by

$$p_{\epsilon} = 1/2\epsilon_{\max} \quad \epsilon \in (-\epsilon_{\max}, \epsilon_{\max}) \tag{28}$$

we get

$$\int_{-\infty}^{E - 2|V|c_{in}} p_{\epsilon} d\epsilon = \begin{cases} 1 & E - 2|V|c_{in} \geq \epsilon_{\max} \\ \frac{(E - 2|V|c_{in} + \epsilon_{\max})}{2\epsilon_{\max}} & -\epsilon_{\max} < E - 2|V|c_{in} < \epsilon_{\max} \\ 0 & E - 2|V|c_{in} \leq -\epsilon_{\max} \end{cases} \text{ for } \begin{cases} E - 2|V|c_{in} \geq \epsilon_{\max} \\ -\epsilon_{\max} < E - 2|V|c_{in} < \epsilon_{\max} \\ E - 2|V|c_{in} \leq -\epsilon_{\max} \end{cases} \tag{29}$$

For the uniform distribution of the probabilities

$$p_V = 1/(V_{\max} - V_{\min}) \quad V \in (V_{\min}, V_{\max}), V_{\min}, V_{\max} > 0 \tag{30}$$

in V -space we have the following result:

$$\int_{\epsilon + 2|V|c_{in} < E} p_V dV = \begin{cases} \Theta(E - \epsilon) & \text{for } c_{in} = 0 \\ 1 & \text{for } E \geq \epsilon + 2V_{\max}c_{in} \text{ and } \\ & c_{in} > 0 \text{ or } E \geq \epsilon + 2V_{\min}c_{in} \text{ and } c_{in} < 0 \\ \frac{E - \epsilon - 2V_{\min}c_{in}}{2(V_{\max} - V_{\min})c_{in}} & \text{for } E \in (\epsilon + 2V_{\min}c_{in}, \epsilon + 2V_{\max}c_{in}) \\ & \text{and } c_{in} > 0 \\ \frac{E - \epsilon - 2V_{\max}c_{in}}{2(V_{\min} - V_{\max})c_{in}} & \text{for } E \in (\epsilon + 2V_{\max}c_{in}, \epsilon + 2V_{\min}c_{in}) \\ & \text{and } c_{in} < 0 \\ 0 & \text{otherwise.} \end{cases} \tag{31}$$

4. Approximate differential density of states

According to equations (16) and (22), the approximate differential density of states given by

$$g_{\text{app}}(E) = d\bar{I}_{\text{app}}(E)/dE \tag{32}$$

equals

$$g_{\text{app}}(E) = \frac{1}{\bar{n}} \sum_{n=1}^{\infty} n \sum_{\epsilon} \sum_V p_{n, \epsilon, V} g_{n, \epsilon, V}(E) \tag{33}$$

where

$$g_{n,\varepsilon,V}(E) = \frac{1}{n} \sum_{i=1}^n \delta(E - \varepsilon - 2|V|c_{in}) \tag{34}$$

is the differential density of states of the finite ordered linear chain corresponding to equations (20).

In the case of the continuous distribution of ε and V we get from equation (26)

$$g_{app}(E) = \frac{1}{\bar{n}} \sum_{n=1}^{\infty} p_n \sum_{i=1}^n \frac{d}{dE} \left(\int_{\varepsilon+2|V|c_{in} < E} p_{\varepsilon,V} d\varepsilon dV \right). \tag{35}$$

This simple expression shows the relation between the electron density $g(E)$ of states and the differential density of states in ε - and V -space.

In a special case of the uniform distribution in ε -space given by equation (28) we have

$$\frac{d}{dE} \left(\int_{\varepsilon+2|V|c_{in} < E} p_{\varepsilon} d\varepsilon \right) = \frac{1}{2\varepsilon_{max}} [\Theta(\varepsilon_{max} - E) - \Theta(-\varepsilon_{max} - E)]. \tag{36}$$

Similarly, for the uniform distribution in V -space (30) we get

$$\begin{aligned} & \frac{d}{dE} \left(\int_{\varepsilon+2|V|c_{in} < E} p_V dV \right) && \delta(E - \varepsilon) && \text{for } c_{in} = 0 \\ & = \frac{1}{[2(V_{max} - V_{min})c_{in}]} \text{sgn}(c_{in}) [\Theta(\varepsilon + 2V_{max}c_{in} - E) && && \tag{37} \\ & \quad - \Theta(\varepsilon + 2V_{min}c_{in} - E)] && && \text{for } c_{in} \neq 0. \end{aligned}$$

Here, $\text{sgn}(\chi)$ denotes the sign of χ .

The upper and lower bounds to $g(E) - g_{app}(E)$ analogous to equation (18) cannot be found directly. In analogy with [9], however, it is possible to derive such bounds for the moments of the density of states:

$$J_k = \int_{E_1}^{E_2} E^k g(E) dE. \tag{38}$$

For example for $k = 0$ we get from equation (19)

$$\begin{aligned} |J_0 - J_0^{app}| &= |\bar{I}(E_2) - \bar{I}(E_1) - \bar{I}_{app}(E_2) + \bar{I}_{app}(E_1)| \leq |\bar{I}(E_2) - \bar{I}_{app}(E_2)| \\ &+ |\bar{I}(E_1) - \bar{I}_{app}(E_1)| \leq 2/\bar{n}. \end{aligned} \tag{39}$$

This equation is valid for arbitrary energies E_1 and E_2 and for $\sum_{\varepsilon,V} p_{n,\varepsilon,V} \geq \sum_{\varepsilon,V} p_{n+1,\varepsilon,V}$. Using the per parts integration, similar results may be derived for the higher moments J_k , too (see [9]).

5. Numerical results

The accuracy of the approximate formulae for the integrated and differential density of states was tested on the following three problems.

(i) The uniform discrete distribution of the probabilities in n -, ε - and V -space. We assumed for simplicity that

$$\begin{aligned} p_n &= 1/n_{\max} && \text{for } n = 1, \dots, n_{\max} \\ p_\varepsilon &= \frac{1}{2} && \text{for } \varepsilon = -2, 2 \\ p_V &= \frac{1}{2} && \text{for } V = 1, 2. \end{aligned} \quad (40)$$

The calculations for case (i) as well as cases (ii) and (iii) were done for the maximum length n_{\max} of the subchains equal to 5, 9, 19 and 39, i.e. for $\bar{n} = 3, 5, 10$ and 20.

(ii) The uniform distribution of the probabilities in n -space and the continuous uniform distribution in ε -space.

$$\begin{aligned} p_n &= 1/n_{\max} && \text{for } n = 1, \dots, n_{\max} \\ p_\varepsilon &= 1/2\varepsilon_{\max} && \text{for } \varepsilon \in (-\varepsilon_{\max}, \varepsilon_{\max}) \end{aligned} \quad (41)$$

where $\varepsilon_{\max} = 1$.

(iii) The uniform distribution of the probabilities in n -space and the continuous uniform distribution in V -space.

$$\begin{aligned} p_n &= 1/n_{\max} && \text{for } n = 1, \dots, n_{\max} \\ p_V &= 1/(V_{\max} - V_{\min}) && \text{for } V \in (V_{\min}, V_{\max}), \end{aligned} \quad (42)$$

where $V_{\min} = 1$ and $V_{\max} = 2$.

The exact integrated and differential densities of states of a disordered infinite linear chain have in general continuous character. The numerically calculated density of states also has a similar character if the chain is sufficiently long. On the other hand, our approximate formulae express the exact density of states in terms of the densities of states of the finite chains with the length $n = 1, \dots, n_{\max}$, which always have a discrete energy spectrum. It is obvious that such an expression cannot describe details of the exact density of states well on an energy scale smaller than the minimum energy interval between the eigenvalues of the subchains. This energy interval is for the investigated problems

$$\Delta E = 2|V|_{\min} \{ \cos[\pi/(n_{\max} + 1)] - \cos[2\pi/(n_{\max} + 1)] \} \quad (43)$$

where $|V|_{\min}$ is the smallest $|V|$ appearing in the problem.

In order to overcome the above-mentioned discreteness of the approximate density of states we replaced the discrete energies of the subchains by the Lorentzian curves following from one of the representations of the δ -function

$$\delta(E) = (1/\pi)\Delta E/(E^2 + \Delta E^2) \quad (44)$$

where ΔE is the half-width of the δ -function. Use of ΔE given by equation (43) should not lead to any substantial loss of accuracy. The integrated density of states corresponding to equation (44) is

$$\Theta(E) = (1/\pi)[\tan^{-1}(E/\Delta E) + \pi/2]. \quad (45)$$

Equations (44) and (45) were used in numerical calculations of the approximate densities of states according to sections 3 and 4.

Numerical calculations were done for the disordered chains with 7000 ($n_{\max} = 5$), 4000 ($n_{\max} = 9$) and 2000 ($n_{\max} = 19$ and 39) subchains. The resulting order of the

Table 1. Numerical results for the integrated density of states. $|\bar{I} - \bar{I}_{\text{app}}|_{\text{max}}$ is the absolute value of the maximum difference of the exact density \bar{I} of states and approximate density \bar{I}_{app} of states over the whole energy spectrum.

Case	n_{max}	n	$1/\bar{n}$	$ \bar{I} - \bar{I}_{\text{app}} _{\text{max}}$
(i)	5	3	0.333	0.056
(i)	9	5	0.2	0.026
(i)	19	10	0.1	0.0099
(i)	39	20	0.05	0.0087
(ii)	5	3	0.333	0.075
(ii)	9	5	0.2	0.043
(ii)	19	10	0.1	0.022
(ii)	39	20	0.05	0.012
(iii)	5	3	0.333	0.082
(iii)	9	5	0.2	0.052
(iii)	19	10	0.1	0.028
(iii)	39	20	0.05	0.015

Hamiltonian H was always at least 20000. The subchains were randomly generated in agreement with the distributions p_n , p_ε and p_V described in cases (i), (ii) and (iii). The exact and approximate densities of states were calculated in 150 energy steps covering the whole energy spectrum. The exact integrated density of states was calculated numerically from equation (2). The approximate integrated density of states was calculated using equations (16), (22), (29) and (31).

The results for the integrated density are summarized in table 1. We see that the maximum difference of the exact integrated density \bar{I} of states and approximate integrated density \bar{I}_{app} of states is on the whole range of the energy spectrum and for all $n_{\text{max}} = 5, 9, 19$ and 39 smaller than 0.082. The actual maximum difference $|\bar{I} - \bar{I}_{\text{app}}|_{\text{max}}$ is in all cases about five times smaller than the upper bound $1/\bar{n}$ following from equation (19). Note that the agreement between the exact and approximate densities of states is relatively good even for $\bar{n} = 3$, i.e. for very short subchains.

The integrated density of states is only a little sensitive to details of the distribution of the eigenvalues in the energy spectrum. Its derivative, the differential density $g(E)$ of states, is more interesting. The exact differential density $g(E)$ of states was calculated numerically using equation (2). The approximate density $g_{\text{app}}(E)$ of states was calculated from equations (33)–(37). The results are shown in figures 1–3.

We see that the agreement between $g(E)$ and $g_{\text{app}}(E)$ is very good in cases (i) and (ii) and $n_{\text{max}} = 19$ and 39. The agreement in case (iii) is good except for the central peak in the approximate density $g_{\text{app}}(E)$ of states. This peak corresponds to the delta function term $\delta(E - \varepsilon)$ in equation (37). This highly degenerate central eigenvalue $E = \varepsilon$ appears in equation (34) for any subchain with an odd number n of atoms and is therefore a consequence of our approximate formula. In general, it does not appear in the exact density of states. If necessary, this peak can be removed by using larger ΔE in equation (44) for this energy. We note also that there is no problem with this peak for combined diagonal and off-diagonal disorder (case (i)) as well as for diagonal disorder only (case (ii)).

The agreement between the exact and approximate density of states is reasonably good even for $n_{\text{max}} = 9$, where the upper bound to the integrated density of states

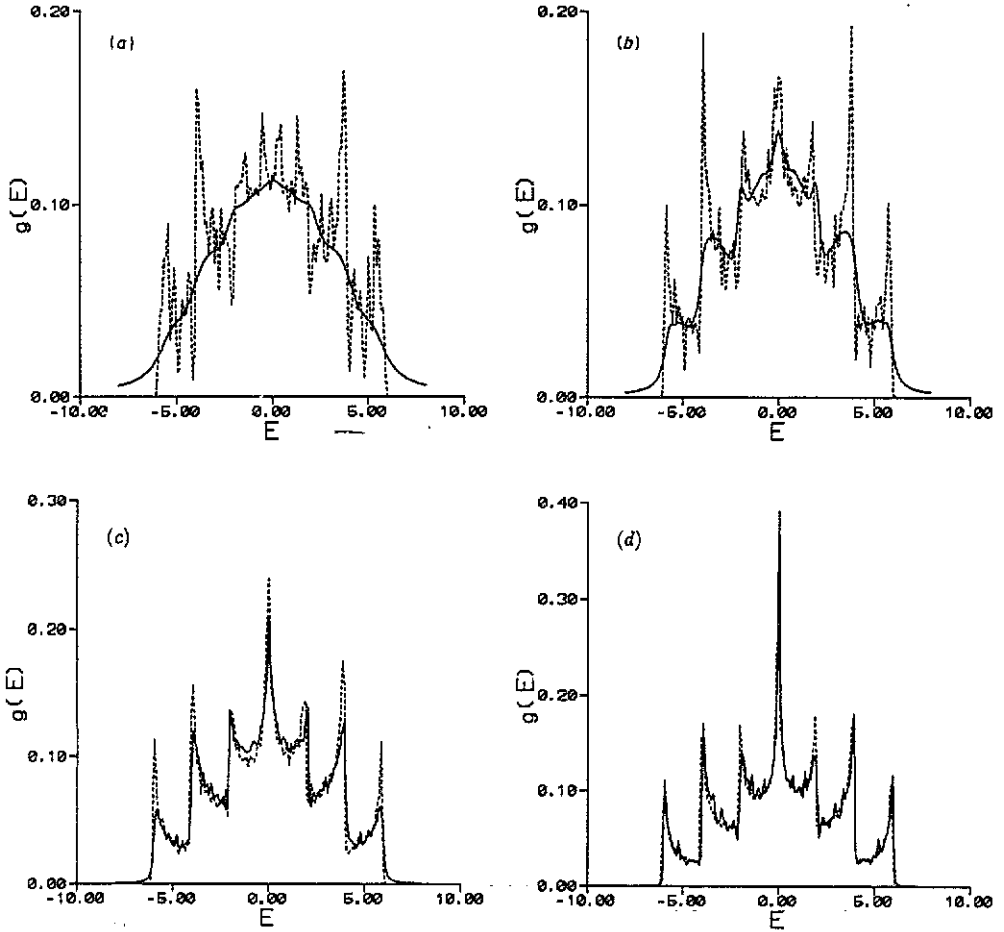


Figure 1. The numerically calculated exact density $g(E)$ of states (-----) and approximate density $g_{app}(E)$ of states (—) for case (i): (a) $n_{max} = 5$; (b) $n_{max} = 9$; (c) $n_{max} = 19$; (d) $n_{max} = 39$.

$1/\bar{n} = \frac{1}{3}$ in equation (19) suggests that the approximation may not be good. We note that some main characteristics of the exact density of states are reproduced by the approximate formula even for $n_{max} = 5$, i.e. for $\bar{n} = 3$. Because of the large ΔE , however, most details of the density of states are lost in this case (see figures 1(a), 2(a) and 3(a)).

6. Conclusions

Using the negative-eigenvalue theorem and partitioning of a disordered linear chain into the ordered linear subchains we have derived approximate formulae for the integrated and differential densities of states of the chain. These formulae express the exact density of states as a sum of analytically known densities for the subchains and show also the relation between the exact density of states and the density of states in ε - and V -space. Upper and lower bounds to the difference of the exact and approximate integrated

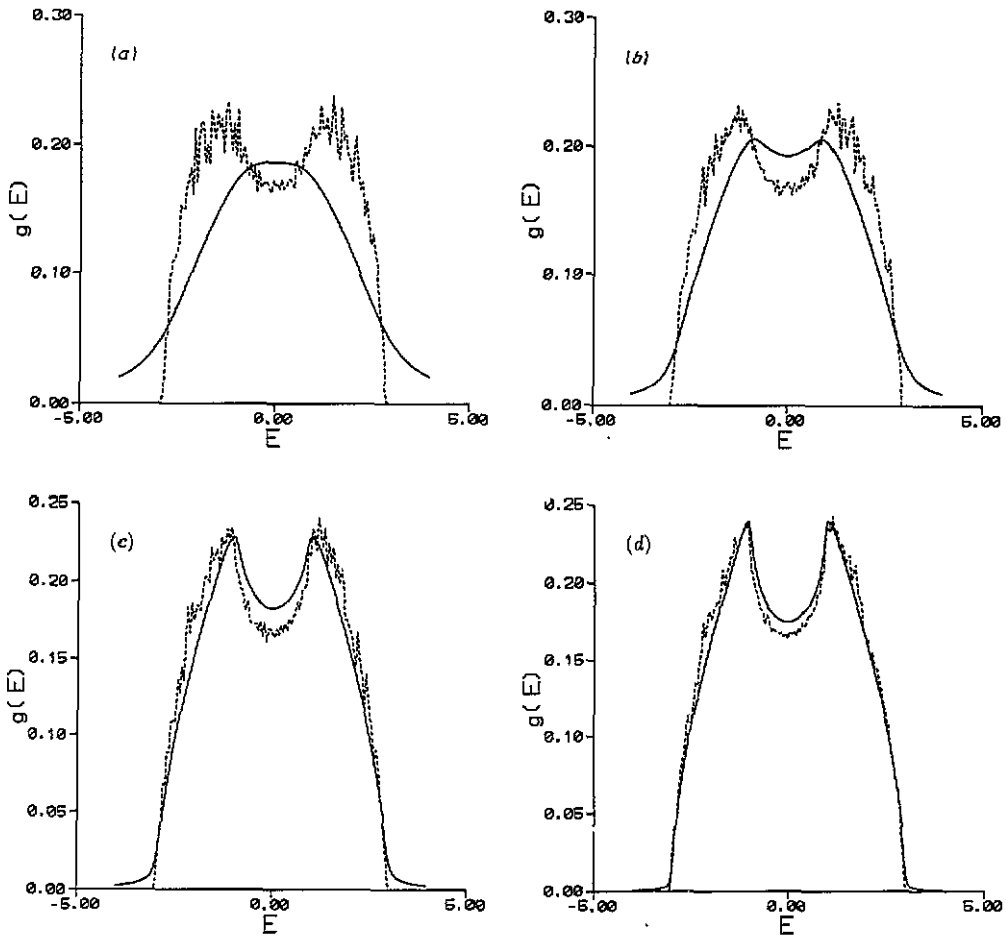


Figure 2. The numerically calculated exact density $g(E)$ of states (----) and approximate density $g_{\text{app}}(E)$ of states (—) for case (ii): (a) $n_{\text{max}} = 5$; (b) $n_{\text{max}} = 9$; (c) $n_{\text{max}} = 19$; (d) $n_{\text{max}} = 39$.

density of states and moments of the differential density of states were also given. The accuracy of the approximation is given by $1/\bar{n}$, where \bar{n} is the average length of the subchains. Numerical tests of the approximate formulae were done for the chains with the uniform distribution of the lengths of the chains from 1 to n_{max} . Three investigated cases correspond to both diagonal and off-diagonal disorder, to diagonal disorder and to off-diagonal disorder only. The agreement between the exact and approximate integrated and differential density of states is very good for the chains with $\bar{n} = 10$ and 20 with the exception of the case with off-diagonal disorder only. The reason for the existence of the central peak in the differential density of states in this case is explained and a method of removing it is suggested. The agreement for the short subchains with $\bar{n} = 3$ and 5 is not as good; however, the basic features of the differential density states are, especially for $\bar{n} = 5$, reproduced.

The results of this paper can be applied to distorted linear polymers, heterostructures and similar systems.

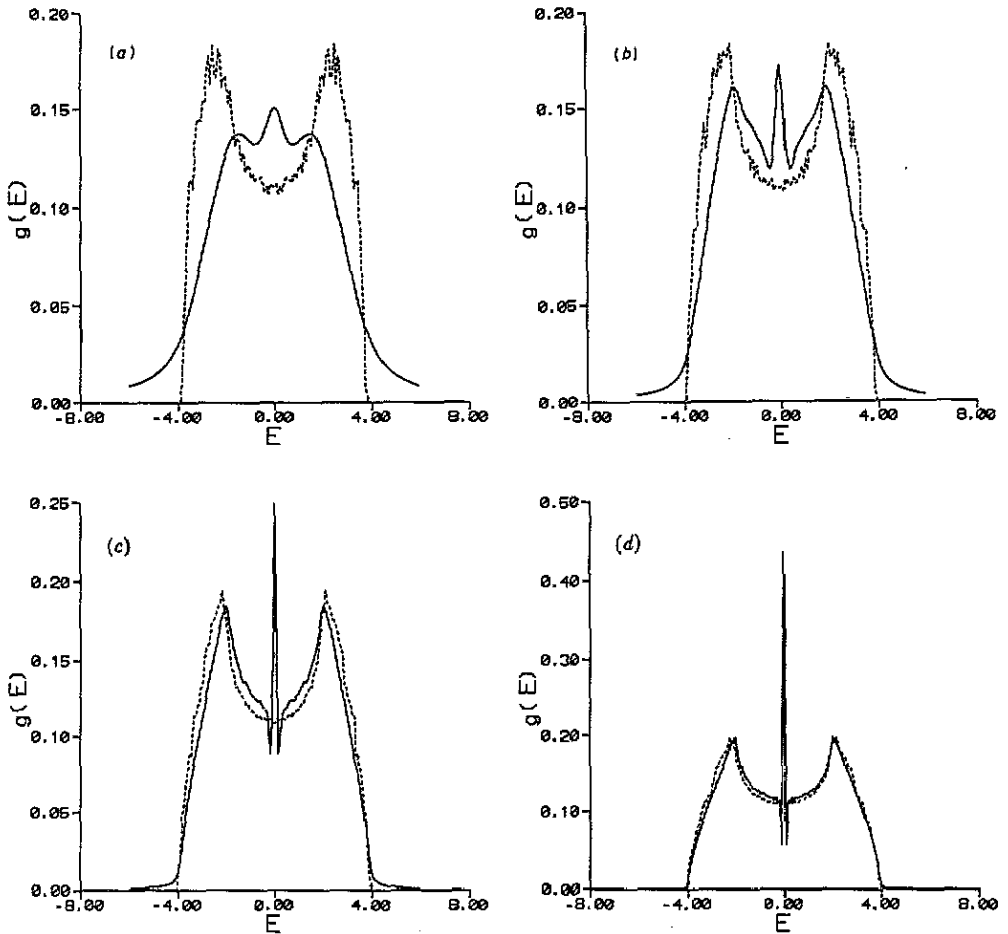


Figure 3. The numerically calculated exact density $g(E)$ of states (-----) and approximate density $g_{app}(E)$ of states (—) for case (iii): (a) $n_{max} = 5$; (b) $n_{max} = 9$; (c) $n_{max} = 19$; (d) $n_{max} = 39$.

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