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1981 J. Phys. C: Solid State Phys. 14 235

(http://iopscience.iop.org/0022-3719/14/3/007)

J. Phys. C: Solid State Phys., 14 (1981) 235–245. Printed in Great Britain

Conductivity of the disordered linear chain

D J Thouless†§ and S Kirkpatrick‡

† Department of Engineering and Applied Science, Becton Center, Yale University, New Haven, CT 06520, USA

‡ IBM Thomas J Watson Research Center, Yorktown Heights, NY 10598, USA

Received 26 June 1980

Abstract. We have developed a fast algorithm for evaluating the Kubo formula for the conductivity of a linear chain, and use it to study the dependence of the conductivity as a function of imaginary frequency. The results for the Anderson model with different degrees of disorder and different energies can all be scaled onto the same curve, which is of the form expected from the theory of localised states. The universal curve obtained provides a simple connection between tight-binding model results and the conductivity which can be calculated for an electron in a white noise potential. Similar, but not identical, results are obtained for tight-binding chains with a Cauchy distribution of site energies.

1. Introduction

In a recent paper Czycholl and Kramer (1979) have presented numerical results for the conductivity of a linear chain that cast doubt on the well established result that electrons are always localised in a disordered one-dimensional system (Mott and Twose 1960, Landauer 1970, Borland 1963, Ishii 1973). In that work the Kubo formula for the conductivity was used for a tight-binding model with random site energies (Anderson model). In view of various recent numerical and theoretical studies of one-dimensional conduction (Berezinskii 1974, Abrikosov and Ryzhkin 1978, Anderson *et al* 1980, Abrahams and Stephen 1980, Andereck and Abrahams 1980, Economou and Soukoulis 1980), mostly based on Landauer's (1970) relation between the conductance and the transmission coefficient of the chain, which support the idea of localisation, it has seemed useful to look at the use of the Kubo formula in more detail.

The Kubo formula involves a sum over squares of all matrix elements of the Green function, so it would seem to involve $O(N^2)$ arithmetical operations for a chain of N sites. However, we have developed a technique that allows a complete evaluation with $O(N)$ operations, so we have been able to study many examples of such a chain with a range of values of the parameters involved. The results have a very simple pattern which for the longer chains can be understood in terms of a frequency-dependent conductivity $\sigma(\omega)$ that goes to zero faster than ω in the low-frequency limit; this is what would be expected for localised electrons. Furthermore, there is a simple scaling law which enables the effect of a change of the degree of disorder or of the energy to be predicted. This scaling law supports the idea that results for a tight-binding model with weak disorder

§ Present address: Department of Physics, FM 15, University of Washington, Seattle, Wash. 98195, USA.

0022-3719/81/030235 + 11 $01.50

have a simple relation to results for the Schrödinger equation in a white noise potential. For shorter chains the results are dominated by boundary effects.

There is a considerable scatter of the calculated results in the region where localisation is important, and so we get quite different results for the mean conductivity and for the reciprocal of the mean resistivity. We have used enough samples that we have been able to study such effects.

We have at least a qualitative understanding of the results of Czycholl and Kramer. It seems that for their least disordered chains they did not take the imaginary part of the frequency small enough to observe the region in which localisation is dominant, and their extrapolation to the infinite chain was unsatisfactory.

2. Kubo formula

The Kubo formula for the conductivity $\sigma(\omega)$ involves matrix elements of the momentum operator between states differing in energy by $\hbar\omega$. In the case of a finite system this gives a set of δ functions, so in order to get a sensible result we need to smooth the results in some way. We follow Czycholl and Kramer by giving an imaginary part to ω, and calculating

$$\sigma(\mathrm{i}\eta) = \frac{2e^2aV^2}{\pi\hbar N} \operatorname{Tr} \operatorname{Im} G(E + \mathrm{i}\eta)\, \hat{D} \operatorname{Im} G(E + \mathrm{i}\eta)\, \hat{D}, \tag{1}$$

for a tight-binding band with Hamiltonian $H_{ij} = \epsilon_i\delta_{ij} - V(\delta_{i,j-1} + \delta_{i,j+1})$, and lattice parameter a, where $\hat{D}$ is the hermitian operator given by $\hat{D}_{jj'} = \mathrm{i}\delta_{j,j'+1} - \mathrm{i}\delta_{j,j'-1}$. This produces a lorentzian average over both the energy and frequency, and gives essentially

$$\sigma(\mathrm{i}\eta) = \int \sigma(\omega)\,(2\eta/\pi)/(\hbar^2\omega^2 + 4\eta^2)\,\hbar\,\mathrm{d}\omega. \tag{2}$$

The effect of non-zero η is to introduce a timescale over which the conductivity is measured, and it is equivalent to introducing an inelastic relaxation process with a relaxation time $\hbar/2\eta$. In some sense the non-zero η simulates the effect of inelastic scattering at non-zero temperatures in a real system, but it must be assumed that the inelastic scattering is an uncorrelated random event (Poisson process), and this is not entirely realistic.

For large ω we expect the Drude formula for degenerate electrons, $\sigma(\omega) = (e^2/\pi\hbar)2v\tau/(1 + \omega^2\tau^2)$, to hold, where τ is the elastic scattering time and the velocity $v = \mathrm{d}E/\mathrm{d}(\hbar k)$ at the Fermi surface. Substitution of this into (2) gives

$$\sigma(\mathrm{i}\eta) = \frac{e^2}{\pi\hbar}\, v \frac{2\tau}{1 + 2\eta\tau/\hbar} \sim \frac{e^2 v}{\pi\eta}. \tag{3}$$

The theory of localisation leads us to expect $\sigma(\omega)$ to go to zero as $\omega^2(\ln\omega)^2$ for small ω, so for small η equation (2) gives

$$\sigma(\mathrm{i}\eta) \approx (2\eta/\hbar\pi)\int \sigma(\omega)/\omega^2\,\mathrm{d}\omega, \tag{4}$$

as Berezinskii (1974) has calculated.

Our method of evaluation depends on the self-energies which are calculated by the iterative schemes

$$\begin{aligned} S_N^{\mathrm{R}} &= 0, \qquad S_j^{\mathrm{R}} = V^2/(E - \mathrm{i}\eta - \epsilon_{j+1} - S_{j+1}^{\mathrm{R}}), \\ S_1^{\mathrm{L}} &= 0, \qquad S_j^{\mathrm{L}} = V^2/(E - \mathrm{i}\eta - \epsilon_{j-1} - S_{j-1}^{\mathrm{L}}). \end{aligned} \tag{5}$$

Some care has to be exercised in these evaluations, as small values of the denominators can lead to large errors, but we found the use of IBM double precision arithmetic at this stage gave plenty of protection against accidentally small denominators. For $j > j'$ the Green function can be written as

$$G_{j'j} = (E - i\eta - \epsilon_{j'} - S_{j'}^{R} - S_{j'}^{L-1}) \prod_{k=j'}^{j-1} (S_k^R/V). \tag{6}$$

Substitution of this in equation (1) gives the result

$$\sigma(i\eta) = \frac{4e^2aV^2}{\pi\hbar N} \sum_{i=2}^{N} \frac{\operatorname{Im} S_i^L}{|E - i\eta - \epsilon_i - S_i^R - S_i^L|^2} \left\{ \eta + \operatorname{Im} S_i^R + 2\left[\operatorname{Im} S_i^R + \sum_{j=i+1}^{W-1} \left(\prod_{k=i}^{j-1} \frac{|S_k^R|^2}{V^2} \right) \operatorname{Im} S_j^R \right] \right\}. \tag{7}$$

The expression in square brackets can be evaluated iteratively at the same time as S_i^R, and all the terms in equation (7) are positive, so this can be evaluated rapidly and accurately.

At the same time as the Kubo formula is evaluated, the logarithm of equation (6) can be used to evaluate $\ln G_{1N}$ in the limit of small η. This is expected to be negative and of order N. G_{1N} is closely related to the transmission coefficient of the chain, and so to its conductance, so that $N^{-1} \ln G_{1N}$ gives a measure of the exponential dependence of resistance on the length of the chain. The results we obtained for this quantity were similar to those found by Andereck and Abrahams (1980) and Economou and Soukoulis (1980), so we do not report them here.

3. Finite-size effects

Because the Green function falls off exponentially with distance, the contributions of the terms with large $j - i$ in equation (7) should be negligible. However, there will be large fluctuations in the distance at which these contributions become negligible, since $\ln G_{ij}$ is essentially the sum of independent random terms. When the distance of i from the boundaries at 1 and N is larger than this distance the contribution to equation (7) should have the value typical of the bulk conductivity, but for i close to the boundary the contribution will be reduced. One can therefore expect the conductivity of a short chain to be less than that of a long chain.

The form of $\sigma(i\eta)$ for a finite chain can be estimated for η small. In terms of the eigenvalues E_α for the chain, equation (1) gives

$$\sigma(i\eta) = \frac{2e^2aV^2}{\pi\hbar N} \sum_{\alpha} \sum_{\beta} \frac{\eta}{(E - E_\alpha)^2 + \eta^2} \frac{\eta}{(E - E_\beta)^2 + \eta^2} |\hat{D}_{\alpha\beta}|^2, \tag{8}$$

where $\hat{D}_{\alpha\beta}$ is zero for $\alpha = \beta$. When η is less than the spacing between energy levels this is of order η^2 with probability close to unity, and is of order unity with probability $\eta N n(E)$, where $n(E)$ is the density of states per site. It would be of order η^{-2} with probability of order η^2, but the repulsion of close energy levels assures that E_α and E_β are only close to one another when $D_{\alpha\beta}$ is negligible. This is another statement of localisation, since $\hat{D}$ is proportional to the commutator $[\hat{H}, \hat{x}]$, and so if the matrix elements of $\hat{x}$ are bounded the matrix elements of $\hat{D}$ between two eigenstates of $\hat{H}$ must be small when the eigenvalues are close. The result is that the average conductivity is dominated by the

terms of order unity, and is proportional to η, but the average of the resistivity is proportional to η^{-2} for $\eta N n(E) \ll 1$.

In the limit of no disorder the conductivity can be calculated directly from equation (1) by using the spectral decomposition of the Green function (Albers and Gubernatis 1978). The amplitudes of the eigenvectors at the site j are of the form $(2/N)^{1/2} \sin[nj\pi/(N+1)]$, and the largest matrix elements of $\hat{D}$ are those between states close in energy. For such states we have

$$\langle n|\hat{D}|n'\rangle \simeq -2\mathrm{i} \sin\frac{n\pi}{N+1}\,[1 + (-1)^{n-n'}]/\pi(n-n') \tag{9}$$

and so we have

$$\begin{aligned}\sigma(\mathrm{i}\eta) &\approx \frac{64e^2aV^2}{\pi^3\hbar N}\sum_m\sum_n \frac{\eta}{\{E - 2V\cos[2m\pi/(N+1)]\}^2 + \eta^2} \\ &\quad\times \frac{\eta}{\{E - 2V\cos[(2n+1)\pi/(N+1)]\}^2 + \eta^2}\,\frac{\sin^2[2n\pi/(N+1)]}{(2m-2n-1)^2} \\ &\approx \frac{e^2a(4V^2 - E^2)}{\pi\eta^2\hbar N}\,\frac{\sinh[\eta N/(4V^2 - E^2)^{1/2}]}{\sin^2[EN/(4V^2 - E^2)^{1/2}] + \sinh^2[\eta N/(4V^2 - E^2)^{1/2}]} \\ &\quad\times\left(\frac{\eta N}{(4V^2 - E^2)^{1/2}}\cosh\frac{\eta N}{(4V^2 - E^2)^{1/2}} - \sinh\frac{\eta N}{(4V^2 - E^2)^{1/2}}\right),\end{aligned} \tag{10}$$

where the sum has been evaluated by contour integral methods. If the average over a narrow range of E is taken we get

$$\overline{\sigma(\mathrm{i}\eta)} = \frac{e^2L}{\pi\hbar}\left(\frac{\hbar v}{L\eta} - \frac{h^2v^2}{L^2\eta^2}\tanh\frac{L\eta}{\hbar v}\right), \tag{11}$$

where $L = Na$ is the length of the chain, and the velocity v for the tight-binding model is given by

$$\hbar v = a(4V^2 - E^2)^{1/2}. \tag{12}$$

This expression has the limiting form given by equation (3) for large η, and is of the form $e^2L^2\eta/3\pi\hbar^2v$ for small η.

If we take the harmonic mean of equation (10) (the inverse of the average resistivity) we get a result which is down by a factor $\tanh(2\eta L/\hbar v)$, and so is proportional to η^2 for small η. If $L\eta$ is held fixed as $L \to \infty$, both the mean and harmonic mean will diverge, as one expects for a system without scattering.

4. Scaling considerations

For the Schrödinger equation in a white noise potential the scaling of results is obvious. There are only two variables, the velocity v, and the localisation length λ (the distance over which the square of the wavefunction decays by a factor of e), which is identical with the mean free path for backward scattering (Thouless 1973) if the scattering is weak. We must have

$$\sigma(\mathrm{i}\eta) = (e^2\lambda/\pi\hbar)\, f(\lambda, \eta/\hbar v) \tag{13}$$

for dimensional reasons.

Far enough away from the band centre the tight-binding model with weak disorder

should correspond to the white noise problem. Indeed a numerical solution of the Schrödinger equation involves replacing the continuum problem by a discrete problem of the tight-binding form. The matrix element V corresponds to $\hbar^2/2ma^2$, and the strength of the white noise potential, the covariance of the potential at two points integrated over one of the points, corresponds to $a(E_i^2 - \bar{E}_i^2)$, the variance of the site energies multiplied by a. We denote the variance of the site energies by $W^2/12$, for consistency with numerical work on the Anderson model. The localisation length λ is given by

$$\lambda = 12\hbar^2 v^2/aW^2, \tag{14}$$

where v is given by equation (12), so the scaling form that should be expected for relatively weak disorder is

$$\sigma(\mathrm{i}\eta) = \frac{e^2}{\pi\hbar}\frac{12\hbar^2 v^2}{aW^2} f\left(\frac{12\hbar v\eta}{aW^2}\right). \tag{15}$$

If the Drude formula, equation (3), were accurate, then $f(x)$ would be

$$f(x) = 2/(1 + 2x). \tag{16}$$

Near the unperturbed band edge there is a maximum in the density of states, the remains of the inverse square root singularity. Because this is a region of strong scattering the velocity and localisation length are no longer appropriate parameters. With $h^2/2m = Va^2$, $aW^2/12$ and η we can construct the dimensionless variable $144h^2\eta^3/2ma^2W^4$, and the scaling form that can be constructed from those variables that occur in the white noise problem at the band edge is

$$\sigma(\mathrm{i}\eta) = (e^2a/\pi\hbar)(12V^2/W^2)^{1/3}\, g[(144V/W^4)^{1/3}\eta]. \tag{17}$$

5. Numerical results

We used equation (7) to carry out an evaluation of the conductivity as a function of η under a wide range of conditions. Except in some cases described below, we have assumed the site energies E_j to be uniformly distributed between $\pm W/2$, so the variance is $W^2/12$. We have varied W/V between 0·25 and 3, with chain lengths N varying from 30 to 2×10^5, and with E varying from the band centre at 0 to the unperturbed band edge at $2V$. We calculated the mean and variance of the conductivity and of its reciprocal. The variances are particularly large for small values of η, but we have not made any systematic use of the results for the variances. Only a sample of the results we have obtained are reported in this paper.

Provided that the system is considerably longer than the localisation length λ given by equation (14), the results for the average conductivity as a function of η all look the same on a log–log plot. The only exceptions occur when η is comparable with the energy scale over which the density of states varies. We have used equation (15), with v given by equation (12), to rescale a wide selection of results for different values of E and W/V onto the same curve; $W = 1$ and $E = 0$ was taken to be the standard curve. This is shown in figure 1. The results for $E = 0$ lie a little above and to the left of the others, and a better fit is obtained if the scaling factor is changed for these by 10–15%. Otherwise the agreement with scaling is strikingly good. The function $f(x)$ tends to $1/x$ for large x, as it must, and is linear in x for small x, in agreement with equation (4); this shows that the AC conductivity $\sigma(\omega)$ tends to zero faster than ω as ω tends to zero. The

coefficient of x, which is related to the integral of $\sigma(\omega)/\omega^2$, is roughly 20. This coefficient is about 16 times smaller than that calculated by Berezinskii (1974). Since the conductivity is proportional to the square of the localisation length, this difference is consistent with a discrepancy of a factor of four in the localisation length as given by other Russian

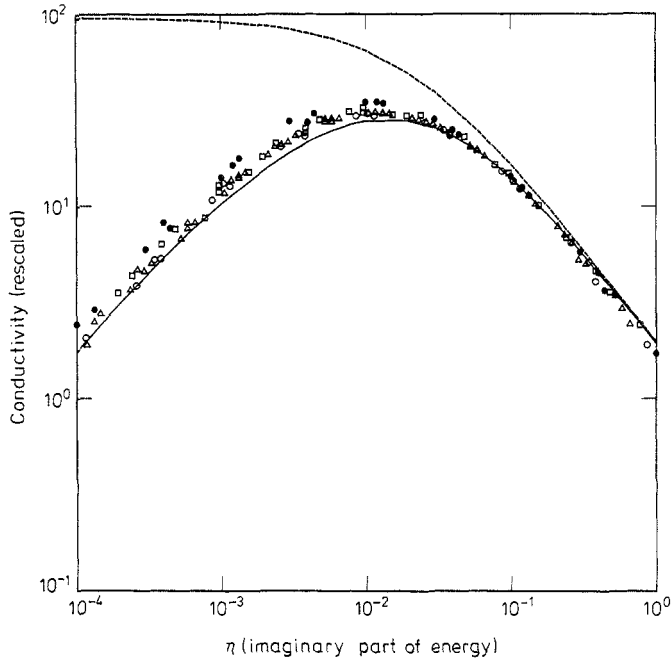

Figure 1. Conductivity, in units of $(e^2a/\pi\hbar)$, as a function of η, the imaginary frequency, for the tight-binding Anderson model with $W = V$, $E = 0$. The broken line indicates the Drude formula (16). Data for other values of W were rescaled onto those for $W = V$, following equation (12), by multiplying σ by $4W^2/V^2$ and η by (V/aW^2). Energies considered are $E = 0$ (dots), 1·0 V (circles), 1·5 V (triangles), and 1·75 V (squares). Values of W from 0·25 to 2·0 V were considered. Results from at least 100 chains of 10000 sites each are averaged for each data point. The full line indicates the phenomenological expression (18).

authors (Thouless 1979). The maximum of $\sigma(i\eta)$ is about $\frac{1}{3}$ of the DC conductivity in the Drude formula. A rough fit for the scaling function is given by taking

$$f(x) \approx [(x + \tfrac{1}{2})^{1/2} + x^{-1/2}/4{\cdot}5]^{-2}. \tag{18}$$

This agrees with the Drude formula for large η, and lies within 10% of our results for small η.

We expect some deviations from the scaling law when W/V is large, so that equations (12) and (14) are no longer valid, and when η is large enough that equation (2) is no longer valid, because the averaging implied by equation (1) covers a range of energies over which there is significant variation in the density of states. In fact the deviation of the large η points in figure 1 from the Drude curve is probably due to this smearing over energy. In the case $E = 2V$, at the unperturbed band edge, this effect is vital. Figure 2 shows the results for the average conductivity as a function of η for various values of W

rescaled to $W = 1$ by the scaling equation (17). Again the data fit well with the scaling theory. To the left of the maximum the curve is similar in shape to figure 1, but to the right it has a slope of 0·5 instead of 1, because for larger values of η the average is taken over a range of energy with substantial variations both of density of states and of conductivity.

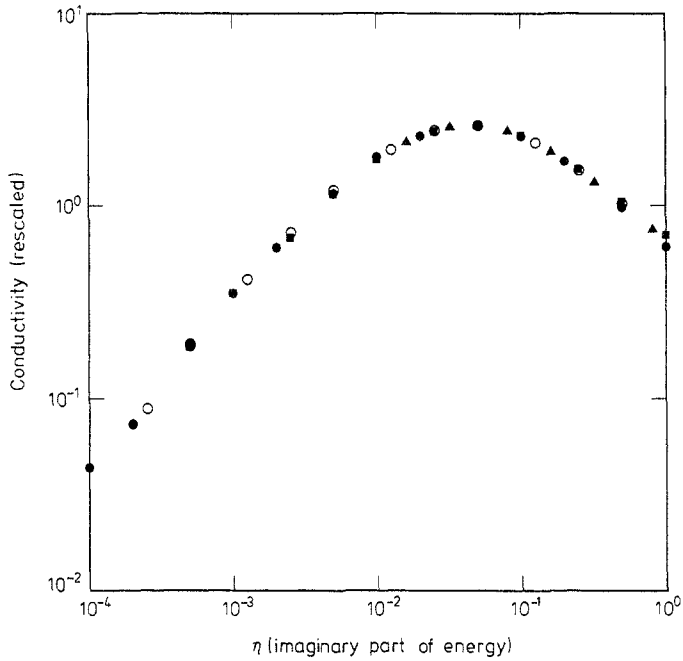

Figure 2. Conductivity as a function of η for $E = 2{\cdot}0\ V$, in the units of figure 1. Results for $W = 0{\cdot}3\ V$ (triangles), $0{\cdot}5\ V$ (squares) and $0{\cdot}7\ V$ (circles) were scaled to agree with the data for $W = V$ by using (17). Each point represents the average conductivity for 100 chains of 10000 sites each.

Several other bounded distributions were studied with results indistinguishable from those of figure 1. For example, in a model with site energies $E_i = W(x_i^2 - \frac{1}{2})$ and x_i uniformly distributed between 0 and 1, $\sigma(E - i\eta)$ could be mapped onto the Anderson model results using (15). The Cauchy distribution, generated by taking

$$E_i = (W/48)\tan(\pi x_i) \tag{19}$$

has infinite variance and requires a slightly different analysis. The localisation length for small W is given by (Hirota and Ishii 1971)

$$\lambda = 12a(4V^2 - E^2)^{1/2}/W. \tag{20}$$

For $W = 1, E = 0$, the same localisation length is obtained as in the Anderson model, but λ^{-1} varies linearly with W, rather than quadratically. We observe precisely this scaling of the conductivities, as demonstrated in figure 3. The peak in $f(x)$ is slightly sharper for the Cauchy distribution than for the distributions with finite variance, leading to larger values of σ at small η.

As the chain is shortened the conductivity is reduced. This is due to the reduction in mean free path by scattering from the ends of the chain. A typical sequence of results is shown in figure 4, for fixed W, E, and varying chain length L. To a first approximation the heights of the maxima can be understood by replacing λ by $\lambda L/(L + 2\lambda)$, but the peak becomes sharper as the chain becomes shorter, so the results cannot be fitted to the

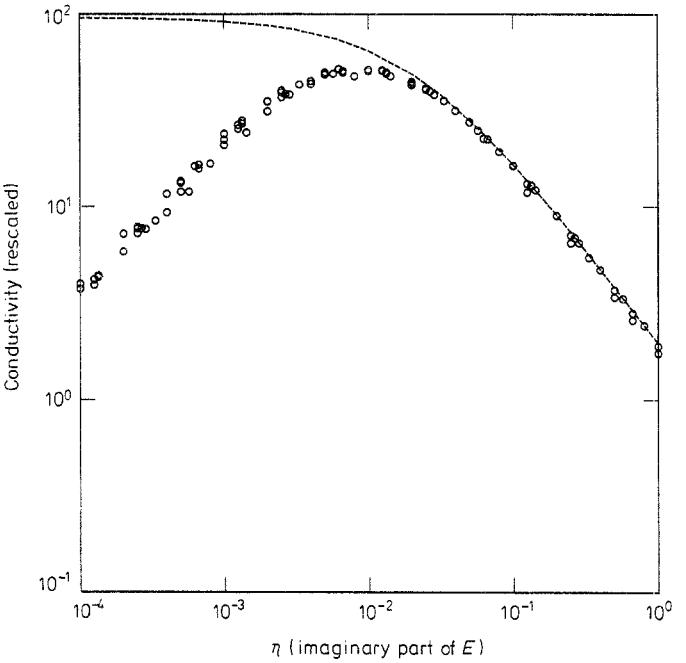

Figure 3. Average conductivity of 1D chains with a Cauchy distribution (19) of random site energies. Results for W = 0·25, 0·35, 0·5, 0·75, 1·5, 2·0, 4·0 and 8·0 V are rescaled by factors linear in W to agree with the $W = V$ data. Each point is the average over 90 samples of 10000 atoms each.

scaling law in this way. In fact the data shown for the shortest chain shown agrees well with equation (11) for the finite perfect chain, which is also shown in figure 4.

In figure 5 are shown some results for the resistivity—the average of the reciprocal of the conductivity—compared with the reciprocal of the average conductivity. Once η is less than the spacing between energy levels, which is $2\pi V/N$ in the band centre, the two curves diverge as expected, with the resistivity rising as η^{-2}.

6. Conclusions

Since all our results for the conductivity fit the same curve of the expected shape there is no reason to doubt that localisation occurs for the one-dimensional Anderson model in just the same way that it does for the white noise problem. Indeed, for the range of parameters we have explored, the results can be mapped onto the results for the white noise problem by a simple scaling transformation.

Some features of the results of Czycholl and Kramer (1979) can be understood from our calculations. For the larger values of W/V they were using values of η small enough to take them onto the low η side of the curve of $f(24V\eta/W^2)$. However, for the lowest value of W/V, equal to 0·6, they chose values of η that were only on the left side of the curve for short chains, and for long chains were on the right side, so that σ increased when η decreased. However we do not agree in detail with their results, and believe that either rounding errors or sampling errors occurred in their work.

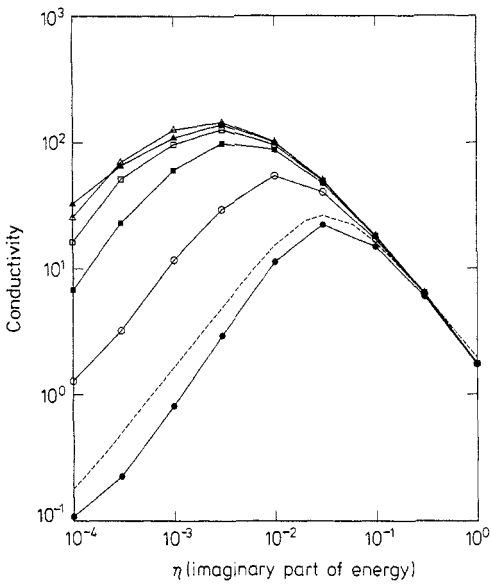

Figure 4. Length dependence of the chain conductivity as a function of η, in the Anderson models with $E = 0$ and $W = 0{\cdot}5\ V$. Chain lengths considered are: 100 sites (dots—1000 cases averaged); 300 sites (circles—600 cases); 1000 sites (squares—400 cases); 3000 sites (open squares —200 cases); 10000 sites (triangles—100 cases); 30000 sites (open triangles—40 cases). The results for the shortest chains ($L = 100$) lie slightly below the broken line representing the conductivity expected for an undisordered chain of the same length.

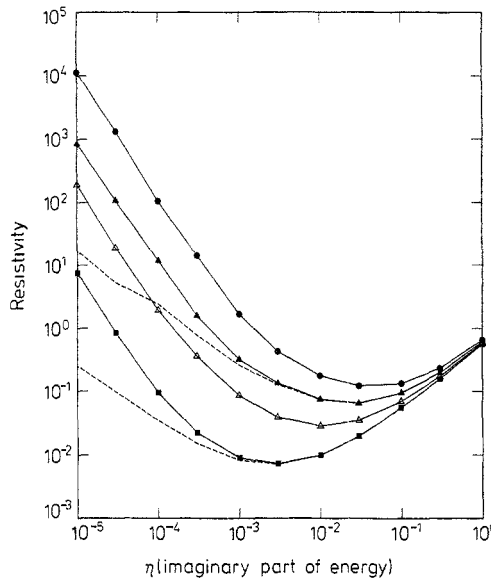

Figure 5. Average resistivity for Anderson model chains at $E = 0$, with $W = 2{\cdot}0\ V$ (dots). $1{\cdot}5\ V$ (triangles), V (open triangles), and $0{\cdot}5\ V$ (squares). The broken lines indicate the inverse of the averaged conductivity for the same parameters. Each data point represents an average over 200 samples of 10000 sites each, except that for $W = 0{\cdot}5\ V$, 300 samples with 20000 sites each were studies.

We have not succeeded in making a direct comparison of our results with those of Anderson *et al* (1980), since we consider the scaling of conductivity as a function of time, whereas they consider conductance as a function of length.

It would obviously be useful to extend this work to systems more than one atom in cross section, so that comparison with thin wire experiments can be made. We would then expect the part of the curve of $\sigma(i\eta)$ proportional to η to be scaled up by a factor of order of the number of atoms in the cross section, so that this part of the curve would meet the Drude formula at a lower value of η. The part of the curve proportional to η, which describes the effects of localisation, would then be separated from the part pro-

portional to η^{-1} by a flat portion of the curve which corresponds to DC metallic conductivity. A possible modification of equation (18) for a chain with A atoms in its cross section, so that the localisation length is of order $A\lambda$ is

$$f(x) \approx [(x + 1/2)^{1/2} + 1/(4{\cdot}5\, Ax^{1/2})]^{-2}. \tag{21}$$

and is plotted in figure 6.

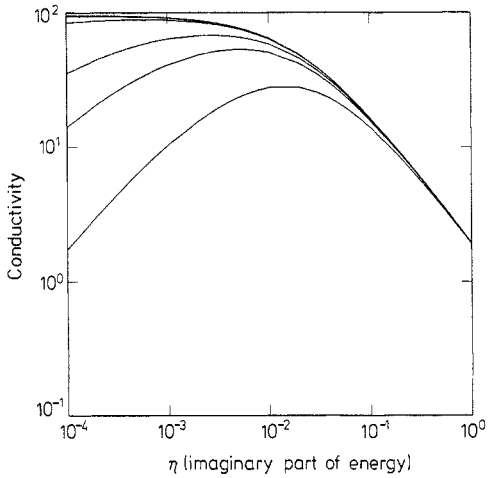

Figure 6. Proposed behaviour of the conductivity in chains of finite cross section, A, using equation (21). A = (bottom to top) 1, 4, 10, 100 and 1000 sites.

This agrees with the Drude formula for η large, is in rough numerical agreement with our results, and gives results for large A and small x in agreement with localisation theory (Thouless 1977, 1980).

Acknowledgments

This work was supported in part by NSF Grant No DMR-7908329.

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