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Electron localisation, Lyapunov exponents and the symmetric group

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Abstract. We use the theory of the symmetric group to construct a generalised transfer matrix from which we can obtain the Lyapunov exponents of the original transfer matrix and the localisation lengths for an electron in a random potential. We compare our results with those of numerical simulations. The generalised transfer matrix has infinite dimensions but can in practice be truncated to finite dimensions. In the limit of an infinite matrix the theory is exact.

1. Introduction

Anderson [1] was the first to show that the presence of disorder introduces not only a mean free path but also a second length scale, the localisation length, which describes the exponential decay in amplitude of localised electron wavefunctions. It is this second length scale that is relevant to the transport problem: when it is infinite the system is delocalised and particles diffuse in a semiclassical manner; when it is finite the system exhibits Anderson localisation.

In general there is a whole set of length scales associated with a system: as many as there are parallel channels. The inverses of these lengths are known as the Lyapunov exponents [2], which characterise the long-length behaviour of the system and are key quantities in a description of the statistics.

One-dimensional systems are relatively well understood. In two and three dimensions the key technique has been numerical simulations [3–5]. In these studies the Lyapunov exponents (or localisation lengths) are calculated for products of random matrices that describe systems of finite cross section. Extrapolation to fully two- and three-dimensional systems is accomplished using finite size scaling. The results are found to be consistent with some of the conclusions of the scaling theory of localisation [6, 7], but several puzzles still remain.

It is the purpose of this paper to introduce a more direct method for calculating all the Lyapunov exponents of a system, one that can be made as accurate as desired by diagonalising a larger matrix in much the same manner as band theory works with truncated secular equations.

The main difficulty confronting a more analytic approach to the problem is that a lack of translational symmetry prevents the use of Bloch's theorem. In this paper we

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continue work which show how to reintroduce symmetry into the problem. This method has already proved very successful in one dimension [8–10] and recently Pendry and Castaño have calculated the density of states for two- and three-dimensional disordered systems [11, 12] using these ideas. Here we show how to calculate the localisation lengths, which are more directly related to the electrical conductivity.

A quasi-one-dimensional disordered system can be studied by dividing it into layers. The scattering properties of a layer are described by a transfer matrix. Localisation effects due to multiple scattering then appear in the multiplication of the transfer matrices. Each transfer matrix will contain random elements corresponding to the disorder in each layer. We assume that the disorder in each layer obeys the same statistics. Using this 'statistical symmetry' we are able to make progress by using the theory of the symmetric group to define generalised transfer matrices. We then make an analytic continuation to obtain the Lyapunov exponents.

2. Symmetry reduction

In this and the following section we show how to use the theory of the symmetric group to obtain the Lyapunov exponents associated with a product of random matrices. Let

$$T_{L_z} = \prod_{n=1}^{L_z} M_n \tag{1}$$

where the M_n are independent, identically distributed random matrices. We calculate the Lyapunov exponents as follows. Let $|w_i\rangle$, $\langle w_i|$ $(i = 1, \ldots, p)$ be a set of orthogonal vectors. Then consider the determinant of the $p \times p$ matrix formed from the elements

$$\langle w_i | T_{L_z} | w_j \rangle \qquad (1 \leqslant [i, j] \leqslant p). \tag{2}$$

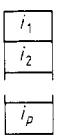
We define $D_p(T_{L_z})$ as the maximum over the set of determinants obtained by taking all distinct sets of p orthogonal vectors. We then obtain the sum of the p largest Lyapunov exponents Γ_p as [13]

$$\Gamma_p = \lim_{L_z \to \infty} (1/L_z) \langle \log |D_p(T_{L_z})| \rangle. \tag{3}$$

We expect our results to be independent of the representation of T_{L_z}. In the following we assume a convenient representation where $|w_i\rangle_j = \delta_{i,j}$, $1 \leqslant [i, j] \leqslant m$ and m is the dimension of T_{L_z}.

The first step in our symmetry analysis is to note that this set of determinants can be obtained as the diagonal elements of the antisymmetric projection of the direct product of T_{L_z} with itself p times. To obtain the projection we must first choose a basis for the antisymmetric subspace. A convenient basis for our purposes can be most easily defined by vertical Young tableaux.

Let $i_1, \ldots, i_p$ be a set of strictly increasing integers



$$1 \leqslant i_1 < i_2 < \ldots < i_p \leqslant m. \tag{4}$$

The vector defined by this tableau has components

$$|u(i_1 \ldots i_p)\rangle_{j_1 \ldots j_p} = \begin{cases} \dfrac{1}{\sqrt{p!}} & j_1 \ldots j_p \text{ an even permutation of } i_1 \ldots i_p \\ \dfrac{-1}{\sqrt{p!}} & j_1 \ldots j_p \text{ an odd permutation of } i_1 \ldots i_p \\ 0 & \text{otherwise} \end{cases} \tag{5}$$

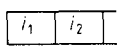
and $\langle u(i_1 \ldots i_p)|$ has the same components. We can write this projection as a matrix $Y_p(T_{L_z})$, with elements

$$\langle u(i_1 \ldots i_p)|T_{L_z} \otimes \ldots \otimes T_{L_z} \ (p \text{ times})|u(j_1 \ldots j_p)\rangle. \tag{6}$$

$D_p(T_{L_z})$ is now the maximum over the diagonal elements of Y_p. Noting that $T_{L_z} \otimes \ldots \otimes T_{L_z}$ (p times) maps the antisymmetric subspace onto itself we can immediately write

$$Y_p(T_{L_z}) = \prod_{n=1}^{L_z} Y_p(M_n). \tag{7}$$

Now consider the direct product of Y_p with itself N times and its projection onto the symmetric subspace. We define a basis for the symmetric subspace using horizontal tableaux:



$$1 \leqslant i_1 \ldots \leqslant i_N \leqslant y \tag{8}$$

where y is the dimension of Y_p. The vector defined by this tableau has components

$$|v(i_1) \ldots i_N)\rangle_{j_1 \ldots j_N} = \begin{cases} \prod \dfrac{\sqrt{l_i!}}{\sqrt{N!}} & j_1 \ldots j_N \text{ a permutation of } i_1 \ldots i_N \\ 0 & \text{otherwise} \end{cases} \tag{9}$$

where l_i ($i = 1, \ldots, y$) is the number of i's in $i_1, \ldots, i_N$, and $\langle v(i_1 \ldots i_N)|$ has the same components. We can thus label each vector in this basis by a set of y positive integers $l_1, \ldots, l_y$ which satisfy

$$\sum_{i=1}^{y} l_i = N. \tag{10}$$

We can now write the projection onto the symmetric subspace, $X(N, Y)$, as

$$X(N, Y)(l_1 \ldots l_y : k_1 \ldots k_y) = \langle v(l_i)|Y \otimes \ldots \otimes Y(N \text{ times})|v(k_i)\rangle$$

$$= \left(\prod_i \sqrt{(l_i!\, k_i!)}\right) \sum_{\{p_{i,j}\}} \prod_{i,j} Y_{i,j}{}^{p_{i,j}} \frac{1}{p_{i,j}} \tag{11}$$

where the sum is over the set of y^2 positive integers $p_{i,j}$ satisfying

$$\sum_{j=1}^{y} p_{i,j} = l_i \qquad \sum_{i=1}^{y} p_{i,j} = k_j$$
$$\sum_{i,j=1}^{y} p_{i,j} = N. \tag{12}$$

The symmetric projection contains D_p^N as the maximum over a subset of diagonal elements, since

$$X(N, Y_p)(l_j = N\delta_{j,i} : k_j = N\delta_{j,i}) = [Y_p]_{i,i}^N. \tag{13}$$

Again noting that $Y \otimes \ldots \otimes Y$ (N times) preserves the symmetric subspace, we see that X has the multiplicative property that

$$X(N, Y_p(T_{L_z})) = \prod_{n=1}^{L_z} X(N, Y_p(M_n)). \tag{14a}$$

This allows us to think of X as a generalised transfer matrix.

The value of the symmetry reduction becomes apparent when we average over the disorder or randomness in M_n

$$\overline{X(N, Y_p(T_{L_z}))} = \overline{X(N, Y_p(M))}^{L_z} \tag{14b}$$

making use of the 'statistical symmetry' mentioned earlier. The problem is then reduced to the consideration of a product of L_z identical matrices.

The main problem with the above analysis is that N is restricted to positive integer values or zero. To make progress we need an analytic continuation for N non-integer. We can then evaluate Γ_p as

$$\Gamma_p = \lim_{L_z \to \infty} \mathrm{Re}\left(\frac{1}{L_z}\frac{\mathrm{d}}{\mathrm{d}N}\overline{D_p(T_{L_z})^N}\right)\Bigg|_{N=0}. \tag{15}$$

3. Analytic continuation

Pendry and Castaño [11, 12] and Kirkman and Pendry [8] have shown how we can analytically continue in N to allow us to define $X(N)$ when N is non-integer. We outline their method below.

Suppose that the (1–1) element is the diagonal element of Y_p with largest modulus (the following is easily generalised to other cases) so that $[Y_p T_{L_z})]_{1,1} = D_p(T_{L_z})$. Let

$$L = l_2 + \ldots + l_y \qquad K = k_2 + \ldots + k_y \tag{16}$$

then we order X so that

$$X(N) = \begin{array}{c} \\ L=0 \\ \\ L=N \end{array} \begin{array}{c} \begin{array}{cc} K=0 & \qquad\qquad K=N \end{array} \\ \begin{bmatrix} & \\ & X(l_i : k_i) \\ & \end{bmatrix} \end{array}. \tag{17}$$

Then

$$D_p(T_{L_z})^N = \langle s|X(N, Y_p(T_{L_z}))|s\rangle \tag{18}$$

where $|s\rangle$ has components $|s\rangle_j = \delta_{j,1}$ and $\langle s|$ has the same components.

So far N is integer and $X(N)$ is finite in size but not necessrily $(N+1)\times(N+1)$ (unless Y is 2×2). This is because for given values of L and K there are in general multiple solutions of (16) for $l_2 \ldots l_y$ and $k_2 \ldots k_y$, each pair of which gives a different matrix element of X.

When N is non-integer we retain (11) for the matrix elements of our new continued X matrix but allow l_1 and k_1 to be non-integer

$$l_1 = N - L \qquad k_1 = N - K \tag{19}$$

and order X as before but now allowing L and K to take any values in the range zero to infinity. This makes X infinite in size. In performing the summation in (11) we sum over all solutions to (12) with p_{11} non-integer but all the other ps positive integers before, so that

$$p_{11} = N - \sum{}' p_{i,j} \tag{20}$$

where Σ' denotes the sum over all ps except p_{11}. The only non-integer factorials appear as a ratio and are easily evaluated as

$$l_1!/p_{11}! = \begin{cases} (n-L)(N-L-1)\ldots(N-L-l_1+p_{11}+1) \\ 1 \qquad \text{if} \quad l_1 = p_{11} \end{cases} \tag{21}$$

and similarly $k_1!$.

So how does the new 'continued' X matrix relate to the previous X matrix when N is a positive integer? The answer is that it is block diagonal

$$X(n) = \begin{array}{c} \\ L=0 \\ \\ \\ L=\infty \end{array} \begin{array}{c} \begin{array}{cc} K=0 & \qquad K=\infty \end{array} \\ \left[\begin{array}{c|c} \begin{array}{l} 0 \leqslant L \leqslant N \\ 0 \leqslant K \leqslant N \end{array} & 0 \\ \hline 0 & L, K > N \end{array}\right] \end{array} . \tag{22}$$

The $0 \leqslant L, K \leqslant N$ block is identical to the previous X matrix at integer N. This means that (18) is automatically valid for the new X matrix. That the continuation is correct and that (18) is valid for non-integer N is argued in more depth in [8]. Ultimately we check the continuation by comparison with published results obtained by alternative methods and indeed excellent agreement is obtained [7–11].

We can obtain a more explicit expression for Γ_p by writing

$$\overline{X(N, Y_p(T_{L_z}))} = \sum_{i=0}^{\infty} \mu_i(N)^{L_z} |N, i\rangle\langle i, N| \tag{23}$$

where $\mu_i(N)$ are the eigenvalues and $|N, i\rangle$, $\langle i, N|$ the right and left eigenvectors of $\overline{X(N, Y_p(M))}$. We now substitute (23) into (18), differentiate with respect to N and note

that $|s\rangle$ and $\langle s|$ are eigenvectors of $X(N=0)$ with eigenvalue unity. If we denote this eigenvalue as $\mu_0(N=0)$ then

$$\Gamma_p = \mathrm{Re}\left(\frac{\mathrm{d}}{\mathrm{d}N}\mu_0(N)\right)\Big|_{N=0}. \tag{24}$$

We can write (24) in a more transparent form by defining a matrix $Z(N, Y)$

$$X(N, Y) = Y_{1,1}^{N} Z(N, Y). \tag{25}$$

Near $N = 0$ we can then write

$$\overline{X(N, Y)} = \overline{Z(N, Y)} + N\,\overline{\ln Y_{11} Z(N, Y)} + \mathrm{O}(N^2). \tag{26}$$

We now use perturbation theory, exact in the limit of small N, to obtain an expansion in powers of N for $\mu_0(N)$, then with reference to (24) we obtain

$$\Gamma_p = \overline{\ln Y_{11}} + \left(\frac{\mathrm{d}}{\mathrm{d}N}\alpha_0(N)\right)\Big|_{n=0} \tag{27}$$

where $\alpha_0(N)$ is the relevant eigenvalue of $\overline{Z(N, Y)}$. Thus our result is that Γ_p is equal to a 'zero-order' estimate plus a correction term.

To generalise to other cases we simply note that if $[Y_p]_{i,i}$ is the maximal diagonal element of Y_p we allow only l_i, k_i and p_{ii} non-integer and set

$$L = l_1 + \ldots + l_{i-1} + l_{i+1} + \ldots l_y \tag{28}$$

are similarly for K.

4. Application to electron localisation

To apply the method to the problem of electron localisation in a random potential we use the usual Anderson model with random site energies (diagonal disorder.) For simplicity we assume a two-dimensional geometry with L_y atoms per layer. Then M_n is a $2L_y \times 2L_y$ matrix

$$M_n = \begin{bmatrix} H_n & -1 \\ I & 0 \end{bmatrix} \tag{29}$$

and H_n is an $L_y \times L_y$ matrix with elements

$$[H_n]_{i,j} = (E - \varepsilon_{n,i})\delta_{i,j} + \beta V \delta_{i,j\pm 1}. \tag{30}$$

Here $\varepsilon_{n,i}$ is the site energy of the ith atom in the nth layer and β is the ratio of the constant hopping matrix elements within a layer to between layers. 'Statistical symmetry' corresponds to the ε's being independently and identically distributed. Before applying the symmetry analysis we transform from a real-space representation to a momentum-space representation

$$M_n \rightarrow Q M_n Q^{-1} \tag{31}$$

where Q and Q^{-1} are the matrices of left and right eigenvectors of M. In the limit of zero disorder this transformation diagonalises Z (and also X)

$$Z(N, Y)(l_i : k_i) = Y_{11}^{-L} \prod_{i=2}^{y} Y_{i,i}{}^{l_i} \delta_{l_i,k_i} \tag{32}$$

and L is given by (16).

We now apply perturbation theory to obtain Γ_p for weak disorder. If we have

$$Y_{11}^{L} \neq \prod_{i=2}^{y} Y_{i,i}{}^{l_i} \tag{33}$$

for any $l_2 \ldots l_y$ satisfying (16), we may apply non-degenerate perturbation theory to order $\langle \varepsilon^2 \rangle$ to obtain $\alpha_0(N) = 1$. So under this condition we have

$$\Gamma_p = \operatorname{Re} \overline{\ln(D_p(M))}. \tag{34}$$

If we expand the logarithm to order $\langle \varepsilon^2 \rangle$ this agrees with the perturbation theory calculations of Derrida *et al* [13] and Slevin [14]. The condition (33) is in general slightly less restrictive than that given in [13].

When condition (33) is not satisfied we must use degenerate perturbation theory. This is a considerable complication. Recently however, Zannon and Derrida [15] have made progress in developing weak disorder expansions for degenerate cases.

5. Numerical results

To go beyond perturbation theory we diagonalise the X matrix, or equivalently the Z matrix, numerically. The simplest non-trivial case to which we can apply the theory is that of a quasi-one-dimensional system with two atoms per layer. For such a system M_n is a 4×4 matrix and H_n has the form

$$H_n = \begin{bmatrix} E - \varepsilon_{n,1} & 2\beta \\ 2\beta & E - \varepsilon_{n,2} \end{bmatrix} \tag{35}$$

and we assume periodic boundary conditions in the transverse direction. We use a binary alloy distribution for the εs

$$p(\varepsilon) = \tfrac{1}{2}\delta(\varepsilon - \tfrac{1}{2}W) + \tfrac{1}{2}\delta(\varepsilon + \tfrac{1}{2}W) \tag{36}$$

and we transform to a momentum representation using

$$Q^{-1} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & -1 & 1 \\ \exp(-i\varphi_1) & \exp(-i\varphi_2) & \exp(i\varphi_2) & \exp(i\varphi_1) \\ \exp(-i\varphi_1) & -\exp(-i\varphi_2) & -\exp(i\varphi_2) & \exp(i\varphi_1) \end{bmatrix} \tag{37a}$$

where

$$E - E_c - 2\beta \cos q_i = 2 \cos \varphi_i \tag{37b}$$

with $q_1 = 0$ and $q_2 = \pi$. E_c is set non-zero to avoid Q becoming singular at the band edges of the pure system. It should be noted that with E_c non-zero neither Z nor X is diagonal for zero disorder. We set $\beta = 1$.

Table 1

Order X	Size $X(Y_p)$ $p = 1, 3$		Size $X(Y_2)$	
0	1	(1)	1	(1)
1	4	(2)	6	(4)
2	10	(6)	21	(13)
3	20	(10)	56	(32)
4	35	(19)	111	(70)
5	56	(28)	—	—
6	84	(44)	—	—
7	120	(60)	—	—

After analytical continuation X is infinite in size. To proceed with numerical calculations we must make an approximation by truncating X to a finite size. To do this we set a maximum value for L and K, which we call the order of the X matrix. We can then diagonalise the matrix numerically and see how μ_0 changes with order. In table 1 we show how the truncation size increases with order for the case where the M_n are 4×4 matrices and we are calculating Γ_p with $p = 1, 2, 3$. We are able to make a reduction in the truncation size by noticing that after averaging the X matrix is block diagonal. It can be shown that when $p = 1$ or 3 it is only necessary to include elements of $X(Y_p)$ for which

$$l_2 + l_3 = k_2 + k_3. \tag{38}$$

When $p = 2$ we need only include elements of $X(Y_2)$ for which

$$l_3 + l_4 = k_3 + k_4. \tag{39}$$

This corresponds to the figures in parentheses in table 1. In general we find that μ_0 converges quickly and in the following calculations we used a maximum order of 4 for Γ_2 and 5 for Γ_1 and Γ_3. Convergence is slowest near $E = 0$. To obtain the maximum exponent, equal to Γ_1, we need only carry out the symmetric projection as Y_1 is the usual transfer matrix. For $E < 0$ we allow p_{11} non-integer and for $E > 0$ we allow p_{22} non-integer.

To obtain Γ_2, the sum of the two largest exponents, we take the antisymmetric projection of $M \otimes M$ with respect to the basis vectors defined by the tableaux

$$\begin{array}{|c|}\hline 1 \\ \hline 2 \\ \hline \end{array} \quad \begin{array}{|c|}\hline 1 \\ \hline 3 \\ \hline \end{array} \quad \begin{array}{|c|}\hline 1 \\ \hline 4 \\ \hline \end{array} \quad \begin{array}{|c|}\hline 2 \\ \hline 3 \\ \hline \end{array} \quad \begin{array}{|c|}\hline 2 \\ \hline 4 \\ \hline \end{array} \quad \begin{array}{|c|}\hline 3 \\ \hline 4 \\ \hline \end{array} \tag{40}$$

Y_2 is a 6×6 matrix and we continue p_{11} at all energies. The smallest positive exponent is found as $\Gamma_2 - \Gamma_1$. This gives the longest localisation length, the length relevant to transport properties. In this case Γ_2 is also the sum of all positive Lyapunov exponents and so the integrated density of states $I(E)$ can be found from its imaginary part. This is developed by Pendry and Castaño [11, 12].

Our results for various values of the disorder parameter W are plotted against results from a numerical simulation provided by A MacKinnon in figures 1–3. Comparison of our results with those of the numerical simulation show good agreement except near $E = 0$. The error arises in the most part from the calculation of the largest exponent, as can be seen by reference to figure 4, where good agreement is obtained for Γ_2 at all energies.

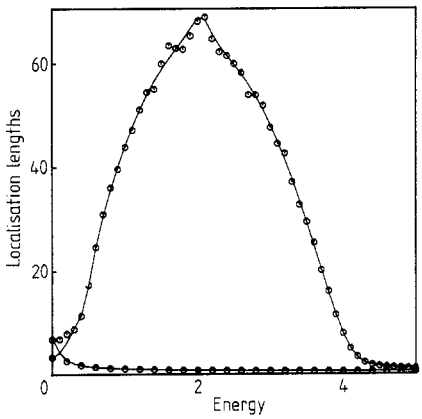


Figure 1. Comparison of localisation lengths obtained from the symmetry reduction (full curves) and numerical simulation (symbols) for disorder $W = 1$. The disagreement near $E = 0$ is discussed in the text.

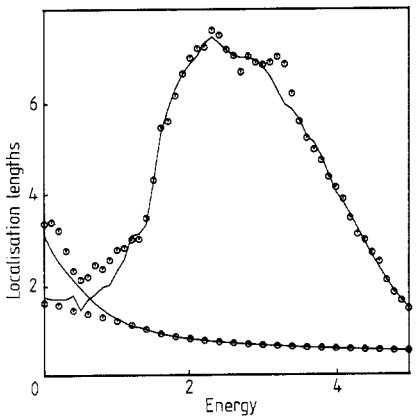


Figure 2. Comparison of localisation lengths obtained from the symmetry reduction (full curves) and numerical simulation (symbols) for disorder $W = 3$.

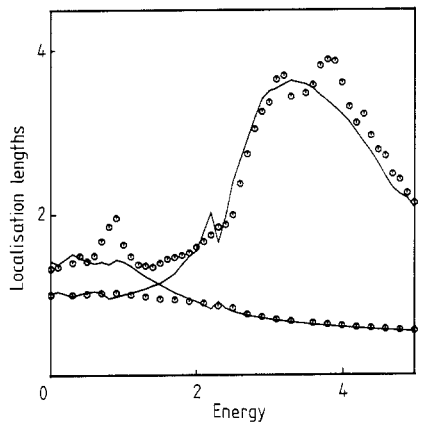


Figure 3. Comparison of localisation lengths obtained from the symmetry reduction (full curves) and numerical simulation (symbols) for disorder $W = 5$.

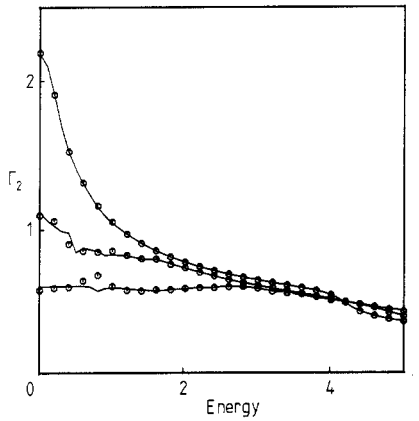


Figure 4. Γ_2 is given correctly at all energies, showing that error in the localisation lengths near $E = 0$ arises for the most part in Γ_1.

So what is going wrong near $E = 0$? One suggestion is a breakdown in the validity of expression (3) for Γ_p. We have been able to rule this out by direct evaluation of (3) using a numerical simulation. To check our theory further, and also equation (3), we note that because T_L is symplectic, Γ_3 is also equal to the largest exponent. We take the antisymmetric projection of $M \otimes M \otimes M$ with respect to the basis

$$\begin{array}{|c|}\hline 1\\\hline 2\\\hline 3\\\hline\end{array}\quad\begin{array}{|c|}\hline 1\\\hline 2\\\hline 4\\\hline\end{array}\quad\begin{array}{|c|}\hline 1\\\hline 3\\\hline 4\\\hline\end{array}\quad\begin{array}{|c|}\hline 2\\\hline 3\\\hline 4\\\hline\end{array} \tag{41}$$

so Y_3 is a 4×4 matrix and we allow p_{11} non-integer for $E < 0$ and p_{22} for $E > 0$. This gives the same results as obtained by calculating Γ_1, with the same problem near $E = 0$.

This seems to leave two further possibilities. The first is that the apparent convergence of our results near $E = 0$ is deceptive. This is a possibility as the zero disorder matrix is highly degenerate at $E = 0$ for the case $L_y = 2$. Another possibility is that there is some form of symmetry breaking which invalidates the analytic continuation near $E = 0$. This would seem very puzzling in view of the accuracy of our results for Γ_2 at all energies, and for Γ_1 and Γ_3 at other energies.

6. Conclusions

We have applied a symmetry analysis and made an analytic continuation to obtain the localisation lengths for an electron in a disordered system. We obtain excellent agreement except in the cases indicated.

Acknowledgments

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