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Transfer matrices and conductivity in two- and three-dimensional systems: I. Formalism

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Abstract. The electronic states responsible for transport constitute a wildly fluctuating minority of the total number of states in a disordered system. These fluctuations are the essence of the problem and demand a rich and powerful formulation if they are to be described accurately. In this paper we introduce a new formalism for treating transport in three-dimensional systems based on the transfer matrix. The method gains its power from the interplay of theory of the symmetric group, which enables irrelevant parts of the mathematics to be thrown out, leaving the essentials intact but simplified. Analogies with replica theory are drawn, and replica symmetry breaking discussed.

1. Introduction

It is the aim of this paper to introduce a formalism for the systematic study of transport properties of disordered systems, using a transfer matrix formulation.

Electronic properties of ordered systems are understood in exhaustive detail. Not only can we understand all the structure and singularities in the densities of states, but also the quantitative study of ordered solids is on a sound footing: spectroscopic studies can be interpreted, and densities of states can be used to calculate total energies and to predict structural arrangement of atoms. All this immense progress is due to the application of group theory in the form of Bloch's theorem, which offers us a complete classification of the electronic states.

If we study electronic transport, that is to say the conductivity of a solid, then either the solid is ordered and the problem is trivial (ordered solids have no electrical resistivity) or the solid disordered, group theory goes out of the window and the theory becomes an unclassified mess. In this paper we show that group theory is still able to help even in the case of disorder, and that a systemic non-perturbative formulation of the problem can be made in terms of a generalisation of the transfer matrices that are used to calculate the band structure of ordered solids.

That is not to deny that progress has been made with the problem. Weakly disordered systems have been investigated by perturbation theory, revealing structure not suspected before in the form of the mesoscopic fluctuations (Stone 1985, Imry 1986). Strong disorder can be addressed by scaling theory (Abrahams *et al* 1979) to investigate the nature of the singularity in conductivity at the mobility edge; or by renormalisation-group techniques (Wegner 1979). Yet another approach has been the application of random matrix theory (Muttalib *et al* 1987, Mello 1988, Zanon and Pichard 1988).

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Powerful and imaginative as these approaches have been, they all demand a physical input in the form of postulates as to the nature of the solution. It is clear from numerical simulations that the rich structure induced in the electron wavefield by disorder goes far beyond what we have been able to classify to date: much remains to be understood. For example, scaling theory suggests that near a mobility edge at E_c the conductance vanishes linearly as

$$G = \text{const}(E - E_c).$$

Yet numerical simulations (MacKinnon and Kramer 1983, Schreiber and Kramer 1989) have so far failed to confirm this result. The whole source of the complication is the nature of fluctuations in the wavefield, which obey an extreme form of statistics and actually get more extreme as the system gets larger. In the case of the conductance in one dimension the current is carried by classes of states that form a vanishing minority of the total number of states (Pendry 1987). Worse still, there is not just one class, but a whole set of them, and which is most effective depends on the circumstances.

Mathematically this is reflected in the fact that a quite different formulation has to be made of the conductivity problem from the one used in calculating density of states; see Kirkman and Pendry (1984a, b) for an explicit demonstration in the 1D case. Transfer matrices have found extensive application to 1D problems (Landauer 1957, 1970, Erdos and Herndon 1982, Pendry 1982) and more recently have been generalised to handle questions concerning correlations in the conductivity of 1D systems.

The idea of a transfer matrix is a simple one; the system is divided into subunits, individual atoms for a 1D systems, planes of atoms for a 3D system. The transfer matrix $\mathbf{T}_n$ for the nth subunit is a function of the elementary properties of the subunit, namely the reflection and transmission coefficients, r_n and t_n, i.e.

$$\mathbf{T}_n = \begin{bmatrix} 1/t_n^* & r_n^*/t_n^* \\ r_n/t_n & 1/t_n \end{bmatrix}. \tag{1}$$

All transfer matrices obey the fundamental theorem, which states that we can construct the transfer matrix for a whole set of L subunits by multiplying together the individual transfer matrices in the correct order, i.e.

$$\mathbf{T}_L = \prod_{n=1}^{L} \mathbf{T}_n \tag{2}$$

where $\mathbf{T}_L$ is the same function of the reflection and transmission coefficients of the complete unit,

$$\mathbf{T}_L = \begin{bmatrix} 1/t_L^* & r_L^*/t_L^* \\ r_L/t_L & 1/t_L \end{bmatrix}. \tag{3}$$

They have one great and overriding virtue, which is that they can be averaged very easily provided that the subunits are statistically independent,

$$\bar{\mathbf{T}}_L = \prod_{n=1}^{L} \bar{\mathbf{T}}_n. \tag{4}$$

There are many other formalisms that give expressions for transmission and reflection, but none exhibits the same simplicity of the averaging process. Why, then, have transfer matrices not solved every question of transport in disordered systems? Because not all

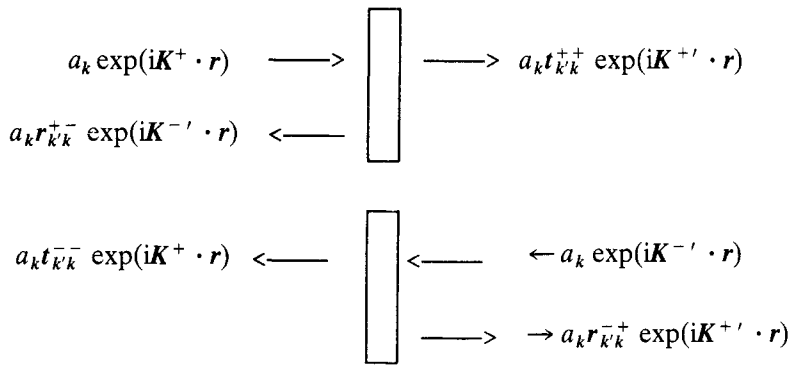


Figure 1. A layer of atoms has scattering properties given by transmission and reflection matrices describing how waves incident from the left or the right scatter into a set of reflected and transmitted beams. Lower-case $\boldsymbol{k}$ is used to label the component of wavevector parallel to the layer, whereas capital $\boldsymbol{K}^{\pm}$ includes a component normal to the layer with sign appropriate to the direction of the wave.

quantities of interest are easily expressed in terms of transfer matrices. The interest in knowing the average of $1/t_L$ is decidedly limited.

Progress was made when it was discovered that transfer matrices could be generalised through the direct products of the elementary $\mathbf{T}_n$ (Pendry 1982). Application of the ideas of the symmetric group enabled questions such as 'What is the average of $|t|^2$?' to be formulated in terms of a transfer matrix. These ideas have solved the problem of finding the distribution of $|t|^2$ for arbitrarily large disorder in 1D systems Kirkman and Pendry 1984a, b).

The method of treatment in 1D does not generalise in a trivial way to higher dimensions; for one thing the transmission and reflection coefficients become non-commuting matrices. Part of the problem was addressed in an earlier paper where we showed how to calculate the density of states in a 2D or 3D disordered system. In this paper we extend the formalism to the transmission and reflection coefficients themselves and hence to the conductivity. First, we shall give the general form of higher-dimensional transfer matrices and a few theorems about them. Then the generalised form of the transfer matrix and its symmetrisation is introduced. Next it is shown how transmission and reflection matrices can be extracted from this generalised form, and some general properties are discussed.

2. Transfer matrices in higher dimensions

The elementary transfer matrix is easily obtained by arguments similar to the 1D case. Consider a layer of atoms; figure 1 defines the transmission and reflection properties. The different beams are distinguished by their momentum parallel to the layer, $\boldsymbol{k} = (\boldsymbol{k}_x, \boldsymbol{k}_y)$, which together with the energy defines the momentum normal to the layer, $\pm\boldsymbol{K}_z$. Thus the complete wavevector is

$$\boldsymbol{K}^{\pm} = (\boldsymbol{k}_x, \boldsymbol{k}_y, \pm\boldsymbol{K}_z). \tag{5}$$

We assume that the z component of the wavevector is always real. This simplifies the

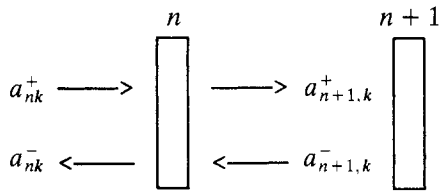


Figure 2. Wave amplitudes around two layers are shown. The self-consistent scattering equations can be used to construct a transfer matrix.

notation, which would otherwise need to distinguish between real and imaginary K_z. The generalisation is straightforward but tedious.

Another important point in defining transmission and reflection matrices is the choice of origin with respect to which the incident and reflected waves are referred. One natural choice is the centre of the scattering layer, but this is not the choice we make here. Instead, different origins are chosen for the waves on the left and right. This choice has the virtue that when several layers are being stacked together we can choose the same origin for waves in between layers 1 and 2. Otherwise our formulae would need to contain a clumsy shift of origin when waves emerging from layer 1 subsequently scatter from layer 2.

The 2D case can be deduced by a trivial specialisation of the formulae.

It is easy to show that these matrices possess some symmetries due to current conservation:

$$\sum_{k''} [V_{k''z}/(V_{zk}V_{zk'})^{1/2}]t^{++}_{k''k'}{}^{*}\, t^{++}_{k''k} + r^{-+}_{k''k'}{}^{*}\, r^{-+}_{k''k} = \delta_{kk'} \tag{6a}$$

$$\sum_{k''} [V_{k''z}/(V_{zk}V_{zk'})^{1/2}]t^{-+}_{k''k'}{}^{*}\, t^{-+}_{k''k} + r^{+-}_{k''k'}{}^{*}\, r^{+-}_{k''k} = \delta_{kk'} \tag{6b}$$

where V_{kz} is the z-component of the group velocity of the kth wave. Note that each of the pairs of matrix products on the left-hand side must commute.

Time reversal gives some more symmetry:

$$\delta_{kk'} = \sum_{k''} (t^{--}_{-k-k''}t^{++}_{k''k}{}^{*} + r^{-+}_{-k-k''}r^{-+}_{k''k}{}^{*}) \tag{7a}$$

$$0 = \sum_{k''} (r^{+-}_{-k-k''}t^{++}_{k''k}{}^{*} + t^{++}_{-k-k''}r^{-+}_{k''k}{}^{*}) \tag{7b}$$

and

$$\delta_{kk'} = \sum_{k''} (t^{++}_{-k-k''}t^{--}_{k''k}{}^{*} + r^{+-}_{-k-k''}r^{+-}_{k''k}{}^{*}) \tag{8a}$$

$$0 = \sum_{k''} (r^{-+}_{-k-k''}t^{--}_{k''k}{}^{*} + t^{--}_{-k-k''}r^{+-}_{k''k}{}^{*}). \tag{8b}$$

We are now in a position to define the transfer matrix. Figure 2 shows waves incident on the nth layer.

The transmission and reflection matrices give us two equations for the amplitudes:

$$a^{+}_{n+1,k} = \sum_{k'} t^{++}_{kk'} a^{+}_{nk'} + r^{+-}_{kk'} a^{-}_{n+1,k'} \tag{9a}$$

$$a^{-}_{nk} = \sum_{k'} r^{-+}_{kk'} a^{+}_{nk'} + t^{--}_{kk'} a^{-}_{n+1,k'}. \tag{9b}$$

These two equations can be written as a single composite matrix equation of twice the size, i.e.

$$\begin{bmatrix} 1 & -r^{+-} \\ 0 & -t^{--} \end{bmatrix} \begin{bmatrix} a^{+}_{n+1} \\ a^{-}_{n+1} \end{bmatrix} = \begin{bmatrix} t^{++} & 0 \\ r^{-+} & -1 \end{bmatrix} \begin{bmatrix} a^{+}_{n} \\ a^{-}_{n} \end{bmatrix}. \tag{10}$$

Inverting this matrix gives

$$\begin{bmatrix} a^{+}_{n+1} \\ a^{-}_{n+1} \end{bmatrix} = \mathbf{T} \begin{bmatrix} a^{+}_{n} \\ a^{-}_{n} \end{bmatrix} \tag{11}$$

where the transfer matrix is defined by

$$\mathbf{T} = \begin{bmatrix} t^{++} - r^{+-}(t^{--})^{-1} r^{-+} & +r^{+-}(t^{--})^{-1} \\ -(t^{--})^{-1} r^{-+} & (t^{--})^{-1} \end{bmatrix}. \tag{12}$$

Making use of the time-reversal symmetry given in equations (7) and (8),

$$(t^{--*})^{-1}_{-k-k'} = t^{++}_{kk'} - \sum_{k''k'''} r^{+-}_{kk''} (t^{--})^{-1}_{k''k'''} r^{-+}_{k'''k'} \tag{13a}$$

$$\sum_{k'} (t^{--*})^{-1}_{-k-k''} r^{+-*}_{-k''-k'} = -\sum_{k'} r^{+-}_{kk''} (t^{--})^{-1}_{k''k'} \tag{13b}$$

the transfer matrix can be re-expressed as

$$\mathbf{T} = \begin{bmatrix} [(t^{*})^{-1}]_{-k-k'} & [(t^{*})^{-1} r^{*}]_{-k-k'} \\ [-(t)^{-1} r]_{kk'} & [(t)^{-1}]_{kk'} \end{bmatrix}. \tag{14}$$

We have dropped the superscripts on t and r since they are now redundant.

3. The story so far

In an earlier paper (Pendry and Castano 1988) several important results were derived, which we shall need. In this section we state these results without proof. The reader is referred to the original paper for details, and to Hammermesh (1962) or Littlewood (1950) for proofs of the group-theoretical results.

In that paper we showed how $\det(t)^{-1}$ could be expressed in terms of a transfer matrix. We can write the determinant of an arbitrary matrix $\mathbf{A}$, dimension d, as

$$\begin{aligned}\sum a_{ijk\ldots} \quad & \mathbf{A}_{ii'} \quad a_{i'j'k'\ldots} = \det \mathbf{A} \\ & \times \\ & \mathbf{A}_{jj'} \\ & \times \\ & \mathbf{A}_{kk'} \\ & \vdots \\ & d \text{ terms}\end{aligned} \tag{15}$$

where $a_{ijk\ldots}$ is the antisymmetric unit tensor. Obviously this has the form of a symmetrised *direct product*, $\langle ad|\mathbf{A}^{\otimes d}|ad\rangle$. The projection we use on this occasion is *completely antisymmetric* in all the subscripts. We could use this method to calculate $\det(t)^{-1}$ simply by choosing $\mathbf{A} = (t)^{-1}$.

Consider the dth-order direct product of the transfer matrix, $\mathbf{T}^{\otimes d}$. We can symmetrise this direct product in the manner discussed in our earlier papers, and in particular we can choose the completely antisymmetric projection corresponding to the Young's tableau

d boxes. (16)

Since the dimensions of $\mathbf{T}$ are $2d$, there is a choice of rows and columns with respect to which we antisymmetrise. The complete set of choices constitute a matrix, $\mathbf{Y}$, which is itself a transfer matrix obeying the fundamental theorem

$$\mathbf{Y}_L = \prod_{n=1}^{L} \mathbf{Y}_n. \tag{17}$$

We shall define the top left-hand element of $\mathbf{Y}$ to correspond to the choice of the first d rows and the first d columns,

$$\mathbf{Y}_{L11} = \det(t_L^*)^{-1}. \tag{18}$$

For solid-state physicists there is a helpful analogy that can be drawn between the $\mathbf{Y}$ matrix and a system of fermions in a half-filled band. If we suppose that the first d rows or columns of $\mathbf{T}$ correspond to the 'lowest-energy' states, and the last d to the 'highest-energy' states, then the 'ground state' of the system is given by an antisymmetrised product of the first d states. The other elements correspond to 'excited states' of the system. For example, we might choose to antisymmetrise on $(d-1)$ states chose from the first set of d and one chosen from the second set of d. Obviously there are d possibilities for each choice, giving a total of d^2 different single excitations. The next most complicated

choice is $(d-2)$ from the first d and two from the second d, and so on. The dimensions of $\mathbf{Y}$ are

$$D = (2d)!/(d!)^2 \tag{19}$$

corresponding to the number of ways of choosing d objects from a set of $2d$.

In the earlier paper we were concerned with the density of states, which is given by

$$\operatorname{Im} \log \det(t)^{-1} = \operatorname{Im} \lim_{N\to 0} \det{}^N(t)^{-1}/N. \tag{20}$$

Hence we showed how to construct a transfer matrix for the Nth power of det. This matrix will also be relevant to the transport properties of the systems as we shall show in a subsequent section.

The Nth power of $\det(t^*)^{-1}$ is contained within the Nth-order direct product of $\mathbf{Y}$. In fact it is contained within the completely symmetric subspace of this direct product, which we obtain in the following manner. The completely symmetric space is labelled by a set of occupation numbers $\{n_i\}$, describing the number of times subscript i occurs in this element. The $\{n_i\}$ obey the sum rule

$$\sum n_i = N. \tag{21}$$

The number of distinct permutations of the N subscripts is

$$N! \Big/ \prod n_i! \tag{22}$$

which is a normalising factor for the symmetrised basis set. We can now write the completely symmetric reduction of $\mathbf{Y}^{\otimes N}$ as

$$\mathbf{X}^{\mathrm{S}}_N(\{n_i\},\{n'_{i'}\}) = \prod_i n_i! \sum_{P_{ii'}} \prod_{ii'} (\mathbf{Y}_{ii'})^{P_{ii'}} \frac{1}{P_{ii'}!} \tag{23}$$

where the product over ii' is over all D^2 values of these subscripts, and the summation over $P_{ii'}$ is over all possible positive integer values of the P subject to the restrictions that they be compatible with the subscripts of $\mathbf{X}$. For example, if $D = 6$ then the table of P would satisfy two-way sum rules:

$$\begin{array}{cccccc}
P_{11} & P_{12} & P_{13} & P_{14} & P_{15} & P_{16} = n_1 \\
P_{21} & P_{22} & P_{23} & P_{24} & P_{25} & P_{26} = n_2 \\
P_{31} & P_{32} & P_{33} & P_{34} & P_{35} & P_{36} = n_3 \\
P_{41} & P_{42} & P_{43} & P_{44} & P_{45} & P_{46} = n_4 \\
P_{51} & P_{52} & P_{53} & P_{54} & P_{55} & P_{56} = n_5 \\
P_{61} & P_{62} & P_{63} & P_{64} & P_{65} & P_{66} = n_6 \\
\| & \| & \| & \| & \| & \| \quad \| \\
n'_1 & n'_2 & n'_3 & n'_4 & n'_5 & n'_6 = N.
\end{array} \tag{24}$$

The quantities we wish to calculate can be expressed in terms of the $\mathbf{X}$ matrix defined in (23). We have already generalised the transfer matrix $\mathbf{T}$ to obtain the $\mathbf{Y}$ matrix. We now go one step further and make a second generalisation by using $\mathbf{Y}$ to construct $\mathbf{X}$. Since $\mathbf{X}$ is another transfer matrix, we can multiply together the $\mathbf{X}$ matrices from

successive slices of the disordered material in exactly the way that the original **T** matrices themselves multiply together. Thus equation (26) shows how to construct the composite transfer matrix for a slab of L layers, and correspondingly for **X**:

$$\mathbf{X}_L = \prod_{n=1}^{L} \mathbf{X}_n^N = \begin{bmatrix} \det{}^N(t_L^*)^{-1} & \cdots \\ \cdot & \cdots \\ \cdot & \cdots \\ \cdot & \cdots \end{bmatrix}. \tag{25}$$

Note that the (1, 1) matrix element is the quantity that we seek in this instance. Therefore we can calculate the average by the usual transfer matrix methods:

$$\overline{\det{}^N(t_L^{*\,-1})} = ([\overline{\mathbf{X}_n^N}]^L)_{11}. \tag{26}$$

We achieve the analytic continuation to fractional N as follows. Suppose in (24) we set $N = -1$. We now wish minimally to extend the restrictions on the P and n to take account of this. First we note that we need to include $\det^N(t_L^{*\,-1})$ in the continued matrix. Therefore we must allow P_{11} to be fractional and/or negative. None of the other P need be anything other than positive integers. This necessarily implies that n_1 and n_1' can also be fractional and/or negative, but none of the other n need be so. Thus our minimal prescription is to allow indices n_1 to take any value subject to the sum rules, and to extend the summation over P to any value of P_{11} subject to the sum rules.

For integer N the new matrix is equivalent to the old one defined by (23) because it takes the following form:

$$\left[\begin{array}{c|c} \text{old matrix} & 0 \\ \hline \multicolumn{2}{c}{\text{new terms}} \end{array}\right]. \tag{27}$$

The top right-hand corner is filled with zeros for integer N because these elements correspond to new elements with negative n_1' but positive integer n_1. Thus in (23) none of the factorials in the numerator is infinite, but at least one of the factorials in the denominator must be so. This ensures that we get the same answers as before for integer N, but have smoothly continued the expression to all values of N. The corresponding terms in the bottom left-hand quadrant are not zero because the normalisation factor also contains factorials that cancel with the $P!$.

4. A transfer matrix for the reflection coefficient

It will make our task a little clearer if we introduce some further notation at this stage. It has been explained how the matrix **Y** consists of all the determinants of order d that can be formed from the $2d \times 2d$ matrix **T**. Let the convention be that subscript '0' corresponds to choosing the first d rows of **T**. In the next class of choice we have $(d - 1)$ terms from the first d rows and one from the last d rows. We label this by the $\boldsymbol{k}$-value omitted from the first set, $\boldsymbol{k}_1$, and the $\boldsymbol{k}$-value chosen from the second set, $\boldsymbol{k}_2$. Similarly in the class consisting of $(d - 2)$ terms from the first d rows and two from the last d rows,

we label using the two k-values missing from the first set, k_1k_2, and the two chosen from the second set, k_3k_4. In this notation $\mathbf{Y}$ appears as

$$\begin{bmatrix} \mathbf{Y}(0;0) & \mathbf{Y}(0;k_1',k_2') & \dots \\ \mathbf{Y}(k_1,k_2;0) & \mathbf{Y}(k_1,k_2;k_1',k_2') & \dots \\ \mathbf{Y}(k_1k_2,k_3k_4;0) & \mathbf{Y}(k_1k_2,k_3k_4;k_1'k_2',k_3'k_4') & \dots \\ \dots & \dots & \dots \\ \dots & \dots & \dots \end{bmatrix}. \tag{28}$$

Some insight into the nature of these matrices can be had by considering the zero-disorder limit, and using a basis set of Bloch waves. Then $\mathbf{T}$ becomes

$$\mathbf{T} = \begin{bmatrix} \exp(\mathrm{i}K_{zk}) & 0 \\ 0 & \exp(-\mathrm{i}K_{zk}) \end{bmatrix} \tag{29}$$

and

$$\mathbf{Y} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \exp(\mathrm{i}K_{zk_1} + \mathrm{i}K_{zk_2})\delta_{k_1k_1'}\delta_{k_2k_2'} & 0 \\ \dots & \dots & \dots \end{bmatrix}. \tag{30}$$

Each successive diagonal block of $\mathbf{Y}$ involves two more K_z in the exponent.

The generalised transfer matrix $\mathbf{X}$ has elements

$$\begin{bmatrix} \mathbf{Y}^N(0;0) & N\mathbf{Y}^{N-1}(0;0)\mathbf{Y}(0;k_1',k_2') & \dots \\ \mathbf{Y}^{N-1}(0;0)\mathbf{Y}(k_1,k_2;0) & \mathbf{Y}^{N-1}(0;0)\mathbf{Y}(k_1,k_2;k_1',k_2') \\ & \quad + (N-1)\mathbf{Y}^{N-2}(0;0)\mathbf{Y}(0;k_1,k_2)\mathbf{Y}(k_1,k_2;0) & \dots \\ \dots & \dots & \dots \end{bmatrix}. \tag{31}$$

Now let us focus on the second block in the first row, i.e.

$$\lim_{N\to 0} N\mathbf{Y}^{N-1}(0;0)\mathbf{Y}0;k_1',k_2')/N = \mathbf{Y}(0;k_1',k_2')/\mathbf{Y}(0;0). \tag{32}$$

We shall show that this is simply the reflection matrix. Consider $\mathbf{Y}(0;0)$: it is given by the determinant of the top left-hand block of $\mathbf{T}$. Let us expand this determinant by the k_1'th column:

$$\mathbf{Y}(0;0) = \delta_{k_1'k}\det(t^*)^{-1} = \sum_k C_{k_1'k}(t^*)^{-1}_{k-k'} \tag{33}$$

where $C_{k_1'k}$ is the cofactor found by taking the determinant of the matrix obtained by

deleting the kth row and k_1'th column of $(t^*)^{-1}$ and multiplying by the appropriate sign. Similarly the prescription for calculating $\mathbf{Y}(0; k_1', k_2')$ is to substitute the k_2'th column of the top right-hand block of $\mathbf{T}$ for the k_1'th column of the top left-hand block. In other words,

$$\mathbf{Y}(0; k_1', k_2') = \sum_k C_{k_1'k}[(t^*)^{-1}r^*]_{-k-k_2'}$$

$$= \sum_{kk'} C_{k_1'k}(t^*)^{-1}_{-k-k'} r^*_{-k'-k_2'}. \tag{34}$$

Note that the same cofactor applies in each case. Substituting from (33) for the part in square brackets gives

$$\mathbf{Y}(0; k_1', k_2') = \det(t^*)^{-1} r^*_{-k_1'-k_2'} \tag{35}$$

and therefore

$$\lim_{N\to 0} N\mathbf{Y}^{N-1}(0;0)\mathbf{Y}(0; k_1', k_2')/N = \mathbf{Y}(0; k_1', k_2')/\mathbf{Y}(0;0) = r^*_{-k_1'-k_2'} \tag{36}$$

which is the result we seek.

We have succeeded in identifying the reflection matrix as a component of the generalised transfer matrix $\mathbf{X}_N$, in the limit $N \to 0$. This is our main result.

The reflection matrix appears in a somewhat unexpected form: its elements are not in fact to be found in a $d \times d$ block of $\mathbf{X}_N$, but strung out as a vector in a $1 \times d^2$ block.

One final step is required to make contact with the transport formalism: we must take the direct product $\mathbf{X}_N \otimes \mathbf{X}^*_{N'}$. This yields a matrix, the first few elements of which are

$$\mathbf{X}_N \otimes \mathbf{X}^*_{N'} = \left[\begin{array}{l|l|l} \mathbf{Y}^N(0;0)\mathbf{Y}^{*N'}(0;0) & N\mathbf{Y}^{N-1}(0;0)\mathbf{Y}(0; k_1', k_2') & \\ & \times N'\mathbf{Y}^{*N'-1}(0;0)\mathbf{Y}^*(0; k_1'', k_2'') & \cdots \\ & = NN' r^*_{-k_1'-k_2'} r_{-k_1''-k_2''} & \\ \hline \mathbf{Y}^{N-1}(0;0)\mathbf{Y}(k_1, k_2; 0) & & \\ \quad \times \mathbf{Y}^{*N-1}(0;0)\mathbf{Y}^*(k_1, k_2; 0) & \cdots & \cdots \\ = r^*_{-k_1-k_2} r_{-k_1-k_2} & & \\ \hline \cdots & \cdots & \cdots \end{array}\right] \tag{37}$$

To complete our prescription we need to find the left and right eigenvalues of the averaged $\mathbf{X}_N \otimes \mathbf{X}^*_{N'}$ for a single layer,

$$\overline{\mathbf{X}_N \otimes \mathbf{X}^*_{N'}}\,|vr_j\rangle = e_j\,|vr_j\rangle \tag{38a}$$

$$\langle vl_j|\,\overline{\mathbf{X}_N \otimes \mathbf{X}^*_{N'}} = e_j\langle vl_j| \tag{38b}$$

then work up to a stack of L layers by raising the eigenvalues to the Lth power, and finally projecting out the components we need:

$$\overline{r^*_{L-k'_1-k'_2} r_{L-k''_1-k''_2}} = \lim_{\substack{N\to 0 \\ N'\to 0}} \sum_j e_j^L \langle 0|\boldsymbol{v}r_j\rangle\langle \boldsymbol{v}l_j|k'_1 k'_2 k''_1 k''_2\rangle/NN' \tag{39}$$

where an obvious notation has been used for the projection operators. Of course, if we are to study transport, we need the transmitted intensity, but this can easily be found from the current conservation requirement discussed in section 2:

$$\sum_{k''} [V_{k''z}/(V_{zk}V_{zk'})^{1/2}](\overline{t^*_{k''k'}t_{k''k}} + \overline{r^*_{k''k'}r_{k''k}}) = \delta_{kk'}. \tag{40}$$

5. An alternative strategy for the transmission matrix

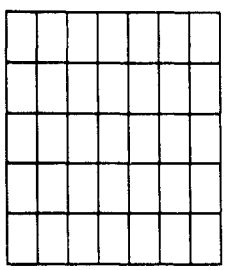
A more straightforward strategy would be to find a generalised transfer matrix that contains the transmission matrix itself. It is not hard to show that such a matrix exists, but there are some formidable group-theoretical difficulties involved in calculating its elements, which we have not completely overcome. It would be worthwhile to set out the problems so that others more skilled in group-theoretical techniques may make progress.

Consider once again the generalised transfer matrix based on dth-order determinants, $\mathbf{Y}$. We have outlined a strategy for extracting

$$\det{}^N(t^*)^{-1} = \mathbf{Y}^N(0;0) \tag{41}$$

from the Nth-order direct product $\mathbf{Y}^{\otimes N}$. We did this by using theory of the symmetric group to reduce the direct product. However, our reduction procedure is incomplete and does not correspond to an irreducible representation.

Consider the Young tableau with d rows and N columns, where d and N are integer for the moment,



d rows, N columns. (42)

It defines an irreducible representation of the symmetric group. Let us use it to reduce the Ndth-order direct product of the transfer matrix with itself, $\mathbf{T}^{\otimes Nd}$, to obtain the

completely reduced matrix $\mathbf{Z}$, which is another transfer matrix. The elements of $\mathbf{Z}$ are defined by the filling of the tableau with subscripts of $\mathbf{T}$, and one such allowed filling is

k_1	k_1	k_1	k_1	k_1	k_1	k_1
k_2	k_2	k_2	k_2	k_2	k_2	k_2
k_3	k_3	k_3	k_3	k_3	k_3	k_3
...	...	...	...	...	...	...
k_d	k_d	k_d	k_d	k_d	k_d	k_d

d rows, N columns. (43)

Let us label this the first element. Then it is easy to show that

$$\mathbf{Z}_{11} = \det{}^{N}(t^*)^{-1}. \tag{44}$$

To be of use to us it is necessary that this expression be analytically continued to fractional and negative values of N. Unfortunately, the reduction procedure is complex and not sufficiently transparent for us to see how to make this continuation. Others may have more insight.

Let us proceed on the assumption that this problem can in principle be solved. Next consider a tableau with $(d-1)$ rows and one column:

$(d-1)$ rows, one column. (45)

It defines another irreducible representation of the symmetric group. Let us use it to reduce the $(d-1)$th-order direct product of the transfer matrix with itself, $\mathbf{T}^{\otimes(d-1)}$, to obtain the completely reduced matrix $\mathbf{A}$, which is yet another transfer matrix. One possible filling of the tableau is a selection of subscripts drawn from the first d of $\mathbf{T}$. Label this filling by the element that is missing. There are thus d possible ways of filling the tableau with this selection. The (kk') element of the reduced matrix is given by the determinant obtained by omitting the kth row and k'th column of $(t^*)^{-1}$, which is related to the inverse of $(t^*)^{-1}$ by

$$\mathbf{A}_{kk'} = t^*_{kk'} S(kk') \det(t^*)^{-1} \tag{46}$$

where S is a factor that is ± 1 according to whether the sum of the row and column positions in the matrix is odd or even: see the standard expression for a matrix inverse.

Next consider the product

$$\mathbf{A}_{kk'}\mathbf{Z}_{11} = t^*_{kk'} S(kk') \det(t^*)^{-N-1}. \tag{47}$$

Then all we need to do is to set $N = -1$ and we have the desired expression for t. In fact,

the product of the elements can again be written as a symmetry-reduced direct product. Consider the non-rectangular tableau:

k_1	k_1	k_1	k_1	k_1	k_1	k_1	k_1
k_2	k_2	k_2	k_2	k_2	k_2	k_2	k_2
k_3	k_3	k_3	k_3	k_3	k_3	k_3	k_3
...	...	...	...	...	...	...	k_4
k_d	k_d	k_d	k_d	k_d	k_d	k_d	

N columns of length d,

one column of length $(d-1)$. (48)

The last column contains all but one of the first d subscripts of $\mathbf{T}$ so that the tableau defines a set of symmetry-reduced matrix elements, which are in fact

$$t^*_{kk'} S(kk') \det(t^*)^{-N+1}.$$

The problem remaining, which we have not yet solved, is to find a sufficiently transparent formula for these elements that they can be analytically continued to fractional and negtive N, in particular to $N = -1$. That would give us our explicit formula for t^* in terms of a transfer matrix.

However, this question is not an urgent one because we do have a transfer matrix, defined in the last section, which can be used to calculate averaged transmitted intensities.

6. Replicas and symmetry breaking

The analogy of the $N \to 0$ limit taken in equations (32) and (36) to the replica trick in spin-glass theory (Edwards and Anderson 1975) has sometimes been drawn: each matrix in the direct product represents a replica, and the disorder introduces an interaction between replicas. In the original version of the replica method, because all the replicas have the same status, it was assumed that the equations would be symmetric in the replicas. The demonstration of symmetry breaking was one of the subtleties of the spin-glass problem (Parisi 1979, 1980). Hence it is natural to ask whether symmetry breaking troubles us here.

Fortunately we have addressed the problem of symmetry from the beginning, in many cases decomposing the direct products into irreducible representations of the symmetric group. Therefore we can address the problem of replica symmetry directly. In the previous section we saw that all questions concerning the transmitted *amplitude* involve a single replica symmetry given by the tableau in equation (48). The solutions have no choice but to take the symmetry defined by this tableau. Only in 1D does this amount to the solution being 'replica symmetric', because there the tableau reduces to a single row corresponding to Bose symmetry of the replicas.

For the transmitted *intensity* used in calculating the conductance, a more complex situation develops because then we must take the direct product of two amplitude matrices: see, for example, equation (37). Group theory tells us that the product contains a number of irreducible representations, and which of them dominates depends on the relative magnitude of the eigenvalues. In 1D we have made a complete analysis of symmetry breaking for the conductance problem (Kirkman and Pendry 1984b), though the language used was that of group theory, not of replica theory. The conclusion is a rather radical and interesting one: the conductance is dominated by replicas of symmetry

corresponding to the permutation of

$$N = -\tfrac{1}{2} + i\alpha \tag{49}$$

particles, and their contribution is proportional to

$$\exp[-\delta'^2 L_z(\tfrac{1}{4} + \alpha^2)] \tag{50}$$

where δ'^2 is a measure of the disorder, and L_z is the length of the 1D system. In 3D we do not have as yet so complete a solution of replica symmetry breaking for the conductance.

7. Conclusions

In this paper we have extended the transfer matrix formalism to the calculation of conductivity in 3D systems. The key element in our theory was application of group-theoretical techniques to symmetry reduction of direct products. The formula we obtain has the same status as the secular determinant in the band structure of solids: it is not a perturbative formulation, but approximations need to be made in terms of truncation of infinite matrices to finite dimensions. This procedure has already been investigated for the case of density-of-states calculations and accurate results found for low-order truncations.

Our result represents a completely new formulation of transport properties and in future papers we shall apply it to a variety of systems.

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