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A rescaling approach to two- and three-dimensional lattice spectra

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Abstract. An exact real-space rescaling transformation is used to calculate the spectral properties of tight-binding Hamiltonians with an arbitrary range of interaction on two- and three-dimensional lattices. The intrinsic problem of the proliferation of initial short-range interactions under rescaling is shown to be tractable numerically. This method provides a direct way of obtaining the local Green functions and local density of states. Singularities of the spectral functions are associated with fixed points or limit cycles of the rescaling transformation. Band edge fixed points and exponents have been found for the square, triangular and cubic lattices. In two and three dimensions there is rapid convergence to accurate numerical results for the Green function outside the band, while good results have been obtained for the in-band (e.g. density of states) spectra in two dimensions by suitable choices of cluster size and attenuation factor. Insight into the relationship between these factors follows from an investigation of finite-cluster approximations to the exact transformation. It is found that the zeros of the Green functions in the complex plane are Julia sets which have a fractal structure. For a given cluster size the attenuation factors must lie outside these zeros in order for the procedure to be convergent.

1. Introduction

In a recent series of papers (Southern *et al* 1983a, b, Langlois *et al* 1983, Tremblay and Southern 1983) a real-space rescaling approach for the study of the spectral properties of tight-binding Hamiltonians was described. The basic idea of the method is to take a system of equations which describe N degrees of freedom and perform a transformation on the system which reduces the number of degrees of freedom to a fraction of N but leaves the equations invariant in form with modified (renormalised) parameters. The relationship between the renormalised parameters and the original set is used to define a scaling transformation on the equations of motion. This procedure can then be repeated indefinitely by simply iterating the transformation many times until there is only one degree of freedom left. In this limit the problem can be trivially solved in terms of the limiting values of the renormalised parameters. The method described in this paper is similar to that proposed by Aoki (1979, 1980, 1982) for the study of Anderson localisation.

Our previous papers concerned 1D systems (with arbitrary range of interaction) which were either ordered or disordered as well as hierarchical and fractal lattices. In all cases the initial range of coupling does not increase under the rescaling transformation. However, for conventional lattices in higher dimensions, even if the couplings are restricted to nearest neighbours initially, each successive elimination causes the

range of interaction to increase. For this reason it is necessary to construct a transformation which is valid for an arbitrary range of the couplings. We have derived a family of transformations which are exact for an arbitrary range on any lattice. Since the transformation is valid for an arbitrary range of the interactions, our procedure provides a simple method of calculating lattice Green functions for lattices with interactions which extend beyond nearest neighbours. The transformation exhibits certain fixed points where the parameters do not change their values under iteration, as well as periodic cycles. The eigenvalues which describe the stability of these fixed points or cycles are associated with singularities of the Green functions.

The intense interest in lattice Green functions (see Katsura *et al* 1971) results from their use in the formulation of many problems in solid state physics. These include impurity problems, e.g. mass, spin or impurity defects (see Economou 1983), where bound states (local modes) may be split off from the bands and can be handled with knowledge of the real part of the lattice Green functions outside the band (i.e. extended Watson integrals); two-magnon bound states, using extended Watson integrals (Wortis 1963), and two-magnon resonances, using the complex in-band lattice Green functions (Loly *et al* 1975, Bahurmuz and Loly 1980).

The paper is organised as follows. In § 2 we describe how to obtain a general rescaling transformation for arbitrary range of interaction. Section 3 gives results for the lattice Green functions for various lattices as well as the fixed points of the rescaling transformation which characterise the singularities of these functions. Section 4 explores finite cluster approximations to the exact transformation. It is shown that the zeros of the Green functions in the complex plane are Julia sets, which have a fractal structure, and these sets provide a useful means of assessing the approximations. Our results are summarised in § 5.

2. Rescaling transformation

Consider a system of N sites described by a model Hamiltonian written in the following tight-binding form

$$H = \sum_r |r\rangle \varepsilon(r) \langle r| + \sum_{r,r'} |r\rangle V(r, r') \langle r'| \quad (1)$$

where $|r\rangle$ represents an atomic-like orbital centred at site r , and $\varepsilon(r)$ and $V(r, r')$ are the diagonal and off-diagonal matrix elements of H in this basis. The solutions of the Schrödinger equation are conveniently described in terms of Green functions which satisfy the following matrix equation

$$(E - H)G = I \quad (2a)$$

where I is the identity matrix and

$$G(r, s) = \langle r | (E - H)^{-1} | s \rangle. \quad (2b)$$

E is a complex energy and the local density of states is obtained from the imaginary part of $G(0, 0)$ in the limit as E approaches the real axis (Economou 1983). In terms of reduced variables, (2a) can be written in the following form

$$G(r, s) = \alpha(r, s) + \sum_{r'} X(r, r') G(r', s) \quad (3a)$$

where

$$\alpha(r, s) = \delta(r, s)/(E - \varepsilon(r)) \quad (3b)$$

$$X(r, r') = V(r, r')/(E - \varepsilon(r)). \quad (3c)$$

Our basic approach to solving these equations for a given element $G(r, s)$ is to apply a transformation to the $N \times N$ matrix $(E - H)$ which brings it to a block diagonal form where each block is of reduced size $\frac{1}{2}N \times \frac{1}{2}N$. If we partition the sites r into two groups which we label 'even' and 'odd', then the transformation effectively eliminates the 'odd' sites and produces new effective interactions between the 'even' sites. The 'even' sites are then further partitioned into two groups and the transformation is repeated. In this way, the Green function $G(r, s)$ eventually belongs to a 1×1 block and its value is trivially obtained from the limiting value of the parameter $\alpha(r, s)$ in (3).

Any element $G(r, s)$ is coupled to the other $G(r', s)$'s in the same column, and these obey a similar equation

$$G(r', s) = \alpha(r', s) + \sum_{r''} X(r', r'')G(r'', s). \quad (4)$$

We multiply the equations (4) by constants $L(r, r')$ and sum over *all* sites $r' \neq r$ and add the result to (3a). Solving for $G(r, s)$ the result can be again expressed in the form

$$G(r, s) = \alpha'(r, s) + \sum_{r'} X'(r, r')G(r', s) \quad (5a)$$

where

$$\alpha'(r, s) = \left(\alpha(r, s) + \sum_{r'} L(r, r')\alpha(r', s) \right) / D(r, r) \quad (5b)$$

$$X'(r, r') = \left(X(r, r') - L(r, r') + \sum_{r''} L(r, r'')X(r'', r') \right) / D(r, r) \quad (5c)$$

and

$$D(r, r) = 1 - \sum_{r'} L(r, r')X(r', r). \quad (5d)$$

The elements $L(r, r')$ are determined such that $X'(r, r') = 0$ when r and r' belong to different groups. There are $N(N-1)$ constants to be determined and only $2(N/2)^2$ constraints. If we choose the $L(r, r') = 0$ when r and r' belong to the same sets, then the solutions for the remaining L 's can be expressed in terms of the inverse of a $\frac{1}{2}N \times \frac{1}{2}N$ matrix. In this case, the transformation is identical to that proposed by Aoki (1979, 1980, 1982). However, if the Hamiltonian is translationally invariant, i.e. $X(r, r') = X(r-r')$, then an alternate solution can be found which does not involve any matrix inversion. The following choice for the L 's produces the desired block form for $(E - H)$

$$\begin{aligned} L(r, r') &= X(r, r') && \text{for } r \text{ and } r' \text{ in different groups} \\ L(r, r') &= -X(r, r') && \text{for } r \text{ and } r' \text{ in the same group.} \end{aligned} \quad (6)$$

The transformation defined by (5) and (6) is valid for any range of the interactions $V(r, r')$ in (1) on any lattice which is translationally invariant. The initial values of $X(r, r')$ and $\alpha(r, s)$ are determined as in (3) with a complex value of the energy E and the transformation is iterated until convergence of the complex quantity $\alpha(r, s)$

is obtained. The Green function $G(r, s)$ is equal to this limiting value. The case of a linear chain has already been discussed by Southern *et al* (1983). In that case the effective range of the interactions does not increase under iteration of the transformation. However, for two- and three-dimensional lattices, even if the initial range in (1) is restricted to nearest neighbours the effective range of the couplings increases under iteration. For real values of E outside the band, the range shrinks after expanding in the early iterations and the Green function converges rapidly. In consequence it is realistic to use a finite-ranged cluster. On the other hand, for values of E inside the band, convergence is only obtained by using an imaginary part in the energy which acts as an attenuation factor. The significant range of the interactions now depends upon the size of the attenuation factor and thereby defines the size of cluster that must be used.

For any lattice, the transformation (5), (6) consists of three steps: (i) partitioning the sites into two groups, (ii) eliminating the 'odd' sites to obtain new effective interactions between the 'even' sites, (iii) relabelling the 'even' sites so that the partitioning can be repeated. The system can be partitioned in more than one way and we will describe various schemes for two- and three-dimensional lattices in § 3.

The exact transformation above was obtained by eliminating a fraction of the degrees of freedom from the equations which determine the Green functions. An equivalent formulation can be constructed in terms of a complex generating function (Tremblay and Southern 1983) which remains invariant under the transformation apart from an additive term. This latter approach clearly exposes the close similarity of our method to the real space renormalisation group approach to critical phenomena which is based on the invariance of the partition function (Niemeijer and van Leeuwen 1976). The renormalisation group approach reduces the problem of phase transitions to the study of maps in a space of Hamiltonians. The various different phases are related to attractive basins of the map and the critical behaviour is related to unstable fixed points of the transformation. In our case, the attractive basins of the transformation describe different regions of energy in which the spectral properties of the system are qualitatively different and the unstable fixed points are related to singularities of the Green functions. In the study of critical phenomena, exact transformations are rare and one usually replaces the map defined in the whole space of Hamiltonians by an approximate map in a subspace of finite dimension. Our exact transformations are infinite-dimensional maps but in obtaining the results in § 3 we have truncated the exact map to allow only interactions up to some maximum range and we set all further interactions equal to zero. However, as we shall demonstrate, the truncated map is adequate to determine the different regions of energy (i.e. phases) and obtain accurate values for the exponents which characterise the singularities of the Green functions at the boundaries between these regions. In § 4 we shall examine in detail the properties of our truncated maps in the complex energy plane. This allows us to see the effect of truncation on the analytic properties of the Green functions since these properties are determined by the map.

3. Two- and three-dimensional lattices

3.1. The square lattice

Consider the square lattice shown in figure 1. In order to calculate the Green function $G(r, s)$ we choose the site r as our origin and the remaining sites can be labelled with

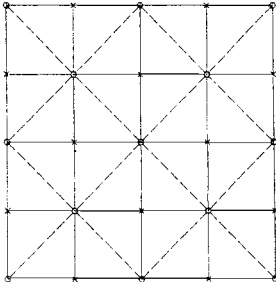


Figure 1. Square lattice: the odd sites (\times) are eliminated and the even sites (\circ) form a new square lattice with a larger lattice spacing.

two integers l, m which specify the x and y coordinates in units of the lattice spacing a . The sites can be partitioned into two equal groups according to whether the sum $(l+m)$ is even or odd. Both the 'even' and 'odd' groups form a 2D square lattice which is rotated by 45° with respect to the original lattice and has a new lattice spacing $a' = (2)^{1/2} a$. The parameters $\alpha(r, s)$ and $X(r, s)$ in (5) can also be labelled in terms of l and m and the transformation becomes

$$X'(p, q) = \left(2X(p-q, p+q) + \sum_{l,m} (-1)^{l+m+1} X(p-q-l, p+q-m) X(l, m) \right) / D$$

$$\alpha'(p, q) = \left(\alpha(p-q, p+q) + \sum_{l,m} (-1)^{l+m+1} \alpha(p-q-l, p+q-m) X(l, m) \right) / D \quad (7)$$

$$D = 1 - \sum_{l,m} (-1)^{l+m+1} X(-l, -m) X(l, m)$$

where p and q label the sites on the new lattice in units of a' .

The transformation above is an exact transformation which can be used to calculate any Green function $G(r, s)$ for any initial range of the interactions. Before we discuss detailed results for the square lattice, we shall make some general comments. For real values of E outside the band of extended states, the iteration process converges rapidly. Although the interaction range initially increases, the $X(p, q)$ soon decrease to zero in a monotonic fashion and $\alpha(r, s)$ reaches a limiting value. For real values of E inside the band, the behaviour of the transformation is chaotic under iteration. The range of the interactions increases indefinitely and $\alpha(r, s)$ does not reach a limiting value. However, for complex values of E this chaotic behaviour is damped out and $\alpha(r, s)$ attains a limiting complex value. These two different regions of energy are separated by the band edges which iterate to fixed points (or limit cycles) of the transformation. The fixed points (or limit cycles) are unstable and the relevant eigenvalues obtained by linearising the transformation about the fixed points can be used to determine the singular behaviour of the Green functions at the band edges.

Figures 2(a) and 2(b) show our results for $G(0, 0)$ and $G(1, 0)$ respectively in the case of the nearest-neighbour square lattice. We have truncated the exact transformation (7) to restrict the range of interactions to eight lattice spacings along the cartesian axes. Outside the band, fewer than ten iterations are required to obtain an accuracy of 10^{-6} . In this energy region, the significant interactions only extend to approximately fifth neighbours. Inside the band, 15 to 30 iterations are required when the imaginary part increases linearly from the band edges to a maximum value of 0.075 at the band

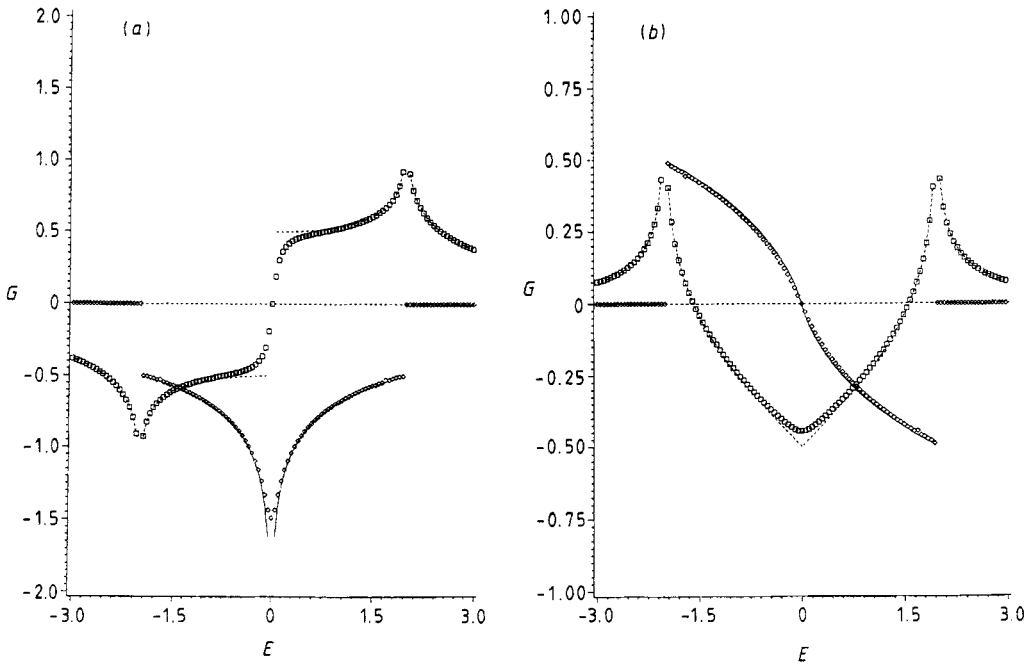


Figure 2. Real and imaginary parts of $G(i, j)$ for the nearest-neighbour square lattice are denoted by the squares and diamonds respectively. The corresponding exact results are indicated by the full and broken curves: (a) $G(0, 0)$, (b) $G(1, 0)$.

centre. The reason for using a variable imaginary part will be discussed further in § 4. The exact analytic results obtained for an infinitesimal imaginary part are shown for comparison (see Economou 1983).

For initial values of the energy corresponding to the band edges, the transformation iterates to the fixed point labelled A in table 1. Near these critical points the density of states has the form $(\Delta E)^{(d-y)/y}$ where d is the dimension and y is an exponent corresponding to the largest eigenvalue of the associated fixed point. For a scaling factor b , the exponents are related to the eigenvalues as $\lambda = b^y$. Fixed point A has one relevant eigenvalue equal to 2.000 which describes the discontinuity in the density of states at these energies.

The Green functions for second and more distant neighbour problems can be calculated using the same transformation (7) by simply changing the initial values of the parameters. This procedure is used in §§ 3.2 and 3.3.

Table 1. Fixed points and exponents for 2- and 3D lattices. The X_n are the coordinates of the n th-neighbour interaction.

| | nth neighbour | | | | | Relevant eigenvalue | y |
|---|---------------|--------|---------|---------|---------|---------------------|---|
| | X1 | X2 | X3 | X4 | X5 | | |
| A | 0.2079 | 0.0432 | -0.0019 | 0.0004 | 0.0000 | 2.000 | 2 |
| B | 0.1630 | 0.0043 | -0.0007 | 0.0000 | 0.0000 | 4.000 | 2 |
| C | -0.2330 | 0.0381 | -0.0265 | 0.0010 | -0.0000 | 4.000 | 2 |
| D | 0.1216 | 0.0194 | 0.0060 | -0.0019 | 0.0001 | 4.000 | 2 |

3.2. The triangular lattice

The triangular lattice can also be treated using the same transformation as for the square lattice but with different initial conditions for the interactions. The nearest-neighbour triangular lattice is topologically equivalent to the square lattice with half of its second neighbour interactions equal to the first neighbours as shown in figure 3. However, the lattice is still translationally invariant and the partitioning and elimination can be carried out in the same way as for the square lattice. One iteration of the transformation does not map the original triangular lattice into a new triangular lattice with larger lattice spacing. However, two iterations of the transformation (7) does constitute a mapping of the original triangular lattice into a new triangular lattice with double the lattice spacing. Figure 4 shows our calculated results for $G(0, 0)$ when the exact transformation is truncated to restrict the interaction range to eight lattice spacings along the cartesian axes. As will be explained in § 4, we have used a variable value for the imaginary part of the energy inside the band. The exact analytic results for the infinitesimal imaginary part obtained by Horiguchi (1972) are shown for comparison. At energies corresponding to the band edges, the transformation does not iterate to a fixed point but instead to a period-two limit cycle. The limit cycle is unstable and is a fixed point of the transformation defined by applying (7) twice. The upper band edge is described by fixed point B in table 1 whereas the lower band edge is described by fixed point C. Both have the same relevant eigenvalue equal to 4.000 which again correctly describes the discontinuity in the density of states at these energies. The eigenvalues for fixed points B and C are the square of that for fixed point A since the former are fixed points of the second iterate of (7).

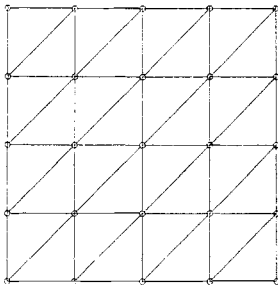


Figure 3. The triangular lattice is topologically equivalent to a square lattice with second neighbour interactions along one diagonal.

3.3. Cubic lattices

For the 2D lattices in §§ 3.1 and 3.2 we chose to partition the sites into two groups according to whether $(l + m)$ is even or odd. This choice is equivalent to eliminating every other plane of sites along the diagonal. A second type of partitioning can be used which leads to a slightly different transformation. If we divide the lattice into two groups according to whether simply l is even or odd, then we can eliminate every other plane of atoms in the x direction. We can now interchange the x and y directions and eliminate sites with m odd. In this way, by first eliminating every other plane along x and then along y , we have performed a transformation to a new lattice which has $a' = 2a$. This two-step transformation is equivalent to applying the one-step

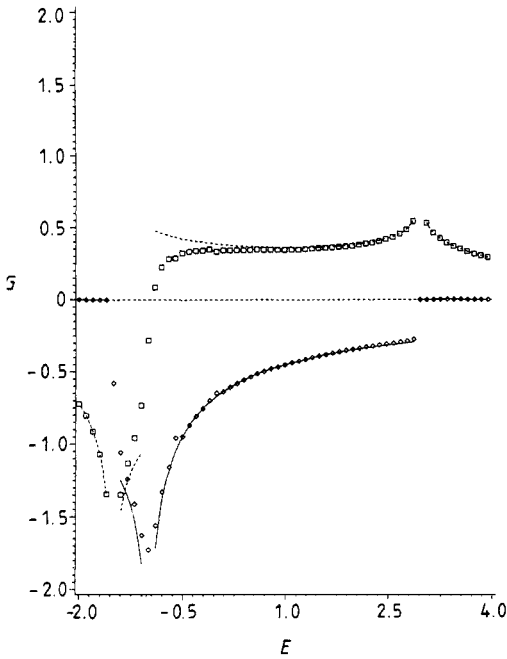


Figure 4. Real and imaginary parts of $G(0,0)$ for the nearest-neighbour triangular lattice are denoted by the squares and diamonds respectively. The corresponding exact results are indicated by the full and broken curves.

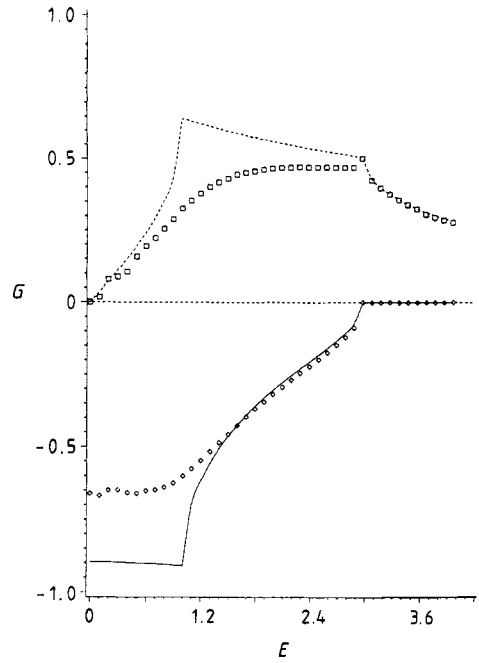


Figure 5. Real and imaginary parts of $G(0,0)$ for the nearest-neighbour simple cubic lattice are denoted by the squares and diamonds respectively. The corresponding exact results are indicated by the full and broken curves.

transformation (7) twice in the case of the square and triangular lattices. However, the two-step transformation can be easily generalised to a d -step transformation in d dimensions.

For example, for the cubic lattices we first eliminate every other plane along the x direction followed by elimination along the y and z directions. After each elimination step we must relabel the sites and the transformation can be written in the following form:

$$\begin{aligned}
 X'(q, r, p) &= \left(2X(2p, q, r) + \sum_{l,m,n} (-1)^{l+1} X(l, m, n) X(2p-l, q-m, r-n) \right) / D \\
 \alpha'(q, r, p) &= \left(\alpha(2p, q, r) + \sum_{l,m,n} (-1)^{l+1} X(l, m, n) \alpha(2p-l, q-m, r-n) \right) / D \quad (8) \\
 D &= 1 - \sum_{l,m,n} (-1)^{l+1} X(l, m, n) X(-l, -m, -n).
 \end{aligned}$$

In the above expressions, the various interactions are labelled with three integers l, m, n . Sites with l odd are eliminated and the even l sites are relabelled. The indices are then cyclically permuted in order to perform the elimination along the other two directions. Hence three iterations of (8) constitutes the scaling transformation which increases the lattice spacing by a factor of two.

All three cubic lattices can be treated using this same transformation but with different initial conditions. The nearest-neighbour simple cubic lattice has the six

$X(1, 0, 0)$ non-zero initially and all others zero. Both the BCC and FCC lattices can be treated as topologically equivalent to a simple cubic lattice with some of the next nearest-neighbour interactions present initially. Figure 5 shows our results for $G(0, 0)$ in the case of the simple cubic lattice when the interactions are restricted to five lattice spacings along the cartesian axes. The numerical results of Oitmaa (1971) for an infinitesimal imaginary part in the energy are also plotted for comparison. Outside the band, fewer than ten iterations of (8) are required to obtain an accuracy of 10^{-4} . The results inside the band required 15 to 30 iterations but are somewhat disappointing. This is due to the fact that, when the transformation is truncated, a rather large imaginary part must be used in the energy for the procedure to converge. This point will be discussed further in § 4. The results can be improved by allowing longer ranged interactions in the truncated expressions but the computation time increases.

The simple cubic band edges are described by fixed point D in table 1. Since the lattice is scaled by a factor of two under three iterations of (8), the eigenvalue 4.000 correctly describes the square root behaviour of the density of states at these energies.

4. Finite-cluster approximations

Maps of a space to itself have been studied in many contexts and even very simple maps may have behaviour which is very complicated (May 1976). There can be fixed points, periodic orbits, chaotic behaviour and strange attractors (see, for example, Collet and Eckmann 1980). Derrida *et al* (1983a, b) have recently examined the consequences of such complicated behaviour on the critical properties of the partition function. They find that when the renormalisation group transformation has more complicated behaviour than only fixed points then the free energy can have an infinite number of critical temperatures and can even be non-analytic over a continuous range of temperatures. In our case it is energy that plays the role of temperature and the Green functions can be non-analytic at many different values of E or over a continuous region of E .

Consider the transformation for the square lattice in (7). If we restrict the range to first neighbours only, then we have a one-dimensional map which can be written in the form

$$Z' = Z^2 - 1 \quad (9)$$

with the change of variable: $Z = \{2X(1, 0)\}^{-1} = (E - \epsilon)/(2V)$. This map is a member of a family of maps that have been studied by many authors both on the real line and in the complex plane. Julia (1918) gave a complete treatment of one-dimensional complex iterative maps of this form. He discovered the existence of an exceptional set, the Julia set, which is the closure of the set of all unstable periodic cycles. This set is a separatrix which separates the attracting domains of the stable fixed points or cycles and becomes an attractor for the inverse map. More recently, Mandelbrot (1980, 1982, 1983) has studied these maps in the complex plane and showed that the Julia sets have a fractal structure. The map (9) has a stable fixed point at infinite Z and an attracting 2-point cycle $Z = \{0, -1\}$ on the real axis. Figure 6 shows the set of points in the complex plane which do not iterate to the infinite energy fixed point. The Julia set is the boundary curve (plus its pre-images) which separates the initial points which are either attracted to infinity or to the stable cycle on the real axis. In our case, the

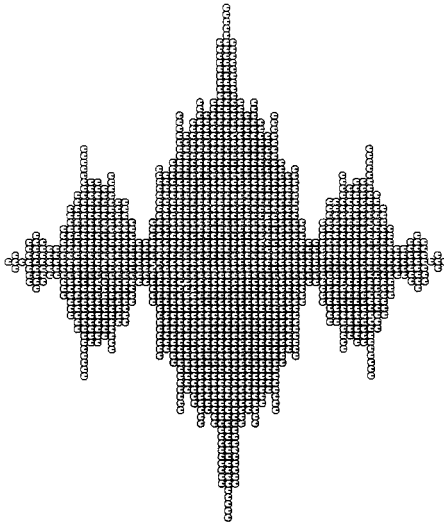


Figure 6. Set of points in the complex energy plane that are not mapped to infinity by (9).

Julia set represents the region in the complex plane where the Green functions are non-analytic.

If we allow the range of interactions to extend to $\pm N$ along the x and y axes, then for $N = 1$ we have only first and second neighbours. The map is a two parameter map:

$$\begin{aligned} X'(1, 0) &= \{2X(1, 1) + 2X(1, 0)^2\} / \{1 - 4X(1, 0)^2 + 4X(1, 1)^2\} \\ X'(1, 1) &= \{X(1, 0)^2 - 2X(1, 1)^2\} / \{1 - 4X(1, 0)^2 + 4X(1, 1)^2\}. \end{aligned} \quad (10)$$

Note that even if $X(1, 1) = 0$ initially, it becomes non-zero under iteration. The truncation of the exact transformation prevents the range from increasing further. Figure 7 shows the same region of the complex energy plane as figure 6 for increasing values of N . As the truncation procedure is improved, the region collapses to a line on the real axis which is the branch cut singularity of the exact Green functions.

For our procedure to converge, the initial values of the complex energy must lie outside these regions and thus there is a minimum value of the imaginary part E_2 required. This function is the Julia set and has a fractal structure. If we use a value of E_2 that is less than this value, then the procedure does not converge. In the calculations in § 3 our best results were obtained when the complex part of E was close to the fractal curve: (a) for the square lattice results in figure 2 we used a linear variation of E_2 from zero at the band edges to a maximum ($E_2\text{MAX}$) at the band centre, (b) in the case of the triangular lattice results in figure 4 we used a square root variation of E_2 from zero at the upper band edge ($E = 3.0$) to a maximum at zero energy and a fourth root variation from the lower band edge ($E = -1.5$), (c) the cubic lattice results in figure 5 were obtained using a square root variation of E_2 from the band edges to the centre.

Knowledge of the exact local density of states allows one to calculate the Green function $G(0, 0)$ anywhere in the complex E plane using the identity (Economou 1983)

$$G(0, 0) = \int_{-\infty}^{\infty} dx \rho(x) / (E - x). \quad (11)$$

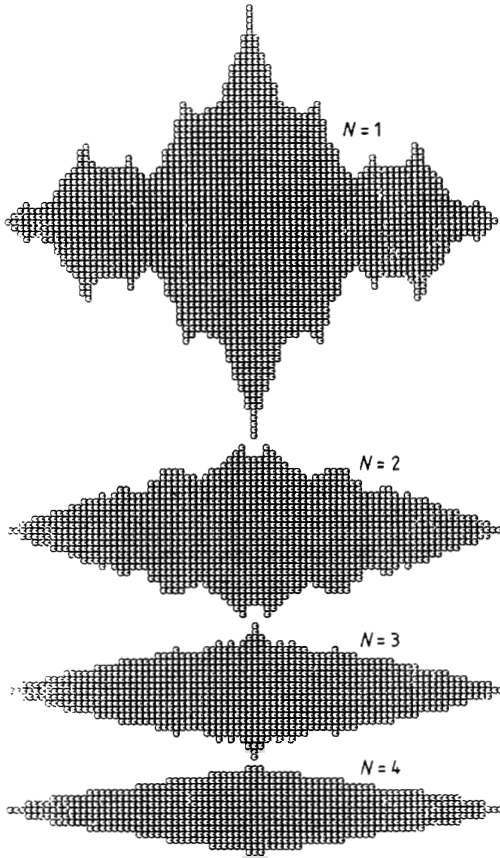


Figure 7. Set of points in the complex energy plane that are not mapped to infinity for truncations with $N = 1, 2, 3$ and 4 .

In each of the cases (a), (b) and (c) above we have evaluated $G(0, 0)$ along the chosen contours using the exact results for the local density of states $\rho(x)$ and we find excellent agreement with the values obtained using the truncated transformation.

5. Summary

An exact real space rescaling transformation for calculating lattice Green functions in two and three dimensions has been presented. The results are primarily concerned with understanding how the scheme performs in practice since truncation approximations are necessary to limit the growth of the interaction range at intermediate stages. We have shown that there is a useful connection between our truncated maps and the fractal patterns shown in figure 7. It is clear that the results improve when longer ranged interactions are allowed in the intermediate iterations but the computer time required rises rapidly. However, the present method could be combined with analytic continuation techniques to improve the results for the 3D lattices (Hass *et al* 1984). We are currently investigating this possibility.

For all lattices in both two and three dimensions the procedure rapidly converges for energies outside the band. Interactions up to fifth neighbours are all that are required to obtain accurate values for the real part of the Green functions in this energy region. Our procedure thus provides a very efficient way of investigating impurity problems which can be expressed in terms of the Green functions outside the band. Inside the band, we can evaluate the Green functions for a minimum value of the imaginary part of the energy which depends upon the range of truncation. Hence integrals over the density of states can be evaluated using our procedure by deforming the integration contour into the complex plane.

Recently, Oliveira *et al* (1984) have proposed a chaotic renormalisation group method for computing the density of states in two and three dimensions. Their method requires knowledge of the dispersion relation and is similar to a random sampling of points in k -space to evaluate Brillouin zone integrals (see Buchheit and Loly 1972 and references therein). In contrast, our procedure only requires the initial values of the tight-binding Hamiltonian matrix elements and leads directly to the complex lattice Green function at all energies and for any range of interaction expressed by the tight binding parameters. It also gives information on the nature of the singularities in contrast to other numerical methods. The transformations obtained in this paper are valid for any lattice that is translationally invariant. However, the technique does not rely upon this fact and can also be applied to systems without translational invariance such as fractal lattices (Tremblay and Southern 1983).

Acknowledgments

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