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On the asymptotic form of the recursion method basis vectors for periodic Hamiltonians

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Abstract. In previous studies of the recursion method, little attention has been paid to the properties of the basis vectors. We present the first detailed study of these for the case of a periodic Hamiltonian. In the examples chosen, the probability density scales linearly with n as $n \to \infty$, whenever the local density of states is bounded. Whenever it is unbounded and the recursion coefficients diverge, different scaling behaviour is found. These findings are explained and a scaling relationship between the asymptotic forms of the recursion coefficients and basis vectors is proposed.

1. Introduction

The recursion method (Haydock 1982) has been applied to a wide range of problems in solid state physics, involving electronic, vibrational and magnetic Hamiltonians, both periodic (perfect crystal) and disordered (amorphous solid, alloy).

The method starts with the choice of an initial vector, often localised at the origin. It proceeds by the recurrence relation

$$b_{n+1}|u_{n+1}\rangle = (H - a_n)|u_n\rangle - b_n|u_{n-1}\rangle \tag{1}$$

to define successive basis vectors $|u_n\rangle$, and coefficients a_n, b_n. This transforms the Hamiltonian into tridiagonal form. In physical terms this corresponds to a linear chain Hamiltonian with diagonal elements a_n and nearest-neighbour coupling b_n. The properties of these recursion coefficients have been widely studied (Turchi *et al* 1982, Beer and Pettifor 1983, Haydock 1982, 1980, etc). On the other hand little attention has been paid to the basis vectors. Hodges *et al* (1980) examined these for the case of a disordered Hamiltonian, in the mistaken belief that the periodic case was well understood. It has indeed been generally assumed that the basis vectors generated for a periodic Hamiltonian move outwards linearly from the origin but nothing approaching a rigorous justification of this assumption has yet been presented. For simple tight-binding Hamiltonians it is true, and trivially obvious, that the *leading edge* of the basis function moves out linearly, since it takes n applications of (1) to generate a non-zero element n steps from the origin (where a step corresponds to a non-zero coupling in the Hamiltonian). The question is—does such a relationship hold for, say, the mean radius of the basis vector, in the limit $n \to \infty$?

We shall address this question in various ways. Firstly, numerical calculations for simple tight-binding Hamiltonians will be shown to exhibit the anticipated linear

scaling, not only for the mean radius but also for the entire profile of the probability distribution (see also Raghavan 1984). However there are some surprises. In particular the probability density has the same anisotropy as the Hamiltonian, even in the asymptotic regime. Also, Hamiltonians with unbounded local densities of states associated with the initial vector will be shown to produce different behaviour, by recourse to a model which can be treated analytically. This leads us to suggest a relation between the scaling behaviour of the recursion coefficients, the basis functions and the form of the local density of states. Finally in § 5 we shall attempt to explain some of these results.

2. Numerical results

We shall look first at a simple tight-binding Hamiltonian of the form

$$H = \sum_{\substack{I,I' \\ \text{neighbours}}} |I\rangle\langle I'|, \tag{2}$$

where I and I' are nearest-neighbour sites of a two-dimensional periodic structure. The initial vector $|u_0\rangle$ has zero elements everywhere except at the origin. The basis vectors are calculated using (1) in the usual way (Haydock 1982).

For the square lattice in two dimensions (with lattice constant taken to be unity), the subsequent basis vectors are contained in a square of side $\sqrt{2}\,n$, oriented as shown in figure 1. Each has a probability density defined by

$$P_n(\boldsymbol{r}) = \sum_I |\langle I|u_n\rangle|^2 \delta(\boldsymbol{r} - \boldsymbol{r}_I) \tag{3}$$

where $\boldsymbol{r}_I$ denotes the position of site I. It is also useful to define the mean radius

$$r_n = \sum_I r_I |\langle I|u_n\rangle|^2, \tag{4}$$

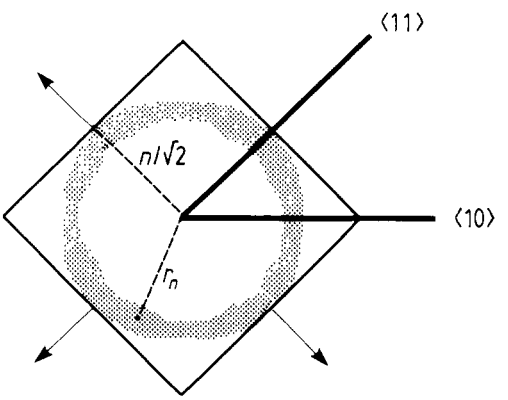

Figure 1. Schematic diagram of the probability density for the nth recursion basis vector $|u_n\rangle$ on a square lattice. The leading edge of the basis vector is shown by the square. All points on this square lie n steps from the origin. The region of substantial probability density is roughly indicated by the shaded area. Note that the probability density is symmetric but not isotropic.

and root-mean-square radius ρ_n according to

$$\rho_n^2 = \sum_I r_I^2 |\langle I|u_n\rangle|^2. \tag{5}$$

Calculation of the two radii gives an immediate indication of scaling behaviour. In the present case, they are both found to vary linearly with n, in the limit $n \to \infty$, for all the structures listed in table 1, which gives the coefficients of proportionality. Also indicated in each case is the corresponding coefficient for the closest point on the leading edge mentioned in § 1. The results listed imply that the probability density is concentrated in a shell close to the leading edge. It remains to examine the form of this shell.

Table 1. Scaling coefficients for the mean radius r_n and RMS radius ρ_n.

Structure	Numerical estimates		Approximate theory
	r_n/n	ρ_n/n	
2D square	0.645	0.653	0.707
triangular	0.710	0.723	0.866
hexagonal	0.615	0.626	0.750
3D simple cubic	0.511	0.517	0.577

Angular and radial distribution functions may be defined according to

$$F_n(\theta)\delta\theta = \sum_{\theta \leqslant \theta_I < \theta + \delta\theta} |\langle I|u_n\rangle|^2 \tag{6}$$

and

$$G_n(r)\delta r = \sum_{r \leqslant r_I < r + \delta r} |\langle I|u_n\rangle|^2. \tag{7}$$

These have been calculated for $1 \leqslant n \leqslant 99$ to investigate the form of $P_n(\boldsymbol{r})$. The radial function behaves as

$$G_n(r) \sim n^{-1} g(r/n) \tag{8}$$

as shown in figure 2. The angular function behaves as

$$F_n(\theta) \to f(\theta) \tag{9}$$

where $f(\theta)$ is as shown in figure 3. Together these results imply that

$$P_n(\boldsymbol{r}) \sim n^{-1} p(n^{-1}\boldsymbol{r}) \tag{10}$$

as anticipated, but the anisotropy of this function ($f(\theta) \neq$ constant) was unexpected.

Equation (8) should be compared with

$$G_n(r) \sim n^{-\alpha} g(n^{-\alpha} r) \tag{11}$$

found by Hodges *et al* (1980) for the disordered case, where

$$\alpha = \tfrac{1}{2} \qquad \text{(two dimensions)} \tag{12}$$

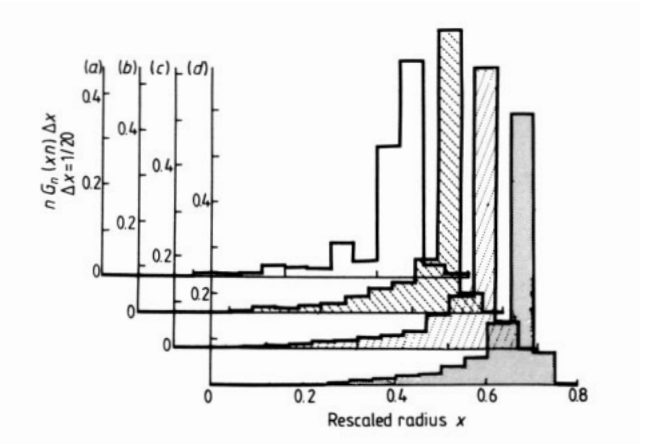

Figure 2. Histograms of the radial distribution function for the square lattice, rescaled as $nG_n(xn)$, to show linear scaling for the cases (a)–(d), $n = 20$, 40, 60, 80 respectively.

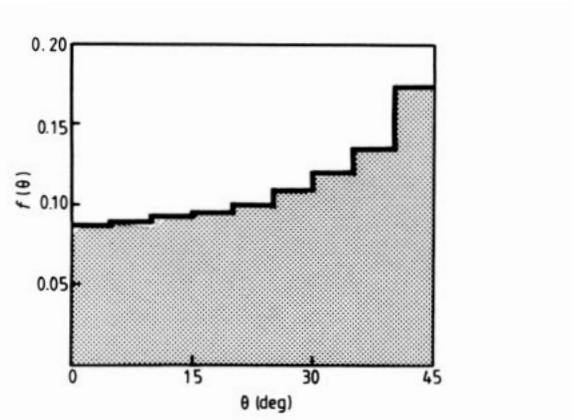

Figure 3. The asymptotic form of the angular distribution function $f(\theta)$ for the square lattice, for θ between 0° (the ⟨10⟩ direction) and 45° (the ⟨11⟩ direction), calculated by averaging $F_n(\theta)$ from $n = 75$ to 99.

and it was suggested that

$$\alpha = d^{-1} \qquad (d \text{ dimensions}). \tag{13}$$

The radial distribution function $G_n(r)$ is even more sharply peaked at the leading edge than is apparent in figure 2. $G_{80}(r)$ is plotted in figure 4 with a smaller bin size. It can be seen that about half of its weight lies between $r = 55$ and $r = 57$. The closest point of the leading edge is at $r = 80/\sqrt{2} = 56.6$.

Such linear scaling implies that the basis vectors do not form a complete set in the original space spanned by the vectors $|I\rangle$. This can be seen as follows.

If the transformation were complete, this would require that

$$\sum_n |u_n\rangle\langle u_n| = \sum_I |I\rangle\langle I| \tag{14}$$

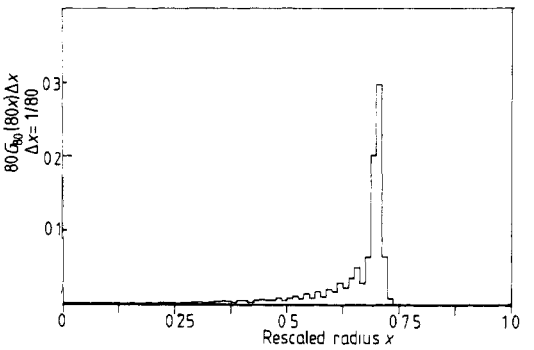

Figure 4. The scaled radial distribution function $nG_n(xn)$ for $n = 80$, plotted with a smaller bin size than in figure 2 to emphasise its sharply peaked structure at $r/n = x = 1/\sqrt{2}$.

and hence

$$\sum_n |\langle u_n | I \rangle|^2 = 1 \tag{15}$$

for all I.

Linear scaling means that

$$\sum_n |\langle u_n | I \rangle|^2 \sim r_I^{-1} \lim_{m\to\infty} \int_0^\infty \frac{m}{r} G_m(r)\, dr \sim r_I^{-1} \int_0^\infty dr\, r^{-1} g(r). \tag{16}$$

Since the integral is just a constant (1.64 for the case at hand—see figure 5), this is incompatible with (15).

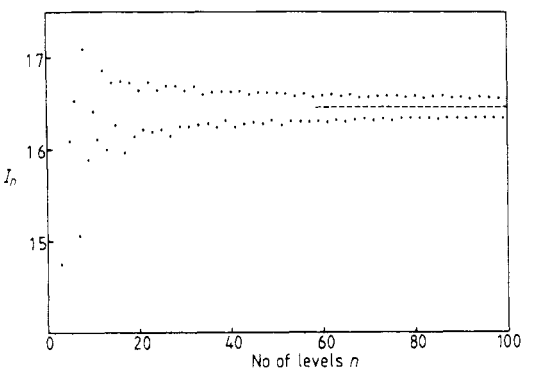

Figure 5. The integral $I_n = \int_0^\infty (n/r) G_n(r)\, dr$, calculated for $n = 1$–99. This approaches the constant value 1.644 as $n \to \infty$, providing further confirmation of linear scaling.

3. Analytic model with bounded density of states

In this section we examine a simple model which is susceptible to a straightforward analytic treatment, and shows similar behaviour to that found in § 2. It consists merely of the free electron model, with an appropriate initial basis function. The Hamiltonian is

$$H = -(\hbar^2/2m)\nabla^2 \tag{17}$$

and the initial function has circular symmetry and the radial dependence

$$u_0(r) = \pi^{-1/2} r^{-1} J_1(\lambda r) \tag{18}$$

where J is a Bessel function, and λ is an arbitrary length. This was obtained by integrating the eigenfunctions of (17) up to a maximum energy $\varepsilon = (\hbar^2/2m)\lambda^2$. The local density of states associated with the initial function is

$$\begin{aligned} n_0(E) &= \varepsilon^{-1}, \qquad 0 < E < \varepsilon, \\ &= 0, \qquad \text{otherwise}, \end{aligned} \tag{19}$$

and the recursion coefficients (Haydock 1980)

$$a_n = \tfrac{1}{2}\varepsilon, \qquad b_n = \tfrac{1}{2}n\varepsilon(4n^2-1)^{-1/2}. \tag{20}$$

The basis functions are

$$u_n(r) = [(2n+1)^{1/2}/\pi^{1/2} r] J_{2n+1}(\lambda r).$$

The corresponding radial probability distribution is given by

$$G_n(r) = [2(2n+1)/r] J_{2n+1}^2(\lambda r). \tag{21}$$

There is of course no angular dependence, since (17) has circular symmetry.

The asymptotic form of this function is given by (8) with

$$\begin{aligned} g(x) &= 0, \qquad \lambda x \leqslant 2, \\ &= 4/\pi\lambda x(\lambda^2 x^2 - 4)^{1/2}, \qquad \lambda x > 2. \end{aligned} \tag{22}$$

This is illustrated in figure 6, which also shows that G converges quite rapidly to its asymptotic form.

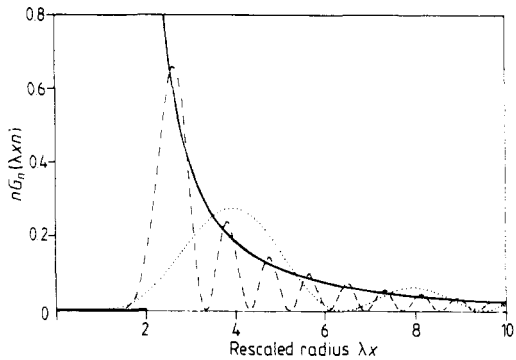

Figure 6. The scaled radial distribution function for the Hamiltonian and starting vector of § 3, for $n = 1$ (· · · ·) and $n = 4$ (– – –). The asymptotic form is shown by the full curve.

The transformation is again not complete. The quantity

$$\sum_{n=0}^{\infty} u_n^2(r) = \frac{1}{\pi r^2} \sum_{n=0}^{\infty} (2n+1) J_{2n+1}^2(\lambda r) = \frac{\lambda^2}{4\pi}[J_0^2(\lambda r) + J_1^2(\lambda r)], \tag{23}$$

which corresponds to (16), falls off as r^{-1} at large r (Abramowitz and Stegun 1965). This is the same behaviour as was noted in § 2.

4. Analytic model with unbounded local density of states

By changing the choice of initial basis function we shall now show that this is critical to the asymptotic properties under study, since these are changed if the local density of states is unbounded.

The Hamiltonian of § 3 is used again. For convenience, we shall discuss the three-dimensional case, since we can avail ourselves of the previous work of Haydock (1980) for this. Similar results apply in two dimensions.

We choose for the initial function the Gaussian

$$u_0(r) = (\lambda/\sqrt{\pi})^{3/2} \exp[-(\lambda r)^2/2] \tag{24}$$

for which the local density of states is

$$\begin{aligned} n_0(E) &= (2/\varepsilon)(E/\varepsilon\pi)^{1/2} \mathrm{e}^{-E/\varepsilon}, && E > 0, \\ &= 0, && E < 0. \end{aligned} \tag{25}$$

The recursion coefficients are

$$a_n = \varepsilon(2n + \tfrac{3}{2}), \qquad b_n = \varepsilon[n(n + \tfrac{1}{2})]^{1/2}, \tag{26}$$

and the basis vectors are

$$u_n(r) = [\tfrac{1}{2}!\, n!/(n + \tfrac{1}{2})!]^{1/2} L_n^{1/2}(\lambda^2 r^2) u_0(r) \tag{27}$$

where $L_n^{1/2}$ is a Laguerre polynomial of order $\frac{1}{2}$.

Note that a_n and b_n diverge linearly, in contrast to the convergence to finite limits in the case of a bounded local density of states.

The mean radius of (27) is

$$r_n = (4/\pi\lambda)(n + \tfrac{1}{2})!/n! \sim (4/\pi\lambda) n^{1/2}, \tag{28}$$

again contrasting with the previous case. Presumably other choices of initial function can generate other powers. It is tempting to speculate on the relation between the indices in the asymptotic forms $r \sim n^{\alpha}$, $a_n, b_n \sim n^{\beta}$, and $n_0(E) \sim \exp(-E^{\gamma})$. The coefficients a_n and b_n can be calculated directly from $n_0(E)$. For $n_0(E) \sim \exp(-E)$, $b \sim n$, while if $n_0(E) \sim \exp(-E^2)$, then $b \sim n^{1/2}$ (Gaspard and Cyrot-Lackmann 1973). We suggest that $\beta = \gamma^{-1}$. The nth basis state corresponds to an energy $a_n \sim n^{\beta}$. As n increases the basis functions move outwards in real space and also, for $\beta > 0$, are composed of states of increasing energy. These higher energy states can be localised in the same region of space as were the previously used states. Hence increasing β should reduce the rate of radial expansion. We suggest $\alpha = (1 + \beta)^{-1}$, which is consistent with the results given above for $\beta = 0$ and 1. It will be interesting to see whether this is sustained by further tests.

5. General theory

We here seek to understand why the probability density function $P_n(r)$ scales linearly with n for asymptotically constant recursion coefficients. We have as yet no explanation for the form of the scaling function but will give an approximate treatment which leads to scaling behaviour. The argument (essentially due to Hodges, private communication) is readily adapted to obtain the result $r_n \sim n^{1/2}$ in the case where a_n and $b_n \sim n$.

Consider a linear chain whose recursion coefficients a_n and b_n approach the constant values a and b as $n \to \infty$. The eigenfunctions of this chain are then asymptotically of the form

$$|\psi_K\rangle = \sum_n \sin(Kn)|u_n\rangle \tag{29}$$

so, for large n,

$$|u_n\rangle = \int_0^\pi \mathrm{d}K \sin(Kn)|\psi_K\rangle. \tag{30}$$

In real space, $|\psi_K\rangle$ is an eigenstate having the symmetry of the starting orbital $|u_0\rangle$ and of the structure under consideration (e.g. the two-dimensional square lattice). Near one of the band edges and for large r, ψ_K must be

$$\psi_K = (\sin kr)/r^{(d-1)/2}, \tag{31}$$

where d is the dimensionality of the lattice.

If we compare energies on the linear chain and in the band structure of the d-dimensional lattice we can relate k and K. For the case of the 2D square lattice $k^2 = 2K^2$. In general $k^2 = cK^2$. So, using (31) as an approximation to ψ_K in (30), we obtain

$$\begin{aligned} u_n(r) &= r^{-(d-1)/2} \int_0^\pi \mathrm{d}K \sin Kn \sin(\sqrt{c}Kr) \\ &= r^{-(d-1)/2} n^{-1} \int_0^{n\pi} \mathrm{d}x \sin x \sin(n^{-1}\sqrt{c}rx). \end{aligned} \tag{32}$$

In the limit $n \to \infty$, the radial probability distribution $G_n(r)$ behaves as

$$G_n(r) \sim \delta(n/\sqrt{c} - r) \tag{33}$$

where $c = 2$ for the square lattice. Hence we have shown that, within the stated approximation, G_n will scale linearly with n and the radial probability function is confined to a shell at the leading edge of the recursion vector. However, this argument fails to account for the detailed form of the function, described in previous sections. Nor is it clear how the argument may be improved. Note also that it fails to explain the anisotropy of the actual function.

To calculate the full form of the scaling function, we should use the exact expression for the basis vector.

This is given by (Haydock 1980)

$$|u_n\rangle = \sum_{\boldsymbol{k}} |\psi_{\boldsymbol{k}}\rangle\langle\psi_{\boldsymbol{k}}|u_0\rangle \mathscr{P}_n(E_{\boldsymbol{k}}) \tag{34}$$

where $|\psi_{\boldsymbol{k}}\rangle$ is a lattice wavefunction, the sum over $\boldsymbol{k}$ is over the full Brillouin zone and $\mathscr{P}_n$ is an orthogonal polynomial of order n, defined by

$$b_{n+1}\mathscr{P}_{n+1}(E) = (E - a_n)\mathscr{P}_n(E) - b_n\mathscr{P}_{n-1}(E). \tag{35}$$

For a Hamiltonian defined on a lattice, the wavefunctions are simply Bloch states and hence (34) becomes

$$u_n(\boldsymbol{r}) = \sum_{\boldsymbol{k}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} \mathscr{P}_n(E_{\boldsymbol{k}}) = \int_{E_{\min}}^{E_{\max}} \mathrm{d}E\, \mathscr{P}_n(E) \int_{E(\boldsymbol{k})=\text{constant}} \mathrm{d}l \frac{\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}}{|\nabla_{\boldsymbol{k}} E|}. \tag{36}$$

We are unable to find the form of (36) in any useful limit, despite the availability of general asymptotic forms for orthogonal polynomials (Szego 1939). It is clear, however, that the anisotropy of the scaling function is associated with the r dependence of the contour integral. It would also appear that the detailed form of the function is dependent on the full band structure and not just the band edges.

6. Conclusion

In our numerical calculations for simple tight-binding Hamiltonians we have found linear scaling of the probability density function in every case. Our approximate theory is consistent with this. However, the scaling function was found to have a much richer structure in the numerical calculations than was expected. It is anisotropic and, while it is sharply peaked at the distance at which it is concentrated in the approximate theory, it has a tail extending back to the origin.

Analytically soluble models, which do not involve a lattice, indicate that this linear scaling is characteristic of an ordered Hamiltonian with a bounded density of states. For an unbounded density of states with recursion coefficients increasing linearly with n, the probability density expands as $n^{1/2}$.

The behaviour described here is to be contrasted with that previously found by Hodges *et al* (1980) for disordered Hamiltonians. In this case the probability density appears to expand as $n^{1/d}$ in d dimensions. The transition between the two regimes, as disorder is increased from zero, remains to be explored.

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