Periodic and quasiperiodic wavefunctions in a class of one-dimensional quasicrystals: an analytical treatment

Periodic and quasiperiodic wavefunctions in a class of one-dimensional quasicrystals: an analytical treatment

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Abstract. The one-dimensional, discrete Schrödinger equation is studied analytically for a class of quasiperiodic Hamiltonians known as the copper mean. The lattice is described by a recursion formula $S_{L+1} = S_{L-1}S_{L-1}S_L$, $L = 2, 3, \ldots$, given the two initial sequences S_0 and S_1. Extended states are shown to exist for energies satisfying $\mathrm{Tr}\,\mathbf{T}_L = 0$ and $\mathrm{Tr}\{(\mathbf{T}_0)^{-2}\mathbf{T}_1\} = 2$ where $\mathbf{T}_L$ is the transfer matrix for the Lth generation of the quasicrystal. Also, periodic states are shown to exist quite generally in a subclass of the copper mean. A specific one-dimensional quasicrystal is given as an example of this, and is shown to have exclusively periodic states.

1. Introduction

Since the experimental discovery (Shechtman *et al* 1984) that the diffraction pattern of a rapidly cooled AlMn alloy can show sharp Bragg peaks of crystallographically forbidden symmetry, and the theoretical work by Levine and Steinhardt (1984) showing that such patterns are to be expected from certain ordered structures without translational symmetry, quasicrystals have been a subject of great interest. The advent of new experimental techniques allowing for the fabrication of high-quality superlattices including quasi-period ones (Merlin *et al* 1985, Karkut *et al* 1986) has further increased the efforts to understand these, in many ways, exotic materials. The physical properties of one-dimensional periodic systems are generally very different from those of disordered systems. For example, the electronic energy spectrum of a periodic lattice is known to consist of absolutely continuous bands (Reed and Simon 1978) and the wavefunctions are all extended. This is in sharp contrast to amorphous one-dimensional solids which have pure point spectrum and exclusively exponentially localised states. The study of quasicrystals has introduced a new class of systems in many ways intermediate between the periodic and amorphous extremes. The by far most studied one-dimensional quasicrystal, the Fibonacci sequence which is best described by the substitution rule A → AB, B → A, is generally believed to have a Cantor set spectrum of zero Lebesgue measure and exclusively critical states (Kohmoto *et al* 1987, Kohmoto *et al* 1983). These states are neither localised nor extended in the classical sense, but something intermediate. The study of other quasicrystals has unveiled a wealth of systems with

properties ranging from crystal-like to random-like and mixtures of the two. For example, the Rudin–Shapiro and the Thue–Morse chains show random-like and crystal-like hopping conduction respectively (Aldea and Dulea 1988) Also, numerical calculations indicate extended 'Bloch-like' electronic states in the Thue-Morse quasicrystal (Riklund *et al* 1987) as well as localised, critical and extended states in the system given by the inflation rule A → ABBB, B → A (Severin and Riklund 1989). Bloch-like spinwaves has also been found (Riklund and Severin 1988) in an aperiodic ferromagnetic crystal of the Thue–Morse type. For some realisations of quasicrystals generated by $S_{L+1} = S_{L-1}S_{L-1}S_L$, $L = 2, 3, \ldots$. numerical analysis shows the existence of localised electronic states (Gumbs and Ali 1988a) and extended magnetic excitations (Kolár and Ali 1989).

   In this paper we study the electronic eigenstates of a class of quasicrystals generated by the inflation scheme

$$S_{L+1} = S_{L-1}^2 S_L \tag{1}$$

where S_L denotes the Lth generation of the quasicrystal. Given two starting sequences S_0 and S_1, the sequence S_L is thus totally determined. The model considered here is the on-site tight-binding model with the equation of motion given by

$$\psi_{n+1} + \psi_{n-1} + V_n\psi_n = E\psi_n \tag{2}$$

where ψ_n denotes the wavefunction on site n, V_n the site energy and E the eigenenergy of the electron. The diagonal elements V_n are given by $V_A(V_B)$ if n is a site of type A (B). The nearest neighbour hopping integral, t, is set equal to unity throughout this paper. The existence of extended states and, in a subclass of (1), periodic states is shown analytically for certain energies.

2. Transfer matrix and trace map formalism

It is very useful to write equation (2) as

$$\begin{bmatrix} \psi_{n+1} \\ \psi_n \end{bmatrix} = \mathbf{M}(n) \begin{bmatrix} \psi_n \\ \psi_{n-1} \end{bmatrix} \qquad \mathbf{M}(n) = \begin{bmatrix} E - V_n & -1 \\ 1 & 0 \end{bmatrix} \tag{3}$$

and to define the total transfer matrix $\mathbf{T}_L$ for a chain of generation L and length N as

$$\mathbf{T}_L = \mathbf{M}(N)\mathbf{M}(N - 1) \ldots \mathbf{M}(2)\mathbf{M}(1).$$

The energy spectrum for a system of length N and periodic boundary conditions is now taken to be the set (Reed and Simon 1978)

$$\{E \mid |X_L| \leqslant 2\} \qquad X_L = \mathrm{Tr}\,\mathbf{T}_L(E)$$

where, for systems satisfying (1), we have the following map.

$$X_{L+1} = X_L(X_{L-1}^2 - 2) - \gamma \qquad \gamma = \mathrm{Tr}[\mathbf{T}_{L-1}^{-2}\mathbf{T}_L]. \tag{4}$$

It should be noted that γ is an invariant of the map (1). The trace map (4) has previously been studied numerically by Gumbs and Ali (1988b) who found a large number of bounded orbits and for the particular choice $\gamma = 2$ a dense set of initial points giving non-escaping orbits. This is in sharp contrast to the maps derived from systems satisfying $L_{L+1} = (S_L)^2S_{L-1}$ where the non-escaping points lie on a set of zero Lebesgue measure

and the wavefunctions are all critical. For the special case $\gamma = 2$, the trace map has the following non-escaping orbit; $X_L = 0$, $X_{L+1} = -2$ and $X_{L+K} = 2$, $K \geq 2$. The aim of this paper is to show that the eigenenergies giving rise to these orbits correspond to extended, and in a special class of systems satisfying (1) even periodic, eigenstates.

3. Solution of the equation of motion

First, we need to observe that an arbitrary generation L of the chain S_L can be constructed as a sequence consisting of only two different sub-sequences S_K and $S_{K-1}S_{K-1}$, where $K < L$, i.e.

$$S_2 = S_0S_0S_1 \qquad S_3 = S_1S_1S_2 = S_1S_1S_0S_0S_1$$

$$S_4 = S_2S_2S_3 = S_0S_0S_1S_0S_0S_1S_1S_1S_0S_0S_1 \text{ etc.}$$

Note that S_K and $S_{K-1}S_{K-1}$ always occur an odd number of times each in S_L. If N is the number of sites in S_L, we can write the periodic boundary conditions as

$$\begin{bmatrix} \psi_{N+1} \\ \psi_N \end{bmatrix} = \mathbf{T}_L \begin{bmatrix} \psi_1 \\ \psi_0 \end{bmatrix} = \begin{bmatrix} \psi_1 \\ \psi_0 \end{bmatrix}. \tag{5}$$

If, for a particular eigenenergy E, $X_K = 0$ then $(\mathbf{T}_K)^2 = -\mathbf{I}$ where $\mathbf{I}$ is the 2×2 identity matrix. This follows since for 2×2 unimodular matrices $\mathbf{T}^2 = \mathbf{T} \, \text{Tr} \, \mathbf{T} - \mathbf{I}$. Furthermore, the following relation holds for 2×2 unimodular matrices satisfying $\text{Tr} \, \mathbf{T} = -2$.

$$\mathbf{T}^n = (-1)^{n+1} n\mathbf{T} + (-1)^{n+1}(n-1)\mathbf{I}. \tag{6}$$

A proof is given in the appendix. Observing then that if $X_K = 0$ then $(\mathbf{T}_K)^2$ and $\mathbf{T}_{K+1}$ commutes and the boundary condition (5) can, using (6), be written

$$\begin{bmatrix} \psi_{N+1} \\ \psi_N \end{bmatrix} = -\begin{bmatrix} n(\mathbf{T}_{K+1})_{11} + (n-1) & n(\mathbf{T}_{K+1})_{12} \\ n(\mathbf{T}_{K+1})_{21} & n(\mathbf{T}_{K+1})_{22} + (n-1) \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_0 \end{bmatrix} = \begin{bmatrix} \psi_1 \\ \psi_0 \end{bmatrix} \tag{7}$$

where n is number of sub-sequences S_{K+1} in the whole chain S_L containing N sites. Equations (7) can also be written

$$(\mathbf{T}_{K+1})_{11} \psi_1 + (\mathbf{T}_{K+1})_{12} \psi_0 = -\psi_1$$
$$(\mathbf{T}_{K+1})_{21} \psi_1 + (\mathbf{T}_{K+1})_{22} \psi_0 = -\psi_0 \tag{8}$$

Given that $\text{Det} \, \mathbf{T}_{K+1} = 1$ and $\text{Tr} \, \mathbf{T}_{K+1} = -2$, equations (8) are actually equivalent and have the solutions

$$\psi_1 = -\frac{(\mathbf{T}_{K+1})_{12}}{((\mathbf{T}_{K+1})_{11} + 1)} \psi_0 \qquad (\mathbf{T}_{K+1})_{11} \neq -1 \tag{9}$$

$$(\mathbf{T}_{K+1})_{12} \psi_0 = 0 \qquad (\mathbf{T}_{K+1})_{21} \psi_1 = 0 \qquad (\mathbf{T}_{K+1})_{11} = -1.$$

Since equations (7)–(9) are all independent of n it is obvious that

$$\begin{bmatrix} \psi_{n+p_1+1} \\ \psi_{n+p_1} \end{bmatrix} = \mathbf{T}_{K+1} \begin{bmatrix} \psi_{n+1} \\ \psi_n \end{bmatrix} = -\begin{bmatrix} \psi_{n+1} \\ \psi_n \end{bmatrix}$$
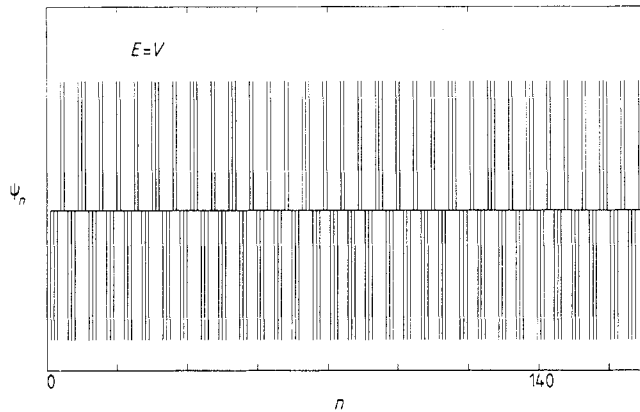
and

Figure 1. The wavefunction with eigenenergy $E = 1.0$ for the copper mean with $S_0 = $ A, $S_1 = $ ABA, $V_A = 1.0$, $V_B = -1.0$. $\gamma(E = 1.0) = 2$ and $X_0 = 0$. The quasiperiodic character of the wavefunction is clearly seen.

$$\begin{bmatrix} \psi_{n+p_0+1} \\ \psi_{n+p_0} \end{bmatrix} = \mathbf{T}_K^2 \begin{bmatrix} \psi_{n+1} \\ \psi_n \end{bmatrix} = - \begin{bmatrix} \psi_{n+1} \\ \psi_n \end{bmatrix}$$

where p_0 and p_1 denote the lengths of $S_K S_K$ and S_{K+1} respectively. The result of $\mathbf{T}_K \mathbf{T}_K$ or $\mathbf{T}_{K+1}$ acting on (ψ_{n+1}, ψ_n) is just $(-\psi_{n+1}, -\psi_n)$. The wavefunction will thus, to within a change of sign, be the same in every block S_{K+1} of the chain, and the same argument holds for the blocks $S_K S_K$. There will thus be no decay of the wavefunctions on length scales of the order of S_{K+1}, i.e. the states are extended. In general these states will not be periodic, instead they will have the same symmetry as the lattice itself. The wavefunction will be quasiperiodic. In figure 1 we show a quasiperiodic wavefunction computed for the system obeying (1) with $S_0 = $ A, $S_1 = $ ABA. The sequence is thus given by AAABAAAABAABAABAAAABA .... The eigenenergy is $E = 1.0$ satisfying $X_0 = 0$. The on-site energies used are $V_A = V$, $V_B = -V$, $V = 1.0$.

4. Systems with periodic solutions

In this section we will describe how periodic solutions to the three term recurrence relation (2) can arise from a quasiperiodic distribution of V_n. The validity of the reasoning is by no means limited to binary sequences but can easily be extended to quasicrystals with three or more different site energies. As an illustration, we shall give one simple example of a binary quasicrystal where all solutions of (2) subject to the boundary conditions (5) or to Dirichlet boundary conditions ($\psi_N = \psi_0 = 0$) will be periodic such that $\psi_{n+p} = \psi_n$, where P is the length of the block S_{K+2} if the eigenenergy, E, satisfies $X_K(E) = 0$. Consider a quasicrystal built according to the inflation rule (1) with the two initial words S_0 and S_1 given by $S_0 = x^0 S^0$, $S_1 = y^0 S^0 x^0 S^0$, where S^0 is an arbitrary word and x^0, y^0 are two arbitrary letters. Then, since $S_2 = S_0 S_0 S_1 = x^0 S^0 x^0 S^0 y^0 S^0 x^0 S^0 = y^1 S^1 x^1 S^1$ and $S_1 = x^1 S^1$ with $S^1 = S^0 x^0 S^0$, $x^1 = y^0$ and $y^1 = x^0$, it follows from induction that

$$S_K = x^K S^K \qquad S_{K+1} = y^K S^K x^K S^K \qquad K = 1, 2, 3 \ldots$$
$$S^{K+1} = S^K x^K S^K \qquad x^{K+1} = y^K \qquad y^{K+1} = x^K. \tag{10}$$
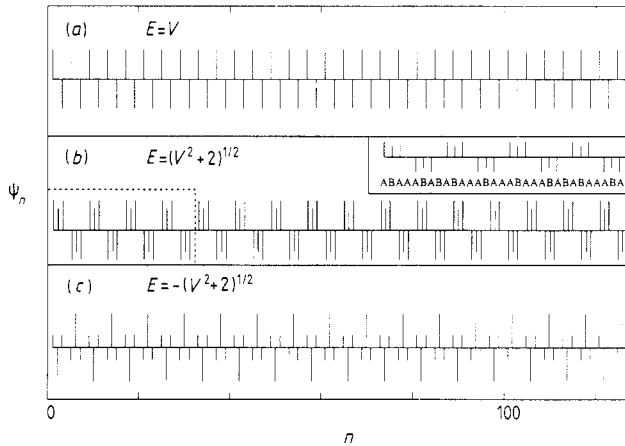
From the map (1), it also follows that the matrix

Figure 2. Periodic wavefunctions for the copper mean lattice with $S_0 = A$, $S_1 = BA$, $V_A = 1.0$, $V_B = -1.0$, $\gamma = 2$. In this model γ is energy independent. The eigenenergies are $E = 1.0$, $E = \sqrt{3.0}$ and $E = -\sqrt{3.0}$ respectively satisfying $X_0 = 0$, $X_1 = 0$ and $X_1 = 0$. The states are periodic with periods 4, 8 and 8 sites. The periods P satisfy $P = 2^{K+2}$ if $X_K(E) = 0$. The inset to figure 2(b) shows ψ_n for $0 \leq n \leq 32$ together with the first 32 letters in the sequence. The physical reason for the periodicity of the solution is that $\psi_n = 0$ on the sites separating the periodically repeated subword. The electron thus 'feels' only the periodic sublattice.

$$\mathbf{W}_K \equiv \mathbf{T}_{K+1}(\mathbf{T}_K)^{-2} = (\mathbf{T}_{K-1})^2(\mathbf{T}_K)^{-1} = [\mathbf{T}_K(\mathbf{T}_{K-1})^{-2}]^{-1} \equiv (\mathbf{W}_{K-1})^{-1}.$$

Notice also from (10) we may write symbolically

$$S_{K+1}(S_K)^{-2} = y^K S^K x^K S^K (S^K)^{-1}(x^K)^{-1}(S^K)^{-1}(x^K)^{-1} = y^K(x^K)^{-1} \tag{11}$$

Assume now $X_K = 0 \Rightarrow (\mathbf{T}_K)^2 = -\mathbf{I}$. Then, from (11), $\mathbf{W}_K = -\mathbf{T}_{K+1} = \mathbf{Y}_K(\mathbf{X}_K)^{-1}$ where $\mathbf{X}_K$ and $\mathbf{Y}_K$ are the transfer matrices corresponding to the letters x^K and y^K respectively.

$$\mathbf{X}_K = \begin{bmatrix} E - V_{x^K} & -1 \\ 1 & 0 \end{bmatrix}, \quad \mathbf{Y}_K = \begin{bmatrix} E - V_{y^K} & -1 \\ 1 & 0 \end{bmatrix}, \quad \mathbf{Y}_K\mathbf{X}_K^{-1} = \begin{bmatrix} 1 & V_{x^K} - V_{y^K} \\ 0 & 1 \end{bmatrix}$$

Observe that the trace map invariant γ is given by $\gamma = \mathrm{Tr}\,\mathbf{W}_K = \mathrm{Tr}\,\mathbf{W}_{K+1} = 2$. Here obviously $(\mathbf{T}_{K+1})_{11} = -1$ and the second of equations (9) apply. Since we are interested in the non-periodic case $x^K \neq y^K$, $(\mathbf{T}_{K+1})_{12} \neq 0 \Rightarrow \psi_0 = 0$. Also, observing that $S_K S_K$ and S_{K+1} contain the same number, p, of letters, and recalling that the effect of $\mathbf{T}_k\mathbf{T}_k$ or $\mathbf{T}_{k+1}$ acting on ψ is only a change of sign, we have

$$\begin{bmatrix} \psi_{np+1} \\ \psi_{np} \end{bmatrix} = (-1)^n \begin{bmatrix} \psi_1 \\ \psi_0 \end{bmatrix} = (-1)^n \begin{bmatrix} \psi_1 \\ 0 \end{bmatrix} \qquad n = 1, 2, 3 \ldots \tag{12}$$

Since the blocks $S_K S_K$ and S_{K+1} are identical except for the last letter and the input values, by (12), alternate only in sign, the solutions in two consecutive blocks are the negative of each other. Therefore the wavefunction clearly obeys

$$\psi_{n+2p} = -\psi_{n+p} = \psi_n$$

and is thus indeed periodic with periodicity $2p$. In figure $2(a)$–(c) the periodic solutions for the quasicrystal $S_0 = A$, $S_1 = BA$, $S_2 = AABA$ with eigenenergies $E = V$, $E =$
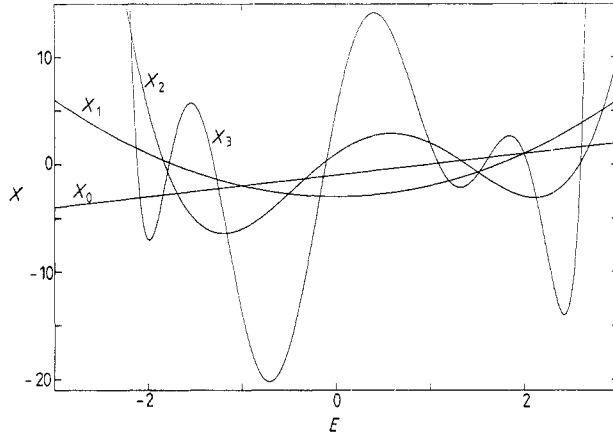
Figure 3. The traces X_0, X_1, X_2 and X_3 for the copper mean with $S_0 = A$, $S_1 = BA$, $V_A = 1.0$, $V_B = -1.0$. The number of zeros of X_K is seen to be 2^K. The cycle $X_0 = 0$, $X_1 = 2$, $X_2 = 2$, $X_3 = 2 \ldots$ is also seen.

$(V^2 + 2)^{1/2}$ and $E = -(V^2 + 2)^{1/2}$ are displayed. The lattice is thus represented by the sequence BABAAABABABAAABAAABAAABABABAAABA .... This quasicrystal can be constructed according to the above scheme by letting S^0 be the empty word, $x^0 = A$ and $y^0 = B$. The energies chosen satisfy $X_0 = 0$, $X_1 = 0$ and $X_1 = 0$ respectively. We therefore expect the corresponding wavefunctions in figure 2(a)–(c) to have the periodicities 4, 8 and 8. From the figure, the origin of periodicity described above, is easily seen. The lattice is, as we have shown, built up from periodic repetition of blocks S^K separated only by one A or B site. Since the wavefunction is zero on those sites it is not affected by the deviation from lattice periodicity introduced by these sites. The electron effectively 'sees' a periodic lattice.

It may seem as the requirement that the energy should satisfy $X_K = 0$ for some K is very strong and that the number of eigenstates for which this treatment is valid therefore in general should be small. This is, however, not the case which is illustrated by the example $S_0 = A$, $S_1 = BA$. Here $X_0 = E - V$ and $X_1 = E^2 - V^2 - 2$ and from (4) we see that $X_K \to \infty$ as $E \to \pm\infty$, $K \geq 1$. Then, assuming $X_0(E_0) = 0 \Rightarrow X_1(E_0) = -2$ and $X_K(E_0) = 2$ $K > 1$, X_1 must have two real roots, one to the left and one to the right of E_0. By the same reasoning X_2 has 4 roots, two roots between the three previous ones, one root to the left of the leftmost and one to the right of the rightmost root of X_1. The argument is illustrated in figure 3 which shows X_0, X_1, X_2 and X_3 as functions of energy. By induction then the number of distinct real roots of X_K is 2^K and the total number of roots of X_0, X_1, $X_2 \ldots X_{L-1}$ satisfying the boundary conditions for a chain S_L of generation L is $\Sigma_{n=0,L-1} 2^n = 2^L - 1$. Note that all roots have multiplicity one since X_K is a polynomial of degree 2^K and that no energy can be the root of more than one X_K since $X_K = 0 \Rightarrow X_{K+1} = -2$, $X_{K+N} = 2$, $N \geq 2$. We may therefore conclude that all wavefunctions satisfying $\psi_N = \psi_0 = 0$ are periodic.

5. Summary

We have performed an analytical treatment of a class of quasicrystals with an inflation rule given by $S_{L+1} = S_{L-1}S_{L-1}S_L$. The existence of extended and in a subclass even

periodic states is shown. A specific example with exclusively periodic states satisfying Dirichlet boundary conditions is given. This class of quasicrystals has previously been studied by Gumbs and Ali under the name copper mean lattices. They performed a numerical study of the trace map for the two classes $S_{L+1} = (S_{L-1})^n S_L$ and $S_{L+1} = S_{L-1}(S_L)^n$ and concluded that in terms of the escape rates the two classes should be considered to be the reverse of each other (Gumbs and Ali 1988b). The latter class above is generally believed to have only critical states whereas numerical calculations has shown electronic localisation (Gumbs and Ali 1988a) and extended magnetic excitations (Kolár and Ali 1989) for copper mean lattices. The analytical results presented in this work agrees with the above conclusion. Considering also the numerical finding that the system $S_{L+1} = (S_{L-1})^3 S_L$ gives rise to both localised, critical and extended states (Severing and Riklund 1989) gives further evidence that the first class above is indeed very different from the second.

Acknowledgments

Appendix. Derivation of equation (6)

We consider 2×2 matrices $\mathbf{T}$ such that Det $\mathbf{T} = 1$ and Tr $\mathbf{T} = -2$, then

Theorem: $\mathbf{T}^n = (-1)^{n+1} n \mathbf{T} + (-1)^{n+1}(n-1)\mathbf{I}, n \geq 1$

Since the theorem is true for $n = 1$ the proof follows by induction.

Assume the theorem is true, then $\mathbf{T}^{n+1} = (-1)^{n+1} n \mathbf{T}^2 + (-1)^{n+1}(n-1)\mathbf{T}$. Using $\mathbf{T}^2 = \mathbf{T}\, \text{Tr}\, \mathbf{T} - \mathbf{I}$ and Tr $\mathbf{T} = -2$ then yields

$$\mathbf{T}^{n+1} = (-1)^{n+1} n(-2\mathbf{T} - \mathbf{I}) + (-1)^{n+1}(n-1)\mathbf{T}$$
$$= (-1)^{n+1}(-2n + n - 1)\mathbf{T} - (-1)^{n+1} n\mathbf{I}$$
$$= (-1)^{n+2}(n+1)\mathbf{T} + (-1)^{n+2} n\mathbf{I}.$$

QED

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