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Quasi-Crystals from a Numerical Point of View

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Abstract

Due to recent results in solid state physics the theory of quasi-crystals has experienced new impetus. First, in the absence of strict mathematical results for the spectrum of the discrete Schrödinger operator, computers were applied to plot it using a recursion formula. An error analysis is presented for this equation, which may be very unstable numerically, to estimate a sound bound for the number of iteration steps given the resolution of the graphical device. Further, a technique is introduced to calculate all periodic points of low orders (≤ 6) to present some examples and counterexamples. Cycles of lenght 12 and 24 are given.

Keywords: quasiperiodic potentials, quasi-crystals, Fibonacci number, Fibonacci string, error analysis for the discrete Schrödinger equation, discrete Schrödinger operator.

Introduction

During the last two decades, the theory of quasiperiodic potentials has attracted renewed attention. The investigation of the characteristic properties of materials in solid state physics has increased the interest in this subject. It has been discussed partly in terms of the theory of dynamical systems and partly using the notion of chaotic sets. For a comprehensive treatment of this field and an extensive bibliography see [1].

A widely used approach consists in the application of the discrete Schrödinger equation to describe the potential between two adjacent points of a one dimensional lattice using a Fibonacci sequence

$$\psi_{n+1} + \psi_{n-1} + V_n \psi_n = E\psi_n, \qquad n \in \mathbf{N}, \quad n \geq 1, \tag{1}$$

where E denotes the energy and the potential V_n assumes its values from a set consisting of two elements only according to the construction scheme of the infinite Fibonacci string. (1) is equivalent to the matrix equation

$$\vec{\psi}_{n+1} = M(n)\vec{\psi}_n. \tag{2}$$

There is a close relationship between the representation of an irrational number as a continued fraction and the potential of a quasi-crystal which is introduced in the sophisticated proofs of [2]. In a sense which becomes clear in the cited paper, the golden mean, the limit value of the quotients of two consecutive Fibonacci numbers, determines a very simple quasi-crystal. It is this special structure which is widely discussed in the literature on quasi-crystals ([3],[4],[5], ect.). However, nearly all the assertions proved in the special case hold in the general case as well. The proofs draw heavily upon number theoretical arguments.

Up to now, a representation of the spectrum of the discrete Schrödinger operator has not been given in a closed analytical form. There are, however, many attempts to represent the spectrum graphically using a recursion formula for the trace of the matrices M_l, which are defined using the matrices $M(n)$. In this paper an error analysis for this equation will be done. It is applied to estimate the maximal number of iterations after which the calculation should be stopped. This should be done when the discretisation error due to the machine arithmetic is large enough so that the stopping criterion can no longer be applied sensibly.

This paper further suggests a method to calculate all periods of lengths ≤ 6, which is used to plot an example. It shows the spectrum in the neighbourhood of a periodic point. It further provides an example where the modulus of a number in the iteration process is greater than one, and where the iteration sequence does not diverge to infinity.

Definitions and Notations

The aim of this section is to introduce the definitions and notations used in the subject. In the literature, Fibonacci strings and sequences are the main tools used to define quasi-crystals and to describe their properties. The present paper joins this tradition: Fibonacci sequences and strings are used to define a quasiperiodic potential.

Definition 1 *Setting* $S_0 = B$ *and* $S_1 = A$, *one defines* $S_{i+1} = S_i S_{i-1}$, $i \geq 1$, $i \in \mathrm{N}$. *The string* S_i *is called the i-th* **Fibonacci string.**

Let F_i denote the length of the string S_i. It is immediately clear from the definition that $F_0 = F_1 = 1$ and $F_{i+1} = F_i + F_{i-1}$. The numbers F_i are called **Fibonacci numbers** and the sequence $(F_i)_{i\in \mathrm{N}_0}$ is called the **Fibonacci sequence.** For $i \geq 2$, the string S_i contains F_{i-1} occurrences of the letter B and F_{i-2} occurences of the letter A. One can show that $\sigma = \lim_{i\to\infty} \frac{F_{i+1}}{F_i}$ exists using induction. This number is called the **golden mean.** It is the smaller root of the quadratic equation $\sigma^2 + \sigma = 1$. In the following the notion of quasiperiodicity is introduced following the lines of [5]. For the purpose of this paper the one dimensional case is sufficient.

Definition 2 *A sequence* $(b_n)_{n\in \mathrm{N}_0}$ *is called* **quasiperiodic** *if* $b_n = n\omega \bmod 1$, *with* $\omega \in \mathrm{R}\backslash\mathrm{Q}$.

Now the relationship between Fibonacci strings and quasiperiodic sequences is explained. The most commonly used irrational number in this context is $\omega = \sigma$, where σ again denotes the golden mean.

Definition 3 *With* $\mathbf{I} := (-\sigma, \sigma^2]$ *one defines*

$$g : \mathbf{I} \longrightarrow \{-1, 1\}, \quad x \longmapsto \begin{cases} 1 : & \text{for} \quad -\omega < x \leq -\omega^3 \\ -1 : & \text{for} \quad -\omega^3 < x \leq \omega^2. \end{cases}$$

The extension of g *from* $\mathbf{I}$ *to* $\mathbf{R}$ *is*

$$V : \mathbf{R} \longrightarrow \{-1, 1\}, \quad x \longmapsto g(x - k),$$

where $k \in \mathbf{N}_0$ *is chosen such that* $x - k \in \mathbf{I}$.

Definition 4 *Setting* $b_n = n\sigma$ *for* $n \in \mathbf{N}_0$, *one defines the sequence* $(a_n)_{n \in \mathbf{N}_0}$ *by* $a_n = V(b_n)$. *With* $S_0 = a_0 = -1$, $S_1 = a_1 = 1$, $S_i = (a_{F_{i-1}}, \ldots, a_0)$ *the string* S_i *is the i-th Fibonacci string.*

The assertion is proven by induction using the construction of the Fibonaccistring $S_{i+1} = S_i S_{i-1} = S_{i-1} S_{i-2} S_{i-1}$.

The one-dimensional quasiperiodic lattice is investigated using a tight-binding model. The potential incorporates the quasiperiodic assumption. It is described by the Hamilton operator H acting on $l_2(\mathbf{Z})$.

$$H = \sum_n (V_n |n\rangle\langle n|) + \sum_n (|n\rangle\langle n+1| + |n+1\rangle\langle n|) \quad . \tag{3}$$

The first summand represents the local energy, the second one the transition between two adjacent vertices in the lattice.

Stressing the Hilbert space aspect, the discrete Schrödinger operator may be represented by an infinite tridiagonal symmetric matrix

$$\begin{pmatrix} V_0 - E & 1 & & & & \\ 1 & V_1 - E & 1 & & & \\ & \ddots & \ddots & \ddots & & \\ & & 1 & V_n - E & 1 & \\ & & & \ddots & \ddots & \ddots \end{pmatrix},$$

where V_n denotes the Fibonacci potential, and E the energy.
Stressing the dynamical system aspect of the discrete Schrödinger operator, the difference equation (ψ_n denotes the amplitude of the probability)

$$\psi_{n+1} + \psi_{n-1} + V_n \psi_n = E \psi_n, \qquad n \in \mathbf{N}, \quad n \geq 1 \tag{4}$$

is written as an iterated matrix equation

$$\vec{\psi}_{n+1} = M(n)\vec{\psi}_n, \tag{5}$$

with

$$M(n) = \begin{pmatrix} E - V_n & -1 \\ 1 & 0 \end{pmatrix}, \quad and \quad \vec{\psi}_n = \begin{pmatrix} \psi_n \\ \psi_{n-1} \end{pmatrix}.$$

Setting $M_l := M(F_l)\cdots M(0)$ one defines the l-th **Fibonacci matrix**. Substituting the matrices $M(0)$ and $M(1)$ for the letters A and B in the definition of the Fibonacci string S_l, M_l may be interpreted as the l-th Fibonacci string. The following lemma holds for the traces of the Fibonacci matrices.

Lemma 1 *With $x_l = 1/2\ Tr\, M_l$, the equation $x_{l+1} = 2x_l x_{l-1} - x_{l-2}$ holds for $l \geq 2$, with $x_0 = 1$, $x_1 = 1/2\ a$, and $x_2 = 1/2\ b$.*

Proof: The matrix M_l satisfies its own characteristic equation

$$M_l^2 - 2x_l M_l + Id = 0.$$

As $\det M_l = 1$, this implies

$$M_l = -(M_l - 2x_l Id)^{-1} = 2x_l Id - M_l^{-1},$$

$$M_{l+1} = M_{l-1}M_l = 2x_l M_{l-1} - M_{l-1}M_l^{-1} = 2x_l M_{l-1} - M_{l-2}^{-1}.$$

One obtains the assertion by taking traces on both sides. □

For the general case of quasiperiodicity the proof may be found in [2]. The spectrum of the quasiperiodic Hamilton operator is often represented graphically. It consists of those values of E for which the sequence $(x_l)_{l\in \mathbf{N}_0}$ is bounded. The next lemma introduces a criterion for when to stop the numerical iteration process. It is easily proven by induction on k.

Lemma 2 *Let l_0 denote the unique minimal l, for which $|x_l| \geq |x_{l-1}| \geq |x_{l-2}| > 1$ holds. The sequence $(|x_{l_0+k}|)_{k\in \mathbf{N}_0}$ grows exponentially.*

Error analysis for the recursion formula $x_{l+1} = 2x_l x_{l-1} - x_{l-2}$

Two types of errors must be distinguished in the following analysis. The first one is due to the fact that the computer uses floating-point arithmetic with a finite precision. The relative error is denoted by ϵ. To represent the spectrum on a graphical device, which usually has a limited resolution only, a maximum of 300 dots per inch on the plotter table is commenly used. This second type of error is not fixed but depends on the scaling. It is denoted by ϵ_d. ϵ_d is usually large in comparison with ϵ.

Theorem 1 *The relative error of x_{l+1} is denoted by ϵ_{l+1}.*

$$\epsilon_{l+1} \approx \left|\frac{2x_l x_{l-1}}{x_l+1}\right| (\epsilon_l + \epsilon_{l-1} + 3\epsilon) + \left|\frac{x_{l-2}}{x_{l+1}}\right| \epsilon_{l-2} + \epsilon.$$

Proof: We begin with the first term. Following the notation of [6] and [7], the symbol ϵ overlined or with subscript denotes the relative error of the term immediately to the left of it. For the relative error $\tilde{\epsilon}_{2l}$ of $2x_l x_{l-1}$ one calculates:

$$\begin{aligned} 2x_l x_{l-1}(1+\tilde{\epsilon}_{2l}) &= \{\, 2(1+\epsilon_2)\,[\,x_l(1+\epsilon_l)x_{l-1}(1+\epsilon_{l-1})\,]\,(1+\bar{\epsilon}_l)\,\}\,(1+\hat{\epsilon}_l) \\ &\approx 2x_l x_{l-1}(1+\epsilon_2+\epsilon_l+\epsilon_{l-1}+\bar{\epsilon}_l+\hat{\epsilon}_l). \end{aligned}$$

With $\epsilon_2 \approx \bar{\epsilon}_l \approx \hat{\epsilon}_l \approx \epsilon$ this implies $\tilde{\epsilon}_{2l} = \epsilon_l + \epsilon_{l-1} + 3\epsilon$.
We now examine the whole expression:

$$x_{l+1}(1+\epsilon_{l+1}) = (2x_l x_{l-1}(1+\tilde{\epsilon}_{2l}) - x_{l-2}(1+\epsilon_{l-2}))\,(1+\hat{\epsilon}_{2l})$$

$$\approx (2x_l x_{l-1} - x_{l-2})\,(1 + \left|\frac{2x_l x_{l-1}}{x_{l+1}}\right| (\epsilon_l + \epsilon_{l-1} + 3\epsilon) + \left|\frac{x_{l-2}}{x_{l+1}}\right| \epsilon_{l-2} + \epsilon). \quad \square$$

Corollary 1 *Defining for a cycle of length d*

$$m := \max_{1\le k\le d} \left\{ \left|\frac{2x_{l+k}x_{l+k-1}}{x_{l+1+k}}\right|,\ \left|\frac{x_{l+k-2}}{x_{l+k+1}}\right| \right\},$$

the estimate reads

$$\epsilon_{l+1} \approx m(\epsilon_l + \epsilon_{l-1} + \epsilon_{l-2}).$$

Note that ϵ is small in comparison with ϵ_l after a few iterations. This estimate is used to calculate the number of iteration steps after which the numerical process should be stopped, i.e. when the criterion of **Lemma 2** can no longer tested sensibly because of the accumulated rounding errors. This occurs when

$$\epsilon_{l-2}\,|x_{l-2}| > 1 \quad\vee\quad \epsilon_{l-2}\,|x_{l-2}| > \big||x_{l-2}| - |x_{l-1}|\big| \quad\vee\quad \epsilon_{l-1}\,|x_{l-2}| > \big||x_{l-2}| - |x_{l-1}|\big|$$
$$\vee\quad \epsilon_{l-1}\,|x_{l-1}| > \big||x_l| - |x_{l-1}|\big| \quad\vee\quad \epsilon_l\,|x_l| > \big||x_l| - |x_{l-1}|\big|.$$

Considering the period (1, 1/3, 1, -1/3, -1, -1/3) of length 6, one obtains $m = 3$, and the iteration should be stopped after 26 steps. Using the individual propagation error for each step, this estimate can be improved to some 48 iterations. In this analysis double precision arithmetic of 14 digits accuracy was assumed.

A useful tool to produce examples and counterexamples is possibly to employ cycles of low orders. Lucky guesses provided three cycles of order 12:

$$\begin{array}{cccccccccccc}
1 & \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & -1 & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -1 & -\frac{1}{2} & \frac{1}{2} & \frac{1}{2}, \\
1 & \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} & 0 & -\frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2} & 1 & -\frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2} & 0 & \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2}, \\
1 & -\frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2} & 0 & \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} & 1 & \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} & 0 & -\frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2},
\end{array}$$

and two cycles of length 24:

$$\begin{array}{ccccccccccccccc}
1 & \frac{\sqrt{3}}{2} & \frac{\sqrt{3}}{2} & \frac{1}{2} & 0 & -\frac{\sqrt{3}}{2} & -\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 & \frac{1}{2} & -\frac{\sqrt{3}}{2} & -\frac{\sqrt{3}}{2} & 1 & -\frac{\sqrt{3}}{2} & -\frac{\sqrt{3}}{2} \\
 & & & & & & \frac{1}{2} & 0 & \frac{\sqrt{3}}{2} & -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 & \frac{1}{2} & \frac{\sqrt{3}}{2} & \frac{\sqrt{3}}{2} \\
1 & -\frac{\sqrt{3}}{2} & -\frac{\sqrt{3}}{2} & \frac{1}{2} & 0 & \frac{\sqrt{3}}{2} & -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 & \frac{1}{2} & \frac{\sqrt{3}}{2} & \frac{\sqrt{3}}{2} & 1 & \frac{\sqrt{3}}{2} & \frac{\sqrt{3}}{2} \\
 & & & & & & \frac{1}{2} & 0 & -\frac{\sqrt{3}}{2} & -\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 & \frac{1}{2} & -\frac{\sqrt{3}}{2} & -\frac{\sqrt{3}}{2}.
\end{array}$$

We now show how to calculate a cycle of length 5 efficiently. Defining

$$T : \mathbf{R}^3 \longrightarrow \mathbf{R}^3, \quad T : \begin{pmatrix} x_2 \\ x_1 \\ x_0 \end{pmatrix} \longmapsto \begin{pmatrix} x_2 x_1 - x_0 \\ x_2 \\ x_1 \end{pmatrix},$$

the conditions are

$$\begin{array}{rl}
(i) & x_2 = x_7 = x_6 x_5 - x_4 = x_1 x_0 - x_4 \\
(ii) & x_1 = x_6 = x_5 x_4 - x_3 = x_0 x_4 - x_3 \\
(iii) & x_0 = x_5 = x_4 x_3 - x_2.
\end{array}$$

Eliminating x_3 and x_4, one finds

$$\begin{array}{rlcl}
(iv) & 4x_2^2 x_1 - x_2 - 3x_1 = 0 & \Longrightarrow & x_1 = \dfrac{x_2}{4x_2^2 - 3} \\
(v) & 8x_2^2 x_1 - 4x_2 - 3x_1 - 2x_2 x_1 + 1 = 0. & &
\end{array}$$

As $x_2 = \pm\sqrt{3}/2$ is not a solution, one obtains, substituting (iv) into (v)

$$(vi) \quad -8x_2^3 + x_2^2 + 9x_2 - 3 = 0.$$

As $x_2 = 1$ is a fixed point, one may divide (vi) by $x_2 - 1$:

$$4x_2^2 + 3x_2 = \frac{3}{2},$$

which has the solutions

$$x_2^+ = \frac{3}{8}\left(\sqrt{\frac{11}{3}} - 1\right) \approx 0.34, \qquad \text{and} \qquad x_2^- = -\frac{3}{8}\left(\sqrt{\frac{11}{3}} + 1\right) \approx -0.61,$$

$$x_1^+ = \frac{1}{8}\left(\sqrt{\frac{11}{3}} - 3\right) \approx -0.14, \qquad \text{and} \qquad x_1^- = -\frac{1}{8}\left(\sqrt{\frac{11}{3}} + 3\right) \approx -1.09.$$

This shows that the sequence $(x_l)_{l \in \mathbf{N}_0}$ does not diverge exponentially if one x_l has a modulus greater than one. In the literature this was used as a criterion for $(x_l)_{l \in \mathbf{N}_0}$ to diverge exponentially. Instead of this **Lemma 2** should be used.

The same example shows that it may happen that the machine arithmetic yields a perfectly periodic cycle of length 5. This holds true for a Tandon AT Computer with a numeric coprocessor using Turbo Pascal and double precision real numbers, whereas with single and extended reals the cycle does not show because of rounding errors.

It is still an open question whether there exist sequences $(x_l)_{l \in \mathbf{N}_0}$ which are bounded, but where traces of the general transfer matrices $M^{(n)}$, with $n \in \mathbf{N_0}$ (where $M^{(n)} = M(n)...M(0)$), are unbounded. Note that $x_l = 1/2\ Tr\ M_l = 1/2\ Tr\ M^{F_l}$.

Using the results derived above, a plot (**fig.1**) was prepared on a NEC P6 printer showing the values (x_1, x_2) for which the sequence $(x_l)_{l \in \mathbf{N}_0}$ possibly does not diverge as black dots. For the reasons mentioned above it does not make sense to use more than some 48 (**fig.1**) iterations. However, to show more than some specks of dust, the iteration process was stopped after 20 steps in **fig.2**, after 25 steps in **fig.3**, and after 30 steps in **fig.4** . **Fig.2** is a part of **fig.1** near the periodic point (-0.61, -1.09) just calculated, as seen through a magnifying glass. It shows a square of length 0.2 on both axes around the periodic point. The following **fig.3** and **fig.4** each are a magnification by a factor of ten in the vicinity of the center of the preceding one.

The above mentioned cycle of length 6 provides an example where $(1/2\ Tr\ M_l)$ with $l \in \mathbf{N_0}$, is bounded, but where $\left(1/2\ Tr\ M^{F_{l-1}}\right)$ with $l \in \mathbf{N_0}$, seems to be unbounded, as the rapidly increasing values suggest. The comparison between the theoretically (using **Lemma 1**) and the numerically (using (5)) calculated values shows that the result is not impaired by rounding errors.

It is not known whether the black dots in the neighbourhood of the periodic point correspond to periodic points of sufficiently high order, or to quasiperiodic (i.e. not diverging) points, or to points which do not diverge after until 30 iterations. A computer with an arbitrary but finite arithmetic is fundamentally inadequate for solving this problem. It is, however, a good tool to obtain sophisticated guesses and hints, which are worthwhile trying an analytical proof.

Summary

This paper is a short and concise introduction to the theory of quasi-crystals using the

notation of Fibonacci theory. Stressing the numerical aspects, it gives an error analysis of the basic recursion formula of the theory for the traces of the Fibonacci matrices. Thus it shows on one side the fundamental limitations in the use on computers in this area, and on the other side their unsurpassed help to obtain intelligent guesses and to prove or refute them.

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The following plots show the energy levels $(a, b,)$ for which the sequence $(x_l)_{l\in\mathbf{N}_0}$ possibly does not diverge as black dots. The sets are calculated in the same manner as Mandelbrot sets.

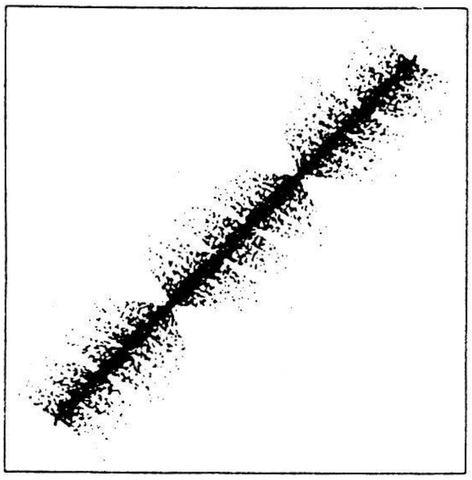

fig.1: 48 iteration steps for the recursion formula $x_{l+1} = 2x_l x_{l-1} - x_{l-2}$. As the initial values of the iteration process, one takes the energy levels a and b in the interval [-2.6, 2.6] respectively.

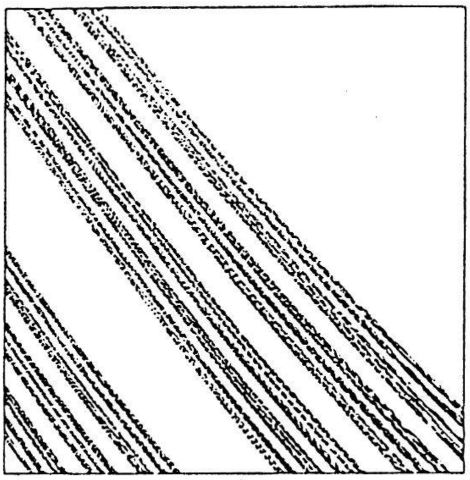

fig.2: Part of **fig.1** near the periodic point (-0.61,-1.09) showing a square of length 0.2 on both axes. One derived the number of iteration steps previously to be 20.

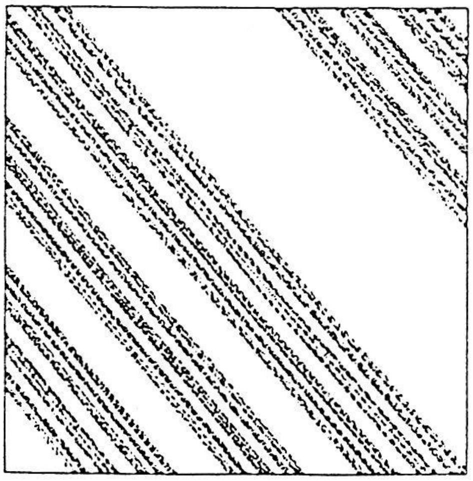

fig.3: Magnification by a factor of ten in the vicinity of the center of **fig.2**. Number of iteration steps: 25.

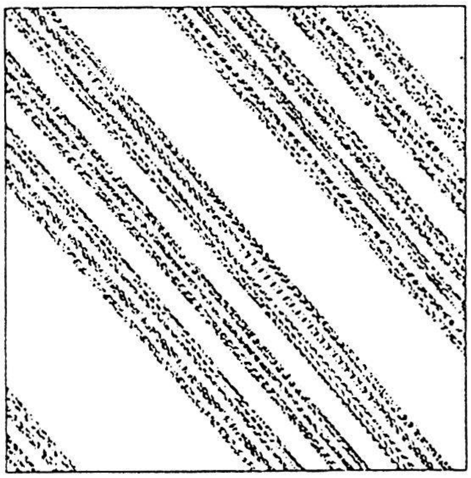

fig.4 Magnification by a factor of ten in the vicinity of the center of **fig.3**. Number of iteration steps: 30.