Journal of Statistical Physics, Vol. 66, Nos. 3/4, 1992

Dynamical System Related to Quasiperiodic Schrödinger Equations in One Dimension

Mahito Kohmoto[1]

Received April 19, 1991; final August 28, 1991

A dynamical map is obtained from a class of quasiperiodic discrete Schrödinger equations in one dimension which include the Fibonacci system. The potentials are constant except for steps at special points.

KEY WORDS: Quasiperiodic Schrödinger equation; dynamical system; Fibonacci sequence; Cantor-set spectrum; localization problem.

1. INTRODUCTION

There has been much interest in the quasiperiodic Schrödinger equation and its finite-difference analogue (for review see, e.g., refs. 1). Since Floquet's theorem holds only for periodic systems, there is an interesting localization problem even in one dimension. There is a tendency for the spectrum to be a Cantor set, i.e., a closed set with no isolated points and whose complement is dense.

A lot of attention has been paid to the study of dynamical systems and much progress has been made in recent years. Some dynamical systems (strange attractor, Smale horseshoe, etc.) also have Cantor sets. Therefore it is desirable to have some connection between these two different areas of physics so that the theories of the dynamical systems can be applied to problems of condensed matter physics.

Kohmoto *et al.*[1] and Ostlund *et al.*[3] showed that the transfer matrices of a special quasiperiodic Schrödinger equation obey the following recursion relation:

$$M_{l+1} = M_{l-1} M_l \tag{1}$$

[1] Institute for Solid State Physics, University of Tokyo, 7-22-1 Roppongi, Minato-ku, Tokyo 106, Japan.

0022-4715/92/0200-0791$06.50/0

where M_l is a 2×2 real matrix with unit determinant. Let us write $M_0 = B$ and $M_1 = A$. Then we have $M_2 = BA$, $M_3 = ABA$, $M_4 = BAABA$, and so on. The sequence of two letters A and B constructed in this way is called a Fibonacci sequence.

One of the purposes of this article is to review the derivation of this dynamical system from the $d=1$ quasiperiodic Schrödinger equation. The other is to present a more general class of equations which eventually can be studied by the same dynamical system.

2. TRANSFER MATRIX FOR THE QUASIPERIODIC MODEL AND ITS RECURSION RELATION

The quasiperiodic (discrete) Schrödinger equation in one dimension is written

$$\psi_{n+1} + \psi_{n-1} + V(n\omega)\,\psi_n = E\psi_n \tag{2}$$

where V is periodic, i.e., $V(t+1) = V(t)$, and ω is an irrational number. It is traditional to introduce a transfer matrix in one-dimensional problems:

$$\Psi_{n+1} = M(n\omega)\,\Psi_n \tag{3}$$

where

$$\Psi_n = \begin{pmatrix} \psi_n \\ \psi_{n-1} \end{pmatrix}$$

and M is the transfer matrix given by

$$M(t) = \begin{pmatrix} E - V(t) & -1 \\ 1 & 0 \end{pmatrix}$$

The matrix satisfies $M(t+1) = M(t)$ and $\det M(t) = 1$. Higher-order transfer matrices are also defined,

$$\Psi_{n+k} = M^{(k)}\Psi_n \tag{4}$$

where

$$M^{(k)}(t) = M(t+(k-1)\omega)\cdots M(t+\omega)\,M(t) \tag{5}$$

For a quasiperiodic system, the evaluation of $M^{(k)}$ for a large value of k is very delicate. The system tries to repeat itself on many length scales. However, it fails to do so and the degree of the failure depends on the incommensurability and the length scale.

We use a recursion relation to calculate $M^{(k)}$. This follows the spirit of the renormalization-group theory. Divide k into two integers k_1 and k_2; then the transfer matrix $M^{(k)}(t)$ is written

$$M^{(k)}(t) = M^{(k_1)}(t + k_2\omega)\, M^{(k_2)}(t) \tag{6}$$

In order to implement the recursive structure in this equation, write $k = F_{l+1}$, $k_1 = F_{l-1}$, $k_2 = F_l$; moreover, $M^{(F_l)} \equiv M_l$. We have

$$M_{l+1}(t) = M_{l-1}(t + F_l\omega)\, M_l(t) \tag{7}$$

where F_l is a Fibonacci number defined by $F_{n+1} = F_{n-1} + F_n$ and $F_0 = F_1 = 1$.

One of the main obstacles to calculating the transfer matrix using (7) is the presence of $F_l\omega$ on the right-hand side. This gives the dependence of M_l on its argument. The first step to overcome this difficulty is to choose an irrational number ω such that $F_l\omega$ is close to an integer. Note that $M_n(t+1) = M_n(t)$, so the argument of M_n is defined on a circle. The best choice of ω is the inverse of the golden mean $\omega^* = (\sqrt{5} - 1)/2 = 0.618...$, since it satisfies

$$F_l\omega^* = F_{l-1} - (-\omega^*)^{l+1} \tag{8}$$

The difference between $F_l\omega^*$ and the integer F_{l-1} becomes geometrically small for large l's. The recursion (7) is then written as $M_{l+1}(0) = M_{l-1}(-(-\omega^*)^{l+1})\, M_l(0)$, where t has been set to be 0 for simplicity.

The second step is to construct potentials $V(t)$ which give

$$M_{l-1}(-(-\omega^*)^{l+1}) = M_{l-1}(0) \tag{9}$$

so that we have the simple recursion relation (1) which does not contain arguments. The condition (9) can be simply satisfied by a constant potential where the incommensurability is lost and the problem is solved trivially. In order to have a nontrivial model, we must allow a potential to have steps. Then, the potential takes a discrete set of values. Recall that (5) is rewritten as

$$M_{l-1}(t) = M(t + (F_{l-1} - 1)\,\omega^*) \cdots M(t + \omega^*)\, M(t) \tag{10}$$

From this we learn that discontinuities must lie *outside* the following intervals:

$$I_l{:}\quad [n\omega^*, n\omega^* - (-\omega^*)^{l+1}]; \qquad n = 0, 1, 2,..., F_{l-1} - 1 \tag{11}$$

in order that (9) be satisfied. The points $n\omega^*$ are always on the edges of the intervals which lie on either side of those points, depending on whether

l is odd or even. In order to control the intervals, it is useful to write (11) in terms of $m = F_{l-1} - n$. A little algebra using (8) gives

$$I_l: \quad [-m\omega^* - (-\omega^*)^l, -m\omega^* - (-\omega^*)^l \omega^{*2}]; \quad m = 1, 2, ..., F_{l-1} \tag{12}$$

Each of these intervals has a length ω^{*l+1} and the edges approach the points $-m\omega^*$ as l becomes large. The points $-m\omega^*$, $m = 1, 2, ..., F_{l-1}$, are clearly outside the "bad" intervals I_l, so we can have discontinuities at those points. Kohmoto *et al.*(2) chose the simplest possible potential, which has two discontinuities at $-\omega^* = \omega^{*2} (\text{mod } 1)$ and $-2\omega^* = -\omega^{*3} (\text{mod } 1)$, i.e.,

$$\begin{aligned} V(t) &= V_0 \qquad \text{for} \quad -\omega^* < t \leqslant -\omega^{*3} \\ &= V_1 \qquad \text{for} \quad -\omega^{*3} < < t \leqslant -\omega^{*2} \end{aligned} \tag{13}$$

For this potential, it can easily be shown that the recursion (1) holds for all $l \geqslant 1$.

Note that the two discontinuities could have been placed on different points. By choosing an appropriate original site for the transfer matrix, one discontinuity can always be placed at $-\omega^*$. Suppose the other discontinuity is at $-m_0\omega^*$; then the recursion (1) holds for $l \geqslant l_0$, where l_0 is the smallest integer which satisfies $F_{l_0 - 1} \geqslant m_0$. In other words, at some earlier steps, the simple recursion (1) does not hold because transfer matrices of different arguments are needed. At the step l_0, the original potential with the discontinuities at $-\omega^*$ and $-m_0\omega^*$ can be regarded as having been renormalized to the potential (13) with appropriate values of V_0 and V_1.

The results described above can easily be generalized to potentials which have more than two discontinuities at points $-k\omega^*$, where k is an integer. Those points are dense on the circle. The intervals between the discontinuities are always commensurate with ω^*, i.e., $n\omega^*$ mod 1 ($n = 1, 2, ...$).

The sequences obtained in this manner are of course not the original Fibonacci sequence. But it looks like a renormalized Fibonacci sequence $A'B'A'A'B'A'B'A'$..., where A' and B' are blocks of more than two different letters. It does not possess the inflation–deflation invariance in terms of the letters.

3. CONCLUDING REMARKS

The trace of the transfer matrix M_l gives the following mapping problem(2):

$$(x_{l+1}, y_{l+1}, z_{l+1}) = (2x_l y_l - z_l, x_l, y_l) \tag{14}$$

where $x_l = 1/2\,\mathrm{Tr}\, M_l$, $y_l = x_{l-1}$, and $z_l = x_{l-2}$. There is a conserved quantity for this map given by

$$I = x_l^2 + y_l^2 + z_l^2 - 2x_l y_l z_l - 1 \tag{15}$$

This determines a two-dimensional manifold on which the dynamical system (14) is defined. The manifold is noncompact and is simply connected for $I > 0$.[4]

The cycles of the map were studied by Kadanoff.[5] Kohmoto and Oono[4] found homoclinic and heteroclinic points for the map. This explains the Cantor-set behavior of the energy spectrum of the quasiperiodic Schrödinger equation. From a fixed point analysis one can derive the scaling behavior of the spectrum, which has previously been found numerically.[6]

The conjecture[4] that the Fibonacci model defined by (2) and (13) has a singular continuous spectrum was recently proven by Suto[7] following the theorem of Kotani.[8] The wave functions corresponding to a singular continuous spectrum are expected to be neither extended nor localized in a standard manner. In fact, the multifractal properties of the wave functions of the Fibonacci model was studied by Fujiwara *et al.*[9]

In summary, we have shown that a class of quasiperiodic discrete Schrödinger equations (2) with periodic function $V(t)$ which is constant and have a number of discontinuities at points $-k\omega^*$ mod 1, where k is an integer and $\omega^* = (\sqrt{5} - 1)/2$, has the same universal properties as the Fibonacci model. Namely, the spectrum is a Cantor set with zero Lebesgue measure and is singular continuous. The wave functions are critical, i.e., neither extended nor localized in a standard manner.

This result may prove useful to understand the problem of interacting electrons on a Fibonacci lattice. Recently Hiramoto[10] studied such a model within the Hartree–Fock approximation. He found numerically that the spectrum remains singular continuous when the electron correlation is introduced. The effective potential function which gives the Hartree–Fock one-body problem is constant except at number of discontinuities. The discontinuities seem to be at points $-k\omega^*$ mod 1, within the numerical accuracy.[11] Thus, the present work explains the numerical result that the singular continuous spectrum is rigid against the effects of electron correlation.

ACKNOWLEDGMENTS

Most of the work reported here has resulted from stimulating conversations with L. P. Kadanoff. It is a pleasure to thank him for a most enjoyable collaboration. I am grateful to H. Hiramoto for discussions on interacting electrons on the Fibonacci lattice.

REFERENCES

1. B. Simon, *Adv. Appl. Math.* **3**:463 (1982); J. B. Sokoloff, *Phys. Rep.* **126**:189 (1985).
2. M. Kohmoto, L. P. Kadanoff, and C. Tang, *Phys. Rev. Lett.* **50**:1870 (1983).
3. S. Ostlund, R. Pandit, D. Rand, H. J. Schellnhuber, and E. Siggia, *Phys. Rev. Lett.* **50**:1873 (1983).
4. M. Kohmoto and Y. Oono, *Phys. Lett.* **102A**:145 (1984).
5. L. P. Kadanoff, unpublished.
6. M. Kohmoto, *Phys. Rev. Lett.* **51**:1198 (1983).
7. A. Suto, *J. Stat. Phys.* **56**:525 (1989).
8. S. Kotani, *Publ. Inst. Math. Sci.* (Kyoto), No. 692 (1989).
9. T. Fujiwara, M. Kohmoto, and T. Tokihiro, *Phys. Rev. B* **40**:7413 (1989).
10. H. Hiramoto, *J. Phys. Soc. Jpn.* **59**:811 (1990).
11. H. Hiramoto and M. Kohmoto, *Int. J. Mod. Phys. B* (to appear).