41 Spectrum of almost periodic quantum systems

41.1 1D lattice Schrödinger equation

Consider a 1D lattice and a discrete version of the Schrödinger equation:

$$\psi_{n+1} + \psi_{n-1} + \lambda V(n\omega)\psi_n = E\psi_n \tag{41.1}$$

with the periodic potential

$$V(t+1) = V(t). \tag{41.2}$$

When $\omega \in \mathbb{Z}$, we have extended states and the usual energy band structure.

What happens if $\omega \notin \mathbb{Z}$? It is known to have complicated Cantor-set like spectrum. An explicitly provable case of self-similar energy band structure can be studied with an Axiom A system.

41.2 Related 2D dynamical system

We can write (41.1) may be rewritten as a 2D map problem:

$$\Psi_{n+1} = M(n\omega)\Psi_n, \tag{41.3}$$

where

$$M(t) = \begin{pmatrix} E - V(t) & -1 \\ 1 & 0 \end{pmatrix}, \quad \Psi_n = \begin{pmatrix} \psi_n \\ \psi_{n-1} \end{pmatrix}. \tag{41.4}$$

Define

$$M^k(t) = M(t + (k-1)\omega) \cdots M(t+\omega)M(t). \tag{41.5}$$

Then, we may write

$$M^k(t)\Psi_n = \Psi_{n+k} \tag{41.6}$$

and

$$M^{k+l}(t) = M^k(t + l\omega)M^l(t). \tag{41.7}$$

If we use the Fibonacci numbers F_m defined as[439]

$$F_{m+1} = F_m + F_{m-1}, \tag{41.8}$$

[439] Perhaps, https://www.math.ksu.edu/~cjbalm/Quest/Day7_slides.pdf is the best elementary page for the Fibonacci numbers.

with $F_0 = F_1 = 1$. Then,[440]

$$M^{F_{m+1}}(t) = M^{F_m}(t + F_{m-1}\omega)M^{F_{m-1}}(t). \tag{41.9}$$

41.3 Discontinuous potential case mappable to dynamical systems

If the periodic potential is two-valued:

$$V(t) = \begin{cases} -1 & \text{for } t \in (-\omega, -\omega^3], \\ +1 & \text{for } t \in (-\omega^3, \omega^2], \end{cases} \tag{41.10}$$

where $\omega = (\sqrt{5} - 1)/2 \simeq= 0.618$.[441] Note $\omega = \lim_m F_{m-1}/F_m$.

Then, (41.9) reads $M_m \equiv M^{F_m}(0)$:

$$M_{m+1} = M_{m-1}M_m \tag{41.11}$$

with $M_0 = M(0)$ and $M_1 = M(-\omega^3)$. Notice that $F_m\omega \simeq F_{m-1}$. This is OK, if, for all $m > 1$,

$$-\omega^3 < F_m\omega \text{ mod } 1 \le \omega^2, \tag{41.12}$$

but $\omega F_m - F_{m-1} = (-\omega)^{m+1}$,[442] this is always true.

Thus, (41.11) may be used to study the spectrum. The 'extended state' implies $|M_m|$ to be bounded from 0 and from above.

41.4 Trace dynamics

Let

$$x_m = \frac{1}{2}\text{Tr}\, M_m. \tag{41.13}$$

From (41.11) $M_m = M_{m-2}M_{m-1} \;\Rightarrow\; M_{m-2}^{-1} = M_{m-1}M_m^{-1}$

$$M_{m+1} + (M_{m-2})^{-1} = M_{m-1}M_m + M_{m-1}M_m^{-1}. \tag{41.14}$$

[440] M. Kohmoto, L. P. Kadanoff and C. Tang, Localization problem in one dimension: mapping and escape, PRL 50 1870 (1983).

[441] $\omega^2 = 0.382$, $\omega^3 = 0.236$; $\omega^2 + \omega = 1$.

[442] $-\omega = (-1/\omega) + 1$, $(-\omega)^2 = 1 + (-\omega)$, $(-\omega)^3 = 2(-\omega) - 1$, etc. gives this formula. Set $(-\omega)^n = A_n(-\omega) + B_n$. Then you see A_n and B_n are Fibonacci numbers F_n and F_{n-1}.

Since $\det M_m = 1$, the trace of the formula may be obtained after explicit matrix calculation as

$$x_{m+1} = 2x_m x_{m-1} - x_{m-2} \tag{41.15}$$

with

$$x_1 = \frac{1}{2}(E+\lambda), x_2 = \frac{1}{2}(E-\lambda), x_3 = 1. \tag{41.16}$$

41.5 Trace dynamics is (likely to be) Axiom A[443]

Thus, the trace of M obeys the 3D diffeo

$$T(x,y,z) = (2xy - z, x, y). \tag{41.17}$$

This has an invariant (with the initial condition (41.16) $I = \lambda^2$)

$$I = x^2 + y^2 + z^2 - 2xyz - 1 \tag{41.18}$$

which determines a 2-mfd (Fig.41.2)

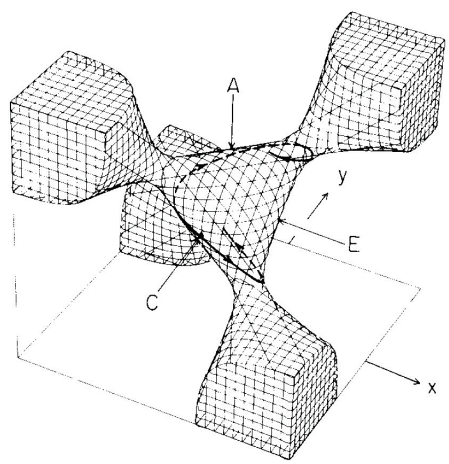

Figure 41.1: An example of the manifolds for $I = 0.2$.

Fig. 41.1 An example of the manifolds for $I = 0.2$. The four parts which are cut by a cube of size 6 actually extend to infinity. There are six saddle points, A, B, C, D, E, and F. The points B, D and F are located at the antipodal positions of E, A and C, respectively. A portion of the unstable manifold of C is drawn schematically. This crosses the stable manifold of A transversally near A.

[443] M Kohmoto and Y Oono, Cantor spectrum for an almost periodic Schrödinger equation and a dynamical map, PL 102A 145 (1984).

41.6 Determination of the spectrum

(41.17) defines a chaotic dynamics on a 2-mfd. It is Anosov if $\lambda = 0$.[444]

The most important periodic orbit of the map T to account for the spectra is the following six cycle:

$$A(0,0,a) \to B(-a,0,0) \to C(0,-a,0)n \to D(0,0,-a) \to E(a,0,0) \to F(0,a,0) \to A, \tag{41.19}$$

where $a = (1+I)^{1/2} = (1+\lambda^2)^{1/2}$. These six points are hyperbolic fixed points of T^6 whose eigendirections are tangent to the manifold:

$$\kappa_\pm = \{[1+4(1+\lambda^2)2]^{1/2} \pm 2(1+\lambda^2)\}^2. \tag{41.20}$$

The initial points are on $y = x - \lambda$, $z = 1$ near the fixed point A. The stable manifold of A crosses this straight line of the initial points. Most orbits starting from these crossings flow into the six cycle. The crossing point specified by the energy ε_0 which is closest to A along its stable manifold is clearly in the spectrum.

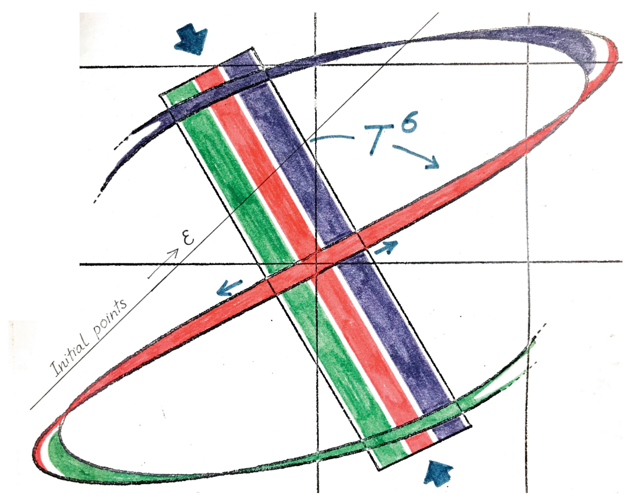

Figure 41.2: Horseshoe structure exhibited by the map T

[444]Pointed out by Y. Takahashi. This was the key observation; this statement immediately suggested a horseshoe, and a horseshoe hunt started.

41.7 Discrete cat map

The second order difference equation like discrete Schrödinger equation can always be rewritten as a first order 2D and vice versa. For example, Thom's map is

$$q_{t+1} = 2q_t + p_t, \tag{41.21}$$
$$p_{t+1} = q_t + p_t. \tag{41.22}$$

Therefore,

$$q_{t+1} = 2q_t + (q_{t-1} + p_{t-1}) = 2q_t + q_{t-1} + (q_t - 2q_{t-1}), \tag{41.23}$$

so

$$q_{t+1} = 3q_t - q_{t-1}. \tag{41.24}$$

This may define a dynamics on $\mathbb{Z}$, but we could impose a mod N condition. Then this defines a dynamics on an integer ring $\mathbb{Z}/N$. Needless to say, all the orbits are periodic (with a period at longest N). This means the discrete version (41.22) mod N is also recursive as illustrated here or here.

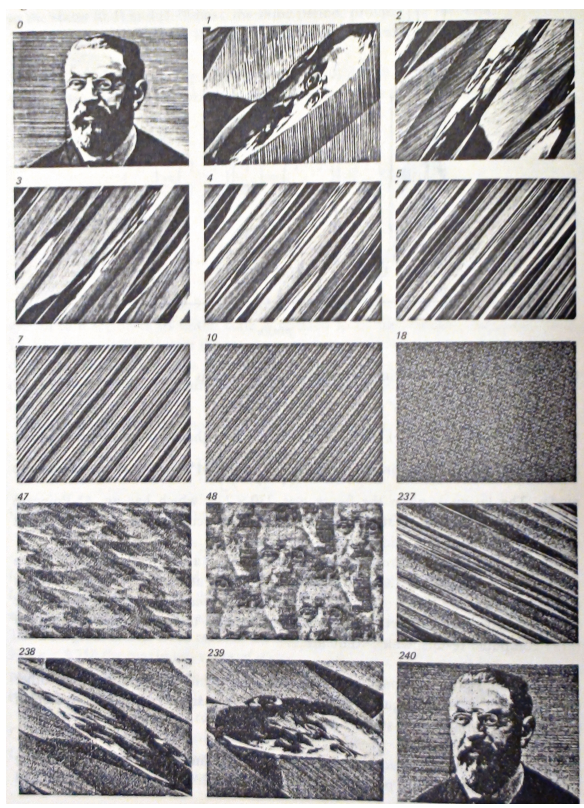

Figure 41.3: Discrete 'cat map' [Fig. 6.107 of Jackson