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LETTER TO THE EDITOR

Ergodicity and density of states in a 1D crystal†

Jorge V José

Physics Department, Northeastern University, Boston, MA 02115, USA

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Abstract. Using a decimation technique, the band structure in a 1D periodic solid is shown to be related to the ergodic Ulam–Von Neumann map, $C_{r+1} = 1 - 2C_r^2$.

The Schrödinger equation with periodic potentials has been the subject of study of many papers in solid state physics. The Kronig–Penny (KP) model (1931) stands out as the original paper that clearly showed how the appearance of bands and gaps leads to the understanding of metals and semiconductors. In this paper we look at this old problem from a different point of view, that makes contact with ideas and results in the theory of dynamical systems, currently an active field of research. We consider the periodic KP model with δ-function interactions in one dimension. The corresponding Schrödinger equation reads

$$\left(-\frac{1}{2}\frac{d^2}{dx^2} + \sum_{n=0}^{L} \beta_0 \delta(x - na)\right)\varphi(x) = E\varphi(x). \tag{1}$$

Here L is the length of the chain, β_0 the strength of the potentials, E the energy, n an integer and a the lattice spacing. Following the dynamical systems theory, instead of studying (1) we study its Poincaré map. This is easily constructed, noting that in between the δ-function potentials the electrons described by (1) are free and that their wavefunction can be written as

$$\varphi_n = \varphi(n^+ a) = A_n e^{iakn} + B_n e^{-iakn},$$

with $[A_n, B_n]$ the amplitudes of the waves in the nth cell, and $k = (2E)^{1/2}$. From the continuity of the wavefunction and its derivative at the lattice site na, we obtain the second-order difference equation (see for example Helleman 1979)

$$\varphi_{n+1} + \varphi_{n-1} - \beta_0[(\sin ka)/ka]\varphi_n = 2\cos ka\, \varphi_n. \tag{2}$$

This is the Poincaré map associated with (1). It involves three sites in the lattice and expresses the relation between the wavefunctions at the three lattice sites.

In the derivation of this equation no approximations are made and therefore it has the same physical content as in (1). We now proceed to study this equation using the renormalisation group (RG) method.

The RG method we use here consists of eliminating every other site in the lattice, leaving the form of the equation of motion unchanged. This procedure is known as decimation and has been used extensively in the theory of critical phenomena. Several

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authors have extended this method to treat tight-binding type problems (Stein and Krey 1978, Domany and Sarker 1979, Aoki 1980, Gonçalves da Silva and Koiller 1981). Here we follow the approach used by us elsewhere (José 1982). Specifically we rewrite (2) as

$$\varphi_{n+1}+\varphi_{n-1}=2C_0(ka)\varphi_n, \tag{3}$$

where

$$C_0(ka)=\cos ka+\beta_0(\sin ka)/2ka. \tag{4}$$

Although (3) looks like a tight-binding equation the specific k dependence of C_0 is different and all important. The decimation procedure is carried out by writing the corresponding equation (3) for φ_{n-1}, and φ_{n+1} on the right-hand side, and then substituting back into (3). As can be easily checked, the resulting equation is of the same form as (3) but with new lattice spacing, $2a$, and a new C. Carrying out this procedure r times the renormalised equation reads

$$\varphi_{n+2^r}+\varphi_{n-2^r}=2C_r\varphi_n, \tag{5}$$

and the recursion formula for C_r is given by

$$C_{r+1}=2C_r^2-1. \tag{6}$$

This is a nonlinear recursion relation of a type studied extensively in the last few years (Collet and Eckmann 1980). The map given in (6) was first introduced by Ulam and Von Neumann (1947), and bears their name. It has also been studied extensively for values of $\lambda\in[0,2]$ in $1-\lambda C_r^2$ by Feigenbaum and others (Collet and Eckmann 1980). The particular value $\lambda=2$ of interest in our analysis is special. Ulam and Von Neumann introduced this map with the aim of finding a random number generator for computer calculations. The map itself is known to be ergodic and mixing (Adler and Rivlin 1964). In order to see how this comes about and how it is connected with the band structure in solids, it is convenient to notice that the right-hand side of (6) is the Chebycheff polynomial of order 2. The general definition of these polynomials is

$$T_n(x)=\cos^{-1} n\cos x,$$

and they satisfy the semigroup property

$$T_n(T_m(x))=T_{mn}(x). \tag{7}$$

Thus if we rewrite (6) as

$$C_{r+1}=T_2(C_r).$$

using (7) we can solve (6), obtaining

$$C_r=T_{2^r}(C_0(ak)). \tag{8}$$

The map $T_n(x)$ has been shown to be strongly mixing and ergodic (Adler and Rivlin 1964). The process being ergodic then allows us to replace averages of the type

$$\frac{1}{N}\sum_r^N\to\int \mathrm{d}C\,\rho(C).$$

Here $\rho(C)$ becomes the probability measure of the ensemble representative of the dynamical process resulting from (6). In the particular case of the Chebysheff polynomials

$$\rho(C) = (1 - C^2)^{-1/2}. \tag{9}$$

We can now make contact with the problem we started with. First notice that if we take as initial condition $|C_0| > 1$, then as we iterate the RG procedure $C_r \to \infty$. On the other hand, if $|C_0| < 1$, then for all r, $C_r \in [-1, 1]$. From the definition of C_0 we see that these are precisely the KP conditions to have bands ($|C_0| < 1$) or gaps ($|C_0| > 1$). This discussion can be made more rigorous (José 1982) in terms of convergence conditions for the self-energy and Green functions for the continued fraction solution of general finite difference equation models. Here this discussion is enough for our purposes. Now, from the ergodicity property of the map we can conclude that (9) gives the density of states for each one of the bands, i.e. for different values of k.

Notice that the way in which we have obtained the density of states differs *fundamentally* from the method used by Gonçalves da Silva and Koiller (1981). They used the standard definition of the density of states as the imaginary part of the Green function. Defining a renormalised Green function after r iterations, they calculate its imaginary part and thus the density of states. Here we have obtained ρ as the probability law associated with the chaotic process described by the deterministic equation of motion (6).

To see how this is connected with our decimation procedure we can take, without loss of generality, $\beta_0 = 0$. In this case (3) acquires a tight-binding form with energy $C_0 = 2 \cos ak$ and hopping constants equal to one. As we change the scale in the model C_0 changes to

$$C_r(ka_r) = \cos ka_r = \cos 2^r ka.$$

This means that the form of the energy relation remains the same at each stage of the RG iterations except for the magnitude of the lattice spacing. Further understanding is gained if we look at figure 1(a). Take the cross as the initial value for C_0.

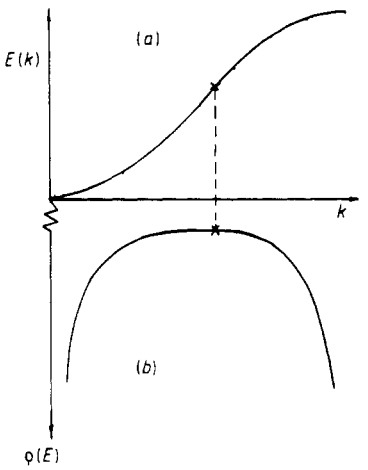

Figure 1. (a) Energy diagram, with the cross indicating the initial value for the RG iteration. (b) Histogram for the number of times the cross in (a) occupies a given point in the renormalised energy diagram.

Then start iterating (6). At each stage of the iteration the curve for C_r is homotopic to the curve for C_0 except that the abscissa is reduced in size by a factor 2^{-r}. If we plot a histogram of the number of times the cross occupies a given point in the renormalised energy diagram, we obtain the curve (b) shown in figure 1, which then gives the density of states for the model with $\beta_0 = 0$. If $\beta_0 \neq 0$ we can repeat the same procedure for all the other bands, getting the same qualitative result.

It is possible that these ideas and results apply as well in higher dimensions as the KP analysis applies to two- and three-dimensional systems. This is of course clear in the case where the higher-dimensional Schrödinger equation is separable.

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