Random walk on a Fibonacci chain

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Abstract. Random walk on a Fibonacci chain is studied both numerically and analytically. We demonstrate that the long-time behaviour is diffusive.

1. Introduction

With the discovery of the quasi-crystalline phase of matter there has been an intense activity in the study of the properties of quasi-periodic systems. Needless to say that one-dimensional quasi crystals have received their share of attention due to the fact that they are the simplest of their kind retaining many features of higher dimensional systems. The study of spectral properties has received the maximum attention (Nori and Rodrigues 1986; Kohomoto and Banavar 1986; Valsakumar and Ananthakrishna 1987; Kumar and Ananthakrishna 1987 to mention only a few). In contrast the problem of diffusion has received much less attention. Numerical evaluation of the diffusion constant has been reported by Kohomoto and Banavar (1986). Kantha and Stinchcombe (1986) have undertaken a renomalization group approach. They show that both diffusive and anomalous behaviour may arise depending upon the choice of initial waiting time distribution.

The purpose of this paper is to show that the method we developed earlier for analysing the spectral properties can be applied here allowing us to demonstrate the diffusive behaviour for long times. We also present an approximate evaluation of the diffusion constant. Further we present a detailed numerical study of the random walk.

2. Model for diffusion on a one-dimensional quasi-periodic lattice

Consider a Fibonacci chain with two length scales L and S arranged in an quasi-periodic sequence. Due to the fact that there are two length scales, we have three types of sites α, β and γ as shown in figure 1, suggesting three distinct jump probabilities W_{α}, W_{β} and W_{γ} corresponding to jumps from W_{n_i+1,n_i}, $i = \alpha$, β and γ. The master equation reads

$$\mathrm{d}P_n/\mathrm{d}t = W_{n,n+1} P_{n+1} + W_{n,n-1} P_{n-1} - P_n. \tag{1}$$

Since the chain is quasi-periodic the W's are distributed quasi-periodically. Further, the random walk is an inhomogeneous random walk. Following our earlier method we can cast (1) in the following form

$$\frac{\mathrm{d}G(k, t)}{\mathrm{d}t} = [\exp(-ik) - 1] G(k, t) + 2i \sin k \int W(k') G(k-k', t) \mathrm{d}k',$$
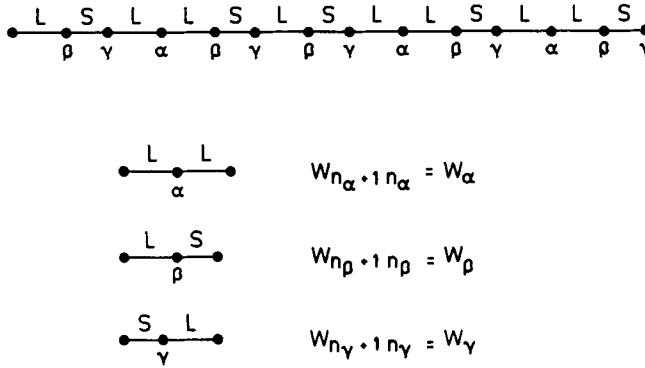
Figure 1. A Fibonacci chain with three distinct sites and the associated jump probabilities.

where,

$$G(k, t) = \sum_n P_n \exp(ikn) \quad \text{and} \quad W(k) = \sum_n W_{n+1,n} \exp(ikn). \tag{3}$$

It can be noted that the relative number of α, β and γ appears in the ratio $\tau^{-1}:1:1$. Therefore we choose the jump probabilities

$$W_{n_\alpha+1, n_\alpha} = W_\alpha, \ W_{n_\beta+1, n_\beta} = W_\beta \ \text{and} \ W_{n_\gamma+1, n_\gamma} = W_\gamma$$

(and their compliments) disbributed in the same quasi-periodic manner as the sites α, β and γ (see figure 1). Following the projection method (Zia and Dallas 1985; Valsakumar and Kumar 1986), the structure factor $W(k)$ can be obtained by choosing the slit widths $S_\alpha = d_1/\tau \sqrt{\tau r}$, $S_\beta = S_\gamma = d_1/\sqrt{\tau r}$, where $r = d_1/d_2$ is the ratio of the two lengths scales chosen (which in principle could be any two lengths) and $\tau = \frac{1}{2}(1 + \sqrt{5})$. Then

$$W(k) = W_\alpha \sum_{n_\alpha} \exp(ikn_\alpha) + W_\beta \sum_{n_\beta} \exp(ikn_\beta) + W_\gamma \sum_{n_\gamma} \exp(ikn_\gamma).$$

The calculations have been carried out for a general d_1 and d_2 (see Valsakumar *et al* 1987). However, since for the present case it is sufficient to have $d_1 = d_2 = 1$, we get a simpler expression for $W(k)$

$$W(k) = \sum_{n,m} \left\{ \frac{W_\alpha \exp\left[-i\phi_{nm}\left(\frac{1+4\tau}{\tau}\right)\right]}{\tau(1+\tau)} \frac{\sin\phi_{nm}/\tau}{\phi_{nm}/\tau} + \frac{W_\gamma \exp(-i3\phi_{nm})}{(1+\tau)} \frac{\sin\phi_{nm}}{\phi_{nm}} \right.$$

$$\left. + \frac{W_\beta \exp(-i\phi_{nm})}{(1+\tau)} \frac{\sin\phi_{nm}}{\phi_{nm}} \right\} \delta(k - k_{nm}), \tag{4}$$

where

$$\phi_{nm} = \frac{\pi(m-n)}{1+\tau} \quad \text{and} \quad k_{nm} = \frac{2\pi(m+n\tau)}{1+\tau}. \tag{5}$$

The wave vectors k_{nm} are bounded between 0 and 2π. Using (4) in (2) we get

$$\frac{dG(k, t)}{dt} = [\exp(-ik) - 1] G(k, t) + 2i \sin k \sum_{n, m} \chi_{nm} G(k - k_{nm}, t),$$

where χ_{nm} is the quantity in curly bracket in (4). For simplicity we take $W_\alpha = \frac{1}{2}$ and $W_\gamma = 1 - W_\beta$ thereby reducing the number of independent jump probabilities to one. (Note this choice is suggested by the symmetry, see figure 1). Then, we have

$$\frac{dG(k, t)}{dt} = (\cos k - 1) G(k, t) + 2i \sin k \sum_{n, m}' \chi_{nm} G(k - k_{nm}, t), \tag{6}$$

where the prime on the summation sign means that the $n = m = 0$ contribution is absorbed in the first term. It is worth noting the similarity of this equation with the harmonically coupled chain with three spring constants. This similarity will be used later to obtain an approximate expression for the diffusion constant. When $W_\alpha = W_\beta = W_\gamma = \frac{1}{2}$ is chosen (6) reduces to the expression for the usual random walk.

3. Numerical results

We have carried out numerical work which we briefly report below. The investigations include the study of the probability distribution (for W_β in steps of 0·1), the mean square distance with and without averaging over the initial configurations. Figure 2 shows a plot of the probability distribution for $W_\beta = 0·1$, time steps 3000 with initial starting point as the β site. The distribution has a feature of the probabilities peaking at (roughly) every eighth site with a general profile of a Gaussian. When $W_\beta (W_\gamma)$ is small then the difference in the occupancy of the $\beta(\gamma)$ sites compared to $\gamma(\beta)$ site is high. As $W_\beta \to \frac{1}{2}$ these differences go to zero restoring a continuous Gaussian profile. The corresponding σ^2 (not averaged over the initial sites) has sawtooth character over successive time steps. A typical plot for three values of W_β up to 50 steps where 5000 to 7000 histories are averaged is shown in figure 3. (It should be mentioned here that $\langle R \rangle$ fluctuates between 1 and -1). However when averaged over initial sites this sawtooth character disappears. In figure 4, we have plotted σ^2 (averaged over initial sites) for several values of W_β (values marked in the figure). It is seen that the diffusion constant shows an increase from small values to maximum at $W_\beta = \frac{1}{2}$ again falling as $W_\beta \to 1$. The diffusion constant we obtained as a function of W_β is shown in figure 5. The shape of this curve is in general agreement with the results of Kohomoto and Banavar (1986). It should be pointed out that the correspondence between the two models is not one to one since we have used all the three distinct sites. This might be the reason why $D(W_\beta)$ is nearly symmetric in our model in contrast to the results of Kohomoto and Banavar (1986) (wherein they use only two types of sites).

4. Perturbative approach

In studying the spectral properties of one-dimensional quasi crystals, it has been shown by a number of authors (including our group) that there is a dense set of gaps
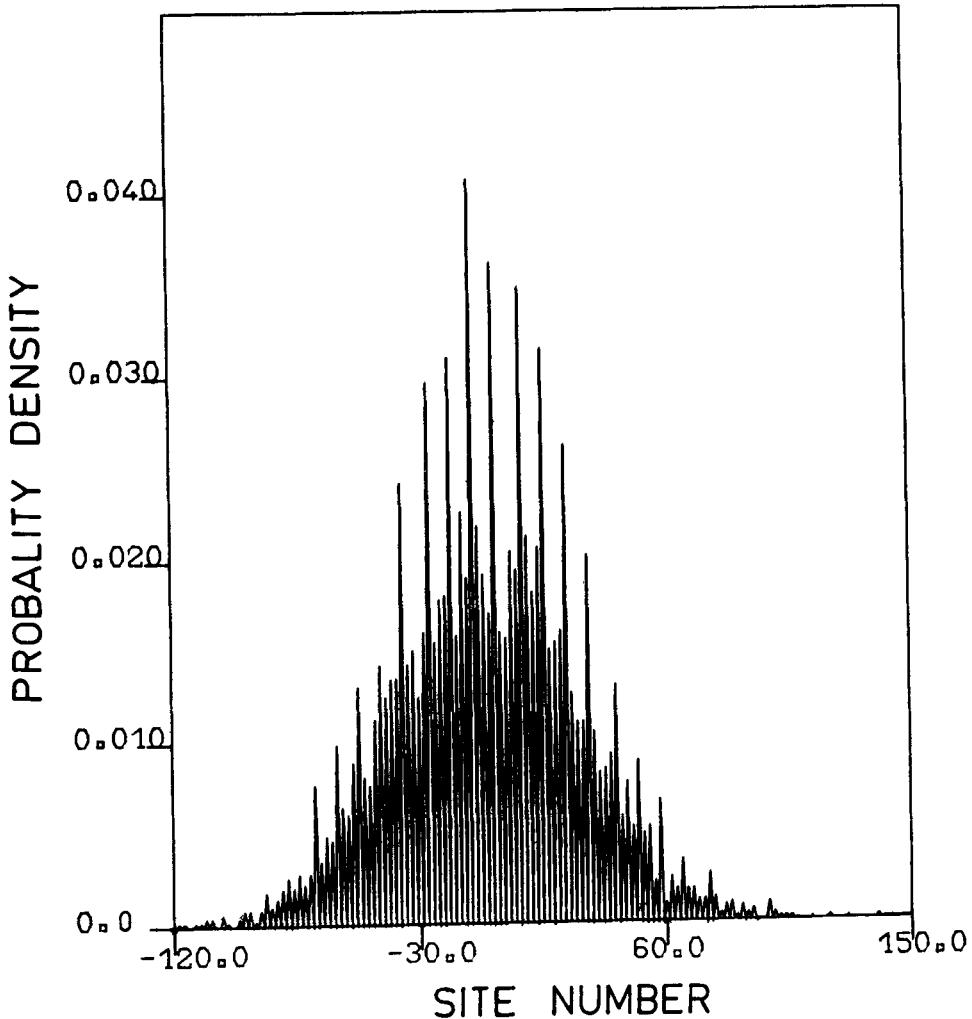
Figure 2.   Probability density for $W_\beta = 0.1$ and 3000 time steps. Origin corresponds to the central peak.

appearing at $k = k_{nm}/2$. Using an approach similar to calculations of the band gap at the band edges, we were able to derive an expression for the gaps (Valsakumar and Ananthakrishna 1987; Valsakumar *et al* 1987). Using this we were able to demonstrate that the magnitude of the gaps goes to zero as $k \to 0$ for the vibrational spectrum. Since the equation of motion for the vibrational problem is formally the same as (1) (if we consider the long-time limit of (1). i.e. the number of sites covered by the random walker is large), this would imply that $z \sim k^2$ where z is the conjugate variable of t. We shall make use of the fact that the eigenvalues exhibit jumps for all values $k = k_{nm}/2$ and the fact that gaps of finite strength affect the coefficient multiplying k^2. Before proceeding to determine the diffusion constant, we first demonstrate that within the perturbative approximation, the long-time limit is linear in t. As mentioned earlier since the gaps occur at $k = k_{nm}/2$ we evaluate the eigenvalues by assuming all other $k_{nm}/2$ do not interfere (for details see Valsakumar and Ananthakrishna 1987). Within this approximation we have
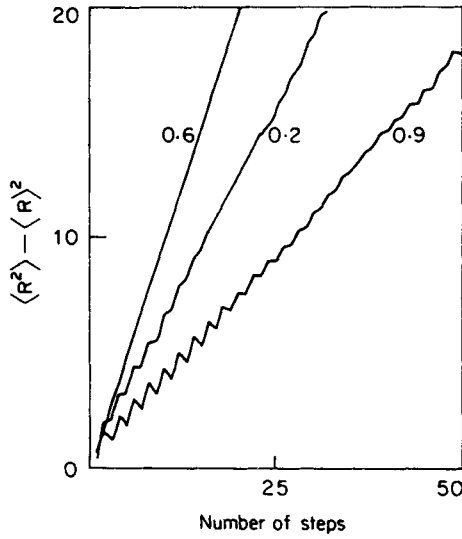
Figure 3. σ^2 as a function of number of steps for various values of W_β. Initial sites are also averaged.
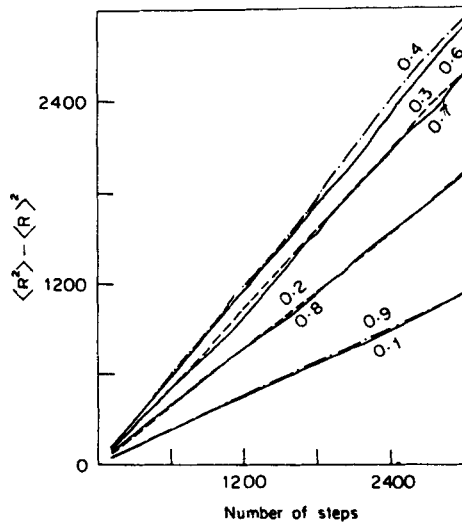

Figure 4. σ^2 as a function of number of steps for a specific choice of site with 5000 histories.

$$(d/dt)\, G = \mathbf{R}\, G,$$

where

$$G^T = (G\,(k_{nm}/2,\, t),\, G\,(-k_{nm}/2,\, t))$$

and

$$\vec{\mathbf{R}} = \begin{pmatrix} \cos\,(k_{nm}/2) - 1 & 2i\,\sin\,(k_{nm}/2)\,\chi_{nm} \\ -2i\,\sin\,(k_{nm}/2)\,\chi_{nm}^{*} & \cos\,(k_{nm}/2) - 1 \end{pmatrix} \tag{7}$$
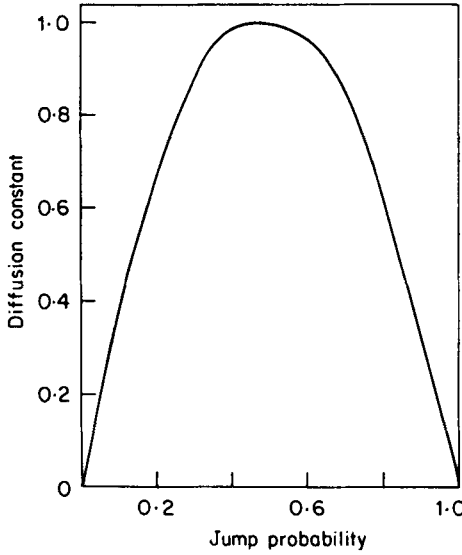
Figure 5. Diffusion constant as a function of W_β.

The two eigenvalues are given by

$$\lambda^{\pm} = (\cos k_{nm}/2 - 1) \pm 2 |\chi_{nm}| \sin k_{nm}/2. \tag{8}$$

By calculating the eigen functions, we obtain

$$G(-k_{nm}/2, t) = \tfrac{1}{2} [\exp(\lambda^{+} t) + \exp(\lambda^{-} t)] - \frac{\chi_{nm}}{2|\chi|} [\exp(\lambda^{+} t) - \exp(\lambda^{-} t)].$$

Here we have used the origin to be the initial starting point. It can be shown that

$$|\chi_{nm}| \sin k_{nm}/2 = \sin k_{nm}/2 \left|(1 - 2 W_\beta) \frac{\sin^2 \phi_{nm}}{\phi_{nm} \tau^2}\right|$$

since $|\sin \phi_{nm}| = |\sin k_{nm}/2|$, this term has a k^3 dependence (for a particular choice of n, m; $k_{nm}/2 \sim \tau^{-r+2}$ and $\phi_{nm} \sim 2/k_{nm}$ then this term has a k^4 dependence). Thus the leading contribution for the long-time behaviour comes from the k^2 term and is linear in t. Further the diffusion constant in this approximation is that of a conventional random walk. Since the numerical results suggest that this is an artifact of the approximation, we outline an argument to obtain an approximate expression for the diffusion constant.

We note that the spectrum is a point spectrum and there is a dense set of gaps. The bigger gaps have an effect of depressing the $k \to 0$ part of the spectrum (in reference to the case $W_\alpha = W_\beta = W_\gamma = \tfrac{1}{2}$) although it retains the k^2 dependence, which means that the coefficient of the k^2 term is altered. This comes about because all modes interact due to the self-similar nature of the wave vectors. The magnitude of the gap is

$$\Delta Z = 4 \sin^2 k_{nm}/2 |1 - 2 W_\beta| (\sin \phi_{nm}/\phi_{nm} \tau^2) \tag{9}$$

This is identical in form with the vibrational problem (see Valsakumar and Ananthakrishna 1987), the first term corresponds to the spectrum of the conventional

chain and the second to the jump at each $k_{nm}/2$. The last factor clearly goes to zero as $k \rightarrow 0$. It is worth noting that if we leave out the jump part, the spectrum has to be a k^2 dependence. The total contribution (for any W_β) from the dominant gaps gives a factor of approximately 0·5. Thus the contribution for modification of the spectrum is $\frac{1}{2} \sin^2 k_{nm}/2 \cdot |1 - 2 W_\beta|$. (It should be emphasized that the prefactor of 0·5 is only an estimate). Thus

$$D \simeq [1 - |1 - 2 W_\beta|].$$

This gives a linear change of D as a function of W_β in contrast to the numerical result. This is the best that could be expected on the basis of a pertubative approach and is expected to hold only for small deviation of W_β (around 0·5). The above arguments are rather heuristic and should be taken with caution. However a better approach would be to use a renormalization group approach where the scale similarity would lead to the renormalization of the jump probabilities. Such an approach should be expected to give the correct form of $D(W_\beta)$.

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