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# Diffusion on a quasiperiodic chain

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**Abstract.** An exact solution to the problem of diffusion on a quasiperiodic chain is provided by a decimation method involving scaling by an irrational length factor.

## 1. Introduction

Considerable interest has recently been focused on various physical phenomena on quasiperiodic lattices [1-5]. These include quasicrystal diffraction patterns [4-6], the stability and elastic properties of incommensurate structures [7], etc. Various construction methods for quasiperiodic lattices such as the grid method [8] and the projection technique from higher-dimensional periodic lattices [4-6] have been shown to be equivalent. The phonon spectra in a one-dimensional quasicrystal [9] reveal a rich structure with scaling properties similar to those observed in tight-binding models with incommensurate (quasiperiodic) potentials [10].

We consider the problem of a random walk (discrete diffusion) on a quasiperiodic chain and obtain an analytic solution. We examine the long-time dynamics of the random walk using the dynamic scaling hypothesis.

A random walk on a quasiperiodic lattice is of interest for several reasons. Quasiperiodic lattices are intermediate between regular Bravais lattices and random (disordered) lattices. Although these structures lack translational invariance and are self-similar by construction, they are, nevertheless, different from fractal or hierarchical lattices. This is easily seen in one dimension where at least two basic lengths or 'tiles' are needed to define a quasiperiodic pattern [1]. Random walks (or diffusion) on dilute (disordered) lattices and on non-random fractals often exhibit anomalous behaviour [11, 12]. It is therefore natural to examine if such behaviour emerges on a quasiperiodic lattice.

The 'geometry' of the problem suggests the use of the position space renormalisation group to study the dynamics of the random walk [12]. In fact, this provides an exact solution to the problem. It turns out that the quasiperiodicity necessitates the introduction of a new 'decimation' scheme. This differs from the conventional method used on regular and fractal lattices where, for example, every other site is eliminated to obtain a lattice with a scaled lattice constant. On a quasiperiodic lattice the decimation involves an irrational length scale and the eliminated sites themselves form a quasiperiodic pattern. This leads to certain interesting consequences in the recursion relations determining the temporal evolution of the random walk. For the sake of analytical tractability we restrict ourselves to a nearest-neighbour random walk on a one-dimensional quasiperiodic chain.

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We begin by describing the general features of one-dimensional quasiperiodic (QP) patterns in § 2. We then define the temporal evolution of a random walk on this set of points in § 3. After setting up the decimation scheme, we write down exact (non-linear) transformation equations for the waiting-time distributions that determine the evolution of the walk at each site. In § 4 we linearise the transformation equations about the fixed point. The 'relevant' eigenvalue then leads to the exponent that relates the distance travelled by a random walker to the time taken (for long times). Depending on the initial waiting-time distributions, the behaviour ranges from that for the 'conventional' random walk to other anomalous forms.

## 2. One-dimensional quasiperiodic lattice

A one-dimensional quasicrystal can be constructed by projecting certain sites of a square lattice on to a line [6]. Alternatively, we can start with two basic tiles A and B (such that the ratio of their lengths is an irrational number) and prescribe a transformation rule by defining a matrix $M$ for the generation of the subsequent pattern [1]. We consider the latter approach here since the transformation rule then gives a clue to the decimation scheme.

The transformation matrix $M$ needs to satisfy certain conditions [1] in order to generate a QP pattern. These are (i) the elements of $M$ are non-negative, and (ii) the characteristic polynomial of $M$ is not factorisable into polynomials with rational coefficients. Certain additional conditions need to be imposed on $M$ if the QP pattern is also required to be self-similar. This is easily written down for the simple case of generating a pattern with just two tiles. Let

$$A/B = r \qquad \text{(an irrational)} \tag{1}$$

and the transformation rule for inflation be given by

$$\begin{bmatrix} A' \\ B' \end{bmatrix} = \begin{bmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix}. \tag{2}$$

Let $\lambda_\pm$ be the irrational roots of the characteristic polynomial of $M$ in (2). For the QP pattern to be self-similar, we require

$$\frac{A}{B} = r = \frac{m_{11}A + m_{12}B}{m_{21}A + m_{22}B}. \tag{3}$$

That is, the ratio of the lengths of the basic tiles should be a fixed point of the transfer matrix. The scale factor that determines by how much the tiles are inflated (or deflated) at every step of iteration is $\lambda_+$ (or $\lambda_-$). For the special class of transformation matrices with $m_{22} = 0$ and $m_{21} = 1$, the self-similarity ratio $r$ is equal to $\lambda_+$.

An oft-quoted example of a 1D QP sequence is one in which the ratio of the tile lengths, $l_a/l_b$, is equal to the 'golden mean', $\tau = (1+\sqrt{5})/2$. Beginning with either tile, one iterates by substituting AB for each A and A for each B, yielding the QP string ABAABABAABAAB .... Each neighbouring pair of sites is separated either by a long (A) or short (B) interval. The sequence of intervals corresponds to the well known Fibonacci sequence. At the $n$th step of iteration of the lattice, the total number of bonds present is $f_n$, where $f_n$ $(n = 0, 1, 2, \ldots)$ represents the Fibonacci numbers $1, 1, 2, 3, \ldots$. The $f$ satisfy the recurrence relation

$$f_n = f_{n-1} + f_{n-2}. \tag{4}$$

## 3. Random walk on the QP chain

It is necessary to formulate the random walk problem on a quasiperiodic chain in a slightly different manner compared with other well known random walk problems in disordered systems [13]. The excitation dynamics on random one-dimensional systems often exhibit anomalous behaviour at low frequencies (or long times). In these systems, the disorder is manifest in the transition rates that govern the individual jumps of a random walker. The random walk itself is assumed to be Markovian. This approach is suitable for diffusion on lattices which are translationally invariant.

The distinctive mark of a QP chain is that the lattice points are distributed neither uniformly nor randomly along the chain. A (Markovian) master equation approach with explicitly site-dependent transition rates with different values at each site depending on the environment becomes tedious and complicated. We find it simpler to use the continuous time random walk (CTRW) approach [14] with distinct waiting-time distributions for jumps across long and short bonds on the QP chain. Machta [15, 16] used a similar approach in studying the long-time properties of a one-dimensional random walk with static disorder using the position space renormalisation group. These results have further been vindicated by an exact calculation [17]. The principal advantage of this method is that it enables us to write down the renormalisation group transformation equations for the Laplace transform of the waiting-time distributions under a site decimation. Since the transformed waiting-time distributions are no longer exponential (corresponding to a Markovian walk), it becomes necessary to work in the framework of non-Markovian continuous time random walks (CTRW).

### 3.1. *The decimation scheme*

Consider a nearest-neighbour CTRW [14] on the infinite QP chain. We assign two distinct waiting-time distributions, $\psi_a(t)$ and $\psi_b(t)$, for jumps across A and B bonds, respectively. $\psi_a(t)\,dt$ ($\psi_b(t)\,dt$) is the probability for the walker to jump across an A (B) bond within $(t, t+dt)$ given that a jump has occurred at $t=0$. The decimation scheme needed to go from one step of the QP sequence iteration to the next lowest is easily found. This corresponds to eliminating those sites which are at the left edge of each B bond. Since the patterns of both the A and B bonds are themselves quasiperiodic within the sequence, the eliminated sites also form a QP sequence. For a given step, $n$, in the iteration process, the $f_{n-2}$ sites that are to be eliminated (corresponding to the $f_{n-2}$ B bonds present) can be enumerated easily. This could be done by writing down the recursion relation that determines them with given initial conditions. The decimation yields the QP sequence at the $(n-1)$th step of iteration, with tile lengths $A'=\tau A$ and $B'=\tau B$. The decimation by the irrational length scale, $\tau$, is a consequence of the quasiperiodicity. (On regular lattices, under decimation, the lattice constant scales to an integer multiple of the original lattice constant.)

A few important points that need to be noted in this irrational QP decimation scheme are as follows.

(i) For every site $i$ that is eliminated (at the $n$th step) its neighbouring sites $i-1$ and $i+1$ are preserved under the decimation.

(ii) There are three distinct possibilities of the 'triplet' of eliminated sites at a given step. The possible triplets are $(i, i-2, i+2)$, $(i, i-2, i+3)$ and $(i, i-3, i+3)$.

Since the QP chain is non-translationally invariant, it is tedious to write down the generalised master equation for the CTRW and keep track of the site indices after the decimation. Instead, it is sufficient if we consider the various possibilities for the immediate environment at any arbitrary site in the QP chain. These are represented in figure 1. The total waiting-time distribution, $\psi_r$, at any arbitrary site $r$ is, therefore, either $2\psi_a$ or $\psi_a+\psi_b$. The normalisation of $\psi_r$ implies the following behaviour for the Laplace transform of $\psi_a$ and $\psi_b$. Let $u$ denote the transform variable and $\tilde{\psi}_a$ and $\tilde{\psi}_b$ denote the Laplace transformed functions. Then, at small $u$,

$$\begin{aligned}
&\tilde{\psi}_a \simeq \tfrac{1}{2}(1-Tu+O(u^2))\\
&\tilde{\psi}_b \simeq \tfrac{1}{2}(1-T'u+O(u^2)).
\end{aligned}\tag{5}$$

Here, $T$ and $T'$ are constants and we have assumed the finiteness of the first moments of the waiting-time distributions.

Consider a typical sequence of decimation on the QP chain represented in figure 2. Figure 2($b$) depicts the sequence after elimination of the encircled sites in figure 2($a$). Let $\Phi^{\pm}$ represent the waiting-time distributions at any site to the right and left, respectively, after the first decimation. These can be expressed in terms of $\psi^{\pm}$ ($\psi_a$, $\psi_b$). This is easily done for the Laplace transformed quantities. We have, for example,

$$\tilde{\Phi}^{+}_{i-1}=\tilde{\psi}^{+}_{i-1}\tilde{\psi}^{+}_{i}\sum_{s=0}^{\infty}(\tilde{\psi}^{+}_{i-1}\tilde{\psi}^{-}_{i}+\tilde{\psi}^{-}_{i-1}\tilde{\psi}^{+}_{i-2})^{s}.\tag{6}$$

The prefactor on the right represents the probability density for jumping directly from site $i-1$ to site $i+1$. The infinite sum represents those contributions in which the walker can make any number of jumps between sites $i$ and $i-1$ and sites $i-2$ and $i-1$ within a time interval $t$, before making a jump to $i+1$. Similar relations can be written for the waiting-time distributions at sites $i+1$ and $i+2$. Carrying out the geometric summation in each case finally yields the following set of transformed waiting-time distributions for the system after one decimation from its initial form:

$$\begin{aligned}
&\tilde{\Phi}^{+}_{i-1}=\tilde{\psi}_a\tilde{\psi}_b(1-\tilde{\psi}^2_a-\tilde{\psi}^2_b)^{-1}=\tilde{\psi}_1\\
&\tilde{\Phi}^{-}_{i-1}=\Phi^{+}_{i+1}\\
&\tilde{\Phi}^{-}_{i+1}=\tilde{\psi}_a\tilde{\psi}_b(1-\tilde{\psi}^2_b)^{-1}=\tilde{\psi}_2\\
&\tilde{\Phi}^{+}_{i+1}=\tilde{\psi}_a(1-\tilde{\psi}^2_b)^{-1}=\tilde{\psi}_3\\
&\tilde{\Phi}^{-}_{i+2}=\tilde{\psi}_a(1-\tilde{\psi}^2_a)^{-1}=\tilde{\psi}_4\\
&\tilde{\Phi}^{+}_{i+2}=\tilde{\psi}_a\tilde{\psi}_b(1-\tilde{\psi}^2_a)^{-1}=\tilde{\psi}_5.
\end{aligned}\tag{7}$$

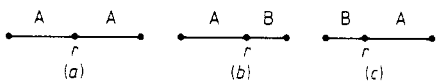


**Figure 1.** The three possible environments at any arbitrary site in the QP chain. ($a$) A long bond (A) to the right and left of a given site; ($b$) a long bond to the left and a short bond (B) to the right; ($c$) a short bond to the left and a long bond to the right.

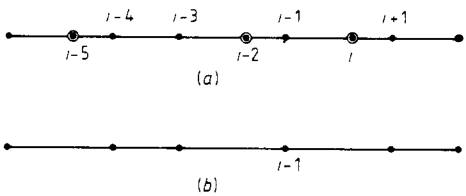


**Figure 2.** ($a$) A typical QP sequence at a given step of iteration. The sites to be eliminated are encircled. ($b$) The sequence obtained after decimation with bond lengths A′ and B′.

The $\tilde{\psi}_i$ $(i = 1, 2, \ldots, 5)$ are the waiting-time distributions after decimation for the three possible environments (figure 3) at any arbitrary site. It is easy to check that the total waiting-time distribution is normalised in each of the three cases. Though $\tilde{\psi}_2$ is different from $\tilde{\psi}_5$, and $\tilde{\psi}_3$ different from $\tilde{\psi}_4$, the transformation equations preserve the following symmetry:

$$\frac{\tilde{\psi}_2}{\tilde{\psi}_3} = \frac{\tilde{\psi}_5}{\tilde{\psi}_4}. \tag{8}$$

If a subsequent decimation is carried out on the transformed lattice using the same prescription we find that the $\psi_i$ $(i = 1, 2, \ldots, 5)$ transform into the following set of functions, $\psi_i'$ $(i = 1, 2, \ldots, 5)$, given by

$$\begin{aligned}
\tilde{\psi}_1' &= \tilde{\psi}_3\tilde{\psi}_5(1 - \tilde{\psi}_2\tilde{\psi}_5 - \tilde{\psi}_3\tilde{\psi}_4)^{-1} \\
\tilde{\psi}_2' &= \tilde{\psi}_4\tilde{\psi}_2(1 - \tilde{\psi}_4\tilde{\psi}_3)^{-1} \\
\tilde{\psi}_3' &= \tilde{\psi}_5(1 - \tilde{\psi}_4\tilde{\psi}_3)^{-1} \\
\tilde{\psi}_4' &= \tilde{\psi}_1(1 - \tilde{\psi}_1\tilde{\psi}_2)^{-1} \\
\tilde{\psi}_5' &= \tilde{\psi}_1\tilde{\psi}_3(1 - \tilde{\psi}_1\tilde{\psi}_2)^{-1}.
\end{aligned} \tag{9}$$

This transformation also preserves the normalisation of the total waiting-time distribution at any arbitrary site. Furthermore, equation (8) is also true for the transformed $\psi_i'$.

Equation (9) represents the exact set of renormalisation group transformation equations for the five distinct waiting-time distributions $\psi_i$ that characterise the random walk on the quasiperiodic chain at a general stage of the decimation process.

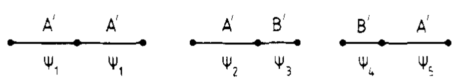


**Figure 3.** The waiting-time distributions for jumps to the right and left from an arbitrary site after the first decimation.

## 4. Linearisation and dynamic scaling

A dynamic scaling form relating the diffusion length $R$ and diffusion time $t$ (analogous to the frequency-wavevector relation) can be found by linearising the non-linear transformation equations about their zero-frequency $(u \simeq 0)$ fixed point. This is done by first writing the linearised forms of the $\psi_i$ near $u \simeq 0$ after many iterations.

An interesting feature of the transformation equations is worth observing at this stage. It turns out that the $u$-independent term in $\tilde{\psi}_2(n)$ near $u \simeq 0$ after $n$ transformations is $f_n/f_{n+2}$, where the $f_n$ represent the Fibonacci numbers. The corresponding constant term in $\tilde{\psi}_3(n)$ near $u \simeq 0$ is $f_{n+1}/f_{n+2}$, which automatically ensures that the normalisation of the total waiting-time distribution is preserved at every stage of decimation. The normalisation check further requires that the constant term in $\tilde{\psi}_1(n)$ near $u \simeq 0$ is $\frac{1}{2}$ for all $n$. By symmetry, the constant term in $\tilde{\psi}_5(n)$ is the same as that in $\tilde{\psi}_2(n)$, with a similar equality between $\tilde{\psi}_3(n)$ and $\tilde{\psi}_4(n)$. As $n\to\infty$, up to the leading $u$-dependent contributions, the $\tilde{\psi}_i$ therefore, take the following forms:

$$\begin{aligned}
\tilde{\psi}_1 &= \tfrac{1}{2}+\delta_1\\
\tilde{\psi}_2 &= \phi^2+\delta_2\\
\tilde{\psi}_3 &= \phi+\delta_3\\
\tilde{\psi}_4 &= \phi+\delta_4\\
\tilde{\psi}_5 &= \phi^2+\delta_5
\end{aligned}\tag{10}$$

where $\phi=(\sqrt{5}-1)/2=1/\tau$. The $\delta_i$ represent the $u$-dependent leading terms. Substituting this in (6) and retaining terms only to the lowest order in $u$ yields the transformation for the $\delta_i$. Since the symmetry expressed by (8) is true to all orders in $u$, one obtains a linear combination of $\delta_i$ that remains invariant to $O(u)$. This is

$$\mu=\delta_5-\delta_2+\phi(\delta_3-\delta_4).\tag{11}$$

Expressing $\delta_5$ in terms of $\mu$, we obtain the following transformation matrix for the $\delta_i$:

$$\begin{pmatrix}\tilde{\delta}_1'\\ \delta_2'\\ \delta_3'\\ \delta_4'\\ \mu'\end{pmatrix}=\begin{pmatrix}0 & 2/\phi^3 & 1/\phi & 1/\phi^4 & 1/\phi^4\\ 0 & 1 & \phi^2 & 1 & 0\\ 0 & 1/\phi & -\phi^2 & 1/\phi & 1/\phi\\ \phi^2 & \phi^2 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 1\end{pmatrix}\begin{pmatrix}\tilde{\delta}_1\\ \delta_2\\ \delta_3\\ \delta_4\\ \mu\end{pmatrix}.\tag{12}$$

Here $\tilde{\delta}_1=4\delta_1$ and $\tilde{\delta}_1'=4\delta_1'$. The eigenvalues of the matrix are

$$\lambda=1,\,1/\phi^2,\,-\phi,\,-1,\,-\phi^2.\tag{13}$$

Out of these, the only relevant eigenvalue ($>1$) is $\lambda=1/\phi^2$. The associated scaling field, $\gamma$, found by using the left eigenvector corresponding to $\lambda=1/\phi^2$ is

$$\gamma=(1-\phi)\delta_1+2(1+\phi)\delta_2+\phi\delta_3+(2+\phi)\delta_4+(2\phi+1)\mu.\tag{14}$$

Under a dilatation by a length factor $\tau=1/\phi$, we have

$$\gamma\to\gamma'=\frac{1}{\phi^2}\gamma.\tag{15}$$

If near $u\simeq 0$, $\gamma$ is assumed to have the scaling form $\gamma\propto(\text{length})^{\tilde{z}}$, then

$$\tilde{z}=\frac{\ln(1/\phi^2)}{\ln(1/\phi)}=2.\tag{16}$$

Because the $\delta_i$ are proportional to $u$, with coefficients dependent on $T$, $T'$ and $\phi$, the scaling field $\gamma$ is in general proportional to $u$. Thus we find that the dynamic exponent $z$ defined by

$$u\propto(\text{length})^z\tag{17}$$

satisfies $z=\tilde{z}=2$. In the present situation, due to the lack of translational invariance, it is more appropriate to write a dynamic scaling form relating $R$ and $t$ [11] rather than $\omega$ and $k$. This is given by

$$R\underset{t\to\infty}{\propto}t^{1/z}F(R^z t).\tag{18}$$

Here, $z=2$ corresponds to the 'conventional' random walk ($R\sim t^{1/2}$). This kind of behaviour in the QP chain is entirely due to the finiteness of the first moment of the waiting-time distributions.

It may be possible for $T$ and $T'$ to be related in such a way that the scaling field $\gamma$ in (14) vanishes. This would imply that $\gamma$ is quadratic in $u$ to lowest order. We then get the behaviour $R \propto_{t\to\infty} t$, since (17) now reads $u^2 \propto (\text{length})^z$. The value of the ratio $T'/T$ required to give the result is not easy to write down. This is because the $\psi_i$ in (9) are non-linearly coupled to each other. Any attempt to obtain the explicit dependence of $\delta_i$ on $T$ and $T'$ after $n$ transformations leads to a complicted set of equations. In spite of the elegant properties of the Fibonacci numbers it is not possible to deduce the analytic dependence for large $n$.

Another interesting case occurs when the waiting-time distributions $\psi_a$ and/or $\psi_b$ do not have finite first moments [14]. If we assume the A bonds to represent higher energy barriers which, therefore, makes them difficult to surmount, the $u\simeq 0$ behaviour of $\tilde{\psi}_a$ could be of the form

$$\tilde{\psi}_a \simeq \tfrac{1}{2}(1 - Tu^\alpha + O(u)) \qquad 0 \leqslant \alpha \leqslant 1. \tag{19}$$

Let $\tilde{\psi}_b$ continue to have the form shown earlier in (2). Substituting these forms in (10), we find that the leading behaviour of all the $\tilde{\psi}_i$ ($i = 1, 2, \ldots, 5$) is of $O(u^\alpha)$. This would then result in anomalous diffusion of the type $R \sim t^{\alpha/z}$. For $z=2$, this implies sub-linear diffusion wherein $R\sim t^{\alpha/2}$. This result is, however, an artefact of the CTRW model assumed for the random walk. Whenever the waiting-time distribution has an infinite first moment there is no long-range diffusion irrespective of the nature of the lattice. This anomalous behaviour is distinct from that observed in random systems [13] which arises due to the divergence of the infinite first moment of the random (site-dependent) transition rates.

## 5. Conclusions

The results obtained in the present paper are based upon the decimation scheme set up for the 1D QP (Penrose) chain. Similar decimation schemes can be set up for other types of transformation rules which generate QP sequences which are self-similar or QP sequences which are not self-similar or self-similar structures which are not quasiperiodic [1]. It may be useful to examine the nature of diffusion on higher-dimensional QP lattices built by projecting hypersurfaces of appropriate periodic lattices.

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