# Diffusion on Archimedean lattices 

Lasko Basnarkov*<br>Saints Cyril and Methodius University, Faculty of Electrical Engineering, P. O. Box 574, Skopje, Macedonia<br>Viktor Urumov ${ }^{\dagger}$<br>Saints Cyril and Methodius University, Faculty of Natural Sciences and Mathematics, P. O. Box 162, Skopje, Macedonia

(Received 26 December 2005; published 12 April 2006)


#### Abstract

We consider random diffusive motion of classical particles over the edges of Archimedean lattices. The diffusion coefficient is obtained by using periodic orbit theory. We also study deterministic motion over a honeycomb lattice without the possibility for an immediate return to the preceding node, controlled by a tent map with the golden ratio slope. Numerical analysis is performed to confirm the theoretical results.


DOI: 10.1103/PhysRevE.73.046116
PACS number(s): 02.50.Ey, 05.40.Jc, 05.40.Fb

## INTRODUCTION

Archimedean lattices are a complete set of infinite tilings of a plane with regular polygons in which all vertices are equivalent (see Fig. 1). Their naming came from Kepler's reference to Archimedes' description of regular solid polyhedra which are related to these two-dimensional lattices. Because of their symmetry they have been studied in mathematics [1], crystallization [2,3], statistical mechanics [4], and percolation $[5,6]$. The most familiar are square, triangular, and honeycomb lattices which are also regular.

By means of periodic orbit theory the averages of observables of a system can be calculated using the properties of the shortest periodic orbits [7]. The theory can be used for analysis of hyperbolic as well as intermittent deterministic systems. Its applications range from calculation of the escape rate for three-disk billiards [7], the diffusion constant for piecewise linear maps [8] or the Lorentz gas [9], to semiclassical quantization of collinear helium [10].

The random motion of particles confined on the edges of an Archimedean lattices is diffusive. This means the meansquare displacement from the starting position of the particles grows linearly with time. The diffusion constant is proportional to the slope of the growth. The dynamics of particles over Archimedean latices can be described using the corresponding fundamental cell (domain). It consists of neighboring nodes selected and assigned in such a way that every possible trajectory can be exactly represented with a sequence of nodes in the fundamental domain only. Then a finite Markov partition of the phase space is possible and movement is expressed with a finite Markov graph. Furthermore we study deterministic motion over the hexagonal lattice. It is assumed that an immediate return to the previous vertex is not possible and the particles are guided by a tent map with the golden ratio slope. Such defined movement is chaotic and diffusive. The diffusion constant can be calculated for both types of movement with periodic orbit theory. We have made a computer simulation of the motion of the

[^0]particles and extracted the diffusion constant from numerical data. We found a very good agreement in the results from the theory and simulation.

As nomenclature we use the general notation of Grünbaum and Shephard [11]. Every lattice label has the form $\left(n_{1}^{\alpha_{1}}, n_{2}^{\alpha_{2}}, \ldots\right)$. In clockwise rotation around the vertex, $n_{i}$ represents the number of sides of the polygon and $\alpha_{i}$ denotes the number of adjacent polygons of the same type. For example, at every vertex in the first lattice in Fig. 1, $\left(3,12^{2}\right)$, one triangle and two consecutive dodecagons are connected.

## PERIODIC ORBIT THEORY: A BRIEF TOUR

In this section we sketch the main lines of the periodic orbit theory in a way similar to Ref. [9] (it is worked out in greater detail in Ref. [7]). We will focus on discrete time systems only, because movement of particles over the edges of the Archimedean lattices can be represented with a mapping. The position of a point in a $d$-dimensional space $\hat{\mathbf{x}}$, changes in (discrete) time $t$, as some function $\hat{\mathbf{f}}(\hat{\mathbf{x}})$. After $t$ iterations it maps to $\hat{\mathbf{f}}^{t}(\hat{\mathbf{x}})=\hat{\mathbf{f}}(\hat{\mathbf{f}}(\cdots \hat{\mathbf{f}}(\hat{\mathbf{x}})))=\hat{\mathbf{x}}_{t}$. The displacement


FIG. 1. Archimedean lattices with notation by Grünbaum and Shephard [11] which is explained in the text. Adapted from [6].
from the starting position $\hat{\mathbf{f}}^{t}(\hat{\mathbf{x}})-\hat{\mathbf{x}}$ is the (integrated) observable we are interested in investigating. For systems exhibiting diffusive transport, as a measure of the growth of the mean-square displacement $\left\langle\left[\hat{\mathbf{f}}^{t}(\hat{\mathbf{x}})-\hat{\mathbf{x}}\right]^{2}\right\rangle$ the spatial diffusion constant appears:

$$
\begin{equation*}
D=\lim _{t \rightarrow \infty} \frac{1}{2 d t}\left\langle\left(\hat{\mathbf{x}}_{t}-\hat{\mathbf{x}}\right)^{2}\right\rangle \tag{1}
\end{equation*}
$$

By means of an auxiliary variable $\beta$ one can consider the following average:

$$
\begin{equation*}
\left\langle e^{\beta\left(\hat{\mathbf{x}}_{t}-\hat{\mathbf{x}}\right)}\right\rangle_{\hat{\mathcal{M}}} \tag{2}
\end{equation*}
$$

carried over all initial points $\hat{\mathbf{x}}$ in the phase space $\hat{\mathcal{M}}$. The average at infinity grows exponentially, with rate

$$
\begin{equation*}
s(\beta)=\lim _{t \rightarrow \infty} \frac{1}{t} \ln \left\langle e^{\beta\left(\hat{\mathbf{x}}_{t}-\hat{\mathbf{x}}\right)}\right\rangle_{\hat{\mathcal{M}}} \tag{3}
\end{equation*}
$$

As a result of symmetry, as is the case for Archimedean lattices, there is no drift

$$
\begin{equation*}
\left.\frac{\partial s}{\partial \beta_{i}}\right|_{\beta=0}=\lim _{t \rightarrow \infty} \frac{1}{t}\left\langle\left(\hat{\mathbf{x}}_{t}-\hat{\mathbf{x}}\right)_{i}\right\rangle_{\hat{\mathcal{M}}}=0 \tag{4}
\end{equation*}
$$

The second derivatives

$$
\begin{equation*}
\left.\frac{\partial}{\partial \beta_{i}} \frac{\partial s}{\partial \beta_{j}}\right|_{\beta=0}=\lim _{t \rightarrow \infty} \frac{1}{t}\left\langle\left(\hat{\mathbf{x}}_{t}-\hat{\mathbf{x}}\right)_{i}\left(\hat{\mathbf{x}}_{t}-\hat{\mathbf{x}}\right)_{j}\right\rangle_{\hat{\mathcal{M}}} \tag{5}
\end{equation*}
$$

form a diffusion matrix which is generally anisotropic. The diffusion constant can be expressed through the rate $s$ with

$$
\begin{equation*}
D=\left.\frac{1}{2 d} \sum_{i=1}^{d} \frac{\partial^{2} s}{\partial \beta_{i}^{2}}\right|_{\beta=0} \tag{6}
\end{equation*}
$$

Assuming uniform initial density of representative trajectories, the mean in Eq. (2) is

$$
\begin{align*}
\left\langle e^{\beta\left(\hat{\mathbf{x}}_{t}-\hat{\mathbf{x}}\right)}\right\rangle_{\hat{\mathcal{M}}} & =\frac{1}{|\hat{\mathcal{M}}|} \int_{\hat{\mathcal{M}}} d \hat{\mathbf{x}} e^{\beta\left(\hat{\mathbf{x}}_{t}-\hat{\mathbf{x}}\right)} \\
& =\frac{1}{|\hat{\mathcal{M}}|} \int_{\hat{\mathcal{M}}} d \hat{\mathbf{x}} d \hat{\mathbf{y}} e^{\beta(\hat{\mathbf{y}}-\hat{\mathbf{x}})} \delta\left(\hat{\mathbf{y}}-\hat{\mathbf{f}}^{t}(\hat{\mathbf{x}})\right) \tag{7}
\end{align*}
$$

where we have used the phase space volume $|\hat{\mathcal{M}}|=\int d \hat{\mathbf{x}}$. The Dirac function checks if $\hat{\mathbf{x}}$ maps to some $\hat{\mathbf{y}}$ in $t$ iterations and makes the dependence of the mean from the map explicit. Systems such as Archimedean lattices which are spatially periodic can be studied in the fundamental domain only. This means that instead of position $\hat{\mathbf{x}}$ in the global phase space $\hat{\mathcal{M}}$, one can take the position $\mathbf{x}$ in the fundamental cell $\mathcal{M}$. The displacement from the starting position $\mathbf{A}^{t}(\hat{\mathbf{x}})=\hat{\mathbf{f}}^{t}(\hat{\mathbf{x}})-\hat{\mathbf{x}}$ can also be obtained from the fundamental cell only, by

$$
\begin{equation*}
\mathbf{A}^{t}=\sum_{k=1}^{t}\left[\hat{\mathbf{f}}^{k}(\hat{\mathbf{x}})-\hat{\mathbf{f}}^{k-1}(\hat{\mathbf{x}})\right]=\sum_{k=1}^{t}\left[\mathbf{f}^{k}(\mathbf{x})-\mathbf{f}^{k-1}(\mathbf{x})\right] . \tag{8}
\end{equation*}
$$

As the $t \rightarrow \infty$ limit behavior of the average [Eq. (7)] is needed, it is calculated with a transfer operator $\mathcal{L}^{t}$ whose kernel is

$$
\begin{equation*}
\mathcal{L}^{t}(\mathbf{y}, \mathbf{x})=e^{\beta \mathbf{A}^{t}(\mathbf{x})} \delta\left(\mathbf{y}-\mathbf{f}^{t}(\mathbf{x})\right) \tag{9}
\end{equation*}
$$

The growth rate $s$ is the leading eigenvalue of the operator $\mathcal{L}^{t}$ because it is dominant for large $t$. In the $t \rightarrow \infty$ limit the double integral is equal to the trace of the operator $\mathcal{L}^{t}$

$$
\begin{equation*}
\operatorname{tr} \mathcal{L}^{t}=\int_{\mathcal{M}} d \mathbf{x} e^{\beta \mathbf{A}^{t}(\mathbf{x})} \delta\left(\mathbf{x}-\mathbf{f}^{t}(\mathbf{x})\right) \tag{10}
\end{equation*}
$$

For hyperbolic systems this trace can be expressed through all $t$-periodic orbits $\mathbf{x}_{t}=\mathbf{x}$ ( $t$ is not necessarily the least period for the orbit),

$$
\begin{equation*}
\operatorname{tr} \mathcal{L}^{t}=\sum_{\mathbf{x}_{t}=\mathbf{x}} \frac{e^{\beta \mathbf{A}^{t}(\mathbf{x})}}{\left|\operatorname{det}\left[\mathbf{1}-\mathbf{J}^{t}(\mathbf{x})\right]\right|}, \tag{11}
\end{equation*}
$$

with Jacobian $\mathbf{J}_{i, j}=\partial f_{i}^{t} / \partial x_{j}$. We denote with $T_{p}, \mathbf{A}_{p}$, and $\mathbf{J}_{p}$ $=\mathbf{J}^{T_{p}}(\mathbf{x})$ the length (duration), displacement, and Jacobian, respectively, that correspond to some periodic orbit $p$ in the fundamental domain $\mathcal{M}$. If its length $T_{p}=t / r$, one has $\mathbf{A}^{t}$ $=r \mathbf{A}_{p}$ and $\mathbf{J}^{t}=\mathbf{J}_{p}^{r}$, because the displacement $\mathbf{A}$ is cumulative and we can apply the chain rule for the Jacobian $\mathbf{J}$. Then the trace can be expressed through prime cycles only,

$$
\begin{equation*}
\operatorname{tr} \mathcal{L}^{t}=\sum_{\mathbf{x}_{T_{p}}=\mathbf{x} ; r T_{p}=t} \frac{e^{\beta r \mathbf{A}_{p}}}{\left|\operatorname{det}\left(\mathbf{1}-\mathbf{J}_{p}^{r}\right)\right|} \tag{12}
\end{equation*}
$$

Prime cycles are those that are not repeats of simpler ones. From the matrix identity $\ln (\operatorname{det} \mathcal{L})=\operatorname{tr}(\ln \mathcal{L})$ which can be found for example in Ref. [12], the trace of the operator $\mathcal{L}$ is related to its spectral determinant

$$
\begin{align*}
\operatorname{det}(1-z \mathcal{L}) & =\exp \left(-\sum_{t=1}^{\infty} \frac{z^{t}}{t} \operatorname{tr} \mathcal{L}^{t}\right) \\
& =\prod_{p} \exp \left(-\sum_{r=1}^{\infty} \frac{z^{r T_{p}}}{r} \frac{e^{\beta r \mathbf{A}_{p}}}{\left|\operatorname{det}\left(\mathbf{1}-\mathbf{J}_{p}^{r}\right)\right|}\right) \tag{13}
\end{align*}
$$

Extraction of the rate $s$ from the determinant can be done with the substitution $z=e^{-s}$ which further leads to the corresponding dynamical $\zeta$ function

$$
\begin{equation*}
\frac{1}{\zeta(\beta, s)}=\prod_{p}\left(1-\frac{e^{\beta \mathbf{A}_{p}-s T_{p}}}{\left|\Lambda_{p}\right|}\right) \tag{14}
\end{equation*}
$$

where $\Lambda_{p}=\Pi \lambda_{e}$ is the product of the expanding eigenvalues of the Jacobian $\mathbf{J}_{p}$. The fractions in the products

$$
\begin{equation*}
t_{p}=\frac{e^{\beta \mathbf{A}_{p}-s T_{p}}}{\left|\Lambda_{p}\right|} \tag{15}
\end{equation*}
$$

are known as local traces of the periodic orbits. As can be seen they contain information about the orbit length $T_{p}$ and the value of the observable $\mathbf{A}_{p}$, as well as the weight of the
orbit $\Lambda_{p}$. Thus averages over chaotic trajectories are stated in terms of prime periodic orbits. Roughly speaking every periodic orbit represents the orbits in its vicinity which is determined by the expanding factor $\Lambda_{p}$. If it is bigger then the neighborhood is smaller, which implies that the weight or "importance" of the orbit is smaller. In this paper we will use the probability of occurrence of a periodic orbit as its weight.

The infinite product in Eq. (14) can be replaced by an infinite sum

$$
\begin{equation*}
\prod_{p}\left(1-t_{p}\right)=1-\sum_{p}(-1)^{k} t_{p_{1}} t_{p_{2}} \cdots t_{p_{k}} \tag{16}
\end{equation*}
$$

The sum is over all nonrepeating combinations of prime cycles. For Archimedean lattices the sum is a polynomial, because their Markov graph is finite. The second derivatives in Eq. (6) can be stated in terms of derivatives of the $\zeta$ function $F(s, \beta)=1 / \zeta=0$

$$
\begin{equation*}
\frac{\partial^{2} s}{\partial \beta_{i}^{2}}=-\left[\frac{\partial^{2} F}{\partial \beta_{i}^{2}}+2 \frac{\partial s}{\partial \beta_{i}} \frac{\partial^{2} F}{\partial \beta_{i} \partial s}+\left(\frac{\partial s}{\partial \beta_{i}}\right)^{2} \frac{\partial^{2} F}{\partial s^{2}}\right] / \frac{\partial F}{\partial s} \tag{17}
\end{equation*}
$$

Finally, the expression for the diffusion constant has the form

$$
\begin{equation*}
D=\frac{1}{2 d} \frac{\left.\left.\langle | \mathbf{A}_{p}\right|^{2}\right\rangle}{\left\langle T_{p}\right\rangle} \tag{18}
\end{equation*}
$$

with mean-square cycle displacement $\left.\left.\langle | \mathbf{A}_{p}\right|^{2}\right\rangle$ and mean cycle length $\left\langle T_{p}\right\rangle$

$$
\begin{align*}
\left.\left.\langle | \mathbf{A}_{p}\right|^{2}\right\rangle & =\sum(-1)^{k} \frac{\left(\mathbf{A}_{p_{1}}+\mathbf{A}_{p_{2}}+\cdots+\mathbf{A}_{p_{k}}\right)^{2}}{\left|\Lambda_{p_{1}} \Lambda_{p_{2}} \cdots \Lambda_{p_{k}}\right|}, \\
\left\langle T_{p}\right\rangle & =\sum(-1)^{k} \frac{\left(T_{p_{1}}+T_{p_{2}}+\cdots+T_{p_{k}}\right)}{\left|\Lambda_{p_{1}} \Lambda_{p_{2}} \cdots \Lambda_{p_{k}}\right|} . \tag{19}
\end{align*}
$$

That is the main result of the periodic orbit theory for the diffusion constant which we will use for Archimedean lattices.

## CALCULATING A DIFFUSION CONSTANT

We study random motion of classical particles confined to the edges of Archimedean lattices. Assuming energy conservation the speed changes only its direction at nodes of the lattice and its modulus can be taken to be 1 . We also suppose that at integer moments particles are located at vertices. Thus the movement can be analyzed with mapping from a vertex to one of its neighbors. For simplicity, the transition probability $p$ to all neighbors is considered equal. Because of conservation $\Sigma p=1$, the probability is the inverse of the coordination number $N$ (the number of edges at every vertex of the lattice) $-p=1 / N$. The full phase space for the mapping is a discrete set containing all vertices. The fundamental cell should be made with as few nodes as possible in order to simplify further calculations. The nodes in it must be denoted in such a way that every trajectory in the lattice can be uniquely determined with the list of corresponding nodes in


FIG. 2. Fundamental cell of the $\left(3^{2}, 4,3,4\right)$ lattice with assignments of the vertices.
the fundamental domain. For example on Fig. 2 is shown the fundamental cell for the most complex lattice for this problem, $\left(3^{2}, 4,3,4\right)$, and the assignment of the vertices. On the basis of the fundamental domain we can make a transition matrix with elements containing information for the transition probability and the displacement of the particle $A_{i, j}$ that is made during that transition

$$
\begin{equation*}
\mathcal{T}_{i, j}=p_{i, j} e^{\beta A_{i, j}-s T} \tag{20}
\end{equation*}
$$

We have attached the term $e^{-s T}$ to obtain as expression similar to the trace [see Eq. (15)] and we note that $T=1$. The 12 possible displacements for all lattices under consideration are given by

$$
\begin{equation*}
A_{k}=\cos \left(\frac{2 \pi k}{12}\right) e_{x}+\sin \left(\frac{2 \pi k}{12}\right) e_{y}, \quad k=0,1, \ldots, 11, \tag{21}
\end{equation*}
$$

where $e_{x}$ and $e_{y}$ are unit vectors on the $x$ and $y$ axes, respectively. For exponentials of the displacements one can assign

$$
\begin{equation*}
\mathcal{A}_{k}=e^{\beta A_{k}} \tag{22}
\end{equation*}
$$

Then the transition matrix $\mathcal{T}$ for the $\left(3^{2}, 4,3,4\right)$ lattice is

$$
\mathcal{T}=p e^{-s}\left(\begin{array}{cccccccc}
0 & \mathcal{A}_{2} & \mathcal{A}_{9} & \mathcal{A}_{4} & \mathcal{A}_{11} & 0 & 0 & \mathcal{A}_{7}  \tag{23}\\
\mathcal{A}_{8} & 0 & \mathcal{A}_{4} & \mathcal{A}_{6} & 0 & \mathcal{A}_{11} & \mathcal{A}_{1} & 0 \\
\mathcal{A}_{3} & \mathcal{A}_{10} & 0 & \mathcal{A}_{8} & \mathcal{A}_{1} & 0 & 0 & \mathcal{A}_{5} \\
\mathcal{A}_{10} & \mathcal{A}_{0} & \mathcal{A}_{2} & 0 & 0 & \mathcal{A}_{7} & \mathcal{A}_{5} & 0 \\
\mathcal{A}_{5} & 0 & \mathcal{A}_{7} & 0 & 0 & \mathcal{A}_{2} & \mathcal{A}_{10} & \mathcal{A}_{0} \\
0 & \mathcal{A}_{5} & 0 & \mathcal{A}_{1} & \mathcal{A}_{8} & 0 & \mathcal{A}_{3} & \mathcal{A}_{10} \\
0 & \mathcal{A}_{7} & 0 & \mathcal{A}_{11} & \mathcal{A}_{4} & \mathcal{A}_{9} & 0 & \mathcal{A}_{2} \\
\mathcal{A}_{1} & 0 & \mathcal{A}_{11} & 0 & \mathcal{A}_{6} & \mathcal{A}_{4} & \mathcal{A}_{8} & 0
\end{array}\right),
$$

with transition probability $p=1 / 5$. Before proceeding with computation of the determinant $\operatorname{det}(1-z \mathcal{T})$, some simplification can be achieved using the relationship between exponentials (22) taking into account the displacements (21). Those relations are

TABLE I. Diffusion constant for Archimedean lattices.

| Lattice | $N(1)^{\mathrm{a}}$ | $N(2)^{\mathrm{a}}$ | $N(3)^{\mathrm{a}}$ | Theoretical result | Theoretical value | Numerical value | Error $\times 10^{-5}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\left(3,12^{2}\right)$ | 3 | 4 | 6 | $(7+4 \sqrt{3}) / 15$ | 0.92855 | 0.92858 | 2.71 |
| $(4,6,12)^{\mathrm{b}}$ | 3 | 5 | 7 | $(2+\sqrt{3}) / 4$ | 0.93301 | 0.93302 | 0.64 |
| $\left(4,8^{2}\right)$ | 3 | 5 | 8 | $(3+2 \sqrt{2}) / 6$ | 0.97145 | 0.97113 | 3.07 |
| Hexagonal | 3 | 6 | 9 | 1 | 1 | 1.00062 | 5.69 |
| $(3,4,6,4)^{\mathrm{b}}$ | 4 | 8 | 12 | $(2+\sqrt{3}) / 4$ | 0.93301 | 0.93298 | 0.64 |
| Square | 4 | 8 | 12 | 1 | 1 | 0.99952 | 3.60 |
| Kagomé | 4 | 8 | 14 | 1 | 1 | 0.99906 | 5.06 |
| $\left(3^{4}, 6\right)^{\mathrm{b}}$ | 5 | 9 | 15 | $14 / 15$ | 0.93333 | 0.93341 | 1.61 |
| $\left(3^{3}, 4^{2}\right)$ | 5 | 10 | 15 | $(11+2 \sqrt{3}) / 15$ | 0.96427 | 0.96544 | 3.52 |
| $\left(3^{2}, 4,3,4\right)$ | 5 | 11 | 16 | $4(2+\sqrt{3}) / 15$ | 0.99521 | 0.99396 | 5.14 |
| Triangular | 6 | 12 | 18 | 1 | 1 | 1.00072 | 3.18 |

${ }^{\mathrm{a}} N(i)$ gives the number of nodes that can be reached from any selected node in not less than $i$ steps.
${ }^{\mathrm{b}}$ Numerical results correspond to averaging from $2 \times 10^{7}$ trajectories.

$$
\begin{array}{cc}
A_{2}=A_{0}+A_{4}, & \mathcal{A}_{2}=\mathcal{A}_{0} \mathcal{A}_{4}, \\
A_{3}=A_{1}+A_{5}, & \mathcal{A}_{3}=\mathcal{A}_{1} \mathcal{A}_{5}, \\
A_{6}=-A_{0}, & \mathcal{A}_{6}=1 / \mathcal{A}_{0}, \\
A_{7}=-A_{1}, & \mathcal{A}_{7}=1 / \mathcal{A}_{1},  \tag{24}\\
A_{8}=-A_{0}-A_{4}, & \mathcal{A}_{8}=1 /\left(\mathcal{A}_{0} \mathcal{A}_{4}\right), \\
A_{9}=-A_{1}-A_{5}, & \mathcal{A}_{9}=1 /\left(\mathcal{A}_{1} \mathcal{A}_{5}\right), \\
A_{10}=-A_{4}, & \mathcal{A}_{10}=1 / \mathcal{A}_{4}, \\
A_{11}=-A_{5}, & \mathcal{A}_{11}=1 / \mathcal{A}_{5} .
\end{array}
$$

Calculation of the determinants is done by means of symbolic mathematics software and they are arranged in polynomial form. The variable $z$ is used as bookkeeping variable and after obtaining the determinant we take $z=1$. For example the determinant $\operatorname{det}(1-z \mathcal{T})$ for the matrix (23) contains terms like

$$
\begin{equation*}
-p^{3} z^{3} e^{-3 s} \frac{4 \mathcal{A}_{0} \mathcal{A}_{1}}{\mathcal{A}_{5}} \tag{25}
\end{equation*}
$$

Then Eqs. (19), (21), and (22) are applied for obtaining the mean-square cycle displacement and mean cycle length. To the term (25), taken as example, corresponds the square displacement $|A|^{2}=(1+\sqrt{3})^{2}$ and length $T=3$, which are used in the sum (19) with a minus sign.

Table I contains diffusion constants of all Archimedean lattices obtained by means of periodic orbit theory in column five as well as their numerical value in column six. The factor $1 / 2 d=1 / 4$ which corresponds to the dimension of the space, was omitted because all shown values are close to unity. To confirm the theoretical results, numerical simulation with $10^{6}$ different trajectories was performed for all lattices. For those having values very close to each other (indicated in Table I) $2 \times 10^{7}$ trajectories were taken instead. The value of diffusion constant is obtained with the best fitting curve. Errors shown in the table are from the least-squares method. As can be seen the results from theory and simulation agree with good accuracy. Columns two, three, and four
in the table contain information on the numbers of nodes $N(i)$ accessible in not less than $i$ steps. From the table it can be seen that among the lattices with the same coordination number $N(1)$ the diffusion constant is larger if the connectivity of the lattice is more pronounced. By better connectivity we mean bigger $N(2)$ or $N(3)$. The exceptions are the square and $(3,4,6,4)$ lattices. However, for square lattices the particle can move for a while in one direction and thus make bigger displacements. The diffusion constant is smallest for the $\left(3,12^{2}\right)$ lattice because it has cavities and thus the displacements are generally smaller for the same number of steps.

## DETERMINISTIC DIFFUSION ON HONEYCOMB LATTICE

Diffusion constant can be calculated with the same theory for some types of deterministic motion over lattices. For simplicity in this section we assume movement on a honeycomb lattice for which the immediate return to the preceding vertex is forbidden. Then six possible states related to directed edges are possible, as it is depicted on Fig. 3.

Because normal diffusion needs a chaotic motion it is simply attainable in the following way. We relate an internal variable $y$ with value in the unit interval $y \in[0,1]$ to every particle. At every vertex the variable changes its value with the tent map


FIG. 3. The six possible states of a particle moving on a honeycomb lattice, which cannot immediately return to the previous node.

$$
g_{\Lambda}(y)= \begin{cases}\Lambda y, & y<1 / 2  \tag{26}\\ \Lambda(1-y), & y \geqslant 1 / 2\end{cases}
$$

with slope $\Lambda$ which plays the role of a weight factor in the trace [Eq. (15)]. The sequence of the values $y_{n}=g_{\Lambda}^{n}(x)$ for almost all $x$ from the unit interval chaotically wanders in the unit interval if the slope is $1<\Lambda \leqslant 2$. From the sequence $y_{n}$ a list $Y_{n}$ of symbols is formed according to the rule

$$
Y_{n}= \begin{cases}L, & y_{n}<1 / 2,  \tag{27}\\ R, & y_{n} \geqslant 1 / 2 .\end{cases}
$$

It simply tells whether the value of the internal variable is $L$ (left) or $R$ (right) from the critical value ( $1 / 2$ ). The node to be visited next is determined by the symbol $Y_{n}$. If it is $L$, the particle proceeds to the left, otherwise it goes to the right. For different starting values $y$, different trajectories are attainable.

The slope $\Lambda$ plays a key role in the dynamics, because it poses restrictions on the sequences $Y_{n}$. For some values the corresponding Markov graph is finite and the diffusion is normal. For example when $\Lambda=2$ all sequences of the symbols $L$ and $R$ are possible and the diffusion constant is $D$ $=3 / 4$. More interesting is the case when the slope has a value equal to the golden ratio $\Lambda=(\sqrt{5}+1) / 2$. The successive repetition of the symbol $L$ is then impossible, which means that after every left turn, a right turn must follow. It implies that the only nonzero matrix elements of the transfer matrix are

$$
\begin{gather*}
L_{i, i}=\frac{\exp \left[\beta\left(A_{i-1}+A_{i}\right)-2 s\right]}{\Lambda^{2}}, \\
L_{i, i-1}=\frac{\exp \left[\beta A_{i-1}-s\right]}{\Lambda} \tag{28}
\end{gather*}
$$

Repeating the same procedure as for the random motion over the Archimedean lattices, one can obtain the diffusion constant $D=3 / 4 \sqrt{5}$.

## CONCLUSION

We have analyzed simple models, both stochastic and deterministic, with diffusive transport. The symmetry, hyperbolicity, and finiteness of the associated Markov graph lead to applicability of the periodic orbit theory for calculating the diffusion constant. Analytic expressions were obtained for the diffusion constants for all Archimedean lattices and they are in good agreement with Monte Carlo simulations. The hexagonal, square, Kagomé, and triangular lattice have equal diffusion constants, which is also the largest. Two other lattices $(4,6,12)$ and $(3,4,6,4)$ share an equal diffusion constant. The smallest diffusion constant is found in the $\left(3,12^{2}\right)$ lattice which is characterized by the lowest connectivity between lattice sites. The model can serve as a tool for studying the basic properties of periodic orbit theory. A higherdimensional lattices can also be analyzed with the same theory.
[1] L. F. Tóth, Acta Math. 11, 363 (1960).
[2] F. C. Frank and J. S. Kasper, Acta Crystallogr. 11, 184 (1958); 12, 483 (1959).
[3] H. Takeda and J. D. H. Donnay, Acta Crystallogr. 19, 474 (1965).
[4] R. Shrock and S. H. Tsai, Phys. Rev. E 56, 4111 (1997).
[5] C. d'Iribarne, G. Rasigni, and M. Rasigni, Phys. Lett. A 209, 95 (1995).
[6] P. N. Suding and R. M. Ziff, Phys. Rev. E 60, 275 (1999).
[7] P. Cvitanović, R. Artuso, R. Mainieri, G. Tanner, and G. Vattay, Classical and Quantum Chaos (Niels Bohr Institute,

Copenhagen, 2005), http://ChaosBook.org
[8] R. Klages and J. R. Dorfman, Phys. Rev. Lett. 74, 387 (1995).
[9] P. Cvitanović, P. Gaspard, and T. Schreiber, Chaos 2, 85 (1992).
[10] G. Tanner, J-M. Rost, and K. Richter, Rev. Mod. Phys. 72, 497 (2000).
[11] B. Grünbaum and G. C. Shephard, Tilings and Patterns (Freeman, New York, 1987).
[12] I. P. Goulden and D. M. Jackson, Combinatorial Enumeration (Wiley, New York, 1983).


[^0]:    *Electronic address: lasko@etf.ukim.edu.mk
    ${ }^{\dagger}$ Electronic address: urumov@iunona.pmf.ukim.edu.mk

