Springer Proceedings in Complexity

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Proceedings of the European Conference on Complex Systems 2012

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ISSN 2213-8684
ISSN 2213-8692 (electronic)
Springer Proceedings in Complexity
ISBN 978-3-319-00394-8
ISBN 978-3-319-00395-5 (eBook)
DOI 10.1007/978-3-319-00395-5
Springer Dordrecht Heidelberg New York London

Library of Congress Control Number: 2013944574

Printed on acid-free paper

Springer is part of Springer Science+Business Media (www.springer.com)

Foreword

The present volume contains contributions presented at the ninth *European Conference on Complex Systems*, held at Université Libre de Bruxelles, Brussels, from 2 to 7 September 2012, under the sponsorship of the Complex Systems Society.

The volume is divided into seven parts. The first six parts comprise contributions to the main conference, whether oral or poster, compiled according to the six conference main tracks. The last part includes contributions to some of satellite meetings hosted at the conference.

We are pleased to acknowledge the invaluable help of the colleagues who assisted in the organization of this event, starting with the *Organizing Committee* members, Vincent Blondel, Timoteo Carletti, Enrico Carlon, Anne De Wit, Pierre Gaspard, Albert Goldbeter, Renaud Lambiotte, and Carlo Vanderzande, and the *Steering Committee*, responsible for the development and support of the ECCS conference series, whose members are Fatihcan Atay, Vittoria Colizza, Thomas Gilbert, Janusz Holyst, Jürgen Jost, Markus Kirkilionis (Chair), Kristian Lindgren, Andras Lorincz, Jorge Louçã, Roberto Serra, Mina Teicher, Stefan Thurner, and Jeff Johnson (President of the Complex Systems Society). The six *Track Committees* were skillfully chaired by Claude Baesens, András Lörincz, Eve Mitleton-Kelly, Jacques Demongeot, Peter Allen, and Sorin Solomon, who benefited from the support of Anne De Wit, Pierre Gaspard, Hugues Bersini, Serge Massar, Annick Castiaux, Stéphane Vannitsem, Geneviève Dupont, Tom Lenaerts, Renaud Lambiotte, Nicolas Vandewalle, Vincent Blondel, Timoteo Carletti, Natasa Golo, as well as of many anonymous referees. The eighteen satellite meetings hosted at the conference were masterfully organized by independent committees to whom we are indebted. In addition, we wish to thank the students and staff members at the Université Libre de Bruxelles, without whom the conference could not have been organized.

We wish to express our gratitude to Theo Geisel who delivered the inaugural talk, as well as to the eight invited keynote speakers Charles H. Bennett, Jean-Louis Deneubourg, Manfred Eigen, Santo Fortunato, Peter Grassberger, Jean-Marie Lehn, Raymond Kapral, and Sylvia Walby.

Finally, it is our pleasure to thank the sponsors who enthusiastically supported this conference: the Université Libre de Bruxelles, the Fonds de la Recherche

Scientifique—FNRS, the Belgian Science Policy Office-Belspo, ASSYST—Action for the Science of complex SYstems and Socially intelligent icT, funded under the CORDIS Seventh Framework Programme, Naxys—Namur Center for Complex Systems, Springer Complexity, Oxford University Press, Cambridge University Press, Groupe De Boeck, World Scientific, Wolfram Research, and Star Alliance.

Thomas Gilbert, Conference Chair
Gregoire Nicolis, Program Chair
Markus Kirkilionis, Chair of the Steering Committee

Contents

Part I
Foundations of Complex Systems

Chapter 1
Aggregation and Emergence in Agent-Based Models: A Markov Chain Approach

Sven Banisch, Ricardo Lima, and Tanya Araújo

Abstract We analyze the dynamics of agent-based models (ABMs) from a Markovian perspective and derive explicit statements about the possibility of linking a microscopic agent model to the dynamical processes of macroscopic observables that are useful for a precise understanding of the model dynamics. In this way the dynamics of collective variables may be studied, and a description of macro dynamics as emergent properties of micro dynamics, in particular during transient times, is possible.

1.1 Introduction

Our work is a contribution to interweaving two lines of research that have developed in almost separate ways: Markov chains and agent-based models (ABMs). The former represents the simplest form of a stochastic process while the latter puts a strong emphasis on heterogeneity and social interactions. The usefulness of the Markov chain formalism in the analysis of more sophisticated ABMs has been discussed by [7], who look at 10 well-known social simulation models by representing them as a time-homogeneous Markov chain. Among these models are the Schelling segregation model [11], the Axelrod model of cultural dynamics [1] and the sugarscape model from [6]. The main idea of [7] is to consider all possible con-

This work has benefited from financial support from the Fundação para a Ciência e a Tecnologia (FCT), under the *13 Multi-annual Funding Project of UECE, ISEG, Technical University of Lisbon*. Financial support of the German Federal Ministry of Education and Research (BMBF) through the project *Linguistic Networks* is also gratefully acknowledged (http://project.linguistic-networks.net).

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T. Gilbert et al. (eds.), *Proceedings of the European Conference on Complex Systems 2012*, Springer Proceedings in Complexity, DOI 10.1007/978-3-319-00395-5_1,

figurations of the system as the state space of the Markov chain. Despite the fact that all the information of the dynamics on the ABM is encoded in a Markov chain, it is difficult to learn directly from this fact, due to the huge dimension of the configuration space and its corresponding Markov transition matrix. The work of Izquierdo and co-workers mainly relies on numerical computations to estimate the stochastic transition matrices of the models.

Consider an ABM defined by a set $\mathbf{N}$ of agents, each one characterized by individual attributes that are taken from a finite list of possibilities. We denote the set of possible attributes by $\mathbf{S}$ and we call the *configuration space* $\mathbf{\Sigma}$ the set of all possible combination of attributes of the agents, i.e. $\mathbf{\Sigma} = \mathbf{S}^N$. This also incorporates models where agents move on a lattice (e.g. in the sugarscape model) because we can treat the sites as "agents" and use an attribute to encode whether a site is occupied or not. The updating process of the attributes of the agents at each time step typically consists of two parts. First, a random choice of a subset of agents is made according to some probability distribution ω. Then the attributes of the agents are updated according to a rule, which depends on the subset of agents selected at this time. With this specification, ABMs can be represented by a so-called random map representation which may be taken as an equivalent definition of a Markov chain [10]. Hence, ABMs are Markov chains on $\mathbf{\Sigma}$ with transition matrix $\hat{P}$. For a class of ABMs we can compute transition probabilities $\hat{P}(x, y)$ for any pair $x, y \in \mathbf{\Sigma}$ of agent configurations. We refer to the process $(\mathbf{\Sigma}, \hat{P})$ as micro chain.

When performing simulations of an ABM we are actually not interested in all the dynamical details but rather in the behavior of variables at the macroscopic level (such as average opinion, number of communities, etc.). The formulation of an ABM as a Markov chain $(\mathbf{\Sigma}, \hat{P})$ enables the development of a mathematical framework for linking the micro-description of an ABM to a macro-description of interest. Namely, from the Markov chain perspective, the transition from the micro to the macro level is a projection of the Markov chain with state space $\mathbf{\Sigma}$ onto a new state space $\mathbf{X}$ by means of a (projection) map Π from $\mathbf{\Sigma}$ to $\mathbf{X}$. The meaning of the projection Π is to lump sets of micro configurations in $\mathbf{\Sigma}$ according to the macro property of interest in such a way that, for each $X \in \mathbf{X}$, all the configurations of $\mathbf{\Sigma}$ in $\Pi^{-1}(X)$ share the same property.

The price to pay in passing from the micro to the macrodynamics in this sense [5, 8] is that the projected system is, in general, no longer a Markov chain: long memory (even infinite) may appear in the projected system. In particular, well known conditions for lumpability [8] make it possible to decide whether the macro model is still Markov. Conversely, this setting can also provide a suitable framework to understand how aggregation may lead to the emergence of long range memory effects.

1.2 Application to the Voter Model

We illustrate these ideas at the example of the Voter Model (VM) (see Refs. [4, 9]). In the VM, $\mathbf{S} = \{0, 1\}$ meaning that each agent is characterized by an attribute x_i,

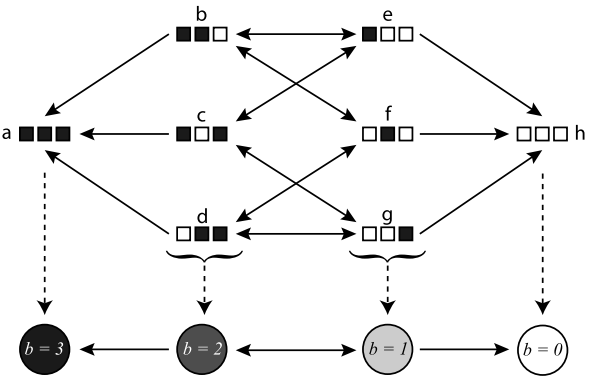

Fig. 1.1 The micro chain for the VM with 3 agents and its projection onto a random walk obtained by agglomeration of states with the same number of black agents b

$i = 1, \ldots, N$ which takes a value among two possible alternatives. The set of all possible combinations of attributes of the agents is $\mathbf{\Sigma} = \{0, 1\}^N$, that is, the set of all bit-strings of length N. At each time step in the iteration process, an agent i is chosen at random along with one of its neighboring agents j. If the states (x_i, x_j) are not equal already, agent i adopts the state of j (by setting $x_i = x_j$). At the microscopic level of all possible configurations of agents the VM corresponds therefore to an absorbing random walk on the N-dimensional hypercube. It is well known that the model has the two absorbing states $(1, \ldots, 1)$ and $(0, \ldots, 0)$. For a system of three agents this is shown in Fig. 1.1.

Opinion models as the VM are a nice examples where our projection construction is particularly meaningful. There, we consider the projection Π_b that maps each $x \in \mathbf{\Sigma}$ into $X_b \in \mathbf{X}$ where b is the number of agents in x with opinion 1. The projected configuration space is then made of the X_b where $0 \leq b \leq N$ (see Fig. 1.1). Markov chain theory, in particular lumpability, allows us to determine conditions for which the macro chain on $\mathbf{X} = (X_0, \ldots, X_b, \ldots, X_N)$ is again a Markov chain. We find that this requires that the probability distribution ω must be invariant under the group $\mathcal{S}_N$ of all the permutations of N agents and therefore uniform. This underlines the theoretical importance of homogeneous or complete mixing in the analysis of the VM and related models.

In this way our method enables the use of Markov chain instruments in the mathematical analysis of ABMs. In Markov chains with absorbing states (and therefore in the ABM) the asymptotic status is quite trivial. As a result, it is the understanding of the transient that becomes the interesting issue. In order to analyze the transient dynamics for the macro dynamics, all that is needed is to compute the fundamental matrix $\mathbf{F}$ of the Markov chain [8]. For the binary VM we are able to derive a closed form expression for the elements in $\mathbf{F}$ for arbitrary N which provides us with all the information needed to compute the mean quantities and variances of the transient dynamics of the model. In addition, we show in the VM with three opinion alternatives ($\mathbf{S} = \{0, 1, 2\}$) how restrictions in communication (bounded confidence) lead to stable co-existence of different opinions because new absorbing states emerge in the macro chain.

1.3 Some Results

The micro chains obtained via the random map representations helps to understand the role of the collection of (deterministic) interaction rules used in the model from one side and of the probability distribution ω governing the sequential choice of the rules used to update the system at each time step from the other side. The importance of this probability distribution is to encode social relations and exchange actions. In our setting it becomes explicit how the symmetries in ω translate into symmetries of the micro chain. If we decide to remain at a Markovian level, then the partition, or equivalently the collective variables to be used to build the macro model must be compatible with the symmetry of the probability distribution ω. In order to account for an increased level of heterogeneity the partition of the configuration space defining the macro-level has to be refined. A first result into this direction is that the symmetry group of agent permutations on ω informs us about ensembles of agent configurations that can be interchanged without affecting the probabilistic structure of micro chain. Consequently, these ensembles can be lumped into the same macro state and the dynamical process projected onto these states is still a Markov chain. It is clear, however, that, in absence of any symmetry, there is no other choice than to stay at the micro-level because no Markovian description at a macro-level is possible in this case.

In our opinion, a well posed mathematical basis for linking a micro-description of an ABM to a macro-description may help the understanding of many of the properties observed in ABMs and therefore provide information about the transition from the interaction of individual actors to the complex macroscopic behaviors observed in social systems. We summarize our main results below:

1. We formulate agent-based models as Markov chains at the micro level with explicit transition probabilities.
2. This allows the use of lumpability arguments to link between the micro and the macro level.
3. In case of a non-lumpable macro description this explains the emergence nontrivial dynamical effects (long memory).
4. In the Voter Model, homogeneous mixing leads to a macroscopic Markov chain which underlines the theoretical importance of homogeneous mixing.
5. This chain can be solved including mean convergence times and variances.
6. The stable co-existence of different opinions with in the bounded confidence model follows from the emergence of new absorbing states in the macro chain.
7. Heterogeneous mixing requires refinement and we show how to exploit the symmetries in the mixing distribution (ω) to obtain a proper refinement.

For further reading, see Refs. [2, 3].

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Chapter 2
Chemically-Driven Miscible Viscous Fingering: How Can a Reaction Destabilize Typically Stable Fluid Displacements?

L.A. Riolfo, Y. Nagatsu, P.M.J. Trevelyan, and A. De Wit

Abstract We experimentally demonstrate that chemical reactions, by producing changes in viscosity at the miscible interface between two fluids, can be the very source of viscous fingering in systems that are otherwise stable in the absence of a reaction. We explain how, depending on whether the reaction product is more or less viscous than the reactants, different patterns develop in the reaction zone.

2.1 Background

Viscous fingering (VF) is the hydrodynamic instability that classically appears when a fluid with a given viscosity displaces another more viscous one in porous media or a Hele-Shaw cell [1]. It has diverse implications in various fields such as hydrology [2], petroleum recovery [1], liquid crystal [3], polymer processing [4], chromatography [5] or CO_2 sequestration to name a few [6].

Experimental [7, 8] and theoretical [9, 10] studies have shown that chemical reactions, by modifying the viscosity of the solutions at hand, can influence miscible VF. Changes in the viscosity profile, induced by a chemical reaction, give rise to variations in the displacement evolution and hence different patterns are observed.

The present work, going further, presents experimental demonstration of reaction-driven viscous fingering of the interface between a more viscous liquid displacing a less viscous one, a displacement that in absence of reaction would typically be stable. It has been theoretically predicted [9, 10] that the necessary condition for such a reactive displacement to undergo fingering is to yield a reaction product with a viscosity either larger or smaller than the viscosity of the reactants. Specifically,

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T. Gilbert et al. (eds.), *Proceedings of the European Conference on Complex Systems 2012*, Springer Proceedings in Complexity, DOI 10.1007/978-3-319-00395-5_2,

if μ_i and μ_d denote the viscosity of the invading solution and that of the displaced solution respectively, purely chemically-driven VF of the classically stable $\mu_i > \mu_d$ situation should occur provided μ_r, the viscosity in the reaction zone, is either larger than μ_i or smaller than μ_d [9, 10].

We study here both scenarios, viscosity maximum ($\mu_r > \mu_i$) and minimum ($\mu_r < \mu_d$), exploiting the viscosity dependence of polymer solutions on pH. From the experimental findings, the different fingering patterns are analyzed as a function of the viscosity contrast generated by the chemical reaction [11].

The article organizes as follows: In the next section we explain the experimental set up and the chemicals utilized in the experiments. Also in this second section we present our experimental findings. In Sect. 2.3 we discuss and explain the evolution on the displacements presented in the second section. Finally, conclusions are drawn while highlighting the possible impact of this experimental work.

2.2 Methods

Experiments are carried out in a horizontal Hele-Shaw cell consisting of two transparent glass plates 100 mm wide, 500 mm long and 14 mm thick separated by a gap width $b = 0.25$ mm. The fluids are injected linearly at a constant flow rate q. As the displacing more viscous fluid, we use aqueous polymer solutions. When these solutions displace a less viscous dyed non-reactive solution, no instability is observed at the miscible interface between the fluids. However, if the displaced fluid reacts with the polymer, generating a maximum or a minimum in the viscosity profile, the interface can become unstable undergoing fingering. In the displacement experiments where the maximum develops, a more viscous aqueous solution of 0.30 %wt polyacrylic acid (PAA—1250000 MW—Sigma Aldrich) displaces a dyed 0.06M sodium hydroxide (NaOH) aqueous solution. The liquids react at the miscible interface. The reaction product, sodium polyacrylate (SPA), typically presents a viscosity larger than that of both reactants. The chemical reaction at the miscible interface is PAA + NaOH → SPA.

On the other hand, in the case where the minimum in viscosity develops, a sodium polyacrylate (SPA—2100000–6600000 MW—Wako) aqueous solution 0.125 %wt pushes a less viscous 60 %wt glycerol aqueous solution containing 0.5M HCl. In this case the polymer reacts with the acid producing PAA, which here has a viscosity lower than that of both reactants. The reaction is then SPA + HCl → PAA + NaCl.

Figure 2.1 shows the temporal evolution of reaction-driven VF observed in a linear displacement for both cases. When the maximum in viscosity develops, fingers grow behind the reactive interface (Fig. 2.1(a)). On the other hand, in the case of a minimum in viscosity, the interface undergoes fingers that grow towards the displaced fluid (Fig. 2.1(b)).

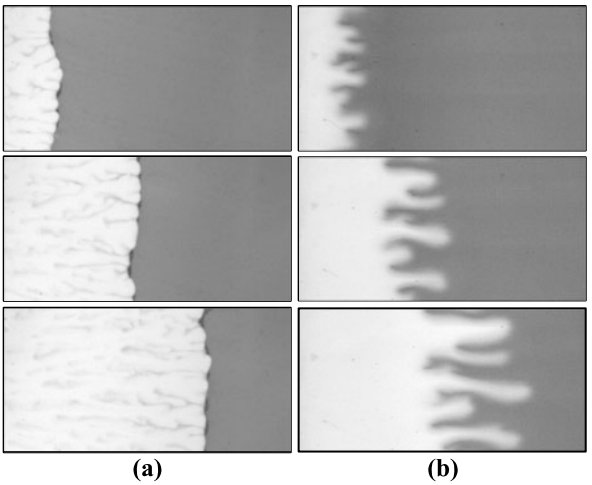

Fig. 2.1 Temporal evolution of reaction-driven VF in a linear displacement. (**a**) A more viscous solution of PAA displaces from left to right a less viscous aqueous dyed solution of NaOH in concentration 0.06M. Flow rate $q = 0.5$ ml/min. Time from top to bottom $t = 75$, 150 and 225 s. (**b**) A more viscous SPA solution displaces from left to right an aqueous dyed solution of 60 %wt glycerol + HCl 0.5M. Flow rate $q = 0.25$ ml/min. Time $t = 140$, 280 and 360 s. Field of view of each image = 4 cm × 8 cm

2.3 Results

In order to understand the systems' evolution we analyze experimentally the viscosity contrasts generated during the displacement experiments. We measure the viscosity of the pure reactants and estimate the viscosity developed in the reaction zone as the viscosity of a mixture of the pure reactants. The respective viscosities are measured with a rotational viscosimeter (Brookfield—Pro Extra II) at the shear rate corresponding to the experimental conditions.

In the displacement experiments with a maximum in viscosity the reactants viscosity are: invading fluid (0.3 %wt PAA) $\mu_i = 870$ cp, displaced fluid (0.06M NaOH) $\mu_d = 1$ cp. Hence, the initial viscosity contrast is stable, because the more viscous fluid displaces the more mobile one. However, in the reaction zone the viscosity developed is approximately $\mu_r = 3880$ cp. Therefore, an unstable contrast of viscosity is developed between the invading fluid and the reaction zone: $\mu_i < \mu_r$ and we have locally a less viscous fluid pushing a more viscous one. As the unstable region is located between the invading fluid and the reaction zone, the fingers should develop in this region. This is consistent with the experiments (Fig. 2.1(a)), where the fingers develop behind the reaction zone toward the invading fluid.

In the displacement with a minimum in viscosity, the viscosities are: invading fluid (0.125 %wt SPA) $\mu_i = 794$ cp, displaced solution (60 % glycerol + 0.5M HCl) $\mu_d = 10$ cp. The viscosity falls to $\mu_r = 5$ cp in the reaction zone. Therefore, even if the initial viscosity contrast is stable, locally an unstable region develops in time between the reaction zone and the displaced fluid ($\mu_r < \mu_d$). The development

of the instability is then predicted to occur in the region between the reaction zone and the displaced fluid. This conjecture from the viscosity profiles agrees with the experimental findings exposed in Fig. 2.1(b).

We show here that depending on the unstable viscosity contrast developed during the displacement different patterns develop, and the interface deforms towards opposite directions, either in the displacement direction if a viscosity minimum develops, or against the displacement direction if a maximum in viscosity is chemically induced.

In this way, we have provided experimental evidence of viscous fingering triggered by a chemical reaction at the miscible interface between a more viscous solution displacing a less viscous one in a Hele-Shaw cell. Such a situation is classically stable in the absence of a reaction as we have a fluid with low mobility invading another more mobile one. The chemical reaction, by generating a product either more or less viscous than both reactants, triggers in time a non-monotonic viscosity profile. A locally unstable configuration with adverse mobility gradient develops around the extremum. This leads to fingers developing respectively behind or ahead of the reaction zone depending whether the viscosity profile exhibits a maximum or a minimum.

This results may help to prevent undesirable mixing during fluids displacements, such in the case of waste management in soils [12, 13], but also could lead to control of mixing enhancement in a unique direction in complex scenarios such as in microfluidics [14].

Acknowledgements We acknowledge JSPS, Prodex, the ITN—Marie Curie—Multiflow network and FNRS for financial support.

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Chapter 3
Dynamical Localization in Kicked Rotator as a Paradigm of Other Systems: Spectral Statistics and the Localization Measure

Thanos Manos and Marko Robnik

Abstract We study the intermediate statistics of the spectrum of quasi-energies and of the eigenfunctions in the kicked rotator, in the case when the corresponding system is fully chaotic while quantally localized. As for the eigenphases, we find clear evidence that the spectral statistics is well described by the Brody distribution, notably better than by the Izrailev's one, which has been proposed and used broadly to describe such cases. We also studied the eigenfunctions of the Floquet operator and their localization. We show the existence of a scaling law between the repulsion parameter with relative localization length, but only as a first order approximation, since another parameter plays a role. We believe and have evidence that a similar analysis applies in time-independent Hamilton systems.

3.1 Introduction

One of the most important manifestations of quantum chaos of low-dimensional classically fully chaotic (ergodic) Hamiltonian systems is the fact that in the (sufficiently deep) semiclassical limit the statistical properties of the discrete energy spectra obey the statistics of Gaussian Random Matrix Theory (RMT). The opposite extreme are classically integrable systems, which quantally exhibit Poissonian spectral statistics (see [1]).

Quantum kicked rotator (QKR) is a typical example in the field of quantum chaos [2]. A typical property of the QKR is the chaos suppression for sufficiently large time scales. The study of the statistical properties of the classical and quantum (semiclassical) parameters in such systems is of great importance. Here we study in detail the semiclassical region where $k > K > 1$, i.e. the regime of full correspondence between quantum and classical diffusion (on the finite time scale $t \leq t_D$) and the manifested quantum dynamical localization for $t > t_D$. Furthermore, we are focused in the probability level spacing distributions in the regime where the system is

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T. Gilbert et al. (eds.), *Proceedings of the European Conference on Complex Systems 2012*, Springer Proceedings in Complexity, DOI 10.1007/978-3-319-00395-5_3,

classically strongly chaotic ($K \geq 7$) but quantally localized, i.e in the *intermediate* or *soft* quantum chaos, as it is described in the literature [5].

3.2 The Quantum Kicked Rotator Model

The QKR model [3] is described by the following function

$$\hat{H} = -\frac{\hbar^2}{2I}\frac{\partial^2}{\partial\theta^2} + \varepsilon_0 \cos\theta \sum_{m=-\infty}^{\infty} \delta(t - mT), \tag{3.1}$$

where $\hbar$ is Planck's constant, I is the moment of inertia of the pendulum and ε_0 is the perturbation strength. The motion after one period T of the ψ wave function then can be described by the following mapping

$$\psi(\theta, t+T) = \hat{U}\psi(\theta, t), \tag{3.2}$$

$$\hat{U} = \exp\left(i\frac{T\hbar}{4I}\frac{\partial^2}{\partial\theta^2}\right)\exp\left(-i\frac{\varepsilon_0}{\hbar}\cos\theta\right)\exp\left(i\frac{T\hbar}{4I}\frac{\partial^2}{\partial\theta^2}\right), \tag{3.3}$$

where the ψ function is determined in the middle of the rotation, between two successive kicks. The evolution operator $\hat{U}$ of the system corresponds to one period. Due to the instant action of the perturbation, this evolution can be written as the product of three non-commuting unitary operators, the first and third of which corresponds to the free rotation during half a period $\hat{G}(\tau/2) = \exp(i\frac{T\hbar}{4I}\frac{\partial^2}{\partial\theta^2})$, $\tau \equiv \hbar T/I$, while the second $\hat{B}(k) = \exp(-ik\cos\theta)$, $k \equiv \varepsilon_0/\hbar$ describes the kick. The system's behavior depends only on two parameters, i.e. τ and k and its correspondence with the classical systems is described by the relation $K = k\tau = \varepsilon_0 T/I$. In the case $K \equiv k\tau \gg 1$ the motion is well-known to be strongly chaotic. The transition to classical mechanics is described by the limit $k \to \infty$, $\tau \to 0$ while $K = \text{const}$. In what follows $\hbar = \tau$ and $T = I = 1$. We shall consider mostly the semiclassical regime $k > K$, where $\tau < 1$.

In order to study how the localization affects the statistical properties of the quasienergy spectra we use the model's representation with a finite number N of levels [4, 5]

$$\psi_n(t+T) = \sum_{m=1}^{N} U_{nm}\psi_m(t), \quad n, m = 1, 2, \ldots, N. \tag{3.4}$$

The finite unitary matrix U_{nm} determines the evolution of a N-dimensional vector (Fourier transform of ψ) of the model

$$U_{nm} = \sum_{n'm'} G_{nm'} B_{n'm'} G_{n'm}, \tag{3.5}$$