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Classical and quantum transport in deterministic Hamiltonian ratchets

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Abstract. We study directed transport in classical and quantum area-preserving maps, periodic in space and momentum. On the classical level, we show that a sum rule excludes directed transport of the entire phase space, leaving only the possibility of transport in (dynamically defined) subsets, such as regular islands or chaotic areas. As a working example, we construct a mapping with a mixed phase space where both the regular and the chaotic components support directed currents, but with opposite sign. The corresponding quantum system shows transport of similar strength, associated to the same subsets of phase space as in the classical map.

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1 Introduction

The concept of ratchets provides a paradigm for how close tangible applications can be to fundamental principles. They have been born out of the desire to achieve a physical explanation for intracellular transport along chain molecules [1]. A surprisingly simple model is sufficient to produce transport: A sawtooth potential (for the interaction with the chain molecule) with a noisy driving (for the internal dynamics of the motor molecules and the coupling to the cell plasma). In order for the ratchet to work, two necessary conditions have to be fulfilled: The potential, while being periodic, must be spatially asymmetric, and the noise has to possess a non-equilibrium character. Otherwise, the functioning of ratchets would violate the Second Law of thermodynamics.

Ironically, the relevance of ratchets for the explanation of directed intracellular transport has been called into question by biologists [1]. On the other hand, the same principle has proven enormously fruitful for the construction of nanoscale devices:

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Artificial ratchets may serve as pumps, rectifiers, and particle selectors, among other applications (for comprehensive reviews, see Refs. [2–4]).

While these applications are interesting enough, the theoretical fascination derives mainly from the fundamental questions raised by this seemingly innocuous gadget. In fact, the ratchet principle was first used by Feynman in his famous series of lectures as a didactical case study of Maxwell's demon [5]. Exactly how the transformation of unbiased, disordered microscopic motion into directed transport escapes the Second Law requires subtle non-equilibrium statistics. A second, related aspect of theoretical interest is the breaking of various symmetries required to generate transport.

In order to make the conditions and limits of transport in ratchets precise, numerous extensions of the original concept have been explored in an already impressive number of publications, a large fraction of which was contributed by the group of Peter Hänggi. For example, a large variety of noise types, as well as of superposed deterministic driving forces, have been studied [2].

A major step towards more rarefied models is the replacement of a noisy driving by a purely deterministic one, thus leaving the realm of "Brownian motors". In order to allow for a non-trivial dynamics, this requires another concomitant generalization: the inclusion of an inertia term in the equation of motion [6]. Since a time-dependent driving amounts to an additional degree of freedom, the deterministic dynamics can now become chaotic even in a one-dimensional model. Transport then requires an asymmetry of the basins of attraction of the (possibly strange) attractors [6].

While for the original biological application, quantum effects play a minor rôle, nanoscale technical applications require to reconsider ratchets in a quantum-mechanical framework [7–9]. Modifications of classical transport are to be expected in particular due to quantum coherence effects: Tunneling can significantly increase transport as compared to the corresponding classical system.

Reducing ratchets further to their conceptual sceleton, one can even abandon dissipation completely. This is a radical step since with dissipation, the most natural mechanism for the breaking of time-reversal symmetry is lost. It can be replaced, however, by choosing the driving function asymmetric in time. As a result, Hamiltonian ratchets turn into laboratories for the study of twofold symmetries and the consequences of their destruction for transport and other properties. At this stage, the study of ratchets starts to overlap strongly with chaos and quantum chaos in Hamiltonian systems, shifting attention from transport as such to the detailed features of nonlinear dynamics responsible for it. Conversely, this also gives a new guise to chaos since the vast majority of models considered up to now in the field is intentionally highly symmetric. Going to the opposite extreme may open the view for unexpected phenomena.

Pioneering work in this direction has recently been done by Flach *et al.* [10]. In many respects, it has stimulated the present study. Addressing an important remaining white patch in the "ratchet phase diagram", we extend that study towards the quantum level. The studies of quantum ratchets mentioned above, both in the overdamped and in the underdamped regime, are based on formalisms which allow only for a very small effective number of eigenstates per unit cell of the potential. While this suffices to establish the feasibility of quantum ratchets and to demonstrate the influence of quantum coherence effects, any connection to the intricate structure of the classical phase space is thereby lost. Our work, by contrast, aims at investigating, in the semiclassical regime, the quantum correlates of the mixed (chaotic and regular) classical dynamics. A directed current in a Hamiltonian system requires a mixed phase space, as we shall argue below.

It has proven fruitful in quantum chaos to study the effects of interest in the simplest possible, paradigmatic models. Usually these are area-preserving maps defined over a two-dimensional compact phase space. Consequently, we shall first uncover the detailed mechanism of directed transport in a suitably defined classical map (Section 2). The insight obtained in this way can easily be transferred to continuously driven systems by a limiting procedure. After a straightforward quantization of the map, the essence of quantum transport induced by an unbiased periodic driving can be studied with relatively low numerical effort (Section 4). We emphasize that this is a report on work in progress: Future perspectives of this project are discussed in Section 5.

2 Transport in classical Maps: General Considerations

Time-periodic systems allow for a concise stroboscopic description in the form of maps, using discrete times n as Poincaré sections. In the simplest case, such a map would take the form

$$p_{n+1} = p_n - V_n'(x_n)\,, \qquad x_{n+1} = x_n + T'(p_{n+1})\,, \tag{1}$$

corresponding to a kicked Hamiltonian

$$H(p,x;t) = T(p) + \sum_{n=-\infty}^{\infty} V_n(x)\,\delta(t-n) \tag{2}$$

with kinetic energy $T(p)$ and a potential which is periodic in both, space and time

$$V_n(x+X) = V_n(x)\,, \qquad V_{n+N}(x) = V_n(x)\,. \tag{3}$$

We allow for several equidistant kicks per time period in order to be able to break time-reversal symmetry. Moreover, the limit $N \to \infty$ corresponds to a continuously driven system. We assume p to be a cyclic variable with period P, i.e., in particular,

$$T(p+P) = T(p)\,, \tag{4}$$

so that the phase space of the map (1) attains the topology of a cylinder. This assumption serves here to avoid some technicalities. It can be dropped if necessary, as will be explained elsewhere [11].

Let us denote the action of the two parts of (1) on a normalized phase-space distribution $\rho(x,p)$ by $\mathcal{M}_n^{(p)}\rho$, $\mathcal{M}_n^{(x)}\rho$. The concatenation $\mathcal{M}_n = \mathcal{M}_n^{(x)}\mathcal{M}_n^{(p)}$ then describes the map for a single time step, and $\mathcal{M}^{(N)} = \mathcal{M}_N \ldots \mathcal{M}_1$ that over a full time period. Besides (1), we consider the restriction of the map to the unit cell, $\mathcal{PM}$, where the projection operator $\mathcal{P}$ acts as

$$[\mathcal{P}\rho](x,p) = \chi_u(x) \sum_{n_x=-\infty}^{\infty} \rho(x + n_x X, p)\,. \tag{5}$$

Here, $\chi_u(x) = \Theta(X/2 + x)\Theta(X/2 - x)/A_u$ is the (normalized) characteristic function of the unit cell u and $A_u = XP$ is its area. The quantities of interest are the mean velocity of step n

$$v_n(\rho_0) = \int \mathrm{d}x\,\mathrm{d}p\,[\mathcal{M}_n \ldots \mathcal{M}_1 \rho_0](x,p)\,T'(p) \tag{6}$$

and its time average

$$v(\rho_0) = \lim_{t\to\infty} \frac{1}{t} \sum_{n=1}^{t} v_n(\rho_0) \tag{7}$$

which depend on the initial conditions expressed by ρ_0. Because of the periodicity of the potential, the mean velocity as defined in (6) is the same for $\mathcal{M}$ and $\mathcal{PM}$. Hence we can focus attention on the restricted map. It follows from (1) and (5) that $\mathcal{PM} : u \to u$ is an area-preserving map. In particular,

$$\mathcal{PM}_n \chi_u = \chi_u \tag{8}$$

for all n and thus from (6)

$$v_n(\chi_u) = \langle T'(p) \rangle_u = 0\,, \tag{9}$$

where $\langle \ldots \rangle_u$ denotes an average over the unit cell u and the vanishing of the r.h.s. is an immediate consequence of (4). This means that there cannot be non-trivial transport in the extended map $\mathcal{M}$ when the initial conditions cover the entire available phase space uniformly. This result is quite general. It applies in particular also to continuous driving and non-compact phase spaces. Note that trivial transport, resulting from a mean force bias or a Galilei transform to a moving frame, was excluded from the outset by (3) and (4).

If any transport is dependent on the initial conditions, can this be interesting at all? The answer is yes, because the mean velocity does not depend on the precise choice of initial conditions but rather only on the (minimal) invariant ergodic manifold of the map $(\mathcal{PM})^{(N)}$ in which it resides. Consider instead of χ_u the normalized characteristic function χ_f of such a manifold f which satisfies $(\mathcal{PM})^{(N)}\chi_f = \chi_f$, for example a torus belonging to the regular component of phase space or a chaotic component. Of course, this excludes systems with a completely regular or homogeneously chaotic phase space from consideration. Along the same lines that led to (9), one can show that

$$v(\chi_f) = \frac{1}{N} \sum_{n=1}^{N} \langle T'(p) \rangle_{(\mathcal{PM})^{(n)} f}\ , \tag{10}$$

where $(\mathcal{PM})^{(n)} f$ denotes the phase-space distribution resulting from f after time n. Equation (9) implies that

$$\sum_f v(\chi_f)\,A_f = 0\,, \tag{11}$$

with f running over all invariant regular and chaotic components of phase space with finite measure $A_f \neq 0$. Clearly, this leaves room for individual contributions $v(\chi_f)\,A_f$ to be non-zero, if they are compensated for by other contributions.

For the question whether some invariant manifolds of $(\mathcal{PM})^{(N)}$ support directed transport, symmetry considerations are important. It was shown in Ref. [10] that twofold symmetries inverting momentum, such as parity or time reversal, respectively,

$$\mathsf{P}\colon p \to -p,\ x \to -x,\ t \to t\,, \qquad \mathsf{T}\colon p \to -p,\ x \to x,\ t \to -t\,, \tag{12}$$

lead to a pair of symmetry-related orbits with opposite mean velocities. Consequently, the transport due to both orbits cancels. Similar to the restriction by the sum rule (11), however, this does not exclude transport on an invariant submanifold, if it is split into two separate, symmetry-related parts and the initial condition is restricted to one of them.

3 A discrete-time Hamiltonian ratchet

In view of the results of the previous section, we seek a model with a completely desymmetrized, mixed phase space. Moreover, in order to facilitate the detection of transport, the chaotic and regular components should each be as compact as possible. We will construct a suitable model on the basis of the standard kicked rotor [12]. It is easy to see that a single kick per period is insufficient to break time-reversal symmetry T. Also for two equidistant kicks, one can always find a phase with respect to which the driving possesses a twofold symmetry, so that a minimum of three equidistant kicks per period is needed to desymmetrize the driving (if the condition of equidistant kicks is dropped, two kicks are sufficient). A systematic way to organize an entire chain of kicks per period of the driving is to consider them as the stroboscopic version of an otherwise rigidly moving, periodic potential,

$$V_n(x) = V(x - nX/N)\,, \tag{13}$$

with N kicks per period. In order to break also spatial parity, we choose the potential

$$V(x) = -K\left(\cos x + \frac{a}{2}\cos(2x+b)\right)\,, \tag{14}$$

which has become a standard in the literature. For this potential, $X = 2\pi$. In view of a later quantization of the map, we enforce periodicity, with period $P = 2\pi$, also for the momentum, i.e., we set $T'(p) = [(p+\pi) \bmod 2\pi] - \pi$. Figure 1 shows a phase-space portrait for the parameter values $N = 4$, $K = 20$, $a = 0.4$, and $b = 0.5$. The most prominent feature are three regular islands, surrounded by a nearly homogeneous chaotic sea. These islands form a period-3 chain, that is, the central periodic orbit jumps from one island to its right neighbour, in an extended representation, at each application of the map (cf. Fig. 2b). In the notation of Eq. (10), the corresponding velocity is $v(\chi_{\text{reg}}) = 2\pi/3$. One obvious way to determine the resulting transport and its chaotic counterpart numerically is to prepare an initial ensemble sharply concentrated in x, and to measure the shift of its mean position as

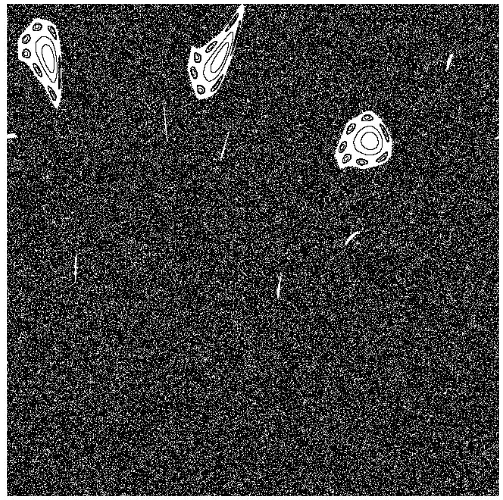

Fig. 1 Phase-space portrait of the map defined by Eqs. (1), (13), (14), for parameter values $K = 20$, $a = 0.4$, $b = 0.5$. The horizontal and vertical axes correspond to $-\pi \leq x, p \leq +\pi$, respectively. The three large islands form a single period-3 chain.

a function of time. Using this technique, we found transport in both, the regular and the chaotic region, which is indeed compatible with Eq. (11) up to a small error due to the finite simulation time for the determination of $v(\chi_{\rm ch})$.

4 Quantum transport

Toroidal phase spaces allow for a particularly simple and transparent quantization [13–16]. We obtain such a topology by requiring cyclic boundary conditions in the x-direction along the boundaries of a single unit cell, or of a chain of several unit cells, as the numerical purpose suggests. In correspondence with our classical model, periodic boundary conditions are imposed in the p-direction at $p = \pm\pi$. A finite total number of M states per unit cell implies discretization of position as well as momentum, say

$$p_l = -\frac{P}{2} + \frac{lP}{M}, \qquad x_m = -\frac{X}{2} + \frac{mX}{M}, \tag{15}$$

so that corresponding bases $\{|\,l\,\rangle; l = 0, \ldots, M-1\}$, $\{|\,m\,\rangle; m = 0, \ldots, M-1\}$, are defined by

$$p|\,l\,\rangle = p_l|\,l\,\rangle, \qquad x|\,m\,\rangle = x_m|\,m\,\rangle\,. \tag{16}$$

Position-momentum uncertainty then requires that

$$XP = 2\pi\hbar M, \tag{17}$$

or specifically in our case, $X = P = 2\pi$, so that $\hbar = 2\pi/M$. If we assume that the space considered accomodates L unit cells, then M must factorize, $M = KL$, where now K is the Hilbert-space dimension per unit cell.

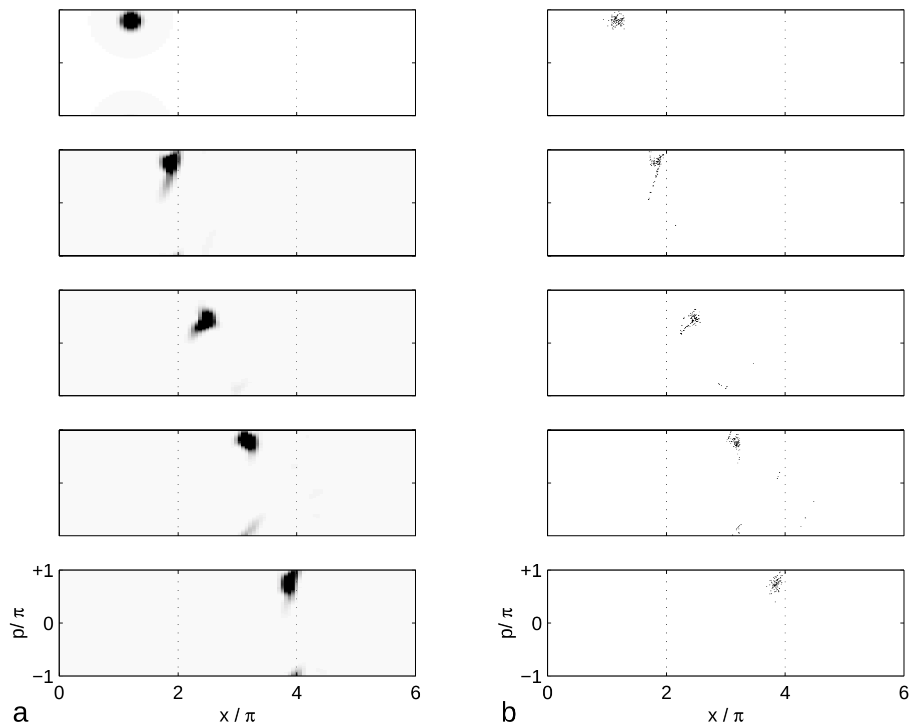

Fig. 2 Time evolution of a classical ensemble (panel b) prepared on the period-3 island chain shown in Fig. 1, and of a quantum wave packet prepared in the same region (a), under the maps defined by Eqs. (1), (13), (14), and by Eq. (18), respectively. Time runs downward over four subsequent kicks (one more than the period of the map).

The big advantage of a kicked dynamics like (2) is that the corresponding quantum time-evolution operator for a single time period from t_n to t_{n+1}, henceforth called the Floquet operator, factorizes into a factor for the kicks and a subsequent one (if $t_n = n - 0^+$) for the free evolution. Moreover, with the bases (16), the change of representation between these factors is equivalent to a discrete Fourier transform. If the time period consists of a concatenation of several kicks, the Floquet operator correspondingly factorizes further. Specifically, in the case of Eq. (13), one has

$$U = \prod_{n=0}^{N-1} U_n \,, \qquad U_n = \exp\left(-\frac{\mathrm{i}}{\hbar}\frac{p^2}{2}\right)\exp\left(-\frac{\mathrm{i}}{\hbar}V_n(x)\right). \tag{18}$$

It is particularly effective to diagonalize the Floquet operator separately for each of the L Bloch-phase subspaces, where it reduces to a $K \times K$ matrix.

For the potential (14) with the classical parameter values given in Fig. 1 and with $\hbar = 2\pi/100$, we computed all eigenfunctions of U. Except for the vicinity of avoided crossings they can all be associated with one of the principal invariant manifolds of classical phase space visible in Fig. 1, i.e., the island chain or the chaotic sea. As an illustrative example, we show in Fig. 2 how a wave packet initialized as a coherent state on one of the regular islands is transported, within a single time period of the potential, by one unit cell to the right. As expected, the quantum time evolution follows essentially the evolution of a classical phase-space distribution prepared as a Gaussian concentrated in the same region.

5 Perspectives

In this state report, we have defined clear conditions for transport in classical Hamiltonian maps on periodic spaces, have presented a working model showing significant classical transport, and studied its quantum counterpart. One result of our investigation, to be further substantiated elsewhere [11], is that quantum transport takes values comparable to the classical, and in particular, that it can clearly be associated to dynamically defined subsets of the classical phase space: Transport in the chaotic component compensates that in the regular one, thus complying with a classical sum rule we derive for Hamiltonian maps.

Directed current due to the breaking of twofold symmetries is a phenomenon not yet studied in the context and from the point of view of quantum chaos. This suggests to follow a number of aspects not immediately implied by the concept of (quantum) ratchets: It has been shown in recent work (for a review, see [17]) that the way wave packets spread over a given, classically chaotic, system is reflected in its the spectral two-point correlations. A naïve expectation then is that also directed transport might have a spectral signature. In particular, the possibility to associate a winding number to classical periodic orbits supporting transport suggests that corresponding quantum states might be classified by a topological quantum number, and thus also show spectral features different from those of non-transporting states.

Studies of quantum ratchets [7, 8] indicate that tunneling may play a major rôle in the type of transport considered here. The deliberate destruction of all twofold symmetries necessary to generate transport of course prevents systematic quasidegeneracies. The influence of tunneling through asymmetric potential maxima, due to random degeneracies, however, is still to be explored in Hamiltonian systems.

Finally, the aim to analyze quantum ratchets in terms of the corresponding classical phase-space structures, calls for being extended to systems with finite damping. The Floquet formalism for dissipative systems, developed during the last years [18], provides an adequate tool for such studies. The intricate structures of classical attractors and their implications for transport suggest a rich repertoire of phenomena originating in the interplay of dissipative dynamics and quantum coherence.

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