



SCRAMBLING IN NEAR-INTEGRABLE AND CHAOTIC SYSTEMS

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“This song is new to me, but I am honored to be a part of it.” — Solanum

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ABSTRACT

This PhD thesis investigates scrambling in near-integrable and chaotic systems. First, we present a quasiclassical formalism of out-of-time-ordered correlators (OTOCs), the main chaos probe that we use, using the semiclassical van Vleck-Gutzwiller propagator and the application of the diagonal approximation. For short evolution times, this quasiclassical approach yields the same result as the Wigner-Moyal formalism, i.e. an exponential growth in a chaotic regime. For long times, for which the semiclassical framework is, in principle, still valid, the diagonal approximation yields an asymptotic saturation value for the quasiclassical OTOC under the assumption of fully developed classical chaos. Numerical simulations in Bose-Hubbard systems show that this estimation strongly underestimates the actual threshold value of the quantum OTOCs. This indicates that genuinely quantum contributions are primarily responsible for describing OTOCs beyond the short-time regime. The thesis then shifts its focus to near-integrable systems, where chaos is present only in the form of a thin chaotic layer. In a fully integrable system, around a fixed point, the dynamics is dictated by a stability exponent, and in a fully chaotic system by a maximal Lyapunov exponent. The question remains open as to how the two compete in near-integrable regimes. We describe this integrability-chaos transition by establishing a description of the dynamics inside the chaotic layer in a universal system: the periodically driven pendulum. We support our claim for the universality of this mechanism by studying two paradigmatic examples of the integrability-to-chaos transition, namely the kicked rotor and the kicked Bose-Hubbard dimer. Finally, we study quantum scars in single- and many-particle systems. For the former, we find that the short-time behaviour of indicators such as the OTOC, computed in the kicked rotor, is not sensitive to the presence of a scar, i.e. to the fulfilment of Heller's criterion. Nonetheless, we show that the OTOC can serve as a probe of unstable periodic orbits. For the latter, we look at the persistent oscillations that manifest in the presence of scars in different observables computed for staggered dimer states in Bose-Hubbard models. As the interaction strength increases, one expects scarring to be a less prevalent phenomenon. This is corroborated by the oscillations that progressively vanish.

RÉSUMÉ

Cette thèse de doctorat étudie le “scrambling”, c’est-à-dire la propagation de l’information, dans des systèmes proches de l’intégrabilité, et dans des systèmes chaotiques. Dans un premier temps, nous présentons un formalisme quasiclassique pour les corrélateurs ordonnés hors temps (OTOCs, de l’acronyme anglais), la sonde du chaos que nous utilisons principalement. Le formalisme est obtenu via le propagateur semiclassique de van Vleck-Gutzwiller combiné à l’approximation diagonale. Pour des temps courts, cette approche quasiclassique donne les mêmes résultats que le formalisme de Wigner-Moyal, c’est-à-dire une croissance exponentielle dans un régime chaotique. Pour des temps longs, où le propagateur semiclassique est en principe valide, l’approximation diagonale nous permet d’obtenir, dans l’hypothèse d’un système complètement chaotique, une valeur de saturation finie. Des simulations numériques dans des systèmes de Bose-Hubbard nous montrent que cette estimation est bien en dessous de la vraie valeur de saturation, celle de l’OTOC quantique. Cela indique que la description des OTOCs au-delà des temps courts doit se faire via un formalisme essentiellement quantique. Ensuite, nous portons notre attention sur des systèmes presque intégrables, où le chaos n’est présent que sous la forme d’une fine couche chaotique. Dans un système intégrable, la dynamique autour d’un point fixe et instable est décrite par l’exposant de stabilité, tandis que celle d’un système complètement chaotique est décrite par l’exposant de Lyapunov maximal. La question de quelle est l’importance de chacun dans la fine couche chaotique d’un système presque intégrable reste ouverte. Nous décrivons cette transition de l’intégrabilité au chaos en établissant une description de la dynamique au sein de la fine couche chaotique d’un système universel : le pendule périodiquement pulsé. Nous étayons notre affirmation de l’universalité de cette transition avec des simulations numériques dans deux systèmes universels : le rotateur pulsé et le système de Bose-Hubbard à deux sites pulsé. Enfin, nous étudions les cicatrices quantiques dans des systèmes à une et plusieurs particules. Pour les premiers, nous montrons que le comportement à temps court des OTOCs n’est pas sensible à la présence de cicatrices, c’est-à-dire si le critère de Heller est satisfait. Cependant, nous montrons qu’une signature d’orbites périodiques instables existe et peut être observée. Pour les seconds, nous nous concentrons sur les oscillations permanentes qui apparaissent, en présence de cicatrices quantiques, dans différentes observables calculées pour des états “staggered dimers” dans

des systèmes de Bose-Hubbard. En augmentant l'interaction dans le système, il est attendu que les cicatrices disparaissent, ce qui est vérifié par les oscillations qui diminuent petit à petit.

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INTRODUCTION

The world as we know it in our daily life seems at the same time fairly regular and predictable, for instance because we all follow our respective routines, and chaotic, due to the unpredictable nature of society. In Physics, the words *regular* and *chaotic* bear a precise meaning that we will study in great detail in this manuscript.

As students, we are presented with the sunny side of physical systems: those are relatively simple, the equations that dictate their motion are solvable, and do not require a computer to have an idea of their behaviour. They are said to be regular, or integrable. As we acquire more knowledge, we start to realise that those systems, although they provide good and pedagogical examples for the application of the tools we learn, are far from realistic and represent only a minority. Indeed, reality is complex, and nothing is truly isolated or in a vacuum, as opposed to what many physicists, myself included, would like. In general, it is impossible to obtain a solution to the equations of a complex system. A good proportion of systems are chaotic: they exhibit a sensitivity to initial conditions which takes the form of an exponential spreading of trajectories that are started nearby in phase space [1]. In other words, any small perturbation will grow exponentially large with time, which is also known as the butterfly effect. As a consequence, predictions are eventually all rendered useless if the starting point of the evolution is not known with infinite accuracy, which is naturally never the case in practice. This does not mean, however, that all hope is lost. As will be seen later on, information can still be extracted. The most well-known being the Lyapunov exponent [2].

Another aspect of reality we are presented with as physics students is the realm of the infinitesimally small scales: quantum mechanics. In this context, the everyday laws of Nature that we know are not valid, and a new physics takes place. Despite being often presented as an alien world, classical and quantum mechanics are not unrelated, as the former must emerge from the latter as the characteristic scales become larger [3]. One of the key ingredients to the complete description of Nature is thus this bridge between the quantum and classical worlds. In addition to the academic need to describe the world, there is also the purely practical necessity to find out how the world behaves at these intermediate scales, as it is the realm of the so-called mesoscopic systems [4, 5]. They are far

too large to find a solution using the quantum formalism, but at the same time still exhibit quantum properties and therefore cannot be described solely with classical mechanics. Some examples are charge transport in high-mobility semiconductor heterostructures [4, 6] and quantum dots [6–8], and quantum wires [6].

SEMICLASSICAL PHYSICS AND QUANTUM CHAOS

Amongst the tools developed to bridge the two descriptions of Nature, and at the same time offer a description of mesoscopic systems, there are effective theories. They consist in a formulation in terms of an effective Planck constant, often written $\hbar_{\text{eff}}$ and proportional to $\hbar$, tending to 0. The literature writes this limit “ $\hbar_{\text{eff}} \rightarrow 0$ ”, or often abusively “ $\hbar \rightarrow 0$ ”. As $\hbar$ is not dimensionless and of course a fundamental constant, the latter must be understood as “ $\hbar/S \rightarrow 0$ ”, with S the typical action of the studied trajectory. The limit corresponds to a situation where this action is much larger than the Planck constant, resulting in very small Planck cells and a phase space that can be considered relatively smooth, similarly to classical dynamics [9, 10]. One of those effective theories is called semiclassical physics, or semiclassics. The “semi” naturally implies that the dynamics obtained from this formalism is not yet classical, as interferences are still considered [11, 12]. Semiclassical physics allows for instance to describe weak localisation [13, 14], resonance-assisted tunneling [15], or even the Aharonov-Bohm effect [16, 17].

Coming back to chaos, we know at this stage that it exists in the classical world. Once quantum mechanics became more familiar, a natural question arose: does this concept have any meaning at the quantum scale? The question was not trivial, as there are fundamental differences between the classical and quantum worlds. Namely, the linearity of the Schrödinger equation, which prevents nonlinearity in the time evolution, and the Heisenberg uncertainty principle that removes the meaning of considering initially close trajectories in phase space. Hence, the correspondence is not so straightforward, but fortunately for this thesis, it exists.

At first, the signatures of quantally chaotic systems were only indirect. For instance, one of those roundabout indicators was the statistics of the energy-level spacings [11, 18, 19]. The distribution they follow is related to the nature of the underlying classical dynamics [18, 20, 21]. In an effort to find more direct indicators, the Loschmidt echo [22, 23] and the out-of-time-ordered correlators [24–27] came to be. The latter will

be central in this manuscript. They probe the quantum correspondence of the exponential spreading of classical trajectories: the spreading, or scrambling, of information in a quantum system [28].

The field studying information spreading, and more specifically, the field studying characteristic quantum signatures that are generally exhibited by systems having a chaotic classical counterpart [18, 20, 21], is naturally named quantum chaos. In addition, it was found that in general, interacting bosonic many-body systems exhibit the same features and, similarly to single-particle systems, possess a chaotic classical limit. As a consequence, the field of quantum many-body chaos was born. In the following, the concept of quantum chaos is used to refer both to single and many-body chaotic quantum systems. Originally rooted in nuclear and atomic physics [29], the subject is now related to many other fields such as mesoscopic physics [6], optics and microwave physics [18], many-body physics [30, 31], as well as black-hole physics [32–35], quantum information [35], and has gained a lot of traction in recent years [26].

OUT-OF-TIME-ORDERED CORRELATORS

As mentioned before, the correspondence between quantum and classical chaos is not direct due to the fundamental differences between the two paradigms to which those concepts belong. One way to connect the two concepts is to link the information spreading to the fact that systems that exhibit this behaviour are chaotic in their classical limit, if this limit exists. One of the most important quantities used to establish that link is the out-of-time-ordered correlator (OTOC). The idea behind it is, given two (local) operators, to probe the propagation of information within a system through the growth of operators.

It was first introduced in the context of superconductivity in 1960 [36] and defined as

$$F(t) = \langle \psi | e^{it\hat{H}/\hbar} \hat{A}^\dagger e^{-it\hat{H}} \hat{B}^\dagger e^{it\hat{H}/\hbar} \hat{A} e^{-it\hat{H}/\hbar} \hat{B} | \psi \rangle. \quad (0.1)$$

In the more contemporary literature, the OTOC is defined as

$$C(t) = \langle \psi | \left| \left[\hat{A}(t), \hat{B} \right] \right|^2 | \psi \rangle, \quad (0.2)$$

with $\hat{A}$, $\hat{B}$ two (local) operators, $\hat{H}$ the Hamiltonian of the system, and t the time [24]. Using $\hat{B}$, the OTOC probes the spreading of operator $\hat{A}$ amongst the degrees of freedom of the system as it is time evolved. The

time evolution of an operator should be understood as in the Heisenberg representation, i.e., $\hat{A}(t) = \hat{U}^\dagger \hat{A} \hat{U}$ with $\hat{U} = \exp(-it\hat{H}/\hbar)$. The two definitions are related. The first definition is one of the 4 terms that appear when carrying out the square modulus of the commutator, and in the particular case of unitary operators, one can show $C(t) = 2 - 2 \operatorname{Re}(F(t))$ [37].

In systems that exhibit information scrambling, the OTOC in equation (0.2) is shown to grow exponentially with time, which makes them a suitable probe for chaos [24, 26, 27, 38, 39]. There are other instances in which the OTOC exhibits an exponential behaviour, but those will be discussed further in this manuscript.

The link between quantum and classical chaos can be established by virtue of the quantum-classical correspondence, which allows us to replace the commutator $[\hat{A}, \hat{B}]$ of two operators by the Poisson bracket, up to a prefactor, of their classical analogue: $i\hbar\{A, B\}$. Considering $\hat{A}$ and $\hat{B}$ to be the position operator $\hat{q}$ in some scrambling system, one would write

$$||\hat{q}(t), \hat{q}||^2 \rightarrow \hbar^2 \{q(t), q\}^2 = \hbar^2 \left(\frac{\partial q(t)}{\partial p} \right)^2 \propto \hbar^2 e^{2\lambda t}, \quad (0.3)$$

with λ corresponding to the Lyapunov exponent of the system if it is chaotic [25, 26, 40]. The proportional relation at the end holds because the derivative is an element of the stability matrix, which is an object that describes the variation of time-evolved coordinates when the initial ones are modified. In a chaotic system, this variation is exponential in time: again, this is the so-called butterfly effect. As a contrast, in an integrable system, this growth is at most polynomial. Let us also note that the transition from the operators to their classical analogues is straightforward in this simple case, but it will be explained for general operators and in more detail in Section 1.3.4.

This approximation is valid up to the so-called Ehrenfest time, the time at which quantum effects become prevalent [41]. In a many-body context, this time is also called the scrambling time [26, 42, 43]. After that time, the quantum OTOC deviates from the exponential growth and saturates, whereas what we will, at this stage, call the classical limit continues to grow exponentially and indefinitely. This implies that before this Ehrenfest time, the quantum and classical dynamics match. In other words, this approximation allows us to link on the one side the Lyapunov exponent, which is a purely classical concept related to chaos, and the exponential growth of the OTOC related to information scrambling, which

is purely quantum.

The exponential growth of the OTOC in scrambling systems possessing a (chaotic) classical limit was numerically observed consistently for both single-particle [40] and many-body [27] systems, providing direct information on the classical dynamics of those systems.

This exponential growth window is, however, not always large enough to clearly observe the scrambling nature of a system in the OTOC. Owing to the unitary dynamics, the growth is limited, meaning that the OTOC can saturate before the hyperbolic dynamics can truly start. The larger the Ehrenfest time, the larger this window. As this time can be seen as the timescale at which a small perturbation of the order of $\hbar_{\text{eff}}$ becomes significant, it can be shown that it behaves as $\log(1/\hbar_{\text{eff}})/\lambda$ [25, 44, 45].

A big part of this manuscript is dedicated to studying in depth the quantum-classical correspondence of the OTOC, and this is done by establishing a formalism that bridges the two realms.

BOSONIC SINGLE- AND MANY-BODY SYSTEMS

A context in which effective theories, in particular semiclassics, are useful and where quantum chaos can be present is bosonic single- and many-body systems, more specifically Bose-Einstein condensates, which will be the framework of all the numerical simulations of this thesis. The first experimental implementations, which were with Rubidium [46] and Sodium [47], were achieved using magnetic trap and laser cooling techniques. More recent advancements are presented in [48–51]. One of the ways to realise the potentials that serve as traps is with pairs of counterpropagating lasers. They allow to create three-[52], two-[53] and one-dimensional [54] lattices, and even ring- and square-shaped lattices [55].

Systems created that way have the advantage of being highly tunable. While the lattices are defect-free, disorder can nonetheless be introduced with an additional laser. The particle-particle interaction can be finely tuned using Feshbach resonance [56], and the hopping from one site to another by the depth of the wells [57].

Similarly to mesoscopic systems, the high number of particles involved in Bose-Einstein condensates means that solving the quantum problem is quite demanding. Resorting to an effective theory thus proves very useful. In the case of bosons, one considers that most atoms are in the ground state, which allows, in the large population limit, approximating the quantum evolution by a mean-field method: the Gross-Pitaevskii

equation [50, 58, 59]. This method is valid in the limit of a large number of particles, while in parallel, the interaction term remains small before the kinetic one [60]. For stronger interactions, contributions beyond the mean field approximation have to be taken into account. One way to go beyond this approximation is the truncated Wigner method [61–66], which takes into account the distribution of the initial state and considers the contributions from points sampled from this distribution, that each evolve according to the aforementioned Gross-Pitaevskii equation [67, 68].

As we now know more about the context, the concepts, and the tools that will be considered and analysed in this manuscript, let us, as the tradition dictates it, present the structure of the thesis.

OUTLINE OF THE THESIS

The thesis is structured into four chapters. The first one is a state of the art of the concepts used in this thesis. The following chapters focus on the work that we built upon these foundations. Let us detail what they contain.

Chapter 1 presents first the fundamental aspects of classical mechanics. It starts with the Hamiltonian formalism, then discusses the stability of a system in terms of the Lyapunov exponent and the stability matrix. It is followed by a presentation of quantum mechanics, starting from the well-known Schrödinger equation and establishing the Feynman path integral. From that starting point, the semiclassical propagator is obtained. Then, the mean-field approximation is presented, followed by the Wigner-Weyl formalism and the truncated Wigner approximation, which will be intensively used in this work. We continue this chapter by exposing the systems in which all the numerical simulations will be run. We conclude by giving an introduction to quantum chaos and the different indicators, namely the out-of-time-ordered correlator, a central object for what is to come.

Chapter 2 establishes a quasiclassical theory of out-of-time-ordered correlators in mixed and fully chaotic systems. It starts from the quantum expression of the correlator, on which are applied the semiclassical and diagonal approximations successively. This results in several contributions that are considered individually. Once the expressions are obtained, an expansion in powers of the Planck constant is then made. The analytical part ends with the derivation of a long-time limit, valid even for chaotic

systems, which gives the dominant contribution to the correlator for long times. Finally, these predictions are tested numerically in different systems.

Chapter 3 focuses on the other end of the spectrum of chaotic systems: near-integrable systems. We study the genesis of chaos around the separatrix linked to an unstable fixed point. The paradigmatic system that is the driven pendulum is used as the framework of our calculations. We study how the system behaves near that separatrix for small perturbations, and establish an analytical expression for the rate of exponential divergence of the dynamics that is neither the Lyapunov nor the stability exponent, but something in between. We verify our predictions numerically in several systems, using the derivations made in this chapter as well as the OTOC formalism from Chapter 2.

Chapter 4 goes back to the realm of fully chaotic systems in order to focus on quantum scarring. We present the concept of quantum scars, their existence criterion called the Heller criterion, and how this concept manifests itself through the lens of out-of-time-ordered correlators in a single-particle system, the kicked rotor, and in a many-body case, Bose-Hubbard models. For the single-particle case, we focus on the short-time behaviour, allowing us to apply the formalism of Chapter 2, whereas for the latter case we look at the long-time persistent oscillations.

CLASSICAL AND QUANTUM CHAOS

Historically, chaos was first a classical concept related to the stability of a system. It has been an active domain of research for many decades [1, 2, 69]. A system was considered chaotic when its dynamics was highly sensitive to initial conditions, despite being dictated by deterministic equations of motion. Numerous examples exist in the literature, with for instance the Lorenz system, used to model the atmosphere [2], or the double pendulum [70]. The chaotic nature of a classical system can be easily highlighted by considering two generic initial conditions that are identical except for an infinitesimal perturbation, and observing that the two phase-space trajectories that are born from those points diverge exponentially with time, rendering any prediction useless. The adjective “generic” is fundamental. Indeed, sensitivity to initial conditions can occur in regular systems as well, but only in particular locations, for instance at an unstable fixed point. Sensitivity at all points, i.e. uniform hyperbolicity, on the other hand, means the system is chaotic.

As Physics matured and quantum mechanics came to be, it was only a matter of time before the concept of chaos was extended to quantum systems [18, 20, 21]. This proved a difficult endeavour, one of the reasons being the fundamental difference between both realms. On the one hand, the classical world, where chaos is defined as the exponential deviation between two initially close trajectories due to nonlinear dynamics. On the other hand, the quantum world, where the notion of close points loses meaning due to the uncertainty principle, and where the dynamics is governed by a linear equation. Because of those differences, quantum chaos cannot be studied with the same tools as its classical equivalent. New probes had to be designed, which will be presented later on.

Since classical and quantum chaos differ in many fundamental aspects, the latter is often referred to as *information scrambling*, or simply *scrambling* [28]. Scrambling is the term used to describe the process through which information is spread throughout a quantum system, which results in its effective loss, in the sense that it cannot be recovered using local probes [71]. This formulation has the advantage of not implying a non-linearity in the time evolution, which is, in principle, forbidden by the

Schrödinger equation. As a consequence, it reflects more accurately what quantum chaos is, in its essence.

However, let us not be too quick to draw the conclusion that the scrambling and classical chaos are totally uncorrelated. As stated in the introduction, those quantum signatures of chaos are exhibited by systems whose classical limit is chaotic [18, 20, 21]. In addition, for short times, more specifically before a time named the Ehrenfest time, the quantum and classical dynamics match, meaning that features of the quantum dynamics can be extracted from the classical one.

To this end, we begin this manuscript by presenting the fundamental concepts of classical Hamiltonian mechanics and chaos to bring an uninitiated reader up to speed, or offer a brief reminder to the seasoned expert in the field. What follows can be found in most textbooks, like references [1, 2, 72], and we will in particular broadly follow what has been done in Josef Rammensee's [73]. We then continue this work with a presentation of quantum mechanics and the concepts relevant to this work. We conclude this chapter by presenting the systems in which numerical simulations will be run, then quantum chaos, more specifically the different indicators that are used to study it.

1.1 CLASSICAL MECHANICS

In the context of the Hamiltonian formalism, a system is entirely described by a function called the *Hamiltonian*, or *Hamilton function*, $\mathcal{H}(\mathbf{q}, \mathbf{p}, t)$. The arguments $\mathbf{q}$ and $\mathbf{p}$ are N -dimensional vectors belonging to spaces called respectively the configuration space and the tangent bundle [74], and t is a scalar representing the time. The two vectors are often named the position and momentum vectors, but it is important to note that, depending on the system that is studied, they do not necessarily bear the same meaning, as will be seen later with the Bose-Hubbard model. We will nonetheless call them that way out of convenience, as in any case they exhibit the same properties. The dimension N is called the number of degrees of freedom.

The state of a system is determined by the position and momentum vectors. They can be combined into a single vector $(\mathbf{q}, \mathbf{p})$ of dimension $2N$. The set of all the vectors built that way is called the *phase space* and is a central notion in both Hamiltonian mechanics and this manuscript.

A phase-space point evolves according to Hamilton's equations of motion, which are given by

$$\begin{cases} \dot{\mathbf{q}}(t) &= \frac{\partial \mathcal{H}}{\partial \mathbf{p}}(\mathbf{q}(t), \mathbf{p}(t), t), \\ \dot{\mathbf{p}}(t) &= -\frac{\partial \mathcal{H}}{\partial \mathbf{q}}(\mathbf{q}(t), \mathbf{p}(t), t), \end{cases} \quad (1.1)$$

with using the usual notation of the dot representing the total time derivative.

An important characteristic of Hamiltonian systems is their symplectic structure. This means that, writing $\mathbf{r} = (\mathbf{q}, \mathbf{p})$ a phase-space vector, the evolution equation can elegantly be formulated as

$$\dot{\mathbf{r}}(t) = J \frac{\partial \mathcal{H}}{\partial \mathbf{r}}(\mathbf{r}, t), \quad (1.2)$$

with J the symplectic matrix

$$J = \begin{pmatrix} 0_{N \times N} & 1_{N \times N} \\ -1_{N \times N} & 0_{N \times N} \end{pmatrix}, \quad (1.3)$$

with $0_{N \times N}$ and $1_{N \times N}$ the $N \times N$ zero and identity matrices respectively.

A consequence is that, as equation (1.2) is a first-order differential equation, there is only one solution corresponding to an initial condition $\mathbf{r}(t_0) = (\mathbf{q}_0, \mathbf{p}_0)$. Finding the solution corresponding to an initial condition is called an initial-value problem. Because of the unique solution of initial-value problems, classical mechanics is deterministic. The ensemble of points that results from the solution of these equations for a given initial condition is called a phase-space trajectory.

In this work, some problems will be formulated not as initial-value problems but as boundary problems: what is set is the initial and final positions as well as the time, but not the momentum. As a consequence, the solution is not guaranteed to be unique or even exist at all. In the context of boundary problems, an important quantity is the action functional $R(\mathbf{r}(t))$, also known as the (on-shell) action, which is defined as the integral of the Lagrangian along a trajectory $\mathbf{r}(t)$ in phase space. If the action functional is evaluated along a path that is not a solution of Hamilton's equations of motion, the quantity is called Hamilton's principal function, or the off-shell action. It is written

$$R_\gamma(\mathbf{q}^f, \mathbf{q}^i, t^f, t^i) \equiv R(\mathbf{r}_\gamma(\mathbf{q}^f, \mathbf{q}^i, t^f, t^i)) \quad (1.4)$$

$$= \int_{t^i}^{t^f} [\mathbf{p}_\gamma(t) \cdot \dot{\mathbf{q}}_\gamma(t) - \mathcal{H}(\mathbf{q}_\gamma(t), \mathbf{p}_\gamma(t), t)] dt, \quad (1.5)$$

with $\mathbf{q}^i$ and $\mathbf{q}^f$ the initial and final positions, $\mathbf{r}_\gamma = (\mathbf{q}_\gamma(t), \mathbf{p}_\gamma(t))$ the phase-space trajectory named γ , t_i and t_f the initial and final times, $t = t_f - t_i$ the elapsed time, and where we omitted the dependence in the initial and final positions for the last line [72]. In the remainder of this manuscript, we will omit the initial and final times and only write the elapsed time along the boundary positions as arguments of the left-hand side of equation (1.4).

Important relations that can be established are the derivatives of Hamilton's principal function with respect to the initial or final position:

$$\frac{\partial R_\gamma}{\partial \mathbf{q}^f}(\mathbf{q}^f, \mathbf{q}^i, t) = \mathbf{p}_\gamma^f(\mathbf{q}^f, \mathbf{q}^i, t), \quad (1.6)$$

$$\frac{\partial R_\gamma}{\partial \mathbf{q}^i}(\mathbf{q}^f, \mathbf{q}^i, t) = -\mathbf{p}_\gamma^i(\mathbf{q}^f, \mathbf{q}^i, t), \quad (1.7)$$

with $\mathbf{p}_\gamma^i(\mathbf{q}^f, \mathbf{q}^i, t)$ and $\mathbf{p}_\gamma^f(\mathbf{q}^f, \mathbf{q}^i, t)$ the initial and final momenta corresponding to the trajectory γ that links the boundaries $\mathbf{q}^i$ and $\mathbf{q}^f$ in a time t . These expressions allow to interpret the off-shell action R_γ as the generating function that sends the point $(\mathbf{q}^i, \mathbf{p}_\gamma^i(\mathbf{q}^f, \mathbf{q}^i, t))$ to $(\mathbf{q}^f, \mathbf{p}_\gamma^f(\mathbf{q}^f, \mathbf{q}^i, t))$ along the path γ [9, 74].

At this point, it is important to introduce the notion of integrability, which will eventually be related to the notion of classical chaos, discussed in the next section. Integrable systems are, according to Liouville's theorem, those that possess as many independent integrals of motion, or first integrals, as there are degrees of freedom¹. They are also called regular systems. This concept is explained through the lens of Poisson brackets. Let f and g be two functions whose domain is the phase space. Their Poisson bracket $\{\cdot, \cdot\}$ is defined as

$$\{f(\mathbf{q}, \mathbf{p}, t), g(\mathbf{q}, \mathbf{p}, t)\} = \sum_{n=1}^N \left[\frac{\partial f}{\partial q_n} \frac{\partial g}{\partial p_n} - \frac{\partial f}{\partial p_n} \frac{\partial g}{\partial q_n} \right], \quad (1.8)$$

with $\mathbf{q} = (q_1, \dots, q_N)$ and $\mathbf{p} = (p_1, \dots, p_N)$ the position and momentum, and where the dependences in the right-hand side have been omitted. Hamilton's equations of motion can be rewritten using the Poisson bracket as

$$\begin{cases} \dot{\mathbf{q}}(t) &= \{\mathbf{q}(t), \mathcal{H}(\mathbf{q}(t), \mathbf{p}(t), t)\}, \\ \dot{\mathbf{p}}(t) &= \{\mathbf{p}(t), \mathcal{H}(\mathbf{q}(t), \mathbf{p}(t), t)\}. \end{cases} \quad (1.9)$$

¹ As it is the consequence of Liouville's theorem, the terms "Liouville-integrable" or "integrable in the Liouville sense" are sometimes used.

A function f is an integral of motion if its Poisson bracket with the Hamiltonian $\mathcal{H}$ is zero, i.e.,

$$\{f(\mathbf{q}, \mathbf{p}, t), \mathcal{H}(\mathbf{q}, \mathbf{p}, t)\} = 0. \quad (1.10)$$

It can be used to perform a change of coordinates to reduce the dimension in which the dynamics takes place. If there are as many independent first integrals in involution as there are degrees of freedom, i.e., for a system of N degrees of freedom, there are N functions $f_1, \dots, f_N$ such that

$$\{f_j(\mathbf{q}, \mathbf{p}), f_k(\mathbf{q}, \mathbf{p})\} = 0 \quad \forall j, k = 1, \dots, N, \quad (1.11)$$

then the system is integrable [74]. The phase-space trajectories then lie on tori and the dynamics is regular and bounded [75]. Nonintegrable systems may, on the other hand, exhibit chaos, which is what will be explained in the coming section.

1.2 SYSTEM STABILITY AND CLASSICAL CHAOS

The deterministic nature of classical mechanics does not, however, mean that everything can be predicted for all systems. While in theory this would be the case, the vast majority of systems exhibit what is called initial value sensitivity. This sensitivity means that any infinitesimal perturbations grow exponentially with time, which is known in the literature as the butterfly effect. This implies that not knowing the initial conditions with infinite precision results in an uncertainty on the prediction that increases exponentially with time. Systems that exhibit such a sensitivity are said to be chaotic, while those that do not are said to be regular. There is, however, a spectrum between regular and chaotic systems. Systems that deviate only a little from integrability are dubbed near-integrable systems. They can be treated using perturbation theory, where their Hamiltonian is written as an integrable part plus a perturbation. The Kolmogorov—Arnold—Mose, or KAM, theorem states that under small perturbations, the phase space continues to contain regular structure and one can thus still make predictions regarding the dynamics [76]. A well-known example is the orbits of planets around the Sun. Stronger deviations from integrability lead to a more predominant chaotic structure in the phase space. Such systems are called mixed systems. Trajectories that lie in the regular region of the phase space are said to be regular, while those in the chaotic region, or chaotic sea, are dubbed chaotic as they present initial-value sensitivity.

As written, chaos leads to uncertainties regarding predictions. This does not mean that this is the end of the road, as information can still be extracted from such systems. One of the most well-known is undeniably the Lyapunov exponent. Often written λ_L , it is the exponential rate of divergence between two initially close phase-space trajectories [1, 2, 77]. As a comparison, regular trajectories deviate at most linearly in time [2].

Consider two phase-space points $\mathbf{r}$ and $\mathbf{r}' = \mathbf{r} + \delta\mathbf{r}$ with $\|\delta\mathbf{r}\| \ll \|\mathbf{r}\|$. The distance between those two points is the usual Euclidean distance

$$d(t; \mathbf{r}, \mathbf{r}') = \sqrt{\sum_{n=1}^{2N} (r_n(t) - r'_n(t))^2} \quad (1.12)$$

$$= \sqrt{\sum_{n=1}^{2N} \delta r_n^2(t)}, \quad (1.13)$$

where $\mathbf{r}(t) = (r_1(t), \dots, r_{2N}(t))$ and $\delta\mathbf{r}(t) = (\delta r_1(t), \dots, \delta r_{2N}(t))$ are the time-evolved vector $\mathbf{r}$ and $\delta\mathbf{r}$, and with $\mathbf{r}'(t) = \mathbf{r}(t) + \delta\mathbf{r}(t)$ the time-evolved vector $\mathbf{r}'$. Using this expression and writing the distance at initial time $d(0; \mathbf{r}, \mathbf{r}') = d_0$, one can define the rate of exponential divergence of two trajectories starting at $\mathbf{r}$ and $\mathbf{r}'$, or Lyapunov exponent, by

$$\lambda_L(\mathbf{r}, \mathbf{r}') = \lim_{t \rightarrow \infty} \lim_{d_0 \rightarrow 0} \log \left(\frac{d(t; \mathbf{r}, \mathbf{r}')}{d_0} \right). \quad (1.14)$$

As indicated by the dependence, the rate of divergence can, in general, depend on the initial point and on the direction of the deviation. Several rates actually exist, and the ensemble of all those rates constitutes the Lyapunov exponent spectrum. For a phase-space of dimension N , there is a set of N Lyapunov exponents $|\lambda_1| \geq |\lambda_2| \geq \dots \geq |\lambda_N|$. Each positive exponent corresponds to a direction of the unstable manifold on which the dynamics takes place. For each unstable direction, there exists a corresponding one in the stable manifold whose Lyapunov exponent is the same but with an opposite sign [2]. For a given phase-space volume, any stretching in a direction is thus balanced out by a contraction in another one, ensuring the validity of Liouville's theorem. If a direction corresponds to a regular motion, the distance grows at most linearly, and the exponent is zero.

If the computation of the Lyapunov exponent is averaged over the whole chaotic sea, which corresponds to the whole phase space for fully chaotic systems, or at least on a sufficiently large region of it because of

the mixing properties, the dynamics will be dominated by the maximum Lyapunov exponent, which we can note λ_L^M . For this reason, in the literature, the Lyapunov exponent λ_L of a system refers to this maximum rate and no spatial dependence is specified. We will follow the same custom in this present work.

To be exhaustive, let us also note that equation (1.14) does not always correspond to λ_L^M . For instance, a regular system can exhibit a nonzero “Lyapunov exponent” if the point $\mathbf{r}_0$ is an unstable fixed point. An example is the highest point of a simple pendulum, which corresponds to the unstable equilibrium position. In this case, a nonzero exponent does not come from a global instability, but rather a local one. The growth rate obtained in this context is called the stability exponent of the associated fixed point, and is written λ_s .

Before going any further, let us introduce the concepts of ergodicity, mixing, and full/uniform hyperbolicity, as some of those terms were already used without having been properly defined, and they are of utmost importance in the study of chaos. A system is said to be ergodic if, given enough time, any trajectory will explore the whole phase space. A direct consequence is that the time and space averages can be freely interchanged. For a given function f defined on the phase space, the ergodic theorem reads

$$\lim_{t \rightarrow \infty} \frac{1}{t} \int_0^t f(\mathbf{q}(t), \mathbf{p}(t)) dt = \frac{1}{\Omega} \int_{\text{phase space}} f(\mathbf{q}, \mathbf{p}) d\mathbf{q} d\mathbf{p}, \quad (1.15)$$

where $\Omega = \int_{\text{phase space}} d\mathbf{q} d\mathbf{p}$ is the phase-space volume. It is important to note that ergodicity, while being a necessary condition for chaos, is not sufficient, as it does not imply a sensitivity to initial conditions. A stronger property, yet not sufficient when it comes to the existence of chaos [9, 11], is the one of mixing.

A system is mixing if, given two phase-space regions A and B , one has [1, 9]

$$\lim_{t \rightarrow +\infty} \mu(A(t) \cap B) = \mu(A)\mu(B), \quad (1.16)$$

with $\mu(A) = \int_A d\mathbf{q} d\mathbf{p}$ the phase-space volume of the region A , with the total phase-space volume set to 1, and $A(t)$ the region obtained by time-evolving² all the points comprised in A for a time t . In other words,

² The time-evolution can be discrete, like for maps, or continuous. More details can be found in Section 2.1 of [9] or Section 2.3.1 of [73].

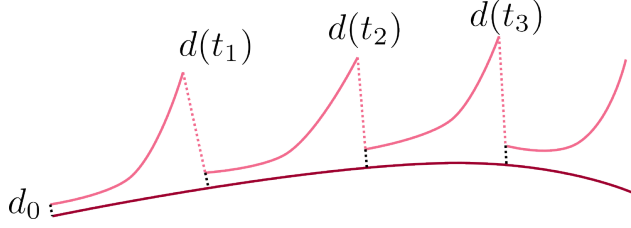


Figure 1.1: Representation of the Wolf algorithm. Two initial conditions are evolved to create phase-space trajectories. One of them is the reference trajectory (dark red), whereas the other one (light red) is “renormalised” at different moments $t_1, t_2, \dots$, to overcome the limitation of more straightforward numerical simulations. More precisely, we mean that the distance between the two trajectories at the renormalisation times, $d(t_1), d(t_2), \dots$, is reset to d_0 .

the volume of the intersection A evolved for a time $t \rightarrow \infty$ and another region B is the same as the product of the volumes of A and B . To understand it, let us give an example that follows the intuitive meaning of the word “mixing”. Consider a cup with a normalised volume, with A the region filled with milk, with $\mu(A) = 0.1$, and B the region filled with coffee, with $\mu(B) = 0.9$. Once the two fluids have been thoroughly mixed ($t \rightarrow \infty$ in our analogy), the fraction of milk in the region that was initially 100% coffee, region B , is given by

$$\frac{\lim_{t \rightarrow +\infty} \mu(A(t) \cap B)}{\mu(B)} = \frac{\mu(A)\mu(B)}{\mu(B)} \quad (1.17)$$

$$= \mu(A) \quad (1.18)$$

$$= 0.1. \quad (1.19)$$

Any phase-space region will, once time-evolved, eventually overlap with any other region.

Finally, the last property that we introduce is the one of complete hyperbolicity. This one is sufficient for chaos. It implies that every point in phase space is subject to a sensitivity to initial conditions, i.e., subject to the butterfly effect [9, 21, 69, 78].

Let us now come back to the concept of Lyapunov exponent. There are a few instances where that quantity can be computed analytically. This is however not the case in all generality, where one must resort to numerical methods. In this case, evaluating equation (1.14) directly is of course not possible. The smallest value of d_0 is limited by machine precision, which would render the other limit wrong, as two initially close

phase-space trajectories cannot grow infinitely apart from each other due to the limitation of the accessible region of phase space. One way to circumvent it is the Wolf algorithm [2, 77]. It consists in taking two initial conditions separated by a very small distance d_0 that is above the machine precision, and thus far from the $d_0 \rightarrow 0$ limit. One of the phase-space points is time-evolved in the usual manner, and the phase-space trajectory that is therefore created is called the reference trajectory. The other initial condition is time-evolved as well, but the distance from the reference trajectory is reset many times during the propagation while keeping the direction of the deviation. This is illustrated in Figure 1.1. Assuming the renormalisation at some time t , the renormalisation can be written

$$\mathbf{r}'(t) = \mathbf{r}(t) + \delta\mathbf{r}(t) \rightarrow \mathbf{r}'(t) = \mathbf{r}(t) + \frac{d_0}{\|\delta\mathbf{r}(t)\|} \delta\mathbf{r}(t). \quad (1.20)$$

The choice as to when or where the distance must be renormalised is usually either after a fixed time has elapsed or after the distance between the two trajectories has reached some threshold. In both situations, the distances at all the renormalisations are saved in memory. After enough renormalisations, the finite-time maximum Lyapunov exponent (FTMLE) is evaluated by computing

$$\lambda_L^{\text{FTMLE}} = \frac{1}{t_M} \sum_{m=1}^M \log\left(\frac{d(t_m)}{d(t_{m-1})}\right), \quad (1.21)$$

where $d(t_m)$ is the distance between the two trajectories before a renormalisation done at a time t_m , and M is the number of renormalisations. This method emulates a propagation for an arbitrary long time without ever reaching the limit of the phase space. A number of renormalisations M large enough so that the exponent has converged allows one to conclude that this estimation is correct and thus write $\lambda_L^{\text{FTMLE}} \simeq \lambda_L$. As is often done in the literature, we will simply use the term Lyapunov exponent without any other qualifier such as FTMLE.

Information about the stability of a system regarding its initial conditions can also be obtained through an object called the stability matrix. Consider $\mathbf{r}(\mathbf{r}_0, t)$, a vector obtained by time-evolving a vector $\mathbf{r}_0$ for a

time t . For short times, a small perturbation $\delta \mathbf{r}_0$ in the initial conditions can be safely linearised:

$$\mathbf{r}(\mathbf{r}_0 + \delta \mathbf{r}_0, t) = \mathbf{r}(\mathbf{r}_0, t) + \frac{\partial \mathbf{r}}{\partial \mathbf{r}_0}(\mathbf{r}_0, t) \delta \mathbf{r}_0 + \mathcal{O}(\delta \mathbf{r}_0^2) \quad (1.22)$$

$$= \mathbf{r}(\mathbf{r}_0, t) + M(\mathbf{r}_0, t) \delta \mathbf{r}_0 + \mathcal{O}(\delta \mathbf{r}_0^2), \quad (1.23)$$

with M the stability matrix, or monodromy matrix, defined as the matrix of the derivatives of the final coordinates with respect to initial ones, i.e.

$$M(\mathbf{r}_0, t) = \frac{\partial \mathbf{r}}{\partial \mathbf{r}_0}(\mathbf{r}_0, t) \quad (1.24)$$

$$= \begin{pmatrix} \frac{\partial r_1(\mathbf{r}_0, t)}{\partial r_{0,1}} & \cdots & \frac{\partial r_1(\mathbf{r}_0, t)}{\partial r_{0,2N}} \\ \vdots & \ddots & \vdots \\ \frac{\partial r_{2N}(\mathbf{r}_0, t)}{\partial r_{0,1}} & \cdots & \frac{\partial r_{2N}(\mathbf{r}_0, t)}{\partial r_{0,2N}} \end{pmatrix}. \quad (1.25)$$

The exponential growth rate of the initial deviation can be obtained through

$$\lambda(\mathbf{r}_0, \delta \mathbf{r}_0) = \lim_{t \rightarrow \infty} \frac{1}{t} \log \frac{\|M(\mathbf{r}_0, t) \delta \mathbf{r}_0\|}{\|\delta \mathbf{r}_0\|}, \quad (1.26)$$

which is equivalent to (1.14). Similarly, this exponent is nonzero if there is an instability, and can correspond to either λ_L or λ_s if it is respectively a global or local one.

Equivalently, one can obtain the exponential growth rate using the eigenvalues of the stability matrix [79, 80]. To illustrate this, and by the same occasion show that one can also extract the exponential growth rate using the trace of the stability matrix, let us consider the particular case of a 1-degree-of-freedom system. Writing explicitly $\mathbf{r}_0 = (q_0, p_0)$, one can write the trace of the stability matrix as

$$\text{Tr}(M(q_0, p_0, t)) = \text{Tr} \begin{pmatrix} \frac{\partial q(t)}{\partial q_0} & \frac{\partial q(t)}{\partial p_0} \\ \frac{\partial p(t)}{\partial q_0} & \frac{\partial p(t)}{\partial p_0} \end{pmatrix}, \quad (1.27)$$

with q and p the position and momentum of the system and q_0 and p_0 the initial position and momentum. As M is symplectic, the determinant of the matrix is 1. Exploiting the fact that the determinant is the product of its eigenvalues, those can be written α and $1/\alpha$ [21]. The trace, being the sum of the eigenvalues, is then given by

$$\text{Tr}(M(q_0, p_0, t)) = \alpha + \frac{1}{\alpha}. \quad (1.28)$$

By defining $\sigma(t) = \pm \log(|\alpha|)/t$, the trace is rewritten as a sum of exponentials, i.e.,

$$\text{Tr}(M(q_0, p_0, t)) = \pm 2 \cosh(\sigma(t)t), \quad (1.29)$$

where $\sigma(t)$ behaves asymptotically as the stability exponent λ . The last equality holds provided that there is an instability at the initial point (q_0, p_0) . The exponent dictating the dynamics can be extracted by

$$\lambda = \lim_{t \rightarrow \infty} \frac{1}{t} \text{arccosh} \left(\frac{|\text{Tr}(M(t))|}{2} \right) \quad (1.30)$$

$$\simeq \lim_{t \rightarrow \infty} \frac{1}{t} \log |\text{Tr}(M(t))|. \quad (1.31)$$

Similarly to the Wolf algorithm, one can work around the numerical limits by performing periodic renormalisations of the distance in the computation of numerical derivatives. More specifically, a numerical derivative, in the sense of a finite-difference derivative, is evaluated as

$$\frac{\partial f}{\partial \mathbf{r}}(\mathbf{r}_0, t) \simeq \frac{f(\mathbf{r}_0 + \delta \mathbf{r}_0, t) - f(\mathbf{r}_0, t)}{\delta \mathbf{r}_0}. \quad (1.32)$$

As $\delta \mathbf{r}_0$ is finite, evaluating the derivatives of the trace that way leads to the wrong behaviour for long times. The idea here is to again reset the distance between the two propagated trajectories, following (1.20), but also keep in mind the total renormalisation that will be done. This means in practice that before any renormalisation, this factor that we can call the renormalisation factor is 1, and at each renormalisation, it gets multiplied by $d(t_m)/d_0$, with as a reminder $d(t_m)$ the distance between the two trajectories at the renormalisation time t_m , and $d_0 = \|\delta \mathbf{r}_0\|$ the initial distance. Multiplying the numerator by the renormalisation factor allows one to obtain the “true” numerator, i.e., the numerator that one would have if the distance between two trajectories could grow indefinitely. It emulates the behaviour of true derivatives and allows to evaluate expression (1.31) at a time large enough so that the exponent converges.

1.3 QUANTUM MECHANICS

1.3.1 *Schrödinger equation and Feynman path integral*

Similarly to a classical system whose time-evolution is dictated by a function called the Hamiltonian, the time-evolution of a quantum system

is given by an operator $\hat{H}$, also called the Hamiltonian of the system. To differentiate the classical from the quantum one, the convention in the literature is to add a hat to indicate that it is an operator.

In the general case, the Hamiltonian is time-dependent. The equation that governs the dynamics is the (time-dependent) *Schrödinger equation*. For an initial state $|\psi(t=0)\rangle = |\psi_0\rangle$, it is given by

$$i\hbar \frac{d|\psi(t)\rangle}{dt} = \hat{H}(t) |\psi(t)\rangle, \quad (1.33)$$

with $\hat{H}$ the Hamiltonian of the system which, in general, is time-dependent. If it is time-independent, the equation is straightforwardly solved as

$$|\psi(t)\rangle = \hat{U}(t) |\psi_0\rangle \quad (1.34)$$

$$\equiv \exp\left(-\frac{i}{\hbar} \hat{H} t\right) |\psi_0\rangle. \quad (1.35)$$

This expression can be formulated in the position representation:

$$\langle \mathbf{r} | \psi(t) \rangle = \langle \mathbf{r} | \hat{U}(t) \int d\mathbf{r}' |\mathbf{r}'\rangle \langle \mathbf{r}' | \psi_0 \rangle \quad (1.36)$$

$$\Leftrightarrow \psi(\mathbf{r}, t) = \int d\mathbf{r}' K(\mathbf{r}, \mathbf{r}', t) \psi_0(\mathbf{r}'), \quad (1.37)$$

where we defined $K(\mathbf{r}, \mathbf{r}', t) = \langle \mathbf{r} | \hat{U}(t) | \mathbf{r}' \rangle$, called the propagator.

Let us for simplicity consider a Hamiltonian made up of a kinetic and potential part:

$$\hat{H} = \hat{T} + \hat{V} \quad (1.38)$$

$$= \frac{\hat{\mathbf{p}}^2}{2m} + V(\hat{\mathbf{r}}). \quad (1.39)$$

To obtain the Feynman path integral, we first look at an infinitesimally small time propagation, i.e., we consider that the time t is a small duration $\delta t \rightarrow 0$. Using the Baker-Campbell-Hausdorff formula, this translates to

$$\hat{U}(\delta t) = \exp\left(-\frac{i}{\hbar} \delta t (\hat{T} + \hat{V})\right) \quad (1.40)$$

$$= \exp\left(-\frac{i}{\hbar} \delta t \hat{T}\right) \exp\left(-\frac{i}{\hbar} \delta t \hat{V}\right) + \mathcal{O}(\delta t^2). \quad (1.41)$$

As the potential operator is diagonal in the position basis, injecting in the propagator yields

$$\langle \mathbf{r} | \hat{U}(t) | \mathbf{r}' \rangle = \langle \mathbf{r} | \exp\left(-\frac{i}{\hbar} \delta t \hat{T}\right) | \mathbf{r}' \rangle \exp\left(-\frac{i}{\hbar} \delta t V(\mathbf{r}')\right). \quad (1.42)$$

The remaining matrix element is treated by inserting a completeness relation in the momentum basis, where the momentum operator is diagonal:

$$\langle \mathbf{r} | \exp\left(-\frac{i}{\hbar} \delta t \hat{T}\right) | \mathbf{r}' \rangle = \int d\mathbf{p} \exp\left(-\frac{i \delta t p^2}{2m\hbar}\right) \langle \mathbf{r} | \mathbf{p} \rangle \langle \mathbf{p} | \mathbf{r}' \rangle \quad (1.43)$$

$$= \int \frac{d\mathbf{p}}{(2\pi\hbar)^L} \exp\left(-\frac{i \delta t p^2}{2m\hbar} + \frac{i}{\hbar} \mathbf{p} \cdot (\mathbf{r} - \mathbf{r}')\right) \quad (1.44)$$

$$= \prod_{j=1}^L \int \frac{dp_j}{(2\pi\hbar)} \exp\left(-\frac{i \delta t p_j^2}{2m\hbar} + \frac{i}{\hbar} p_j (r_j - r'_j)\right), \quad (1.45)$$

with L the number of degree of freedom, $p^2 = \mathbf{p} \cdot \mathbf{p}$, and using the overlap between the position and momentum eigenstates

$$\langle \mathbf{r} | \mathbf{p} \rangle = \frac{1}{\sqrt{(2\pi\hbar)^L}} \exp\left(\frac{i}{\hbar} \mathbf{r} \cdot \mathbf{p}\right). \quad (1.46)$$

In order to evaluate the Fresnel integral (1.45), we rewrite the argument of the exponential as

$$\begin{aligned} & -\frac{i \delta t p^2}{2m\hbar} + \frac{i}{\hbar} \mathbf{p} \cdot (\mathbf{r} - \mathbf{r}') \\ &= \sum_{j=1}^L \left[-\frac{i \delta t}{2m\hbar} \left(p_j + 2m \frac{r_j - r'_j}{\delta t} \right)^2 + \frac{i m}{2\hbar} \frac{(r_j - r'_j)^2}{\delta t} \right]. \end{aligned} \quad (1.47)$$

We then use

$$\int_{\mathbb{R}} e^{i\alpha x^2} dx = \lim_{\varepsilon \rightarrow 0^+} e^{-(\varepsilon - i\alpha)x^2} \quad (1.48)$$

$$= \lim_{\varepsilon \rightarrow 0^+} \sqrt{\frac{\pi}{\varepsilon - i\alpha}} \quad (1.49)$$

$$= \sqrt{\frac{\pi}{|\alpha|}} e^{i\pi \text{sgn}(\alpha)/4}, \quad (1.50)$$

which, once particularised for our integral, yields

$$\int dp_j \exp\left(-\frac{i \delta t}{2m\hbar} \left(p_j + 2m \frac{r_j - r'_j}{\delta t} \right)^2\right) = \sqrt{\frac{2m\pi\hbar}{\delta t}} e^{-i\pi/\hbar}, \quad (1.51)$$

which in turn enables us to write the matrix element (1.45) as

$$\langle \mathbf{r} | \exp\left(-\frac{i}{\hbar} \delta t \hat{T}\right) | \mathbf{r}' \rangle = \prod_{j=1}^L \sqrt{\frac{m}{2\pi i \hbar \delta t}} \exp\left(\frac{i}{\hbar} \frac{(r_j - r'_j)^2 m}{2\delta t}\right). \quad (1.52)$$

The propagator (1.42) is then written

$$\langle \mathbf{r} | \hat{U}(\delta t) | \mathbf{r}' \rangle = \left(\frac{m}{2\pi i \hbar \delta t}\right)^{L/2} \exp\left(\frac{i\delta t}{\hbar} \left(\frac{m}{2} \left(\frac{\mathbf{r} - \mathbf{r}'}{\delta t}\right)^2 - V(\mathbf{r}')\right)\right). \quad (1.53)$$

We can note that the argument of the exponential consists basically of the classical Lagrangian function

$$\mathcal{L}\left(r'_{j-1}, \frac{r_j - r'_{j-1}}{\delta t}\right) = \frac{m}{2} \left(\frac{\mathbf{r} - \mathbf{r}'}{\delta t}\right)^2 - V(\mathbf{r}'). \quad (1.54)$$

To obtain an evolution to arbitrary time, one has to use the composition property of the evolution operator, which reads

$$\hat{U}(t_2 + t_1) = \hat{U}(t_2) \circ \hat{U}(t_1). \quad (1.55)$$

For the propagator, it translates to

$$K(\mathbf{r}, \mathbf{r}', t_2 + t_1) = \langle \mathbf{r} | \hat{U}(t_2) \circ \hat{U}(t_1) | \mathbf{r}' \rangle \quad (1.56)$$

$$= \int d\mathbf{r}'' \langle \mathbf{r} | \hat{U}(t_2) | \mathbf{r}'' \rangle \langle \mathbf{r}'' | \hat{U}(t_1) | \mathbf{r}' \rangle \quad (1.57)$$

$$= \int d\mathbf{r}'' K(\mathbf{r}, \mathbf{r}'', t_2) K(\mathbf{r}'', \mathbf{r}', t_1). \quad (1.58)$$

For a path of an arbitrary duration, one can thus divide it in $N \rightarrow +\infty$ parts of duration δt and express the full propagator as a composition of all the smaller parts:

$$K(\mathbf{r}, \mathbf{r}', t) = \int d\mathbf{r}_1 \dots \int d\mathbf{r}_{N-1} K(\mathbf{r}_N = \mathbf{r}, \mathbf{r}_{N-1}, \delta t) \dots K(\mathbf{r}_2, \mathbf{r}_1, \delta t) \\ \times K(\mathbf{r}_1, \mathbf{r}_0 = \mathbf{r}', \delta t) \quad (1.59)$$

$$\xrightarrow{N \rightarrow +\infty} \int d\mathbf{r}_1 \dots \int d\mathbf{r}_{N-1} \prod_{j=1}^N \left(\frac{m}{2\pi i \hbar \delta t}\right)^{\frac{L}{2}} \exp\left(\frac{i\delta t}{\hbar} \mathcal{L}\left(\mathbf{r}_{j-1}, \frac{\mathbf{r}_j - \mathbf{r}_{j-1}}{\delta t}\right)\right) \quad (1.60)$$

$$= \left(\frac{m}{2\pi i \hbar \delta t}\right)^{\frac{NL}{2}} \int d\mathbf{r}_1 \dots \int d\mathbf{r}_{N-1} \exp\left(\frac{i\delta t}{\hbar} \sum_{j=1}^N \mathcal{L}\left(\mathbf{r}_{j-1}, \frac{\mathbf{r}_j - \mathbf{r}_{j-1}}{\delta t}\right)\right). \quad (1.61)$$

In other words, this last equation means that the propagator is written as an integral over all classical and non-classical paths that link $\mathbf{r}'$ and $\mathbf{r}$ in time t . A more compact way to write it is

$$K(\mathbf{r}, \mathbf{r}', t) = \int \mathcal{D}(\mathbf{q}) \exp\left(\frac{i}{\hbar} \int_0^t \mathcal{L}(\mathbf{q}(t'), \dot{\mathbf{q}}(t')) dt'\right), \quad (1.62)$$

where $\mathbf{q} : [0, t] \rightarrow \mathbb{R}^L$ denotes a (non-)classical path that links $\mathbf{q}(0) = \mathbf{r}'$ to $\mathbf{q}(t) = \mathbf{r}$ and $\int \mathcal{D}(\mathbf{q})$ denotes the integral over all of those.

1.3.2 Semiclassical physics and the van Vleck-Gutzwiller propagator

In order to obtain the van Vleck-Gutzwiller propagator, also known as the semiclassical propagator, one has to resort to the stationary phase, or saddle point, approximation.

Let us consider a simple case. Let g be a real, well-behaved function, and f an integrable function. We define the integral

$$\int_a^b g(x) e^{\frac{i}{\hbar} f(x)} dx. \quad (1.63)$$

The dominant contributions originate from points where the first derivative of f vanishes, i.e., for x_j such that $\partial_x f(x_j) = 0$. Expanding f around such point yields

$$f(x) = f(x_j) + \partial_x^2 f(x_j) \frac{(x - x_j)^2}{2} + \mathcal{O}((x - x_j)^3). \quad (1.64)$$

There are as many such contributions to (1.63) as there are such stationary points:

$$\int_a^b g(x) e^{\frac{i}{\hbar} f(x)} dx \xrightarrow{\hbar \rightarrow 0} \sum_j g(x_j) e^{\frac{i}{\hbar} f(x_j)} \sqrt{\frac{2\pi\hbar}{|\partial_x^2 f(x_j)|}} e^{\frac{i\pi}{4} \alpha_j} + \mathcal{O}(\hbar), \quad (1.65)$$

with $\alpha_j = \text{sgn}(\partial_x^2 f(x_j))$, keeping only the 0th order in $(x - x_j)$ after expanding g around the saddle points x_j and where we used (1.50). This saddle point approximation can easily be generalised to L dimensions:

$$\int g(\mathbf{x}) e^{\frac{i}{\hbar} f(\mathbf{x})} d\mathbf{x} \xrightarrow{\hbar \rightarrow 0} \sum_j g(\mathbf{x}_j) e^{\frac{i}{\hbar} f(\mathbf{x}_j)} \sqrt{\frac{2\pi\hbar}{\left| \det \frac{\partial^2 f(\mathbf{x}_j)}{\partial x_m \partial x_n} \right|}} e^{\frac{i\pi}{4} \alpha_j} + \mathcal{O}(\hbar), \quad (1.66)$$

with $\alpha_j = \sum_{l=1}^L \text{sgn}(\lambda_l^{(j)})$, and where $\lambda_l^{(j)}$ are the eigenvalues of the matrix $\left(\det \frac{\partial f(x_j)}{\partial x_m \partial x_n}\right)_{L \times L}$. We now want to apply this saddle-point approximation to the Feynman propagator (1.61). As we use the limit $N \rightarrow +\infty$, the argument of the exponential can be rewritten as a continuous sum, i.e., an integral:

$$\frac{i\delta t}{\hbar} \sum_{j=1}^N \mathcal{L}\left(\mathbf{r}_{j-1}, \frac{\mathbf{r}_j - \mathbf{r}_{j-1}}{\delta t}\right) \rightarrow \int_0^t \mathcal{L}(\mathbf{q}(t'), \dot{\mathbf{q}}(t')) dt'. \quad (1.67)$$

Finding extremal points of the phase means looking for trajectories that satisfy

$$\frac{\delta}{\delta \mathbf{q}(t)} \int_0^t \mathcal{L}(\mathbf{q}(t'), \dot{\mathbf{q}}(t')) dt' = 0, \quad (1.68)$$

which is equivalent to the Euler-Lagrange equation of classical mechanics. This result is of utmost importance as it highlights a key point of semiclassical physics: in the semiclassical limit, the main contribution to the propagator originate from classical trajectories with the boundary conditions $\mathbf{q}(0) = \mathbf{r}'$ and $\mathbf{q}(t) = \mathbf{r}$, i.e., the trajectories that link $\mathbf{r}'$ and $\mathbf{r}$ in time t .

Expanding the phase of (1.61) around those trajectories yields the semiclassical, or van Vleck-Gutzwiller, propagator, which is expressed as a coherent sum over all classical paths:

$$K(\mathbf{q}^f, \mathbf{q}^i, t) \equiv \langle \mathbf{q}^f | \hat{U}(t) | \mathbf{q}^i \rangle \simeq \sum_{\gamma: \mathbf{q}^i \rightarrow \mathbf{q}^f} A_\gamma(\mathbf{q}^f, \mathbf{q}^i, t) e^{iR_\gamma(\mathbf{q}^f, \mathbf{q}^i, t)/\hbar}, \quad (1.69)$$

with

$$A_\gamma(\mathbf{q}^f, \mathbf{q}^i, t) = \frac{1}{(2\pi\hbar)^{L/2}} \left| \det \frac{\partial^2 R_\gamma}{\partial \mathbf{q}^f \partial \mathbf{q}^i}(\mathbf{q}^f, \mathbf{q}^i, t) \right|^{1/2} e^{-i\mu_\gamma \pi/4}, \quad (1.70)$$

$$R_\gamma(\mathbf{q}^f, \mathbf{q}^i, t) = \int_0^t dt' (\mathbf{p}_\gamma(t') \cdot \dot{\mathbf{q}}_\gamma(t') - H_{cl}(\mathbf{q}_\gamma(t'), \mathbf{p}_\gamma(t'))), \quad (1.71)$$

respectively the amplitude of the propagator and the action of the trajectory, with μ_γ is the Morse index related to the trajectory γ [74, 81], and $H_{cl}(\mathbf{q}, \mathbf{p}) \equiv (\hat{H})_W(\mathbf{q}, \mathbf{p})$. It is important to highlight that this approximation preserves the coherent aspect of quantum mechanics [25, 26, 82]. Details on this derivation can be found in Section 4.3.2 of [9] and the particular details of the determination of the amplitudes in (1.69) can be found in Section 10.2 of [21].

1.3.3 Mean-field approximation: the Gross-Pitaevskii equation

Let us consider the general case of a Bose-Einstein condensate trapped in a potential $V(\mathbf{r}, t)$ and where the bosons of mass m interact with each other according to a two-body interaction potential $U(|\mathbf{r} - \mathbf{r}'|)$. The many-body Hamiltonian dictating the dynamics of the system is

$$\begin{aligned} \hat{H} = & \int \hat{\psi}^\dagger(\mathbf{r}, t) \left(\frac{\hbar^2}{2m} \Delta + V(\mathbf{r}, t) \right) \hat{\psi}(\mathbf{r}, t) \\ & + \frac{1}{2} \int \int \hat{\psi}^\dagger(\mathbf{r}, t) \hat{\psi}^\dagger(\mathbf{r}', t) U(|\mathbf{r} - \mathbf{r}'|) \hat{\psi}(\mathbf{r}, t) \hat{\psi}(\mathbf{r}', t) d\mathbf{r} d\mathbf{r}', \end{aligned} \quad (1.72)$$

where $\hat{\psi}(\mathbf{r}, t)$ and $\hat{\psi}^\dagger(\mathbf{r}, t)$ are the annihilation and creation field operators that remove or add a particle at position $\mathbf{r}$ and time t . As they belong to the class of bosonic operators, they obey a bosonic algebra that reads

$$[\hat{\psi}(\mathbf{r}, t), \hat{\psi}^\dagger(\mathbf{r}', t)] = \delta(\mathbf{r} - \mathbf{r}'), \quad (1.73)$$

$$[\hat{\psi}(\mathbf{r}, t), \hat{\psi}(\mathbf{r}', t)] = 0, \quad (1.74)$$

$$[\hat{\psi}^\dagger(\mathbf{r}, t), \hat{\psi}^\dagger(\mathbf{r}', t)] = 0. \quad (1.75)$$

The field operators are defined as

$$\hat{\psi}(\mathbf{r}) = \sum_{k=0}^{\infty} \langle \mathbf{r} | \varphi_k \rangle \hat{a}_k, \quad (1.76)$$

$$\hat{\psi}^\dagger(\mathbf{r}) = \sum_{k=0}^{\infty} \langle \mathbf{r} | \varphi_k \rangle^* \hat{a}_k^\dagger, \quad (1.77)$$

with $\{|\varphi_k\rangle, k \in \mathbb{N}\}$ the basis of single-particle states, and $\hat{a}_k, \hat{a}_k^\dagger$ the annihilation and creation operators respectively. Those are defined by their action on Fock states by

$$\hat{a}_k |n_0, \dots, n_k, \dots\rangle = \sqrt{n_k} |n_0, \dots, n_k - 1, \dots\rangle, \quad (1.78)$$

$$\hat{a}_k^\dagger |n_0, \dots, n_k, \dots\rangle = \sqrt{n_k + 1} |n_0, \dots, n_k + 1, \dots\rangle \quad (1.79)$$

with n_k the occupation of the k^{th} mode, defined as the eigenvalue of the population operator $\hat{n}_k = \hat{a}_k^\dagger \hat{a}_k$ [60, 73, 83, 84]. The total population operator is defined as

$$\hat{N} = \sum_k \hat{a}_k^\dagger \hat{a}_k. \quad (1.80)$$

The creation and annihilation operators obey the commutation rules

$$[\hat{a}_k, \hat{a}_{k'}^\dagger] = \delta_{kk'}, \quad (1.81)$$

$$[\hat{a}_k, \hat{a}_{k'}] = 0, \quad (1.82)$$

$$[\hat{a}_k^\dagger, \hat{a}_{k'}^\dagger] = 0. \quad (1.83)$$

It can be noted that one can express a Fock state as a vacuum state $|0, 0, \dots\rangle$ on which successive creation operators have been applied:

$$|n_0, n_1, \dots\rangle = \prod_k \frac{(a_k^\dagger)^{n_k}}{\sqrt{n_k!}} |0, 0, \dots\rangle. \quad (1.84)$$

We can introduce the quadrature operators $\hat{q}_k$ and $\hat{p}_k$ [25, 73] with the relations:

$$\hat{q}_k = \sqrt{\frac{\hbar_{\text{eff}}}{2}} (\hat{a}_k^\dagger + \hat{a}_k) = \frac{1}{\sqrt{2N}} (\hat{a}_k^\dagger + \hat{a}_k), \quad (1.85)$$

$$\hat{p}_k = i\sqrt{\frac{\hbar_{\text{eff}}}{2}} (\hat{a}_k^\dagger - \hat{a}_k) = \frac{i}{\sqrt{2N}} (\hat{a}_k^\dagger - \hat{a}_k), \quad (1.86)$$

where $\hbar_{\text{eff}}$ plays the role of a Planck constant. It is identified with $1/N$, with N the total population of the system, and $\hbar_{\text{eff}} \rightarrow 0$ indicates the classical limit [26]. They are linked to occupation operators through

$$\frac{1}{N} \left(\hat{n}_k + \frac{1}{2} \right) = \frac{\hat{q}_k^2 + \hat{p}_k^2}{2}. \quad (1.87)$$

The conditions to go further are the following. One must consider a low enough temperature so that there is only s -wave scattering between particles, and the dilute limit, where the typical interaction length is much lower than the distance between particles. As the interaction process between bosons can be approximated by a s -wave scattering, i.e., a hard-sphere model, the exact van der Waals interaction potential U can be replaced by $g\delta(\mathbf{r} - \mathbf{r}')$ with $g = 4\pi\hbar^2 a/m$ with a the s -wave scattering length [17, 50, 60]. The Hamiltonian (1.72) can be replaced by

$$\begin{aligned} \hat{H} = & \int \hat{\psi}^\dagger(\mathbf{r}, t) \left(\frac{\hbar^2}{2m} \Delta + V(\mathbf{r}, t) \right) \hat{\psi}(\mathbf{r}, t) \\ & + \frac{g}{2} \int \hat{\psi}^\dagger(\mathbf{r}', t) \hat{\psi}^\dagger(\mathbf{r}', t) \hat{\psi}(\mathbf{r}', t) \hat{\psi}(\mathbf{r}', t) d\mathbf{r}'. \end{aligned} \quad (1.88)$$

The time-evolution equation of the field operator is given by the Heisenberg equation

$$i\hbar \frac{\partial}{\partial t} \hat{\psi}(\mathbf{r}, t) = [\hat{\psi}(\mathbf{r}, t), \hat{H}] \quad (1.89)$$

$$\Leftrightarrow i\hbar \frac{\partial}{\partial t} \hat{\psi}(\mathbf{r}, t) = \left(-\frac{\hbar^2}{2m} \Delta + V(\mathbf{r}, t) + g \left| \hat{\psi}(\mathbf{r}, t) \right|^2 \right) \hat{\psi}(\mathbf{r}, t), \quad (1.90)$$

by using the commutation relations (1.73) and the notation $\left| \hat{\psi}(\mathbf{r}, t) \right|^2 = \hat{\psi}^\dagger \hat{\psi}$ [60].

From this point, in the limit of large populations, often written $1/N \rightarrow 0$ while keeping the typical interaction energy much lower than the kinetic one, the dynamics can be described using the mean-field equations. This amounts to replacing the field operator by a classical field. The approximation is justified because in those conditions, most of the bosons are in the same quantum state: the ground state of a Bose-Einstein condensate [50]. One can write $N = N_0 + \delta N$, with N_0 the number of particles in the ground state, and δN the population of the excited states, such that $\delta N \ll N_0$. This allows us to consider $N \simeq N_0$.

The first step consists thus in separating the ground-state from the excited-state contribution in equation (1.76):

$$\hat{\psi}(\mathbf{r}, t) = \varphi_0(\mathbf{r}, t) \hat{a}_0 + \sum_{k=1}^{\infty} \varphi_k(\mathbf{r}, t) \hat{a}_k, \quad (1.91)$$

with $\langle \mathbf{r} | \varphi_k \rangle = \varphi_k(\mathbf{r}, t)$. Because the ground state is dominantly populated, the contributions from the excited states can be treated as a perturbation that is neglected. This amounts to do the replacement $\hat{\psi}(\mathbf{r}, t) \rightarrow \varphi_0(\mathbf{r}, t) \hat{a}_0$. As the goal is to replace operators by complex numbers, neglecting the perturbation is not enough. Looking at the expectation value of operators associated to the ground state that would originate from (1.89), one has

$$\langle \varphi_0 | \hat{a}_0^\dagger \hat{a}_0 | \varphi_0 \rangle = N, \quad (1.92)$$

$$\langle \varphi_0 | \hat{a}_0^\dagger \hat{a}_0 \hat{a}_0^\dagger \hat{a}_0 | \varphi_0 \rangle = N^2, \quad (1.93)$$

which allows to conclude that the operators $\hat{a}_0$ and $\hat{a}_0^\dagger$ can be replaced by the complex number $\sqrt{N}$. Another way to see it is from equations (1.78) and (1.79). The annihilation and creation operators introduce respectively the prefactors $\sqrt{N}$ and $\sqrt{N+1}$, which can be considered to

both be $\sqrt{N}$ in the limit of large populations. The replacement $\hat{\psi}(\mathbf{r}, t) \rightarrow \sqrt{N}\varphi_0(\mathbf{r}, t) \equiv \psi(\mathbf{r}, t)$ leads to the well-known Gross-Pitaevskii equation:

$$i\hbar \frac{\partial}{\partial t} \psi(\mathbf{r}, t) = \left(-\frac{\hbar^2}{2m} \Delta + V(\mathbf{r}, t) + g|\psi(\mathbf{r}, t)|^2 \right) \psi(\mathbf{r}, t). \quad (1.94)$$

Due to its form, it is often referred to as a non-linear Schrödinger equation, owing to the additional term $g|\psi(\mathbf{r}, t)|^2\psi(\mathbf{r}, t)$.

This equation is a good approximation when the s -wave scattering length is much smaller than the average distance between the atoms of the system and when the number of atoms is much larger than 1. This is the case, for instance, at very low temperatures in the context of Bose-Einstein condensates. The mean field approximation has many times proved to be a very efficient method to study such objects [60].

1.3.4 Wigner-Weyl formalism

Quantum mechanics is usually introduced in terms of operators belonging to Hilbert spaces. Nonetheless, one can exactly reformulate it in terms of smooth functions living in phase space using the so-called Wigner-Weyl formalism [65, 85, 86]. It presents the advantages of being more intuitive as well as easier to deal with in the context of this work.

In the Wigner-Weyl formalism, operators are represented by Weyl symbols. For any operator $\hat{A}$, one defines its Weyl symbol as

$$A(\mathbf{q}, \mathbf{p}) \equiv (\hat{A})_W(\mathbf{q}, \mathbf{p}) = \int d\xi \left\langle \mathbf{q} - \frac{\xi}{2} \left| \hat{A} \right| \mathbf{q} + \frac{\xi}{2} \right\rangle e^{i\mathbf{p} \cdot \xi / \hbar}, \quad (1.95)$$

with $\mathbf{q} = (q_1, \dots, q_L)$, $\xi = (\xi_1, \dots, \xi_L)$ position vectors and $\mathbf{p} = (p_1, \dots, p_L)$ a momentum vector, with L the number of degrees of freedom. A state $|\psi\rangle$ is represented by the Wigner function, or quasidistribution, defined by the Weyl symbol associated with the density operator of the system, up to a global prefactor:

$$W(\mathbf{q}, \mathbf{p}) \equiv \frac{1}{(2\pi\hbar)^L} \int d\xi \left\langle \mathbf{q} - \frac{\xi}{2} \left| \psi \right\rangle \left\langle \psi \right| \mathbf{q} + \frac{\xi}{2} \right\rangle e^{i\mathbf{p} \cdot \xi / \hbar} \quad (1.96)$$

$$= \frac{1}{(2\pi\hbar)^L} \int d\xi \psi^* \left(\mathbf{q} + \frac{\xi}{2} \right) \psi \left(\mathbf{q} - \frac{\xi}{2} \right) e^{i\mathbf{p} \cdot \xi / \hbar}. \quad (1.97)$$

The designation “quasidistribution” stems from the fact that it is normalised such that

$$\int d\mathbf{q} d\mathbf{p} W(\mathbf{q}, \mathbf{p}) = 1 \quad (1.98)$$

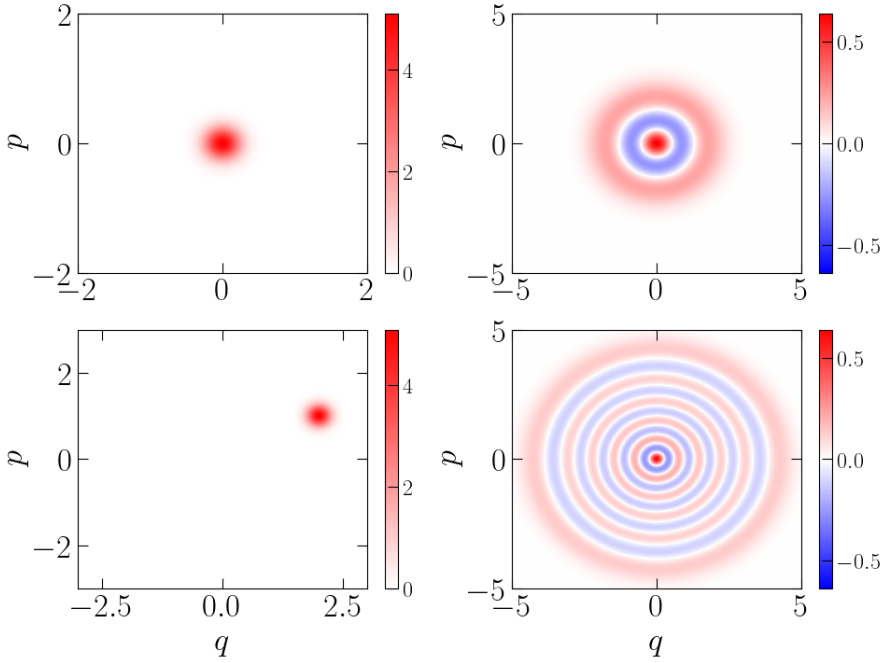


Figure 1.2: Gallery of Wigner functions. The left column shows Wigner functions of coherent states, centred on $(0, 0)$ (top), which corresponds to a vacuum state, and $(2, 1)$ (bottom), with $\hbar$ set to 2^{-4} . The right column shows Wigner functions of Fock states for $N = 2$ (top) and $N = 5$ (bottom) particles.

but not necessarily positive. As a sidenote, the negative regions can be interpreted as an indicator of quantumness, or non-classicality [87–89]. Taking the classical limit $\hbar \rightarrow 0$ erases those negative regions, further corroborating that fact. This is also why coherent states, that will be introduced hereafter, are labelled *classical states*: they are the only states whose Wigner function is always positive [88, 90].

Let us take this opportunity to present a gallery of Wigner functions, which allows us at the same time to introduce two types of states that will be used in this manuscript: coherent states and Fock states. The former are ideal states for investigating the quantum-classical correspondence, because they minimise the Heisenberg uncertainty relation, and have already proven to be experimentally relevant, since they describe accurately a Bose-Einstein condensate [50, 91–93]. Moreover, their Wigner

function W_{CS} is a Gaussian, which is positive everywhere, and thus can be considered to be a probability distribution. Its expression is [94]

$$W_{CS}(\mathbf{q}, \mathbf{p}) = \prod_{l=1}^L \frac{1}{\pi \hbar} e^{-2(q_l - \varepsilon_q \alpha_{R,l})^2 / \varepsilon_q^2} e^{-2(p_l - \varepsilon_p \alpha_{I,l})^2 / \varepsilon_p^2}, \quad (1.99)$$

where the coherent state is defined by complex numbers $(\alpha_{R,1} + i\alpha_{I,1}, \dots, \alpha_{R,L} + i\alpha_{I,L})$, and $\varepsilon_q, \varepsilon_p$ depends on experimental parameters [94]. In the left column of Figure 1.2, we show the Wigner function for two coherent states, the first one centred on $(0, 0)$ and corresponding to a vacuum state, and the second one centred on $(2, 1)$.

However, these states are not the ones that naturally emerge when working within the framework of second quantisation. Those are Fock states, or number states, which were already mentioned above when introducing the creation and annihilation operators. Incidentally, they coincide with states obtained when the parameters of the studied system correspond to a regime yielding Mott insulators, for instance in the low-hopping limit of the Bose-Hubbard model [95]. Their Wigner function contains negativities, which bear no classical meaning, but these can be considered to be strictly quantum as they disappear when looking at the classical limit [87, 88]. The Wigner quasidistribution of a Fock state W_{Fock} is given by [94]

$$W_{\text{Fock}}(\mathbf{q}, \mathbf{p}) = \prod_{l=1}^L \frac{4}{\pi} (-1)^{n_l} e^{-|q_l^2 + p_l^2|} L_{n_l}(2|q_l^2 + p_l^2|), \quad (1.100)$$

with n_l the occupation of site l and L_n the n^{th} Laguerre polynomial. In the large occupation limit, it can be approximated by a Dirac delta on the occupation level. We will later consider it to be the classical limit, as all negativities disappear that way:

$$W_{\text{Fock,cl}}(\mathbf{q}, \mathbf{p}) = \prod_{l=1}^L \frac{1}{2\pi} \delta\left(\frac{q_l^2 + p_l^2 - 1}{2} - n_l\right). \quad (1.101)$$

We represent the Wigner function of the Fock states corresponding to 2 and 5 particles on respectively the first and second line of the second column of Figure 1.2. Now that the states that we will use are introduced, let us go back to our presentation of the Wigner-Weyl formalism.

Using this formalism, the expectation value of observable $\hat{A}$ can be written exactly:

$$\langle \hat{A} \rangle = \int d\mathbf{q} d\mathbf{p} A(\mathbf{q}, \mathbf{p}) W(\mathbf{q}, \mathbf{p}). \quad (1.102)$$

As the goal is to compute the Weyl symbol of a commutator, it is necessary to introduce the Weyl symbol of a product of operators. It is given by the Moyal product

$$(\hat{A}\hat{B})_W(\mathbf{q}, \mathbf{p}) = A(\mathbf{q}, \mathbf{p}) \exp \left(i\hbar \sum_l^L \left(\overleftarrow{\partial}_{q_l} \overrightarrow{\partial}_{p_l} - \overleftarrow{\partial}_{p_l} \overrightarrow{\partial}_{q_l} \right) / 2 \right) B(\mathbf{q}, \mathbf{p}), \quad (1.103)$$

where the arrows indicate the side on which the derivative operators are applied [65]. It follows that the symbol of a commutator is

$$[\hat{A}, \hat{B}]_W(\mathbf{q}, \mathbf{p}) = 2A(\mathbf{q}, \mathbf{p}) \sin \left(\frac{\hbar}{2} \sum_l^L \overleftarrow{\partial}_{q_l} \overrightarrow{\partial}_{p_l} - \overleftarrow{\partial}_{p_l} \overrightarrow{\partial}_{q_l} \right) B(\mathbf{q}, \mathbf{p}). \quad (1.104)$$

where $[\cdot, \cdot]_W$, sometimes written $\{\{\cdot, \cdot\}\}$, is called the Moyal bracket. As it will be relevant later, it is important to note that, when performing an expansion in powers of $\hbar$, the dominant contribution to the Moyal bracket is a Poisson bracket:

$$[\hat{A}, \hat{B}]_W(\mathbf{q}, \mathbf{p}) = i\hbar \{A(\mathbf{q}, \mathbf{p}), B(\mathbf{q}, \mathbf{p})\} + \mathcal{O}(\hbar)^2. \quad (1.105)$$

Finally, let us focus on the particular case of a time-evolved operator, as this will be at the centre of this thesis. The evolution of $\hat{A}$ is given, in the Heisenberg picture, by

$$\frac{d}{dt} \hat{A}(t) = \frac{i}{\hbar} [\hat{H}, \hat{A}(t)] + \left(\frac{\partial}{\partial t} \hat{A} \right) (t), \quad (1.106)$$

where the last term is the partial derivative of $\hat{A}$ (in the Schrödinger picture) evolved for a time t in the Heisenberg picture. Taking the leading order of the Wigner-Weyl transform of the equation yields

$$\frac{d}{dt} A_W(\mathbf{q}, \mathbf{p}, t) = \{A_W(\mathbf{q}, \mathbf{p}, t), H(\mathbf{q}, \mathbf{p})\} + \frac{\partial}{\partial t} A_W(\mathbf{q}, \mathbf{p}) + \mathcal{O}(\hbar). \quad (1.107)$$

Neglecting the contribution in $\hbar$ means that (1.107) has the same form as the classical equation of motion for a phase-space quantity that we can label $A(\mathbf{q}^f(\mathbf{q}, \mathbf{p}, t), \mathbf{p}^f(\mathbf{q}, \mathbf{p}, t), t)$ where $\mathbf{q}^f(\mathbf{q}, \mathbf{p}, t)$ and $\mathbf{p}^f(\mathbf{q}, \mathbf{p}, t)$ are the position and momentum evolved for a time t according to the classical equations of motion³ for the initial conditions $(\mathbf{q}, \mathbf{p})$. Choosing the initial conditions for the function A as $A(\mathbf{q}, \mathbf{p}, 0) = A_W(\mathbf{q}, \mathbf{p}, 0)$, we can write

$$A_W(\mathbf{q}, \mathbf{p}, t) = A(\mathbf{q}^f(\mathbf{q}, \mathbf{p}, t), \mathbf{p}^f(\mathbf{q}, \mathbf{p}, t), t) + \mathcal{O}(\hbar). \quad (1.108)$$

In other words, in leading order, the Weyl symbol of the time-evolved operator $\hat{A}(t)$ is given by the Weyl symbol of the unevaluated operator $\hat{A}$ evaluated at the classically-time-evolved coordinates $\mathbf{q}^f(\mathbf{q}, \mathbf{p}, t)$ and $\mathbf{p}^f(\mathbf{q}, \mathbf{p}, t)$ [73]. For this reason, in the following, we refer to the truncated Wigner approximation that will be explained hereafter as a form of classical, or more precisely quasiclassical, approximation, bearing in mind that some aspects of quantum mechanics are still considered by sampling the initial wave packet. The short-time correspondence between the quantum and classical expectation value is often called the “quantum-classical correspondence”. This agreement is, of course, not eternal. The breakdown of the correspondence occurs at the so-called Ehrenfest time. It can be seen as the time at which quantum effects become nonnegligible [41].

1.3.5 *Truncated Wigner and diagonal approximation*

Similarly to the evolution of a symbol, one can derive the evolution equation of the Wigner function. In the classical limit, this equation can be approximated and yield the so-called truncated Wigner method, or approximation [62, 63].

The original way it has been introduced is the following. Considering the general case of mixed states, one can introduce a more general definition of the Wigner-Weyl formalism, and thus of the Wigner function. The evolution equation of the latter is obtained by taking the Wigner-Weyl transform of the von Neumann equation, which dictates how the density matrix representing the state evolves. The resulting partial differential equation proves to be very hard to solve. Nonetheless, in the limit of large occupation, i.e., $1/N \rightarrow 0$, one can safely neglect the highest-order

³ The Hamiltonian used for those classical equation is the Weyl symbol of the quantum Hamiltonian where $\hbar$ contributions have been neglected. Mathematically, it means doing the replacement $\hat{\mathbf{q}} \rightarrow \mathbf{q}$ and $\hat{\mathbf{p}} \rightarrow \mathbf{p}$

derivatives (here, third-order ones). Doing so amounts to neglecting the quantum noise in the time-evolution [62] and turns the equation into a Fokker-Planck equation which can, in turn, be mapped to a set of coupled Langevin equations that correspond to classical equations of motion following Hamiltonian formalism. This allows one to express the expectation value of a time-evolved observable as a phase-space average of the time-evolved symbol (1.108) weighted by the unevolved Wigner function, i.e.,

$$\langle \hat{A}(t) \rangle \simeq \int d\mathbf{q}d\mathbf{p} A(\mathbf{q}^f(\mathbf{q}, \mathbf{p}, t), \mathbf{p}^f(\mathbf{q}, \mathbf{p}, t), t) W(\mathbf{q}, \mathbf{p}). \quad (1.109)$$

Let us note that while neglecting the third-order derivatives means getting rid of some noise, all the quantum aspects are not removed. The Wigner function of the initial state still contains quantum noise, as it takes into account the uncertainty principle. This translates to the function being a quasidistribution and not simply a point. More details can be found in [17, 62, 73, 96].

In this thesis, we will not follow this path. Rather, we establish equation (1.109) using what is called the *diagonal approximation*, which is introduced in the context of the semiclassical formulation of the Feynman path integral.

Let us consider again the expectation value of a time-evolved observable $\hat{A}$ for an initial state $|\psi\rangle$ and formulate it using the Wigner-Weyl formalism:

$$\langle \hat{A}(t) \rangle = \langle \psi | \hat{U}^\dagger(t) \hat{A} \hat{U}(t) | \psi \rangle \quad (1.110)$$

$$= \int d\mathbf{x}_1 d\mathbf{x}_2 d\mathbf{y}_1 d\mathbf{y}_2 \langle \psi | \mathbf{x}_1 \rangle \langle \mathbf{x}_1 | \hat{U}^\dagger(t) | \mathbf{y}_1 \rangle \langle \mathbf{y}_1 | \hat{A} | \mathbf{y}_2 \rangle \\ \times \langle \mathbf{y}_2 | \hat{U}(t) | \mathbf{x}_2 \rangle \langle \mathbf{x}_2 | \psi \rangle \quad (1.111)$$

$$= \int d\mathbf{x}_1 d\mathbf{x}_2 d\mathbf{y}_1 d\mathbf{y}_2 d\mathbf{p} \psi^*(\mathbf{x}_1) K^*(\mathbf{y}_1, \mathbf{x}_1, t) A\left(\frac{\mathbf{y}_1 + \mathbf{y}_2}{2}, \mathbf{p}\right) \\ \times e^{\frac{i}{\hbar} \mathbf{p} \cdot (\mathbf{y}_1 - \mathbf{y}_2)} K(\mathbf{y}_2, \mathbf{x}_2, t) \psi(\mathbf{x}_2), \quad (1.112)$$

using

$$\langle \mathbf{y}_1 | \hat{A} | \mathbf{y}_2 \rangle = \int \frac{d\mathbf{p}}{(2\pi\hbar)^L} A\left(\frac{\mathbf{y}_1 + \mathbf{y}_2}{2}, \mathbf{p}\right) e^{i\mathbf{p} \cdot (\mathbf{x}_1 - \mathbf{x}_2)/\hbar}, \quad (1.113)$$

derived from equation (1.95) and the definition of the propagator $K(\mathbf{x}_2, \mathbf{x}_1, t) = \langle \mathbf{x}_2 | \hat{U}(t) | \mathbf{x}_1 \rangle$.

Using then the semiclassical approximation of the propagator (1.69), one obtains

$$\begin{aligned} \langle \hat{A}(t) \rangle^{sc} = & \int d\mathbf{x}_1 d\mathbf{x}_2 d\mathbf{y}_1 d\mathbf{y}_2 d\mathbf{p} \sum_{\substack{\alpha: \mathbf{x}_1 \rightarrow \mathbf{y}_1 \\ \beta: \mathbf{x}_2 \rightarrow \mathbf{y}_2}} \psi^*(\mathbf{x}_1) \psi(\mathbf{x}_2) A_\alpha^*(\mathbf{y}_1, \mathbf{x}_1, t) \\ & \times A_\beta(\mathbf{y}_2, \mathbf{x}_2, t) A\left(\frac{\mathbf{y}_1 + \mathbf{y}_2}{2}, \mathbf{p}_1\right) e^{\frac{i}{\hbar}(-R_\alpha(\mathbf{y}_1, \mathbf{x}_1) + R_\beta(\mathbf{y}_1, \mathbf{x}_1) + \mathbf{p} \cdot (\mathbf{y}_1 - \mathbf{y}_2))}. \end{aligned} \quad (1.114)$$

At this point, the expression is semiclassical. The stationary-phase approximation has been made, but interference is still taken into account. To extract the dominant contribution from the last equation, we exploit the following. The two-fold sum runs over all classical paths that link $\mathbf{x}_1$ to $\mathbf{y}_1$ and $\mathbf{x}_2$ to $\mathbf{y}_2$. We call the ensemble of those paths families and label the paths belonging to each family α and β respectively. Two trajectories are said to belong to the same family if, upon continuous and smooth transformation of the initial and final coordinates of one trajectory to match those of the other, both trajectories become identical. In general, the actions of two trajectories belonging to two different families are uncorrelated. Since the difference of those actions appears in a complex exponential, most semiclassical contributions to $\langle \hat{A}(t) \rangle$ are highly oscillating terms that average out. The dominant contributions are given by pairs of trajectories that are correlated in action. In other words, the non-vanishing contributions are given by $\alpha \sim \beta$. Restricting the sum to this is called the *diagonal approximation*. Doing so gets rid of interference, and the expression is now quasiclassical⁴.

As the trajectories are now correlated, they can be developed around a central one. Doing a change of variables to centre-and-relative coordinates

$$\begin{aligned} \mathbf{x}_1 &= \mathbf{X} + \frac{\mathbf{x}}{2}, & \mathbf{y}_1 &= \mathbf{Y} + \frac{\mathbf{y}}{2}, \\ \mathbf{x}_2 &= \mathbf{X} - \frac{\mathbf{x}}{2}, & \mathbf{y}_2 &= \mathbf{Y} - \frac{\mathbf{y}}{2}, \end{aligned} \quad (1.115)$$

yields

$$\begin{aligned} \langle \hat{A}(t) \rangle^{qcl} = & \int d\mathbf{x}_1 d\mathbf{x}_2 d\mathbf{y}_1 d\mathbf{y}_2 d\mathbf{p} \sum_{\alpha} \psi^*(\mathbf{X} + \frac{\mathbf{x}}{2}) \psi(\mathbf{X} - \frac{\mathbf{x}}{2}) \\ & \times |A_\alpha(\mathbf{Y}, \mathbf{X}, t)|^2 A(\mathbf{Y}, \mathbf{p}) e^{\frac{i}{\hbar}(-R_\alpha(\mathbf{Y} - \frac{\mathbf{y}}{2}, \mathbf{Y} - \frac{\mathbf{y}}{2}) + R_\alpha(\mathbf{Y} + \frac{\mathbf{y}}{2}, \mathbf{X} + \frac{\mathbf{x}}{2}) + \mathbf{p} \cdot \mathbf{y})}, \end{aligned} \quad (1.116)$$

⁴ The expression is sometimes said to be classical due to the absence of interference, but it is important to keep in mind that it is still a wavefunction that is studied.

where only the dominant order for the amplitudes of the propagators is kept. Expanding now the actions

$$R_\alpha(\mathbf{Y} + \frac{\mathbf{y}}{2}, \mathbf{X} + \frac{\mathbf{x}}{2}) \simeq R_\alpha(\mathbf{Y}, \mathbf{X}) + \frac{\partial R_\alpha}{\partial \mathbf{Y}}(\mathbf{Y}, \mathbf{X}) \frac{\mathbf{y}}{2} + \frac{\partial R_\alpha}{\partial \mathbf{X}}(\mathbf{Y}, \mathbf{X}) \frac{\mathbf{x}}{2} \quad (1.117)$$

$$\simeq R_\alpha(\mathbf{Y}, \mathbf{X}) + \mathbf{p}_\alpha^f(\mathbf{Y}, \mathbf{X}) \cdot \frac{\mathbf{y}}{2} - \mathbf{p}_\alpha^i(\mathbf{Y}, \mathbf{X}) \cdot \frac{\mathbf{x}}{2}, \quad (1.118)$$

where we used $\partial R_\alpha / \partial \mathbf{Y}(\mathbf{Y}, \mathbf{X}) = \mathbf{p}_\alpha^f(\mathbf{Y}, \mathbf{X})$ and $\partial R_\alpha / \partial \mathbf{X}(\mathbf{Y}, \mathbf{X}) = -\mathbf{p}_\alpha^i(\mathbf{Y}, \mathbf{X})$, allows to write

$$\begin{aligned} \langle \hat{A}(t) \rangle^{\text{qcl}} &= \int d\mathbf{X} d\mathbf{x} d\mathbf{Y} d\mathbf{y} d\mathbf{p} \sum_\alpha \psi^*(\mathbf{X} + \frac{\mathbf{x}}{2}) \psi(\mathbf{X} - \frac{\mathbf{x}}{2}) |A_\alpha(\mathbf{Y}, \mathbf{X}, t)|^2 \\ &\quad \times A(\mathbf{Y}, \mathbf{p}) e^{\frac{i}{\hbar}((\mathbf{p}-\mathbf{p})_\alpha^f(\mathbf{Y}, \mathbf{X}) \cdot \mathbf{y} + \mathbf{p}_\alpha^i(\mathbf{Y}, \mathbf{X}) \cdot \mathbf{x})} \end{aligned} \quad (1.119)$$

$$\begin{aligned} &= \int d\mathbf{X} d\mathbf{Y} \sum_\alpha W(\mathbf{X}, \mathbf{p}_\alpha^i(\mathbf{Y}, \mathbf{X})) \\ &\quad \times |A_\alpha(\mathbf{Y}, \mathbf{X}, t)|^2 A(\mathbf{Y}, \mathbf{p}_\alpha^f(\mathbf{Y}, \mathbf{X})). \end{aligned} \quad (1.120)$$

Using the definition (1.70) of the amplitude of the propagator, one has

$$|A_\alpha(\mathbf{Y}, \mathbf{X}, t)|^2 = \frac{1}{(2\pi\hbar)^L} \det \left| \frac{\partial R_\alpha}{\partial \mathbf{Y} \partial \mathbf{X}}(\mathbf{Y}, \mathbf{X}) \right| \quad (1.121)$$

$$= \frac{1}{(2\pi\hbar)^L} \det \left| \frac{\partial \mathbf{p}_\alpha^i}{\partial \mathbf{Y}}(\mathbf{Y}, \mathbf{X}) \right|. \quad (1.122)$$

In conjunction with the sum, this is the expression that would appear if one performed a change of integration variables from initial momentum $\mathbf{p}^i$ to final position $\mathbf{Y}$. Performing the inverse change would consume this Jacobian, resulting in

$$\langle \hat{A}(t) \rangle^{\text{qcl}} = \int d\mathbf{X} d\mathbf{p}^i A(\mathbf{Y}(\mathbf{X}, \mathbf{p}^i), \mathbf{p}^f(\mathbf{X}, \mathbf{p}^i)) W(\mathbf{X}, \mathbf{p}^i), \quad (1.123)$$

with $\mathbf{Y}^f(\mathbf{X}, \mathbf{p}^i)$ and $\mathbf{p}^f(\mathbf{X}, \mathbf{p}^i)$ the final position and momentum obtained from evolving the initial condition $(\mathbf{X}, \mathbf{p}^i)$ for a time t , the time-dependence being omitted in the right-hand side of (1.123). In other words, when computing expectation values, keeping only the dominant and classical contribution amounts to the truncated Wigner approximation, as expressions (1.109) and (1.123) are the same [67].

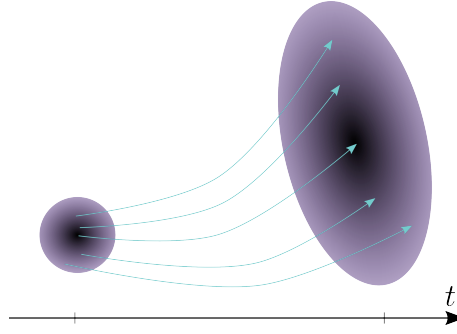


Figure 1.3: Schematic representation of the truncated Wigner method. The Wigner distribution of the wavepacket is represented in purple. Trajectories starting from points sampled from the quasidistribution are shown in blue. For short times, they allow to reconstruct the quantum evolution.

Expression (1.123) can be evaluated numerically by sampling the initial wavepacket, given by the Wigner distribution, propagating each point from the sampling, and summing all the contributions⁵. We represent in Figure 1.3 how the evolution of the wavepacket, in purple, is reconstructed from the sampled points and the trajectories born from them.

1.4 MODEL SYSTEMS

In the remainder of this chapter and the others that follow, numerical simulations will be presented to either verify analytical derivations made in a general context or to support findings in paradigmatic systems. To this end, we introduce the systems in which the simulations will be run. Rather than particular examples, they must actually be considered as universal: what is observed in those systems is also observed in any system. As the goal is to always compare the quantum and classical dynamics, we will introduce for each system the classical limit along its initial quantum formulation.

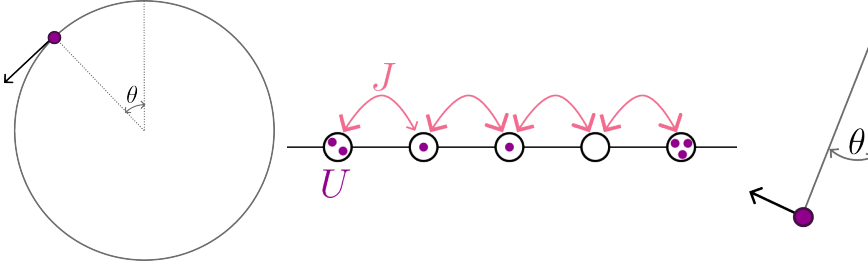


Figure 1.4: Visual representation of different systems. *Left*: kicked rotor: a particle moving on a circle. *Centre*: 1D Bose-Hubbard system. The hopping, represented by the arrows and the J , can be either a permanent feature of the dynamics, or be present only at discrete times, i.e., in the form of kicks. *Right*: simple pendulum.

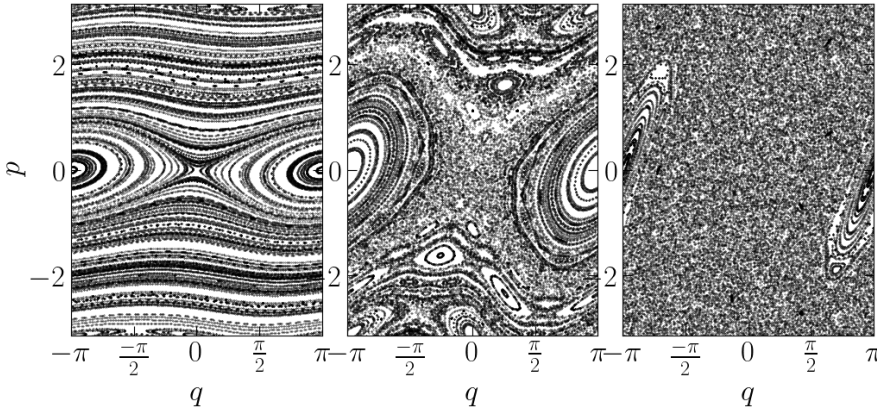


Figure 1.5: Stroboscopic sections of the kicked rotor for different kicking strength K . From left to right: $K = 0.2$, $K = 1$, and $K = 3.5$. The larger the kicking strength, the more chaotic the phase space

1.4.1 *Kicked rotor*

Complex systems often exhibit, naturally, complicated dynamics. To avoid probing intricate features, it is wise to start with simple models. A very well-known one is the quantum kicked rotor, whose first introduction dates back to 1979 [97]. It consists of a particle that moves freely on a circle, and that is subject to periodic kicks [98]. A schematic representation is shown in the left of Figure 1.4. While it is a very simple model, it is nonetheless a textbook case to study chaos, both from the quantum and classical perspectives. The quantum kicked rotor can be used to model general quantum phenomena like dynamical localization [99, 100] and quantum resonances in rotational excitation [99, 101], or systems such as cold atoms in optical lattices [102] and microwave ionization of hydrogen atoms [100], to name a few. Experimental realisations have been made using for instance ultracold sodium [99, 102] and cesium [103] atoms.

It is defined by the Hamiltonian

$$\hat{H}(t) = \frac{\hat{p}^2}{2} + K \cos \hat{\theta} \sum_{n=-\infty}^{\infty} \delta(t - n), \quad (1.124)$$

where K is the kicking strength [97, 98, 102]. Its classical limit, known as the standard map, can be written

$$\begin{cases} p_{n+1} &= p_n + K \sin \theta_n, \\ \theta_{n+1} &= \theta_n + p_{n+1}. \end{cases} \quad (1.125)$$

K is the only parameter. The larger its value, the more chaotic the phase space, as is shown in Figure 1.5. The chaotic region are those that lack apparent order and look like noise.

As its Hamiltonian is time-dependent, the total energy is not conserved. Nonetheless, as there is only one degree of freedom, which is why the phase space can be entirely visualised, the kicked rotor will prove a powerful tool to verify universal behaviours of chaos indicators.

1.4.2 *Bose-Hubbard systems*

We here present the Bose-Hubbard model, which consists of interacting bosons trapped in a lattice, and where the bosons can hop from one site to

⁵ One must also divide the result by the number of sampling points to ensure the normalisation of the Wigner function.

another adjacent site. It is used to describe ultra-cold gas of bosons [49] as well as superconducting qubits [104] and is described by the Hamiltonian

$$\hat{H} = \sum_{l=1}^L \left(E_l(t) \hat{n}_l + \frac{U}{2} \hat{n}_l (\hat{n}_l - 1) \right) - J \sum_{l=1}^{L-1} \left(\hat{a}_l^\dagger \hat{a}_{l+1} + \hat{a}_{l+1}^\dagger \hat{a}_l \right), \quad (1.126)$$

with L the number of sites, E_l is the on-site energy that can in general depend on time, U the 2-body interaction strength, J the hopping between adjacent sites, $\hat{a}_l$ and $\hat{a}_l^\dagger$ the annihilation and creation operators on site l , and $\hat{n}_l = \hat{b}_l^\dagger \hat{b}_l$ the population operator on site l . A schematic representation is shown in the middle of Figure 1.4. We distinguish 2 cases for the on-site energies. If the number of sites $L = 2$, the system is integrable, and we add a periodic driving to end up with a chaotic system. We refer to this system as the *driven dimer*. If the number of sites is $L \geq 3$, the system is chaotic, and the on-site energy can simply be set to 0. Mathematically, this reads

$$\begin{cases} L = 2 : E_1(t) = -E_2(t) = \delta \cos(\omega t), \\ L \geq 3 : E_l(t) = 0 \quad \forall l, \end{cases} \quad (1.127)$$

where δ and ω are the amplitude and the frequency of the driving in the case of the dimer.

The classical equations of motion are obtained by taking the Weyl symbol of the Hamiltonian (1.126), which yields

$$\mathcal{H}(\mathbf{q}, \mathbf{p}) \equiv \left(\hat{H} \right)_W(\mathbf{q}, \mathbf{p}) \quad (1.128)$$

$$\begin{aligned} &= \sum_{l=1}^L \left(E_l(t) n_l(\mathbf{q}, \mathbf{p}) + \frac{U}{2} n_l(\mathbf{q}, \mathbf{p}) (n_l(\mathbf{q}, \mathbf{p}) - 1) \right) \\ &\quad - J \sum_{l=1}^{L-1} (q_l q_{l+1} + p_l p_{l+1}), \end{aligned} \quad (1.129)$$

with $n_l(\mathbf{q}, \mathbf{p}) \equiv (\hat{n})_W(\mathbf{q}, \mathbf{p}) = (q_l^2 + p_l^2 - 1)/2$ the symbol of the population operator.

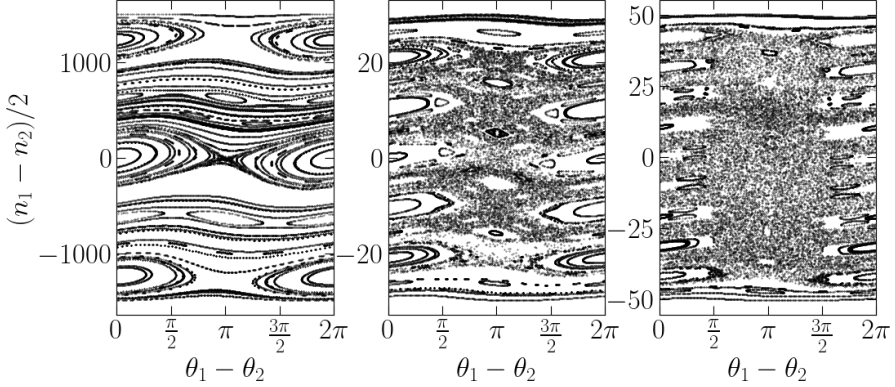


Figure 1.6: Stroboscopic maps of the classical kicked Bose-Hubbard dimer described by the equations (1.135) for different sets of parameters. *Left:* $N = 3000$ particles, interaction parameters $U = 0.025J$, kicking strength and period $\tau = 0.2J$. *Centre:* $N = 60$, $U = 3.0J$, $\tau = 0.2J$. *Right:* $N = 100$, $U = 3.0J$, $\tau = 0.2J$.

One can define complex vectors $\psi = (\mathbf{q} + i\mathbf{p})/2$, in which case the Hamiltonian takes the form

$$\begin{aligned} \mathcal{H}(\psi, \psi^*) \equiv & \sum_{l=1}^L \left(E_l(t) \left(|\psi_l|^2 - \frac{1}{2} \right) + \frac{U}{2} \left(|\psi_l|^4 - 2|\psi_l|^2 + \frac{3}{4} \right) \right) \\ & - J \sum_{l=1}^{L-1} (\psi_l^* \psi_{l+1} + \psi_l \psi_{l+1}^*). \end{aligned} \quad (1.130)$$

This allows to derive the time-evolution of ψ :

$$i\hbar \frac{d}{dt} \psi_k = \frac{\partial H}{\partial \psi^*}(\psi, \psi^*) \quad (1.131)$$

$$= E_k(t) \psi_k + U \left(2|\psi_k|^2 \psi_k - \psi_k \right) - 2J(\psi_{k-1} + \psi_{k+1}), \quad (1.132)$$

which is a type of non-linear Schrödinger equation.

1.4.3 Kicked Bose-Hubbard dimers

Two subcases of Bose-Hubbard models were introduced above: the driven dimer and the drivenless N -site systems. One can introduce a slight variation of the former by introducing a dimer where the hopping is done in the form of kicks, with a hoppingless propagation between kicks: the

kicked Bose-Hubbard dimer [105–107]. Experimentally, this would mean setting up a regular Bose-Hubbard system without any hopping, and then modifying the lattice potential depth so that for a very short time, bosons can hop from one site to another.

The Hamiltonian that describes this system is

$$\begin{aligned} \hat{H} = & \frac{U}{2} (\hat{n}_1 (\hat{n}_1 - 1) + \hat{n}_2 (\hat{n}_2 - 1)) \\ & - J \left(\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1 \right) \tau \sum_{n=-\infty}^{\infty} \delta(t - n\tau), \end{aligned} \quad (1.133)$$

with τ the period and strength of the hopping kicks. The classical Hamiltonian can be obtained by taking its Weyl symbol:

$$\begin{aligned} \mathcal{H}(\mathbf{q}, \mathbf{p}, t) = & \frac{U}{2} (n_1(n_1 - 1) + n_2(n_2 - 1)) \\ & - J (q_1 q_2 + p_1 p_2) \tau \sum_{n=-\infty}^{\infty} \delta(t - n\tau). \end{aligned} \quad (1.134)$$

The corresponding classical equations of motion are

$$\begin{aligned} \text{Between kicks:} \quad & \begin{cases} \dot{q}_i = \frac{U}{2} (p_i (q_i^2 + p_i^2 - 2)), \\ \dot{p}_i = -\frac{U}{2} (q_i (q_i^2 + p_i^2 - 2)), \end{cases} \quad \text{with } i = 1, 2, \end{aligned} \quad (1.135)$$

$$\begin{aligned} \text{At a kick:} \quad & \begin{cases} \dot{q}_1 = \frac{-J p_2 \tau}{m\omega}, & \dot{q}_2 = \frac{-J p_1 \tau}{m\omega}, \\ \dot{p}_1 = -J m\omega q_2, & \dot{p}_2 = -J m\omega q_1, \end{cases} \end{aligned} \quad (1.136)$$

where the time resolution is 1 kick, and the evolution from right after a kick to right after the next one is given by an interaction-only propagation that lasts for a time τ , followed by an instantaneous hopping-only propagation. This can be understood as a regularisation of the Dirac δ 's by a function that is locally constant around the kicks, such that for a very short time, it is the hopping term that dominates. Phase-space visualisations are shown in Figure 1.6 for different sets of parameters.

1.4.4 Driven pendulum

The last system that will be used in this work is the driven pendulum. For this system only, it makes more sense to introduce the classical framework

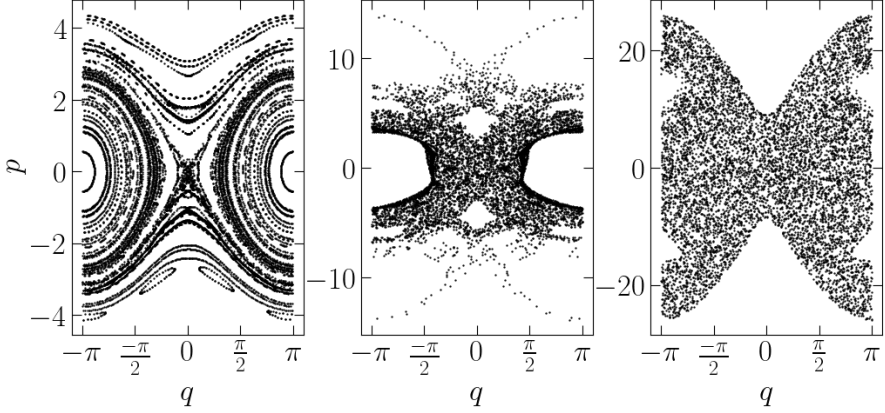


Figure 1.7: Stroboscopic maps of the classical driven pendulum described by the equations (1.138) for different sets of parameters. *Left:* $\lambda_s = \sqrt{2.5}$, 0.0632 , $\omega = 10$. *Centre:* $\lambda_s = \sqrt{6}$, $\kappa = 0.245$, $\omega = 10$. *Right:* $\lambda_s = \sqrt{6}$, $\kappa = 4.08$, $\omega = 10$.

first. A pendulum can be driven in several ways. The Hamiltonian we use proves to be the one that reproduces the effective behaviour of the dynamics of a system in the vicinity of a resonance, making it universal [15, 108]. More details can be found in [69] as well as Appendix B for the two-degree-of-freedom case.

The driven pendulum is classically described by

$$\mathcal{H}(q, p, t) = \frac{p^2}{2} + \lambda_s^2 \cos(q) + \kappa \omega \lambda_s \cos(q) \cos(\omega t + \varphi), \quad (1.137)$$

with the first two terms being the regular pendulum Hamiltonian, $\kappa \omega \lambda_s$ the amplitude of the perturbation, ω its frequency, and λ_s the stability exponent associated with the hyperbolic fixed point at $(q, p) = (0, 0)$ of the Hamiltonian. The dimensionless parameter κ characterises the strength of the perturbation. For the following, we assume a weak driving amplitude with a high frequency. In other words, the system must satisfy $\kappa \ll \lambda_s \ll \omega$ and $\kappa \omega \sim 1$.

The classical Hamilton equations of motion are given by

$$\ddot{q}(t) = \lambda_s^2 \sin(q(t)) + \kappa \omega \lambda_s \sin(q(t)) \cos(\omega t + \varphi). \quad (1.138)$$

A schematic representation is shown in the right of Figure 1.4. Phase-space visualisations are shown in Figure 1.7 for different sets of parameters.

Quantum calculations will be made only in the undriven case. The Hamiltonian is then simply

$$\hat{H} = \frac{\hat{p}^2}{2} + \lambda_s^2 \cos(\hat{q}). \quad (1.139)$$

As it was written, these systems will serve not only as examples to present numerical simulations, but also as models exhibiting universal dynamics, meaning that what will be presented is the generic behaviour of any system. In particular, their first utility will come in the last section of this chapter, dedicated to quantum chaos.

1.5 QUANTUM CHAOS

The end of this chapter is dedicated to the introduction of quantum chaos. As it was already stated, there are fundamental differences between quantum and classical chaos. New indicators thus had to be investigated. At first, indirect signatures of quantum chaos were found. The most well-known, which we will present here, is the statistics of the energy-level spacing. Eventually, more direct indicators of the instability of the dynamics were found, allowing to link quantum and classical chaos. We will review here the Loschmidt echo as well as the out-of-time-ordered correlator, the latter being at the heart of this thesis.

1.5.1 *Level spacing and random matrix theory*

As explained above, studying the stability of a quantum system by investigating its sensitivity to initial conditions is not possible. Alternative ways, which were first more indirect, had to be designed. The first indicator that is usually introduced in the literature is obtained by looking at the distribution of the energy-level spacings [18]. The reason why this indicator is important comes from what is called random matrix theory. This theory was introduced in the fifties and sixties by Wigner, Dyson and Mehta, to name a few [18]. It received renewed interest when this theory was applied to quantum chaotic systems.

The first system that students encounter when they start to learn about quantum mechanics is usually the harmonic oscillator. Its energy level, and thus its spectrum, is described by the simple and well-known formula $E_n = \hbar\omega(n + 1/2)$ with ω the angular frequency and n a positive integer [9]. An important feature is that the energy levels are all equally

spaced. More generic and thus more complex systems have in general more elaborate spectra that, at least at first sight, lack regularity [18]. To organise this apparent anarchy, random matrix theory was introduced to describe complex systems qualitatively. It is a theory used to study matrices, in this case Hamiltonians, obeying some symmetries. Depending on those, the matrix will belong to one of the so-called universality classes. It has proved extremely effective to describe Hamiltonians in the sense that the statistical properties of their level spacing can be known [18, 19]. In addition, as it works for chaotic systems as well and because the level spacing statistics associated with those types of systems exhibit characteristics different from the integrable ones, it is also used as a chaos probe.

It is important to note that directly studying the distribution of the spacings will not work in general. What matters is actually the relationship between energy levels, in other words, their local behaviour. Computing the differences between consecutive energy levels directly will not only probe this, but also the global trend they follow, which is system-dependent. One must thus perform what is called an *unfolding* of the spectrum in order to make the analysis local only. In this context, this means not taking into account the general trend of the level distribution and assuming that the average spacing between two consecutive levels is one. Details of the procedure can be found in [9], and the steps are highlighted here.

Let us assume that we study a system described by the Hamiltonian $\hat{H}$. To unfold the spectrum, the steps are the following.

- Compute the eigenvalues E_n , $n = 1, 2, \dots$, i.e., the energies, of $\hat{H}$, and order them so that $E_1 < E_2 < \dots$.
- From those data, build the integrated density of states $\mathcal{N}(E)$, the function that returns how many states have an energy equal to or below E . Analytically, it corresponds to $\mathcal{N}(E) = \sum_n \Theta(E - E_n)$ with Θ the Heaviside function. Numerically, this is simply the index of the energy as a function of the energy.
- Fit a smooth function $\mathcal{N}_{fit}$ to $\mathcal{N}$. We chose a polynomial of degree 8. As long as the fit is reasonably accurate, the function itself has no particular importance⁶.

⁶ Bear in mind, however, that some references use the word “interpolate” instead of “fit”, which could be understood as “find a function that passes by all the points of the set”.

- Replace the energies E_n , $n = 1, 2, \dots$ by the fit function evaluated at those energies $\{\mathcal{N}_{\text{fit}}(E_n), n = 1, 2, \dots\}$.
- Compute the “level spacing” using those new quantities: $s_n = \mathcal{N}_{\text{fit}}(E_{n+1}) - \mathcal{N}_{\text{fit}}(E_n)$ and build a histogram with them.

The unfolding procedure is not unique, but the results are essentially equivalent. For instance, as long as the function is a sufficiently good fit, its exact expression has no appreciable effect on the end result [9, 21].

Random matrix theory tells us that the distribution that the s_n follow informs us whether the dynamics is regular or chaotic. The correspondence with classical regular and chaotic motion is obtained by looking at the dynamics associated with the classical limit of the studied system, if one exists [9, 18, 21]. The question is more complicated with systems that do not possess such a limit, for instance fermionic systems, and we will not tackle this problem in this work.

Let us investigate why the integrability and the level spacing statistics are related. A continuous symmetry gives rise to a constant of motion in a classical system, and to a good quantum number in a quantum system. The symmetries can be used to express the Hamiltonian in a block-diagonal form, and by extension constrain its shape. In the particular case where there are as many symmetries as there are degrees of freedom, the Hamiltonian can be completely diagonalised using only those properties. Its eigenvalues, in other words the energy levels, are thus uncorrelated and there is no limit to how close they can be to each other. In this case, they will follow what is called a Poisson distribution, whose expression is given hereafter. If there are fewer symmetries than degrees of freedom, the system does not, in general, follow a regular dynamics. Consequently, the Hamiltonian will at best be reduced to a block-diagonal representation by using those symmetries, meaning that in a given block, there are matrix elements linking the energy levels, forcing them to be in general different. This will lead to what is called the energy-level repulsion. There are 3 distributions falling in this category, all labelled under the name Wigner-Dyson. Depending on the symmetries of the system, the distribution corresponds to the Gaussian Orthogonal Ensemble (GOE) if the Hamiltonian is real, the Gaussian Unitary Ensemble (GUE) if it is complex, and the Gaussian Symplectic ensemble (GSE) for instance for

Doing so would result not only in the average spacing between levels being one, but also the exact value of the spacing itself, and this between all levels. The consequence is that no analysis is possible in this case as the distribution becomes trivial.

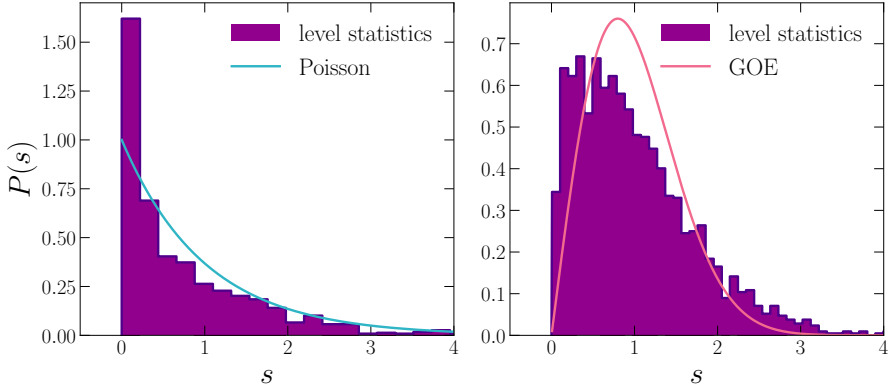


Figure 1.8: Histogram of the unfolded level-spacing distribution of the 3-site disordered Bose-Hubbard model (purple) and the corresponding distribution. *Left*: $N = 30$ particles, $U = 0.05J$, disorder range $= 0.1J$. The Poisson distribution (1.140) is shown in blue. *Right*: $N = 30$ particles, $U = 0.5J$, disorder range $= 1J$. The GOE distribution (1.141) is shown in pink. The Hamiltonian of the system is given by (1.126)

half-integer spin systems. More details can be found in [9] and [21]. The distributions that were mentioned are given by

$$P(s) = \begin{cases} e^{-s} & \text{(Poisson),} & (1.140) \\ s \frac{\pi}{2} e^{-s^2 \pi / 4} & \text{(GOE),} & (1.141) \\ s^2 \frac{32}{\pi} e^{-s^2 4 / \pi} & \text{(GUE),} & (1.142) \\ s^3 \frac{2^{18}}{36 \pi^3} e^{-s^2 64 / 9 \pi} & \text{(GSE).} & (1.143) \end{cases}$$

Whereas the maximum of the Poisson distribution is located at the origin, highlighting the absence of correlation between energy levels, the maximum of each distribution lies at a nonzero spacing, illustrating the level repulsion.

We illustrate the aforementioned procedure for the disordered Bose-Hubbard model described in equation (1.126) by showing histograms of the level spacings in Figure 1.8. In the left plot, the interaction is small compared to the hopping. This results in a dynamics tending to the superfluid state [54], which is integrable, and thus a Poissonian distribution of the level spacing. In the right plot, the interaction is larger,

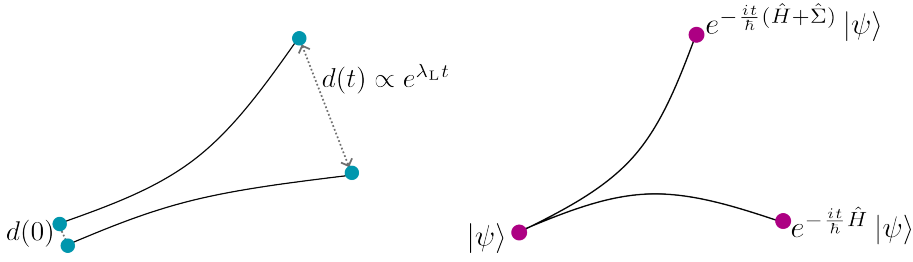


Figure 1.9: Representation of the parallel to be made between the exponential divergence of classical trajectories and the Loschmidt echo. *Left:* Two initially close phase-space points on the left that diverge exponentially from one another with time, with $d(t)$ the distance between the two points at time t , and λ_L the classical Lyapunov exponent. *Right:* Representation of the propagation of the same initial state according to two slightly different Hamiltonians $\hat{H}$ and $\hat{H} + \hat{\Sigma}$. The Loschmidt echo is the overlap between the two resulting states. The farther apart the final states, the smaller the overlap between the two, the smaller the echo.

making the dynamics chaotic, resulting in a GOE distribution of the level spacings.

It is important to note that the spectrum will not exactly follow one distribution or another. For instance, the edges of the spectrum usually correspond to an integrable dynamics. One way to circumvent this is to restrict the spectrum to a window small enough to avoid those “boundary effects”. Here, we removed 10% of the energy levels from each edge.

Finally, it is important to note that there exists another, more modern, indicator, related to the ratio of consecutive levels [109]. It offers the considerable advantage that no unfolding procedure is required, making it a more transparent probe of chaos than the level-spacing distribution.

However, as was explained before, this indicator is only indirect in the sense that it does not directly probe the scrambling nature of the system. To this end, new tools were introduced, which will be the focus of the following sections.

1.5.2 Loschmidt echo

As it was stated already multiple times, classical chaos is characterised by a high sensitivity of a system to a change in the initial conditions, i.e., the butterfly effect. One can thus investigate this sensitivity by propagating

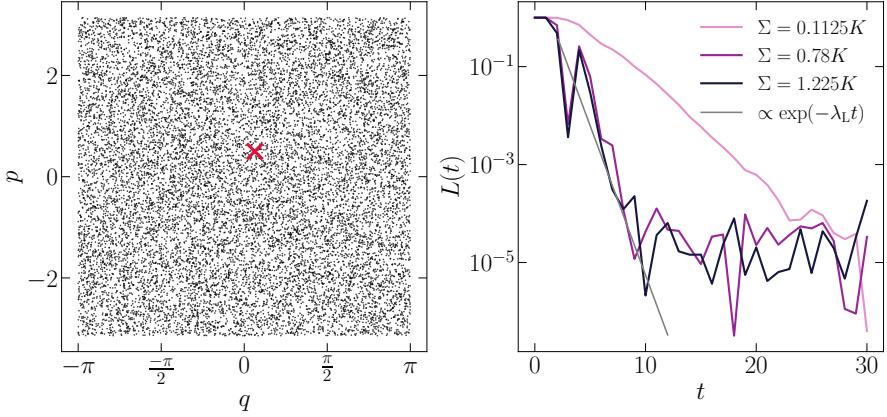


Figure 1.10: Loschmidt echo in the kicked rotor. *Left*: Phase space of the classical kicked rotor (standard map) for a kicking strength $K = 8$. The centre of the initial coherent state is represented by a red cross at $(q, p) = (0.2, 0.5)$, with $\hbar = 2\pi/N$, with $N = 2^{14}$. *Right*: Loschmidt echo of the quantum kicked rotor for the coherent state centred on the red cross for 3 different perturbations Σ to the kicking strength K , expressed as a function of K .

two initially very close initial conditions and see how fast they diverge from each other. This concept is not applicable to quantum systems, but a relatively similar one exists in the name of the Loschmidt echo. The main difference is that the perturbation lies in the propagation itself, in other words, in the Hamiltonian [22, 110]. Mathematically, it is computed as the overlap of two initially identical wavefunctions $|\psi\rangle$ that evolve according to slightly different Hamiltonians $\hat{H}$ and $\hat{H} + \hat{\Sigma}$, with $\hat{\Sigma}$ a perturbation:

$$L(t) = \left| \langle \psi | \exp\left(\frac{it}{\hbar}(\hat{H} + \hat{\Sigma})\right) \exp\left(-\frac{it}{\hbar}\hat{H}\right) | \psi \rangle \right|^2. \quad (1.144)$$

We illustrate this parallel in Figure 1.9. On the left, we show two initially close trajectories in phase space that diverge exponentially in the presence of chaos. The analogue is the exponential decrease of the overlap in (1.144), represented schematically on the right of the figure. The Loschmidt echo can also be seen as a characterisation of how well a system can forward and backward evolve in time when a perturbation is introduced. A chaotic dynamics translates into an exponential decrease in echo, which highlights the unstable nature of the system.

If a system admits a classical limit, or analogue, then an exponential

decrease in the echo implies a chaotic classical dynamics. However, the link between quantum and classical chaos goes further than that. Indeed, in this case, the classical system can be characterised by a Lyapunov exponent λ_L , and the exponential decrease rate of the Loschmidt echo can be shown to be precisely that exponent, up to the Ehrenfest time.

As already stated, it is the time at which quantum effects become prevalent [41]. In a chaotic system, when a small perturbation of the order of $\hbar$ grows to the typical action S , the classical and quantum dynamics do not match anymore. The timescale at which it happens is called the Ehrenfest time and can be estimated by

$$\hbar e^{\lambda t_E} \sim S \quad (1.145)$$

$$t_E \sim \frac{1}{\lambda} \log\left(\frac{S}{\hbar}\right). \quad (1.146)$$

As $\hbar/S$ plays the role of an effective Planck constant $\hbar_{\text{eff}}$, this can be rewritten

$$t_E \sim \frac{1}{\lambda} \log\left(\frac{1}{\hbar_{\text{eff}}}\right). \quad (1.147)$$

Coming back to the Loschmidt echo, the exponential decrease observed in chaotic systems is a generic behaviour and is expected to hold true for any system, provided that the perturbation is large enough with respect to the mean-level spacing. This regime is called the non-perturbative, or exponential, regime [22]. In the eventuality of a smaller perturbation, the rate is perturbation-dependent, and the Loschmidt echo is in the so-called perturbative, or Gaussian, regime. We show this in Figure 1.10 in the context of the kicked rotor. The quantum Hamiltonian, which will be detailed further, is given by (1.124) and the corresponding classical mapping is (1.125). On the left, we show the classical phase space of the kicked rotor, which is entirely chaotic, as well as the centre of the coherent state chosen as the initial state, here $(q, p) = (0.2, 0.5)$. On the right, we show the Loschmidt echo for that initial state, for 3 different perturbations Σ of the kicking strength K , expressed as a function of K . The smallest one, in pink, falls into the Gaussian regime. The behaviour looks exponential, at least in the time window during which the decay occurs, but clearly the decay rate is perturbation-dependent, as going to larger perturbations modifies it. However, the increase in the perturbation strength between the purple and dark blue curves does not translate into an increase in the decay rate, indicating that the perturbation is now

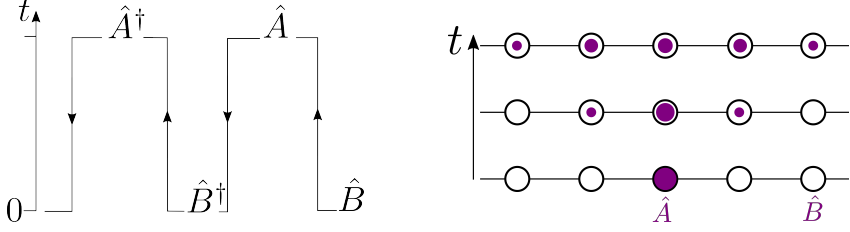


Figure 1.11: Schematic representations of OTOCs. *Left*: Representation of the forward and backward evolution as well as the operator application involved in the OTOC. *Right*: representation of the spreading of operator $\hat{A}$ with time on a 1D lattice.

in the exponential regime. In addition, we show a curve proportional to $\exp(-\lambda_L t)$ where the Lyapunov exponent has been obtained with the classical dynamics. We can note that the decay rate of the Loschmidt echo is equal to this classical exponent. Should the reader be interested in a more in-depth analysis, we redirect them to [111].

Although the Loschmidt echo can be related to information scrambling, there exist other indicators whose connection to scrambling is more direct. With that in mind, we can now introduce the most important one in the context of this thesis, which has the advantage of not having the constraint of choosing the right perturbation.

1.5.3 Out-of-time-ordered correlators

As it was stated before, one can consider that the quantum counterpart of the exponential spreading of trajectories that are started close to one another in phase space is information scrambling. A quantity that analyses exactly this exists in the name of the out-of-time-ordered correlator, often shortened to OTOC. It will be of utmost importance for this thesis and thus deserves a more thorough introduction.

First introduced in 1969 in the context of superconductivity [36], the OTOC has since been used in various fields of physics like the study of black holes [32, 34] and quantum information, to name a few [112, 113], and several experimental realisations exist [114–116]. The idea behind the OTOC is, given two (local) operators, to probe the propagation of information within a system through the growth of operators [24]. Initially, it was introduced as follows. Take an initial state $|\psi\rangle$ in a system defined by a Hamiltonian $\hat{H}$, and two operators $\hat{A}$ and $\hat{B}$. With these

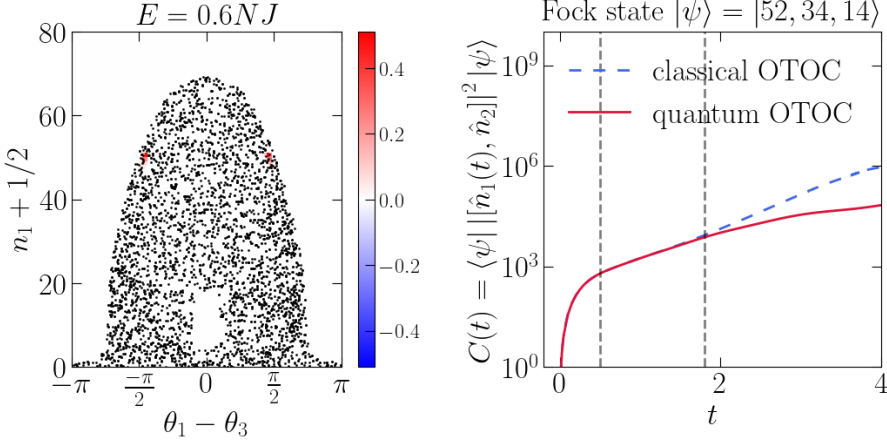


Figure 1.12: OTOC in a fully chaotic case: the Bose-Hubbard trimer. *Left:* Poincaré surface of section of the Bose-Hubbard trimer for the set of parameters $U = 0.06J$, $N = 300$, at energy $E = 0.6NJ$. The vertical axis represents the population of the first site n_1 and the horizontal one the difference between the phase of the first site θ_1 and the third one θ_3 . In the Poincaré surface of section, the Wigner function of the initial state is represented in arbitrary units. *Right:* quantum and classical OTOC (Poisson bracket) in respectively the solid red and the dashed blue curve for the Fock state $|\psi\rangle = |52, 34, 14\rangle$, $U = 0.06J$. The vertical dashed lines separate the different growth regimes. The first one is the power-law regime, followed by the exponential region, then the saturation region.

ingredients, create two states. The first one is obtained by applying $\hat{B}$, time-evolving the system to a time t , applying the other operator $\hat{A}$, and finally backward evolving the resulting state to the initial time. The other state is obtained the same way, except that the application of $\hat{B}$ is done at the end of the procedure instead of the beginning. Computing the overlap of those two states yields

$$F(t) = \langle \psi | e^{it\hat{H}/\hbar} \hat{A}^\dagger e^{-it\hat{H}} \hat{B}^\dagger e^{it\hat{H}/\hbar} \hat{A} e^{-it\hat{H}/\hbar} \hat{B} | \psi \rangle. \quad (1.148)$$

Because this is, in essence, a correlator that involves a sequence of operators that is not time-ordered, this was the first definition of the OTOC [36]. Alternatively, this can be seen as the overlap between the initial state and another that is obtained by a sequence of applications of operators and time evolution. On the left part of Figure 1.11, we show a visual representation of the forward and backward propagations.

Another more contemporary definition of the OTOC exists [24]. It is given by

$$C(t) = \langle \psi | \left| [\hat{A}(t), \hat{B}] \right|^2 | \psi \rangle. \quad (1.149)$$

Using $\hat{B}$, it probes the spreading of operator $\hat{A}$ amongst the degrees of freedom of the system as it is time-evolved. The time-evolution of an operator should be understood as in the Heisenberg representation, i.e., $\hat{A}(t) = \hat{U}^\dagger \hat{A} \hat{U}$ with $\hat{U} = \exp(-it\hat{H}/\hbar)$.

Expressions (1.148) and (1.149) are not unrelated. The first definition is one of the 4 terms that appear when carrying out the square modulus of the commutator, and in the particular case of unitary operators, one has

$$C(t) = 2 - 2\text{Re}(F(t)), \quad (1.150)$$

which is why studying one or the other is essentially equivalent [37]. The definition (1.149) is the one we used for all of our work, and consequently that will be used for the remainder of this thesis.

As written above, the OTOC is used to probe information scrambling. If the system in which the OTOC is computed is chaotic, information will spread ballistically, rather than only diffusively or not at all. The speed at which information propagates within the system is called the butterfly velocity. Its name was chosen to make an explicit allusion to the classical butterfly effect. This velocity determines the boundary of

the light-cone of a given perturbation, which grows linearly in time [71]. This ballistic spreading usually translates into an exponential growth⁷ of the OTOC. The exponential growth rate is considered to be a quantum analogue of the classical Lyapunov exponent [24, 26, 27, 38, 39]. Evidence supporting this claim will be established in the following.

It has been shown that an upper bound exists for this exponent, known as the Maldacena bound [42]. For a system at a non-zero temperature T , the OTOC is defined as a thermal expectation value, i.e.,

$$C_\beta(t) = \left\langle \left| [\hat{A}(t), \hat{B}] \right|^2 \right\rangle_\beta \quad (1.151)$$

$$= \frac{1}{Z} \text{Tr} \left(e^{-\beta \hat{H}} \left| [\hat{A}(t), \hat{B}] \right|^2 \right), \quad (1.152)$$

with $\beta = 1/k_B T$, k_B the Boltzmann constant and Z the canonical partition function [39, 42, 119, 120]. The quantum Lyapunov exponent λ_L must satisfy $\lambda_L \leq 2\pi k_B T/\hbar$. Interestingly, in the context of the anti-de Sitter/conformal field theory, often abbreviated AdS/CFT, it was proven that black holes saturate this bound and were thus the fastest scramblers in Nature [32, 34].

There are mechanisms that can prevent the thermalisation of a system, amongst which is the presence of disorder. More specifically, the presence of disorder modifies the time-dependence of the light-cone boundary, which goes from linear in time to a fractional power in time, and eventually logarithmically in time [71]. The latter is characteristic of a phenomenon called many-body localisation. This results in a power-law increase of the OTOC, meaning that the correlator is sensitive to the growth speed of operators as well as the presence or absence of thermalisation, and the consequences are shown in the time-dependence [71, 119]. Other mechanisms can prevent thermalisation, trivial ones like integrability, and more elaborate ones like quantum scarring [121].

Finally, in addition to their initial interest as a quantum chaos probe, one can use the OTOC to analyse other aspects of a system. It is related to the variance of the correlator $[\hat{A}(t), \hat{B}]$, meaning it can be used to analyse out-of-equilibrium fluctuations after saturation [39].

Out-of-time-ordered correlators do not exist solely as theoretical objects. They were experimentally realised in several contexts, such as nuclear

⁷ The word “usually” here is employed because there exist what are called *slow scramblers*. They are system whose OTOC grow only polynomially in time, despite the presence of chaos [117, 118].

magnetic resonance to probe the chaotic dynamics in small systems as well as the localisation in larger ones [114], spin systems [115, 116], and momentum states in a Bose-Einstein condensate [122].

For the remainder of this introduction, let us focus on the chaotic case. Consider a system with a completely chaotic classical phase space, and an initial state randomly chosen inside this chaotic sea. In this framework, the OTOC follows three regimes. For very short times, up to the Lyapunov time $1/\lambda_L$, it follows a power-law regime. Indeed, before this time, the hyperbolic nature of the dynamics hasn't manifested yet, resulting in a behaviour reminiscent of the absence of chaos. Between the Lyapunov time and the Ehrenfest time $t_E \sim \log(1/\hbar)/\lambda_L$ [25, 44, 45], the OTOC follows an exponential regime whose exponential growth rate is $2\lambda_L$. After that, it saturates with or without oscillations [25, 26]. For this reason, the Ehrenfest time is also called the scrambling time in a many-body context [25, 42, 123]. In Figure (1.12), we show in red the OTOC computed for a Fock state in a Bose-Hubbard timer, and the three aforementioned regimes are separated by vertical dashed lines. The different regimes are separated by vertical dashed lines.

To conclude this introduction of OTOCs, it is important to present the typical quasiclassical limit used in the literature, which allows making a bridge between classical and quantum chaos. The limit consists in reexpressing the OTOC using the Wigner-Weyl formalism, then taking the $\hbar \rightarrow 0$ limit of the Moyal bracket. As it was shown in equation (1.105) in Section 1.3.4, the dominant contribution is a Poisson bracket of the Weyl symbols multiplied by $i\hbar$. Using for instance $\hat{A} = \hat{q}_i$, $\hat{B} = \hat{p}_j$, this becomes

$$\begin{aligned} \langle \psi | [[\hat{q}_i(t), \hat{p}_j]]^2 | \psi \rangle &= \int d\mathbf{q} d\mathbf{p} \left([\hat{q}_i(t), \hat{p}_j]^2 \right)_W(\mathbf{q}, \mathbf{p}) W(\mathbf{q}, \mathbf{p}) \\ &= \hbar^2 \int d\mathbf{q} d\mathbf{p} \{q_i(t), p_j\}^2 W(\mathbf{q}, \mathbf{p}) + \mathcal{O}(\hbar^3) \\ &\simeq \hbar^2 \int d\mathbf{q} d\mathbf{p} \left(\frac{\partial q_i}{\partial q_j}(t) \right)^2 W(\mathbf{q}, \mathbf{p}) \propto \hbar^2 e^{2\lambda t}, \end{aligned} \tag{1.153}$$

where λ is the classical Lyapunov exponent of the system, considered fully chaotic [25, 26]. This approximation, sometimes called the Wigner-Moyal approximation, is valid until the Ehrenfest time, where the OTOC saturates due to interferences [25]. Wigner-Moyal does not account for this effect, but results in a never-ending exponential growth. As there is a quantum-classical correspondence before t_E , this allows us to conclude

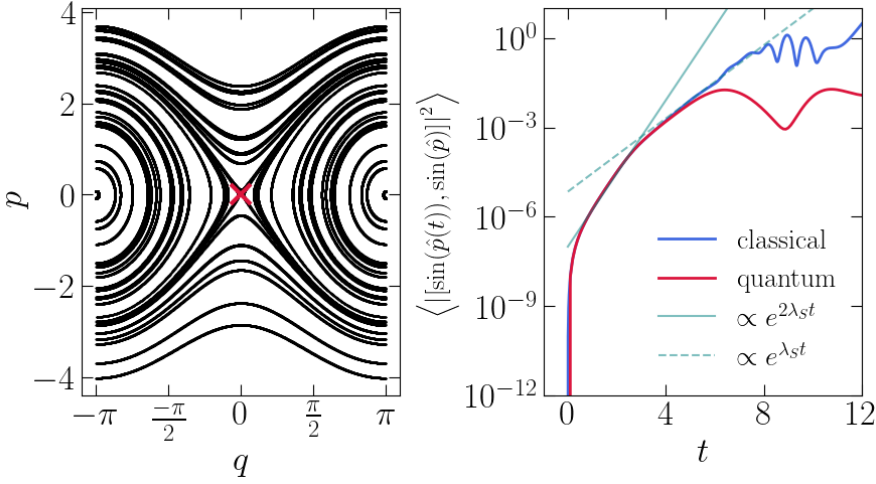


Figure 1.13: OTOC at the unstable fixed point of the simple pendulum. *Left:* Phase space of the simple pendulum. The centre of the initial coherent state is indicated by a red cross located on the fixed point $(0, 0)$. *Right:* Quantum (red) and quasiclassical (blue) out-of-time-ordered correlator. The initial state is the coherent state centred on the red cross, and the operators involved in the OTOC are specified on the vertical axis.

that the quantum and classical Lyapunov exponents are the same. This can be observed in Figure 1.12, where the Poisson bracket (in dashed blue) matches with the quantum curve (in red) for short time.

While this is the typical way the classical limit of the OTOC is obtained, it is as stated valid only for short times. Additionally, it offers no control in the transition from the quantum to the classical realm, and there is no guarantee that some terms of the same order were neglected as well, terms that could push the quantum-classical correspondence beyond the Ehrenfest time. A more elaborate formalism will be established and discussed in Chapter 2.

Before going further, it is important to nuance the link with the Lyapunov exponent of the system. The λ appearing in (1.153), in the case of an initial state in the chaotic sea of a fully chaotic system, is indeed the classical Lyapunov exponent, as it was just written. However, there exist instances in which the OTOC can exhibit an exponential behaviour in the absence of chaos. In the context of a completely integrable system, there can be local instabilities: hyperbolic fixed points. If the initial wavepacket

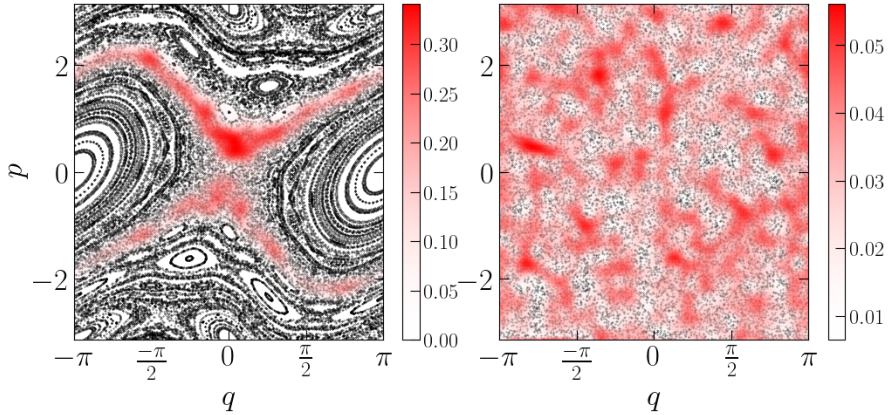


Figure 1.14: Husimi distribution in the kicked rotor. The parameters are a kicking strength $K = 1$ and an initial coherent state centred on $(q, p) = (1, 0.7)$ (left), and $K = 9$ and an initial coherent state centred on $(q, p) = (2.4, 5.8)$ (right). The distribution is shown in a colour scale in arbitrary units. In both instances, the initial states were propagated for 1000 kicks, and the Husimi distributions were averaged over the 10 kicks that follow.

is sufficiently localised on such a point, the OTOC will grow exponentially. The exponential growth rate λ is, in this case, the stability exponent λ_s associated with the fixed point [124–126]. In addition, there is a crossover to half that rate after some time [107, 127]. This is shown in Figure 1.13. On the left, we show the classical phase space, which is entirely regular, and the centre of the initial coherent state, which is located on the unstable fixed point. On the right, we show the corresponding quantum OTOC in red, which is shown to exhibit not only an exponential behaviour, but a crossover to half the initial exponential growth rate. In addition, we also plot the quasiclassical OTOC associated to the quantum one in blue. Again, the correspondence holds for short times, but the classical curve fails to saturate.

The last indicator we will focus on is a type of quantum phase space visualisation called the Husimi distribution.

1.5.4 Husimi distribution

Throughout this introduction, several phase-space visualisations have been shown. Those can show the whole phase space, as is the case with the

simple pendulum (in the left of Figure 1.13), while others are stroboscopic sections, in other words a point in the representation is obtained from a periodic snapshot of a trajectory, as is the case with the kicked rotor (see Figure 1.5) or other Floquet systems (see e.g. Figure 1.6 for the kicked dimer). When it comes to quantum mechanics, one cannot obtain such a straightforward visualisation since “a point in phase space” is a concept that does not make sense anymore. One quantum phase-space visualisation was already introduced before in Section 1.3.4: the Wigner function. Another one, that is positive everywhere, is called the Husimi distribution, or Q function. It is defined as

$$Q(\alpha) = \frac{1}{\pi} \langle \alpha | \hat{\rho} | \alpha \rangle, \quad (1.154)$$

where α is a complex number, $|\alpha\rangle$ is a coherent state centred on α such that $\hat{a}|\alpha\rangle = \alpha|\alpha\rangle$, and $\hat{\rho}$ is the density matrix of a state. For a pure state, $\hat{\rho} = |\psi\rangle\langle\psi|$ and the Husimi distribution takes the form

$$Q(\alpha) = \frac{1}{\pi} |\langle\psi|\alpha\rangle|^2. \quad (1.155)$$

In Figure 1.14, we show the Husimi distribution in the context of the kicked rotor for different kicking parameters and initial states. In the two cases, the initial states were propagated for 1000 kicks, and the Husimi distributions were averaged over the 10 kicks that follow in order to smooth the background. On the left, the phase space is mixed, and we can observe that the distribution follows the domain delimited by the chaotic sea. On the right, the phase space is entirely chaotic, and the distribution is spread on the whole chaotic sea.

A natural question that arises is: why would one distribution be preferred over another? There is no definitive answer, as it all depends on the context. Both functions allow one to compute expectation values, but there are two main differences. Firstly, as stated above, the Wigner function is not necessarily positive, whereas the Husimi function is. Secondly, the former gives the correct marginal probabilities, whereas the latter does not [64, 89, 128, 129].

In this thesis, both phase-space visualisations will be used, but not in the same context. The Wigner distribution will be relevant when using the truncated Wigner approximation, and the Husimi distribution will be of use when visualising the presence or absence of a quantum scar.

QUASICLASSICAL THEORY OF OUT-OF-TIME-ORDERED CORRELATORS

2.1 MOTIVATIONS

As the focus of this thesis is to study scrambling in near-integrable and chaotic systems, objects that are particularly suited to this goal are the already-introduced out-of-time ordered correlators [24, 28, 36]. They can be applied to a variety of systems, ranging from simple models to complex many-body systems. Similarly, as for the Loschmidt echo [22], the concept of OTOCs allows, in a semiclassical context, for the appearance of the classical Lyapunov exponent in the framework of a quantum observable. More specifically, for systems with a chaotic classical counterpart, OTOCs can be shown to grow exponentially for short times, with the exponential growth rate being determined by the maximum Lyapunov exponent of the system [25, 40, 42]. This exponential growth is not unlimited but turns into a saturation of the OTOC observable beyond the Ehrenfest time t_E of the chaotic system. It can be reproduced, but without saturation, by means of a quasiclassical approach based on the Wigner-Moyal formalism, which is strictly perturbative in $\hbar$ and not suited for being applied to time scales larger than t_E .

Proper semiclassical reasoning, applied to generic systems with chaotic behaviour, allows one to quantitatively explain the occurrence of saturation in terms of trajectory pairs that exhibit low-angle crossing [25, 73]. In a very similar manner as for loop corrections to the spectral form factor [130], those trajectory pairs give rise to contributions to the OTOC that are intrinsically nonclassical, in the sense that they do not arise in the framework of a diagonal approximation [131] and thus cannot be incorporated into a quasiclassical numerical simulation scheme based on the Truncated Wigner approximation [62, 63]. A gap occurs thus between this perfectly coherent semiclassical approach [25, 73] on the one hand, and the incoherent Wigner-Moyal approach on the other hand. The former is, in principle, of general validity for fully chaotic systems but cannot be exploited in practice for the development of a numerical tool to study OTOCs beyond the Ehrenfest time. An important reason is that it relies on the explicit knowledge of the system's Lyapunov exponent,

whose precise determination is a formidable problem in the generic case of mixed regular-chaotic phase space. The latter is limited to short times but does not require fully developed chaos and yields the Truncated Wigner method as a practical tool to calculate OTOCs under various circumstances. Due to the presence of this gap, it is, in particular, not obvious to what extent the OTOC growth near the Ehrenfest time is of classical, i.e., incoherent, nature or does imply quantum coherence to hold.

This latter question is most properly addressed by invoking Berry's diagonal approximation [131], which provides the standard method to extract the classical contribution to quantum mechanical observables. This is precisely the method that we use in the first part of the present chapter in order to yield this missing information that is related to the presence of the above-mentioned gap. To this end, we start from a full-fledged semiclassical theory of OTOCs based on the van Vleck-Gutzwiller propagator [20, 132], which is then used to derive a quasiclassical description via a diagonal approximation. The approach presented here can be seen as an extension (and, in some key aspects, a correction) of two previous attempts towards this aim [120, 133]. In [120], both short- and long-time behaviour of the OTOC are calculated in the framework of the van Vleck-Gutzwiller propagator, using extra assumptions that extend beyond the bare semiclassical propagator. For the short-time regime, the propagation is approximated by free evolution (a step justified only for billiard systems) while ergodic arguments are invoked to explain the saturation at long times. Similarly, the calculation presented in [133] bypasses these restrictions for the short-time dynamics by addressing only the dynamics of a particle on a Riemannian manifold of constant negative curvature, which is again a particular type of chaotic system. Avoiding any additional assumption, our calculation yields a quasiclassical description of OTOCs that is valid for general Hamiltonian systems in the short-time regime where the exponential increase of the OTOC is recovered, exactly as predicted by the Wigner-Moyal approach.

Once the incoherent nature of the short-time dynamics is fully established by means of the diagonal approximation, we turn our arguments into the opposite direction and ask whether quantum interference is indeed the sole mechanism responsible for the saturation of the OTOCs for late times. The hope here is that a (possibly improved) version of the diagonal approximation could explain the saturation, thus providing a useful tool to efficiently access numerically the late-time regime, which otherwise is essentially inaccessible to even state-of-the-art semiclassical simulations.

We will show that, indeed, our quasiclassical framework based on the combination of diagonal approximation and classical ergodicity ideas also allows us to obtain a prediction for an asymptotic long-time value of the OTOC. However, comparisons with numerical simulations, which are carried out in the framework of periodically driven Bose-Hubbard dimers and undriven Bose-Hubbard trimers, reveal that this particular long-time value strongly underestimates the true threshold value of the OTOC. We conclude from this finding that the genuinely nonclassical contributions stemming from trajectory pairs with low-angle crossing play a dominant role for times beyond the Ehrenfest time, as was also conjectured in [25].

The chapter is structured as follows. Section 2.2 presents the state of the art of OTOCs in chaotic systems. We give here a brief account of the Wigner-Moyal approach and explain the general ideas behind the reasoning developed in [25]. In Section 2.3, we present the general quasiclassical expression for the OTOC as it is derived from the semiclassical van Vleck-Gutzwiller propagator through the application of the diagonal approximation. We then particularise this expression to the different contributions. In Sections 2.4 and 2.5, we respectively discuss the short-time and the long-time limit of the quasiclassical OTOC. Comparisons with numerical simulations carried out within Bose-Hubbard systems are presented and discussed in Section 2.6.

2.2 OUT-OF-TIME-ORDERED CORRELATOR IN CHAOTIC SYSTEMS

Despite the fact that the definition of OTOCs was already mentioned in the Introduction and Chapter 1, we will still recall it one last time here, as the chapter is entirely dedicated to the study of this particular object. The out-of-time-ordered correlator is defined as

$$C(t) = \langle \psi | \left| [\hat{A}(t), \hat{B}(0)] \right|^2 | \psi \rangle. \quad (2.1)$$

Here $\hat{A}$, $\hat{B}$ are local operators, $\hat{A}(t)$ is the time-evolved operator $\hat{A}$ in the Heisenberg representation, given by

$$\hat{A}(t) = \hat{U}^\dagger(t) \hat{A} \hat{U}(t), \quad (2.2)$$

with $\hat{U}(t)$ the evolution operator, and $|\psi\rangle$ is the initial state of the system [24, 25]. The operators are assumed to be Hermitian to simplify the derivations.

The formalism that we developed is applicable to generic one- or multi-dimensional quantum systems that possess a classical limit. Since our goal is to look at the classical limit, we will naturally use the Wigner-Weyl formalism introduced in Section 1.3.4. In Section 1.5.3, we presented the very direct power expansion in $\hbar$ of the OTOC, which allows the appearance of a Poisson bracket that, in turn, translates into an exponential, hence making the connection between the quantum and classical Lyapunov exponent [25, 27]. It was written

$$\langle \psi | |[\hat{q}_i(t), \hat{p}_j]|^2 | \psi \rangle = \hbar^2 \int d\mathbf{q} d\mathbf{p} \{q_i(t), p_j\}^2 \propto \hbar^2 e^{2\lambda t}, \quad (2.3)$$

with λ is the classical Lyapunov exponent of the system [26]. The exponential growth holds provided that the system is chaotic. This approximation is valid until the Ehrenfest time, where the OTOC saturates due to interferences. Wigner-Moyal does not account for this effect, but results in a never-ending exponential growth.

In order to obtain an expression that is not necessarily time-restricted, we use the semiclassical approximation that we introduced as the van Vleck-Gutzwiller propagator in 1.3.2 and whose expression is given by (1.69). Let us recall that at this point, the coherent aspect of quantum mechanics is still preserved [25, 26, 82].

Our work follows what has been done in [25], although in a slightly different fashion. In Rammensee *et al.*'s paper, the path integral is expressed as a coherent sum over mean-field solutions of the time evolution. Then, the dominant many-body interference terms are computed, which results in contributions that can be represented by 4 diagrams, as is shown in Figure 2.1. Quantum interference is thus considered to some degree in so-called *encounter regions*, which are regions where the four trajectories are in the vicinity of each other, such as in the leftmost part of Figure 2.1a.

In our work, we start from the same path integral but restrict ourselves to strict quasiclassical contributions which do not involve any interference term. Both formalisms predict a finite and non-trivial long-time value. [25] identifies two contributions, Figures 2.1b and 2.1d, whereas our formalism does not enable us to capture the latter. This allows us to identify the importance of interference quantitatively, as our long-time value is purely quasiclassical.

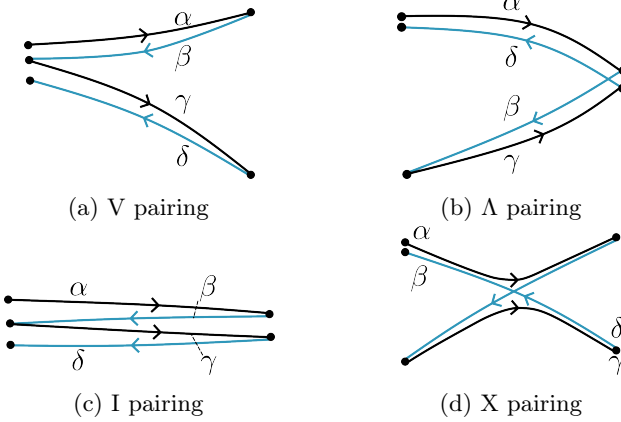


Figure 2.1: The four semiclassical contributions to the OTOC: (a) V pairing, (b) Λ pairing, (c) I pairing, and (d) X pairing. The time axis is assumed horizontal, with the future on the right. The black trajectories (α , γ) are forward-propagating, whereas the blue trajectories (β , δ) are backward-propagating.

2.3 GENERIC TERM OF THE OUT-OF-TIME-ORDERED CORRELATORS

The OTOC is an object whose mathematical expression can quickly become tedious to manipulate, despite having a relatively compact definition. To circumvent that and offer a more pedagogical introduction to our formalism, let us first consider what we name as the generic term of an OTOC:

$$O_{CDEFG}(t) = \langle \psi | \hat{C} \hat{D}(t) \hat{E} \hat{F}(t) \hat{G} | \psi \rangle, \quad (2.4)$$

where each of the 5 indices corresponds to the operator with the same letter. The OTOC can be built by replacing $\hat{D}$, $\hat{F}$ by $\hat{A}$ and $\hat{C}$, $\hat{E}$, $\hat{G}$ by either the identity operator $\hat{1}$, $\hat{B}$ or $\hat{B}^2$ depending on the term of the OTOC. (2.1) can then be written:

$$C(t) = O_{BA1AB}(t) - O_{BABA1}(t) - O_{1ABAB}(t) + O_{1AB^2A1}(t). \quad (2.5)$$

2.3.1 Semiclassical expression

By introducing completeness relations of position eigenstates $\hat{1} = \int d\mathbf{x} |\mathbf{x}\rangle \langle \mathbf{x}|$ between each operators, one can reexpress the expectation value (2.4) as a phase-space integral of matrix elements and propagators:

$$\begin{aligned} O_{CDEFG}(t) &= \int \prod_{i=1}^6 d\mathbf{x}_i \prod_{j=2}^5 d\mathbf{y}_j K^*(\mathbf{y}_2, \mathbf{x}_2, t) K(\mathbf{y}_3, \mathbf{x}_3, t) K^*(\mathbf{y}_4, \mathbf{x}_4, t) \\ &\times K(\mathbf{y}_5, \mathbf{x}_5, t) \langle \mathbf{x}_1 | \hat{C} | \mathbf{x}_2 \rangle \langle \mathbf{y}_2 | \hat{D} | \mathbf{y}_3 \rangle \langle \mathbf{x}_3 | \hat{E} | \mathbf{x}_4 \rangle \langle \mathbf{y}_4 | \hat{F} | \mathbf{y}_5 \rangle \langle \mathbf{x}_5 | \hat{G} | \mathbf{x}_6 \rangle, \end{aligned} \quad (2.6)$$

with $K(\mathbf{q}^f, \mathbf{q}^i, t) = \langle \mathbf{q}^f | \hat{U}(t) | \mathbf{q}^i \rangle$ the propagator from $\mathbf{q}^i$ to $\mathbf{q}^f$ in time t [18, 73].

We then use (1.113) to make the Weyl symbols appear from the matrix elements, and the semiclassical approximation of the propagator given by (1.69) and (1.70). As a result, the phase contains actions related to four different trajectories and expression (2.6) becomes:

$$\begin{aligned} O_{CDEFG}(t) &= \frac{1}{(2\pi\hbar)^{5L}} \int \prod_{i=1}^6 d\mathbf{x}_i \int \prod_{j=2}^5 d\mathbf{y}_j d\mathbf{P} W\left(\frac{\mathbf{x}_1 + \mathbf{x}_6}{2}, \mathbf{P}\right) \\ &\times \sum_{\substack{\alpha: \mathbf{x}_2 \rightarrow \mathbf{y}_2 \\ \beta: \mathbf{x}_3 \rightarrow \mathbf{y}_3}} \sum_{\substack{\gamma: \mathbf{x}_4 \rightarrow \mathbf{y}_4 \\ \delta: \mathbf{x}_5 \rightarrow \mathbf{y}_5}} A_\alpha^* A_\beta A_\gamma^* A_\delta \\ &\times \exp\left(\frac{i}{\hbar} [R_\beta(\mathbf{y}_3, \mathbf{x}_3, t) - R_\alpha(\mathbf{y}_2, \mathbf{x}_2, t) - R_\gamma(\mathbf{y}_4, \mathbf{x}_4, t) + R_\delta(\mathbf{y}_5, \mathbf{x}_5, t)]\right) \\ &\times \int \prod_{k=1}^5 d\mathbf{p}_k C\left(\frac{\mathbf{x}_1 + \mathbf{x}_2}{2}, \mathbf{p}_1\right) D\left(\frac{\mathbf{y}_2 + \mathbf{y}_3}{2}, \mathbf{p}_2\right) \\ &\times E\left(\frac{\mathbf{x}_3 + \mathbf{x}_4}{2}, \mathbf{p}_3\right) F\left(\frac{\mathbf{y}_4 + \mathbf{y}_5}{2}, \mathbf{p}_4\right) G\left(\frac{\mathbf{x}_5 + \mathbf{x}_6}{2}, \mathbf{p}_5\right) \\ &\times \exp[i(\mathbf{p}_1 \cdot (\mathbf{x}_1 - \mathbf{x}_2) + \mathbf{p}_2 \cdot (\mathbf{y}_2 - \mathbf{y}_3) + \mathbf{p}_3 \cdot (\mathbf{x}_3 - \mathbf{x}_4))/\hbar] \\ &\times \exp[i(\mathbf{p}_4 \cdot (\mathbf{y}_4 - \mathbf{y}_5) + \mathbf{p}_5 \cdot (\mathbf{x}_5 - \mathbf{x}_6) - \mathbf{P} \cdot (\mathbf{x}_1 - \mathbf{x}_6))/\hbar], \end{aligned} \quad (2.7)$$

using the shorthand notation $\sum_{\alpha: \mathbf{x} \rightarrow \mathbf{y}} A_\alpha \equiv \sum_{\alpha: \mathbf{x} \rightarrow \mathbf{y}} A_\alpha(\mathbf{y}, \mathbf{x}, t)$. This expression is the starting point of the derivations that follow.

The next step is to use the diagonal approximation, which was introduced in Section 1.3.5. This results in four contributions that are shown in Figure 2.1, but in practice, the last one is related to phenomena beyond quasiclassics and thus does not contribute. A quick reminder of

the diagonal approximation is as follows. One can make the reasonable assumption that uncorrelated paths, with uncorrelated actions, translate into highly oscillatory terms that average out. In other words, the only non-vanishing contributions to the integral are paths that have correlated actions. Inside the phase, the action of a forward-propagating (respectively a backward-propagating) trajectory appears with a plus (respectively a minus) sign. The diagonal approximation consists in identifying pairs of forward- and backward-propagating trajectories that result in a vanishing action difference at the 0th order¹ for a given pair. Interferences are now neglected, and the theory is, in this sense, classical. Nonetheless, as no hypothesis on $\hbar$ has been made thus far, we will refer to this framework as quasiclassical. It also means that this approximation can, in principle, be valid beyond the Ehrenfest time. The three resulting pairings of the diagonal approximation are shown in Figure 2.1a, 2.1b, and 2.1c and are named according to their respective shape. We will be calling them the V , Λ , I pairings. In the framework of the V pairing, we consider that the trajectories α and β , respectively γ and δ , belong to the same family. The Λ pairing pairs the trajectories α with δ , and β with γ . Finally, the I pairing groups all the trajectories together. In order to go further and account for quantum effects, the first correction is the X pairing, represented by 2.1d [25].

Applied on (2.7), the diagonal approximation reads

$$G_{\text{qcl}}(t) = G^V(t) + G^\Lambda(t) - G^I(t), \quad (2.8)$$

which eventually translates to

$$C_{\text{qcl}}(t) = C^V(t) + C^\Lambda(t) - C^I(t), \quad (2.9)$$

for the OTOC, where the subscript qcl stands for quasiclassical. As the I pairing is already contained within the V and Λ pairing, we must remove the overcounting, hence the minus. The complete expression of all the terms of the last two equations is detailed in the following.

2.3.2 V pairing

The first pairing corresponds to the situation where $\alpha \sim \beta$ and $\gamma \sim \delta$, meaning that α and β are actually the same family, likewise for γ and δ .

¹ The development is in the deviation in phase-space between the forward- and backward-propagating trajectories when those are developed around a central one. As will be seen later, this deviation parameter will always be proportional to $\hbar$, thus the development can be considered as an $\hbar$ expansion, and will be referred to as such later in the text.

The first step is to exploit the fact that when two trajectories belong to the same family, they can be linearised around a central one. We thus switch to some centre-of-mass and relative coordinates:

$$\begin{aligned} \mathbf{x}_1 &= \mathcal{X} + \frac{\hbar \mathbf{x}}{2}, & \mathbf{x}_2 &= \mathbf{R}_2 + \frac{\hbar \mathbf{r}_2}{2}, & \mathbf{x}_4 &= \mathbf{R}_4 + \frac{\hbar \mathbf{r}_4}{2}, \\ \mathbf{x}_6 &= \mathcal{X} - \frac{\hbar \mathbf{x}}{2}, & \mathbf{x}_3 &= \mathbf{R}_2 - \frac{\hbar \mathbf{r}_2}{2}, & \mathbf{x}_5 &= \mathbf{R}_4 - \frac{\hbar \mathbf{r}_4}{2}, \\ \mathbf{y}_2 &= \mathbf{S}_2 + \frac{\hbar \mathbf{s}_2}{2}, & \mathbf{y}_4 &= \mathbf{S}_4 + \frac{\hbar \mathbf{s}_4}{2}, \\ \mathbf{y}_3 &= \mathbf{S}_2 - \frac{\hbar \mathbf{s}_2}{2}, & \mathbf{y}_5 &= \mathbf{S}_4 - \frac{\hbar \mathbf{s}_4}{2}. \end{aligned} \quad (2.10)$$

The amplitudes of the propagator are considered at the 0th order only. More specifically

$$A_\alpha^*(\mathbf{S} + \frac{\hbar \mathbf{s}}{2}, \mathbf{R} + \frac{\hbar \mathbf{r}}{2}) A_\alpha(\mathbf{S} - \frac{\hbar \mathbf{s}}{2}, \mathbf{R} - \frac{\hbar \mathbf{r}}{2}) \simeq |A_\alpha(\mathbf{S}, \mathbf{R})|^2, \quad (2.11)$$

up to corrections that scale as $\hbar^2$. The first non-vanishing terms when expanding the actions in the phase are of the 1st order:

$$\begin{aligned} &R_\alpha \left(\mathbf{S}_2 + \frac{\hbar \mathbf{s}_2}{2}, \mathbf{R}_2 + \frac{\hbar \mathbf{r}_2}{2}, t \right) - R_\alpha \left(\mathbf{S}_2 - \frac{\hbar \mathbf{s}_2}{2}, \mathbf{R}_2 - \frac{\hbar \mathbf{r}_2}{2}, t \right) \\ &\simeq \hbar \mathbf{s}_2 \cdot \mathbf{p}_\alpha^f(\mathbf{S}_2, \mathbf{R}_2, t) - \hbar \mathbf{r}_2 \cdot \mathbf{p}_\alpha^i(\mathbf{S}_2, \mathbf{R}_2, t), \end{aligned} \quad (2.12)$$

where we have used $\partial R_\gamma / \partial \mathbf{q}^i(\mathbf{q}^f, \mathbf{q}^i, t) = -\mathbf{p}_\gamma^i(\mathbf{q}^f, \mathbf{q}^i, t)$ and $\partial R_\gamma / \partial \mathbf{q}^f(\mathbf{q}^f, \mathbf{q}^i, t) = \mathbf{p}_\gamma^f(\mathbf{q}^f, \mathbf{q}^i, t)$. This yields

$$\begin{aligned} O_{CDEFG}^V(t) &= \frac{1}{(2\pi)^{5L}} \int d\mathbf{R}_2 d\mathbf{R}_4 d\mathbf{r}_2 d\mathbf{r}_4 d\mathbf{S}_2 d\mathbf{S}_4 d\mathbf{s}_2 d\mathbf{s}_4 d\mathcal{X} d\mathbf{x} \\ &\sum_{\substack{\alpha: \mathbf{R}_2 \rightarrow \mathbf{S}_2 \\ \gamma: \mathbf{R}_4 \rightarrow \mathbf{S}_4}} |A_\alpha|^2 |A_\gamma|^2 W(\mathcal{X}, \mathbf{P}) \int \prod_{i=1}^5 d\mathbf{p}_i C \left(\frac{\mathcal{X} + \mathbf{R}_2}{2} + \frac{\hbar(\mathbf{x} + \mathbf{r}_2)}{4}, \mathbf{p}_1 \right) \\ &\times D(\mathbf{S}_2, \mathbf{p}_2) E \left(\frac{\mathbf{R}_2 + \mathbf{R}_4}{2} + \frac{\hbar(\mathbf{r}_4 - \mathbf{r}_2)}{4}, \mathbf{p}_3 \right) F(\mathbf{S}_4, \mathbf{p}_4) \\ &\times G \left(\frac{\mathcal{X} + \mathbf{R}_4}{2} - \frac{\hbar(\mathbf{x} + \mathbf{r}_4)}{4}, \mathbf{p}_5 \right) \exp \left[i \left(\mathbf{s}_2 \cdot (\mathbf{p}_2 - \mathbf{p}_\alpha^f) \right) \right] \\ &\times \exp \left[i \left(\mathbf{r}_2 \cdot (\mathbf{p}_\alpha^i - \frac{\mathbf{p}_1 + \mathbf{p}_3}{2}) + \mathbf{s}_4 \cdot (\mathbf{p}_4 - \mathbf{p}_\gamma^f) + \mathbf{r}_4 \cdot (\mathbf{p}_\gamma^i - \frac{\mathbf{p}_3 + \mathbf{p}_5}{2}) \right) \right] \\ &\times \exp \left[i \left(\mathcal{X} \cdot (\mathbf{p}_1 - \mathbf{p}_5) + \mathbf{x} \cdot \frac{\mathbf{p}_1 + \mathbf{p}_5}{2} + \mathbf{R}_2 \cdot (\mathbf{p}_3 - \mathbf{p}_1) + \mathbf{R}_4 \cdot (\mathbf{p}_5 - \mathbf{p}_3) \right) \right] \\ &\times \exp[-i\mathbf{P} \cdot \mathbf{x}]. \end{aligned} \quad (2.13)$$

In order to make the last step towards the symplectic formalism, we will introduce a symmetry between the position and momentum arguments of a given symbol, and between two pairs of symbols as well. To this end, we will perform several changes of variables to some new centre-of-mass and relative coordinates. First, we do it for the position argument of symbols C and G :

$$\begin{aligned} \mathbf{Y} &= \frac{1}{2} \left(\frac{\mathbf{X} + \mathbf{R}_2}{2} + \frac{\hbar(\mathbf{x} + \mathbf{r}_2)}{4} + \frac{\mathbf{X} + \mathbf{R}_4}{2} + \frac{\hbar(\mathbf{x} + \mathbf{r}_4)}{4} \right) \\ \mathbf{y} &= \frac{1}{2} \left(\frac{\mathbf{X} + \mathbf{R}_2}{2} + \frac{\hbar(\mathbf{x} + \mathbf{r}_2)}{4} - \frac{\mathbf{X} + \mathbf{R}_4}{2} - \frac{\hbar(\mathbf{x} + \mathbf{r}_4)}{4} \right) \\ \mathbf{p}_1 &= \mathbf{\Pi}_1 + \frac{\hbar\omega_1}{2}, \quad \mathbf{p}_5 = \mathbf{\Pi}_1 - \frac{\hbar\omega_1}{2}. \end{aligned} \quad (2.14)$$

We then use the amplitudes of the propagator as a Jacobian of a change of variables to change the integration with respect to the final positions $\mathbf{S}_2, \mathbf{S}_4$ to initial momenta $\mathbf{p}_\alpha^i, \mathbf{p}_\beta^i$:

$$\sum_\alpha |A_\alpha|^2 = \sum_\alpha \frac{1}{(2\pi\hbar)^L} \left| \det \frac{\partial^2 R}{\partial \mathbf{S}_2 \partial \mathbf{R}_2}(\mathbf{S}_2, \mathbf{R}_2) \right| = \sum_\alpha \frac{1}{(2\pi\hbar)^L} \left| \frac{\partial \mathbf{p}_\alpha^i}{\partial \mathbf{S}_2} \right|, \quad (2.15)$$

where we have used this time $\partial R_\gamma / \partial \mathbf{q}^i(\mathbf{q}^f, \mathbf{q}^i, t) = -\mathbf{p}_\gamma^i(\mathbf{q}^f, \mathbf{q}^i, t)$. We then go to centre-of-mass and relative coordinate for the symbols D and F :

$$\begin{aligned} \mathbf{R}_2 &= \mathbf{R} + \frac{\hbar\mathbf{r}}{2}, \quad \mathbf{p}_\alpha^i = \mathbf{\Pi}_2 + \frac{\hbar\omega_2}{2}, \\ \mathbf{R}_4 &= \mathbf{R} - \frac{\hbar\mathbf{r}}{2}, \quad \mathbf{p}_\beta^i = \mathbf{\Pi}_2 - \frac{\hbar\omega_2}{2}. \end{aligned} \quad (2.16)$$

We perform the integral with respect to $\mathbf{x}$ and obtain

$$\begin{aligned} O_{CDEFG}^V(t) &= \frac{1}{(2\pi)^{4L}} \int d\mathbf{X} d\mathbf{x} d\mathbf{Y} d\mathbf{y} d\mathbf{R} d\mathbf{r} d\mathbf{P} d\mathbf{\Pi}_1 d\mathbf{\Pi}_2 d\omega_1 d\omega_2 \\ &\exp(i(\omega_2 \cdot (2\mathbf{Y} - \mathbf{X} - \mathbf{R}))) \\ &\times \exp(i(\omega_1 \cdot (\mathbf{X} - \mathbf{R}) + \mathbf{y} \cdot (\mathbf{\Pi}_1 - \mathbf{P}) + \mathbf{r} \cdot (\mathbf{P} + \mathbf{\Pi}_2 - 2\mathbf{\Pi}_1))) \\ &\times C \left(\mathbf{Y} + \frac{\hbar\mathbf{y}}{4}, \mathbf{\Pi}_1 + \frac{\hbar\omega_1}{4} \right) D \left((\mathbf{R}_t, \mathbf{P}_t) \left(\mathbf{R} + \frac{\hbar\mathbf{r}}{4}, \mathbf{\Pi}_2 + \frac{\hbar\omega_2}{4} \right) \right) \\ &\times E(\mathbf{X} - 2\mathbf{Y} + 2\mathbf{R}, \mathbf{P} - 2\mathbf{\Pi}_1 + 2\mathbf{\Pi}_2) \\ &\times F \left((\mathbf{R}_t, \mathbf{P}_t) \left(\mathbf{R} - \frac{\hbar\mathbf{r}}{4}, \mathbf{\Pi}_2 - \frac{\hbar\omega_2}{4} \right) \right) \\ &\times G \left(\mathbf{Y} - \frac{\hbar\mathbf{y}}{4}, \mathbf{\Pi}_1 - \frac{\hbar\omega_1}{4} \right) W(\mathbf{X}, \mathbf{P}), \end{aligned} \quad (2.17)$$

where we used the notation $(\mathbf{R}_t, \mathbf{P}_t)(\mathbf{R}, \mathbf{\Pi}) = (\mathbf{R}_t(\mathbf{R}, \mathbf{\Pi}), \mathbf{P}_t(\mathbf{R}, \mathbf{\Pi}))$ to shorten the expression, and where $\mathbf{R}_t(\mathbf{R}, \mathbf{\Pi})$ and $\mathbf{P}_t(\mathbf{R}, \mathbf{\Pi})$ means respectively the position and momentum after an evolution for t time, having started from $(\mathbf{R}, \mathbf{\Pi})$.

In the expression for all the pairings, there is eventually a symmetry between the position and momentum arguments, which allows us to regroup them in a single vector, called a symplectic vector. We introduce the symplectic (or wedge) product $\wedge$ that is defined as follows: if $X = (\mathbf{q}_1, \mathbf{p}_1)$ and $Y = (\mathbf{q}_2, \mathbf{p}_2)$, then

$$X \wedge Y = X J Y = \mathbf{q}_1 \cdot \mathbf{p}_2 - \mathbf{q}_2 \cdot \mathbf{p}_1, \quad (2.18)$$

with J the symplectic matrix [86].

Using this newly introduced notation, the general term of the V pairing is

$$\begin{aligned} O_{CDEFG}^V(t) &= \int \frac{dX_1 dX_2 dX_3 d\Delta_1 d\Delta_2}{(2\pi)^{4L}} e^{i\Delta_1 \wedge (X_2 - X_3)} e^{i\Delta_2 \wedge (X_1 - 2X_2 + X_3)} \\ &\times C\left(X_2 + \frac{\hbar\Delta_1}{4}\right) D\left(X_t\left(X_1 + \frac{\hbar\Delta_2}{4}\right)\right) E(2X_1 - 2X_2 + X_3) \\ &\times F\left(X_t\left(X_1 - \frac{\hbar\Delta_2}{4}\right)\right) G\left(X_2 - \frac{\hbar\Delta_1}{4}\right) W(X_3), \end{aligned} \quad (2.19)$$

where $X_1 = (\mathbf{Y}, \mathbf{\Pi}_1)$, $X_2 = (\mathbf{R}, \mathbf{\Pi}_2)$, $X_3 = (\mathbf{X}, \mathbf{P})$, $\Delta_1 = (\mathbf{y}, \boldsymbol{\omega}_1)$, $\Delta_2 = (\mathbf{r}, \boldsymbol{\omega}_2)$, and X_t indicates the evolution to time t .

Using this general term to build the OTOC, as prescribed by (2.5), yields the following expression for the V pairing:

$$\begin{aligned} C^V(t) &= \int \frac{dX_1 dX_2 dX_3 d\Delta_1 d\Delta_2}{(2\pi)^{4L}} e^{i\Delta_1 \wedge (X_2 - X_3)} e^{i\Delta_2 \wedge (X_1 - 2X_2 + X_3)} \\ &\times A_t\left(X_1 + \frac{\hbar\Delta_2}{4}\right) A_t\left(X_1 - \frac{\hbar\Delta_2}{4}\right) \left[B\left(X_2 + \frac{\hbar\Delta_1}{4}\right) B\left(X_2 - \frac{\hbar\Delta_1}{4}\right) \right. \\ &- B(2X_1 - 2X_2 + X_3) \left(B\left(X_2 + \frac{\hbar\Delta_1}{4}\right) + B\left(X_2 - \frac{\hbar\Delta_1}{4}\right) \right) \\ &\left. + (\hat{B}^2)_W(2X_1 - 2X_2 + X_3) \right] W(X_3). \end{aligned} \quad (2.20)$$

The OTOC has thus been rewritten as an initial value problem in the form of phase space integrals weighed by the Wigner function.

2.3.3 Λ pairing

The second pairing follows the same steps as the first one, although with some changes when it comes to the integration variables. The main difference is that one naturally ends up with integrals with respect to final conditions instead of initial ones.

Starting from (2.7), this time the pairs of trajectories are $\alpha \sim \delta$ and $\beta \sim \gamma$. Similarly to the V pairing, we go to some new centre-of-mass and relative coordinates:

$$\begin{aligned}
 \mathbf{x}_1 &= \mathcal{X} + \frac{\hbar \mathbf{x}}{2}, & \mathbf{x}_2 &= \mathbf{R}_2 + \frac{\hbar \mathbf{r}_2}{2}, & \mathbf{x}_3 &= \mathbf{R}_3 + \frac{\hbar \mathbf{r}_3}{2}, \\
 \mathbf{x}_6 &= \mathcal{X} - \frac{\hbar \mathbf{x}}{2}, & \mathbf{x}_5 &= \mathbf{R}_2 - \frac{\hbar \mathbf{r}_2}{2}, & \mathbf{x}_4 &= \mathbf{R}_3 - \frac{\hbar \mathbf{r}_3}{2}, \\
 \mathbf{y}_2 &= \mathbf{S}_2 + \frac{\hbar \mathbf{s}_2}{2}, & \mathbf{y}_3 &= \mathbf{S}_3 + \frac{\hbar \mathbf{s}_3}{2}, \\
 \mathbf{y}_5 &= \mathbf{S}_2 - \frac{\hbar \mathbf{s}_2}{2}, & \mathbf{y}_4 &= \mathbf{S}_3 - \frac{\hbar \mathbf{s}_3}{2}.
 \end{aligned} \tag{2.21}$$

We can then linearise the action around these new centre-of-mass coordinates, which calls for some other changes of variables, this time related to the momenta:

$$\begin{aligned}
 \mathbf{p}_1 &= \mathbf{\Pi}_1 + \frac{\hbar \boldsymbol{\omega}_1}{2}, & \mathbf{p}_2 &= \mathbf{\Pi}_2 + \frac{\hbar \boldsymbol{\omega}_2}{2}, \\
 \mathbf{p}_5 &= \mathbf{\Pi}_1 - \frac{\hbar \boldsymbol{\omega}_1}{2}, & \mathbf{p}_4 &= \mathbf{\Pi}_2 - \frac{\hbar \boldsymbol{\omega}_2}{2}.
 \end{aligned} \tag{2.22}$$

By performing the integration with respect to $\mathbf{r}_3$ one can rewrite (2.7) as

$$\begin{aligned}
O_{CDEFG}^\Lambda(t) = & \int d\boldsymbol{\mathcal{X}} d\boldsymbol{\Delta\mathcal{X}} d\mathbf{R}_2 d\mathbf{R}_3 d\mathbf{r}_2 d\mathbf{S}_2 d\mathbf{S}_3 ds_2 ds_3 d\boldsymbol{\Pi}_1 d\boldsymbol{\Pi}_2 d\boldsymbol{\omega}_1 d\boldsymbol{\omega}_2 \\
& \times W(\boldsymbol{\mathcal{X}}, \mathbf{P}) \sum_{\alpha, \beta} \frac{|A_\alpha|^2 |A_\beta|^2}{(2\pi)^{4L}} \exp \left[i \left(\mathbf{s}_2 \cdot (\boldsymbol{\Pi}_2 - \mathbf{p}_\alpha^f) + \mathbf{r}_2 \cdot (\mathbf{p}_\alpha^i - \boldsymbol{\Pi}_1) \right) \right] \\
& \times \exp \left[i \left(\mathbf{s}_3 \cdot (\mathbf{p}_\beta^f - \boldsymbol{\Pi}_2) + (\boldsymbol{\mathcal{X}} - \mathbf{R}_2) \cdot \boldsymbol{\omega}_1 + (\mathbf{S}_2 - \mathbf{S}_3) \cdot \boldsymbol{\omega}_2 - \mathbf{P} \cdot \mathbf{x} \right) \right] \\
& \times C \left(\frac{\boldsymbol{\mathcal{X}} + \mathbf{R}_2}{2} + \frac{\hbar(\boldsymbol{\Delta\mathcal{X}} + \mathbf{r}_2)}{4}, \boldsymbol{\Pi}_1 + \frac{\hbar\boldsymbol{\omega}_1}{2} \right) \\
& \times D \left(\frac{\mathbf{S}_2 + \mathbf{S}_3}{2} + \frac{\hbar(\mathbf{s}_2 + \mathbf{s}_3)}{4}, \boldsymbol{\Pi}_2 + \frac{\hbar\boldsymbol{\omega}_2}{2} \right) E(\mathbf{R}_3, \mathbf{p}_\beta^i) \\
& \times F \left(\frac{\mathbf{S}_2 + \mathbf{S}_3}{2} - \frac{\hbar(\mathbf{s}_2 + \mathbf{s}_3)}{4}, \boldsymbol{\Pi}_2 - \frac{\hbar\boldsymbol{\omega}_2}{2} \right) \\
& \times G \left(\frac{\boldsymbol{\mathcal{X}} + \mathbf{R}_2}{2} - \frac{\hbar(\boldsymbol{\Delta\mathcal{X}} + \mathbf{r}_2)}{4}, \boldsymbol{\Pi}_1 - \frac{\hbar\boldsymbol{\omega}_1}{2} \right). \tag{2.23}
\end{aligned}$$

In order to obtain an expression that is writable in symplectic formalism, one must perform additional changes of variables that consist of shifts to symmetrise the position and momentum arguments of a given symbol. Again, one uses the amplitudes of the propagator as a Jacobian of a change of variables, this time from initial position $\mathbf{R}_2, \mathbf{R}_3$ to final momenta $\mathbf{p}_\alpha^f, \mathbf{p}_\beta^f$:

$$\sum_\alpha |A_\alpha|^2 = \sum_\alpha \frac{1}{(2\pi\hbar)^L} \left| \frac{\partial \mathbf{p}_\alpha^f}{\partial \mathbf{R}_2} \right|, \tag{2.24}$$

where we have used $\partial R_\gamma / \partial \mathbf{q}^f(\mathbf{q}^f, \mathbf{q}^i, t) = \mathbf{p}_\gamma^f(\mathbf{q}^f, \mathbf{q}^i, t)$. The final expression is then

$$\begin{aligned}
O_{CDEFG}^\Lambda(t) = & \frac{1}{(2\pi)^{4L}} \int d\mathbf{X} d\mathbf{r}_2 d\mathbf{S}_2 d\mathbf{S}_3 d\mathbf{s}_2 d\mathbf{p}_\alpha^f d\mathbf{p}_\beta^f d\mathbf{\Pi}_1 d\mathbf{\Pi}_2 d\boldsymbol{\omega}_1 d\boldsymbol{\omega}_3 \\
& \times \exp \left[i \left(\mathbf{s}_2 \cdot (\mathbf{p}_\beta^f - \mathbf{p}_\alpha^f) \right) + \mathbf{r}_2 \cdot (\mathbf{P}_{-t}(2\mathbf{S}_2 - \mathbf{S}_3, 2\mathbf{p}_\alpha^f - \mathbf{p}_\beta^f) - \mathbf{\Pi}_1) \right] \\
& \times \exp \left[i \left((\mathbf{X} - \mathbf{R}_{-t}(2\mathbf{S}_2 - \mathbf{S}_3, 2\mathbf{p}_\alpha^f - \mathbf{p}_\beta^f) \cdot \boldsymbol{\omega}_1 + (\mathbf{S}_2 - \mathbf{S}_3) \cdot \boldsymbol{\omega}_2 \right) \right] \\
& \times C \left(\mathbf{X} + \frac{\hbar \mathbf{r}_2}{4}, \mathbf{\Pi}_1 + \frac{\hbar \boldsymbol{\omega}_1}{4} \right) D \left(\mathbf{S}_2 + \frac{\hbar \mathbf{s}_2}{4}, \mathbf{p}_\alpha^f + \frac{\hbar \boldsymbol{\omega}_2}{4} \right) \\
& \times E \left(\mathbf{R}_{-t}(\mathbf{S}_3, \mathbf{p}_\beta^f), \mathbf{P}_{-t}(\mathbf{S}_3, \mathbf{p}_\beta^f) \right) F \left(\mathbf{S}_2 - \frac{\hbar \mathbf{s}_2}{4}, \mathbf{p}_\alpha^f - \frac{\hbar \boldsymbol{\omega}_2}{4} \right) \\
& \times G \left(\mathbf{X} - \frac{\hbar \mathbf{r}_2}{4}, \mathbf{\Pi}_1 - \frac{\hbar \boldsymbol{\omega}_1}{4} \right) \\
& \times W \left(2\mathbf{X} - \mathbf{R}_{-t}(2\mathbf{S}_2 - \mathbf{S}_3, 2\mathbf{p}_\alpha^f - \mathbf{p}_\beta^f), 2\mathbf{\Pi}_1 - \mathbf{P}_{-t}(2\mathbf{S}_2 - \mathbf{S}_3, 2\mathbf{p}_\alpha^f - \mathbf{p}_\beta^f) \right), \tag{2.25}
\end{aligned}$$

where $\mathbf{R}_{-t}(\mathbf{S}, \mathbf{P})$ and $\mathbf{P}_{-t}(\mathbf{S}, \mathbf{P})$ are the position and momentum obtained from the backward evolution of $(\mathbf{S}, \mathbf{P})$ for time t .

The symplectic notation reads

$$\begin{aligned}
O_{CDEFG}^\Lambda(t) = & \int \frac{dX dS_2 dS_3 d\Delta_2 d\Delta_3}{(2\pi)^{4L}} e^{i\Delta_1 \wedge (X - X_{-t}(2S_2 - S_3))} e^{i\Delta_2 \wedge (S_3 - S_2)} \\
& \times C \left(X + \frac{\hbar \Delta_1}{4} \right) D \left(S_2 + \frac{\hbar \Delta_2}{4} \right) E(X_{-t}(S_3)) F \left(S_2 - \frac{\hbar \Delta_2}{4} \right) \\
& \times G \left(X - \frac{\hbar \Delta_1}{4} \right) W(2X - X_{-t}(2S_2 - S_3)), \tag{2.26}
\end{aligned}$$

where $X = (\mathbf{X}, \mathbf{\Pi}_1)$, $S_2 = (\mathbf{S}_2, \mathbf{p}_\alpha^f)$, $S_3 = (\mathbf{S}_3, \mathbf{p}_\beta^f)$, $\Delta_1 = (\mathbf{r}_2, \boldsymbol{\omega}_1)$, $\Delta_2 = (\mathbf{s}_2, \boldsymbol{\omega}_2)$, and $X_{-t}(S)$ is the backward evolution from S for time t .

The Λ contribution to the OTOC reads

$$\begin{aligned}
C^\Lambda(t)(t) = & \int \frac{dX dS_2 dS_3 d\Delta_1 d\Delta_2}{(2\pi)^{4L}} e^{i\Delta_1 \wedge (X_{-t}(2S_2 - S_3) - X)} e^{i\Delta_2 \wedge (S_3 - S_2)} \\
& \times A \left(S_2 + \frac{\hbar \Delta_2}{4} \right) A \left(S_2 - \frac{\hbar \Delta_2}{4} \right) \left[B \left(X + \frac{\hbar \Delta_1}{4} \right) B \left(X - \frac{\hbar \Delta_1}{4} \right) \right. \\
& - B(X_{-t}(S_3)) \left(B \left(X + \frac{\hbar \Delta_1}{4} \right) + B \left(X - \frac{\hbar \Delta_1}{4} \right) \right) \\
& \left. + \left(\hat{B}^2 \right)_W(X_{-t}(S_3)) \right] W(2X - X_{-t}(2S_2 - S_3)). \tag{2.27}
\end{aligned}$$

Let us note that, contrarily to (2.20), this contribution is expressed as a mix between phase-space integrals with respect to initial values (the coordinates X , Δ_1 , and Δ_2) and final values (S_1 and S_2).

2.3.4 I pairing

Finally, let us consider the third pairing. When summing the contributions from both the V and Λ pairing, we are overcounting the subcase where all four trajectories are near one another, i.e., $\alpha \sim \beta \sim \gamma \sim \delta$. Therefore, we actually have to subtract this contribution to account for it only once. Intuitively, one would try to linearise all four trajectories around a global central one. However, using the same set of variables as for the Λ pairing seems far more suitable for the derivation. One can thus follow the same steps as for the last pairing and obtain

$$\begin{aligned}
O_{CDEFG}^I(t) = & \frac{1}{(2\pi)^{4L}2^{2L}} \int d\mathcal{X} d\mathbf{R}_2 \mathbf{R}_3 d\mathbf{r}_2 d\mathbf{S}_2 d\mathbf{S}_3 d\mathbf{s}_2 d\mathbf{\Pi}_1 d\mathbf{\Pi}_2 d\boldsymbol{\omega}_1 d\boldsymbol{\omega}_2 \\
& \times \sum_{\alpha} \left| \det \frac{\partial^2 R_{\alpha}(\mathbf{S}_2, \mathbf{R}_2)}{\partial \mathbf{S}_2 \partial \mathbf{R}_2} \right| \left| \det \frac{\partial^2 R_{\alpha}(\mathbf{S}_3, \mathbf{R}_3)}{\partial \mathbf{S}_3 \partial \mathbf{R}_3} \right| \\
& \times \exp \left(i(\mathbf{s}_2 \cdot (\mathbf{\Pi}_2 - \mathbf{p}_{\alpha}^f(\mathbf{S}_2, \mathbf{R}_2))) \right) \\
& \times \exp \left[\left(\mathbf{r}_2 \cdot (\mathbf{p}_{\alpha}^i(\mathbf{S}_2, \mathbf{R}_2) - \mathbf{\Pi}_1) + (\mathcal{X} - \mathbf{R}_2) \cdot \boldsymbol{\omega}_1 + \frac{\mathbf{S}_2 - \mathbf{S}_3}{2} \cdot \boldsymbol{\omega}_2 \right) \right] \\
& \times C \left(\mathcal{X} + \frac{\hbar \mathbf{r}_2}{4}, \mathbf{\Pi}_1 + \frac{\hbar \boldsymbol{\omega}_1}{4} \right) \\
& \times D \left(\frac{\mathbf{S}_2 + \mathbf{S}_3}{2} + \frac{\hbar \mathbf{s}_2}{4}, \frac{\mathbf{p}_{\alpha}^f(\mathbf{S}_2, \mathbf{R}_2) + \mathbf{p}_{\alpha}^f(\mathbf{S}_3, \mathbf{R}_3)}{2} + \frac{\hbar \boldsymbol{\omega}_2}{4} \right) \\
& \times E \left(\mathbf{R}_3, \mathbf{p}_{\alpha}^f(\mathbf{S}_3, \mathbf{R}_3) \right) \\
& \times F \left(\frac{\mathbf{S}_2 + \mathbf{S}_3}{2} - \frac{\hbar \mathbf{s}_2}{4}, \frac{\mathbf{p}_{\alpha}^f(\mathbf{S}_2, \mathbf{R}_2) + \mathbf{p}_{\alpha}^f(\mathbf{S}_3, \mathbf{R}_3)}{2} - \frac{\hbar \boldsymbol{\omega}_2}{4} \right) \\
& \times G \left(\mathcal{X} - \frac{\hbar \mathbf{r}_2}{4}, \mathbf{\Pi}_1 - \frac{\hbar \boldsymbol{\omega}_1}{4} \right) W(2\mathcal{X} - \mathbf{R}_2, 2\mathbf{\Pi}_1 - \mathbf{p}_{\alpha}^i(\mathbf{S}_2, \mathbf{R}_2)).
\end{aligned} \tag{2.28}$$

To introduce the symplectic notation, we add integration over Dirac deltas for the two initial and the two final momenta, resulting in

$$\begin{aligned}
O_{CDEFG}^I(t) = & \int \frac{dX dR_2 dR_3 dS_2 dS_3 d\Delta_1 d\Delta_2}{2^{2L} (2\pi)^{4L}} \\
& \times \sum_{\alpha} \left| \det \frac{\partial^2 R_{\alpha}(\mathbf{S}_2, \mathbf{R}_2)}{\partial \mathbf{S}_2 \partial \mathbf{R}_2} \right| \left| \det \frac{\partial^2 R_{\alpha}(\mathbf{S}_3, \mathbf{R}_3)}{\partial \mathbf{S}_3 \partial \mathbf{R}_3} \right| \\
& \times e^{i\Delta_1 \wedge (R_2 - R)} e^{i\Delta_2 \wedge (S_3 - S_2)/2} \\
& \times C \left(\frac{X + R_2}{2} + \frac{\hbar \Delta_1}{4} \right) D \left(\frac{S_2 + S_3}{2} + \frac{\hbar \Delta_1}{4} \right) E(R_3) \\
& \times F \left(\frac{S_2 + S_3}{2} - \frac{\hbar \Delta_1}{4} \right) G \left(\frac{X + R_2}{2} - \frac{\hbar \Delta_1}{4} \right) \\
& \times \delta(\mathbf{\Pi}_2 - \mathbf{p}_{\alpha}^i(\mathbf{S}_2, \mathbf{R}_2)) \delta(\mathbf{\Pi}_3 - \mathbf{p}_{\alpha}^i(\mathbf{S}_3, \mathbf{R}_3)) \\
& \times \delta(\mathbf{P}_2 - \mathbf{p}_{\alpha}^f(\mathbf{S}_2, \mathbf{R}_2)) \delta(\mathbf{P}_3 - \mathbf{p}_{\alpha}^f(\mathbf{S}_3, \mathbf{R}_3)) W(2X - R_2), \quad (2.29)
\end{aligned}$$

where part of the expression cannot be put in symplectic formalism. The symplectic vectors are $X = (\mathcal{X}, \mathbf{\Pi}_1)$, $R_2 = (\mathbf{R}_2, \mathbf{\Pi}_2)$, $R_3 = (\mathbf{R}_3, \mathbf{\Pi}_3)$, $S_2 = (\mathbf{S}_2, \mathbf{P}_2)$, $S_3 = (\mathbf{S}_3, \mathbf{P}_3)$, $\Delta_1 = (\mathbf{r}_2, \boldsymbol{\omega}_1)$, $\Delta_2 = (\mathbf{s}_2, \boldsymbol{\omega}_2)$, and the four δ 's at the end are introduced to write the expression as phase-space integrals.

The I-pairing contribution to the OTOC is

$$\begin{aligned}
C^I(t) = & \int \frac{dX dR_2 dR_3 dS_2 dS_3 d\Delta_1 d\Delta_2}{(2\pi)^{4L} 2^{2L}} \sum_{\alpha} \left| \det \frac{\partial^2 R_{\alpha}(\mathbf{S}_2, \mathbf{R}_2)}{\partial \mathbf{S}_2 \partial \mathbf{R}_2} \right| \\
& \times \left| \det \frac{\partial^2 R_{\alpha}(\mathbf{S}_3, \mathbf{R}_3)}{\partial \mathbf{S}_3 \partial \mathbf{R}_3} \right| e^{i\Delta_1 \wedge (R_2 - X)} e^{i\Delta_2 \wedge (S_3 - S_2)/2} A \left(\frac{S_2 + S_3}{2} + \frac{\hbar \Delta_2}{4} \right) \\
& \times A \left(\frac{S_2 + S_3}{2} - \frac{\hbar \Delta_2}{4} \right) \left[B \left(\frac{X + R_2}{2} + \frac{\hbar \Delta_1}{4} \right) B \left(\frac{X + R_2}{2} - \frac{\hbar \Delta_1}{4} \right) \right. \\
& \left. - B(R_3) \left(B \left(\frac{X + R_2}{2} + \frac{\hbar \Delta_1}{4} \right) + B \left(\frac{X + R_2}{2} - \frac{\hbar \Delta_1}{4} \right) \right) + (\hat{B}^2)_W(R_3) \right] \\
& \times \delta(\mathbf{\Pi}_2 - \mathbf{p}_{\alpha}^i(\mathbf{S}_2, \mathbf{R}_2)) \delta(\mathbf{\Pi}_3 - \mathbf{p}_{\alpha}^i(\mathbf{S}_3, \mathbf{R}_3)) \delta(\mathbf{P}_2 - \mathbf{p}_{\alpha}^f(\mathbf{S}_2, \mathbf{R}_2)) \\
& \times \delta(\mathbf{P}_3 - \mathbf{p}_{\alpha}^f(\mathbf{S}_3, \mathbf{R}_3)) W(X). \quad (2.30)
\end{aligned}$$

Note that since there is only one family of trajectories, there is not a double sum $\sum_{\alpha, \gamma} |A_{\alpha}|^2 |A_{\gamma}|^2$ as prefactor, but rather $\sum_{\alpha} |A_{\alpha}|^2 |A_{\alpha}|^2$, which requires extra steps to be dealt with when looking at the $\hbar \rightarrow 0$ limit.

2.4 $\hbar$ EXPANSION

Let us now discuss the classical limit $\hbar \rightarrow 0$ of each contribution to the OTOC. As a reminder, the crude limit tells us that the integrand of the OTOC should become a Poisson bracket. What results from the $\hbar$ expansion should thus give this same expression. It is important to note that the contributions (2.20), (2.27), and (2.47) are quasiclassical expressions where no $\hbar$ expansion has been made, so they are in principle valid beyond the Ehrenfest time. Once the expansion is made, the Ehrenfest time, which behaves as $\log(1/\hbar)/\lambda_L$, tends to infinity. As it corresponds to the saturation time [25, 26], it implies that the OTOC never saturates and thus that the expansion is valid for short times only.

2.4.1 V pairing

Starting from expression (2.20), the 0th order in $\hbar$ corresponds to neglecting any $\hbar$ dependencies. It becomes

$$\begin{aligned} C^V(t) = & \int \frac{dX_1 dX_2 dX_3 d\Delta_1 d\Delta_2}{(2\pi)^{4L}} e^{i\Delta_1 \wedge (X_2 - X_3)} e^{i\Delta_2 \wedge (X_1 - 2X_2 + X_3)} \\ & \times A_t^2(X_1) \left[B(X_2) - B(2X_1 - 2X_2 + X_3) \right]^2 W(X_3) + \mathcal{O}(\hbar). \end{aligned} \quad (2.31)$$

We then perform the integral with respect to Δ_1 and Δ_2 , which yields Dirac deltas:

$$\begin{aligned} \int \frac{d\Delta_1 d\Delta_2}{(2\pi)^{4L}} e^{i\Delta_1 \wedge (X_2 - X_3)} e^{i\Delta_2 \wedge (X_1 - 2X_2 + X_3)} = & \delta(X_2 - X_3) \\ & \times \delta(X_1 - X_2). \end{aligned} \quad (2.32)$$

This will make the square bracket vanish, and thus so will the OTOC at the 0th order.

The 1st order term in $\hbar$ vanishes as well owing to the $\hbar \longleftrightarrow -\hbar$ symmetry of the expression (2.20) and to the fact that the 1st order of the symbol of a square operator vanishes. To evaluate the 2nd order in $\hbar$, one splits the problem into two parts by considering only the expansion up to $\hbar^2$ in the symbol of $\hat{A}$, and in a separate term, only the expansion of the symbol of $\hat{B}$. The two contributions to the OTOC will be labelled

C_A^V and C_B^V respectively.

For the first term, one can write

$$\begin{aligned} C_A^V(t) &= \frac{\hbar^2}{4} \int \frac{dX_1 dX_2 d\Delta_2}{(2\pi)^{2L}} e^{i\Delta_2 \wedge (X_1 - X_2)} \sum_{k,l}^{2L} \Delta_{2,k} \Delta_{2,l} \\ &\quad \times [A_t(X_1) \partial_{kl}^2 A_t(X_1) - \partial_k A_t(X_1) \partial_l A_t(X_1)] \\ &\quad \times [B(X_2) - B(2X_1 - X_2)]^2 W(X_2), \end{aligned} \quad (2.33)$$

where we have already performed the integration with respect to Δ_1 . The procedure is then similar to that of the symbol of a squared operator, see (A.5). The Δ_2 's will be transformed into derivative operators with respect to components of X_1 acting on the exponential, followed by an integration by parts that will move said operators to the rest of the integrand. For some generic function f of symplectic vectors X and Y such that f vanishes at the integration boundaries, this translates to

$$\begin{aligned} \int dX dY d\Delta e^{i\Delta \wedge (X - Y)} \Delta_k f(X, Y) \\ &= \int dX dY d\Delta \frac{\sigma_k}{i} \frac{\partial e^{i\Delta \wedge (X - Y)}}{\partial X_{\bar{k}}} f(X, Y) \\ &= (2\pi\hbar)^{2L} \int dX dY \frac{-\sigma_k}{i} \delta(X - Y) \frac{\partial f}{\partial X_{\bar{k}}} (X, Y), \end{aligned} \quad (2.34)$$

where we integrated by parts to obtain the last line. Applying this to (2.33) leads to

$$\begin{aligned} C_A^V(t)(t) &= -\frac{\hbar^2}{2} \int dX \sum_{k,l=1}^{2L} \sigma_k \sigma_l \partial_{\bar{k}} B(X) \partial_l B(X) \\ &\quad [A_t(X) \partial_{kl}^2 A_t(X) - \partial_k A_t(X) \partial_l A_t(X)] W(X). \end{aligned} \quad (2.35)$$

In this development, and those that follow, we assumed that the observables vanish at the integration boundaries so that all the expressions that appear are integrable. While this is technically not the case for operators that we will use, such as the standard population operator $A(Y) = (Y_k^2 + Y_{\bar{k}}^2)/2$, we consider this operator to be amended, *e.g.* $A(Y) = \exp\left(-\varepsilon \sum_{k=1}^{2L} Y_k^2\right) (Y_k^2 + Y_{\bar{k}}^2)/2$ for sufficiently small ε . This reflects the experimental limitations for the detection of such an observable.

Equivalently, one could have transformed the $\Delta_{2,k}\Delta_{2,l}$ as derivatives with respect to X_2 . The vanishing of the integrated term is then assured by the Wigner function. A similar approach for C_B^V yields

$$C_B^V(t)(t) = \frac{\hbar^2}{2} \int dX \sum_{k,l=1}^{2L} \frac{\sigma_k \sigma_l}{i^2} \partial_{\bar{k}} B(X) \partial_{\bar{l}} B(X) \\ \times [-A_t(X) \partial_{kl}^2 A_t(X) - \partial_k A_t(X) \partial_l A_t(X)] W(X). \quad (2.36)$$

The classical OTOC of the V pairing C_{cl}^V , i.e., the first non-vanishing contribution to the OTOC, is written

$$C_{cl}^V(t) = C_A^V(t) + C_B^V(t) \\ = \hbar^2 \int dX \sum_{k,l=1}^{2L} \sigma_k \sigma_l \partial_k A_t(X) \partial_l A_t(X) \partial_{\bar{k}} B(X) \partial_{\bar{l}} B(X) W(X) \\ = \hbar^2 \int dX \{A_t(X), B(X)\}^2 W(X). \quad (2.37)$$

2.4.2 Λ pairing

We start from expression (2.27). We follow the same procedure as before, i.e., we look at the 0th, 1st and 2nd order in $\hbar$. The 0th and 1st order vanish for the same reason as in the V pairing. The first non-vanishing contribution to the out-of-time-ordered correlator is again the 2nd order in $\hbar$. As the lower orders are shown to be zero, one can once again look separately at the expansion of the A and B symbols.

The second-order expansion of the A symbols yields

$$C_A^\Lambda(t) = \frac{\hbar^2}{16} \int \frac{dX dS_2 dS_3}{(2\pi)^{2L}} d\Delta_1 d\Delta_2 e^{i\Delta_1 \wedge (X_{-t}(2S_2 - S_3) - X)} \\ \times e^{i\Delta_2 \wedge (S_3 - S_2)} \sum_{i,j=1}^{2L} \Delta_{2i} \Delta_{2j} [A(S_2) \partial_{ij}^2 A(S_2) - \partial_i A(S_2) \partial_j A(S_2)] \\ \times [B(X) - B(X_{-t}(S_3))]^2 W(2X - X_{-t}(2S_2 - S_3)). \quad (2.38)$$

One can perform the integration with respect to Δ_1 and transform the perturbation variables Δ_{2i} and Δ_{2j} into derivation operators acting on

the exponential, remove them from said exponential by integrating by parts, and end up with

$$C_A^\Lambda(t) = \frac{\hbar^2}{4} \int dS \sum_{i,j=1}^{2L} \frac{\sigma_i \sigma_j}{i^2} [A(S) \partial_{ij}^2 A(S) - \partial_i A(S) \partial_j A(S)] \\ \times \frac{\partial B}{\partial S_{\bar{i}}}(X_{-t}(S)) \frac{\partial B}{\partial S_{\bar{j}}}(X_{-t}(S)) W(X_{-t}(S)). \quad (2.39)$$

For the perturbation in the B symbols, one obtains at first

$$C_B^\Lambda(t) = \frac{\hbar^2}{16} \int \frac{dX dS_2 dS_3}{(2\pi)^{2L}} d\Delta_1 d\Delta_2 e^{i\Delta_1 \wedge (X_{-t}(2S_2 - S_3) - X)} e^{i\Delta_2 \wedge (S_3 - S_2)} \\ \times A^2(S_2) \sum_{i,j=1}^{2L} \Delta_{1i} \Delta_{1j} [B(X) \partial_{ij}^2 B(X) - \partial_i B(X) \partial_j B(X) \\ + B(X_{-t}(S_3)) \partial_{ij}^2 B(X)] \\ \times W(2X - X_{-t}(2S_2 - S_3)) \\ + \frac{\hbar^2}{8} \int dX A_t^2(X) \sum_{i,j=1}^{2L} \frac{\sigma_i \sigma_j}{i^2} \partial_{ij}^2 B(X) \partial_{ij}^2 B(X) W(X), \quad (2.40)$$

and when following the same guidelines as above, ends up with

$$C_B^\Lambda(t) = \frac{\hbar^2}{4} \int dX \sum_{i,j=1}^{2L} \frac{\sigma_i \sigma_j}{i^2} A_t^2(X) \left[\partial_{ij}^2 B(X) \partial_{ij}^2 B(X) W(X) \right. \\ \left. + 2\partial_i B(X) \partial_{ij}^2 B(X) \partial W_{\bar{j}}(X) + \partial_i B(X) \partial_j B(X) \partial_{ij}^2 W(X) \right] \quad (2.41)$$

$$= \frac{\hbar^2}{4} \int dX \sum_{i,j=1}^{2L} \sigma_i \sigma_j A_t^2(X) \frac{\partial^2}{\partial X_{\bar{i}} \partial X_{\bar{j}}} [\partial_i B(X) \partial_j B(X) W(X)]. \quad (2.42)$$

When integrating by parts, this last term and putting everything together, we end up with the classical OTOC of the Λ pairing

$$\begin{aligned}
C_{cl}^\Lambda(t) &= C_A^\Lambda(t) + C_B^\Lambda(t) \\
&= \int dS \, \hbar^2 \sum_{i,j} \sigma_i \sigma_j \partial_i A(S) \partial_j A(S) \frac{\partial B}{\partial S_i}(X_{-t}(S)) \frac{\partial B}{\partial S_j}(X_{-t}(S)) W(X_{-t}(S)) \\
&\quad - \frac{\hbar^2}{2} \int dS \sum_{i,j=1}^{2L} \sigma_i \sigma_j A(S) \partial_{ij}^2 A(S) \frac{\partial B}{\partial S_i}(X_{-t}(S)) \frac{\partial B}{\partial S_j}(X_{-t}(S)) W(X_{-t}(S)) \\
&\quad + \frac{\hbar^2}{2} \int dX \sum_{i,j=1}^{2L} \sigma_i \sigma_j A_t \frac{\partial^2 A_t}{\partial X_i \partial X_j}(X) \partial_i B(X) \partial_j B(X) W(X) \\
&= \hbar^2 \int dX \, \{A(S(X)), B(X)\}^2 W(X) \\
&\quad - \frac{\hbar^2}{2} \int dS \sum_{i,j=1}^{2L} \sigma_i \sigma_j A(S) \partial_{ij}^2 A(S) \frac{\partial B}{\partial S_i}(X_{-t}(S)) \frac{\partial B}{\partial S_j}(X_{-t}(S)) W(X_{-t}(S)) \\
&\quad + \frac{\hbar^2}{2} \int dX \sum_{i,j=1}^{2L} \sigma_i \sigma_j A(S) \frac{\partial^2 A}{\partial X_i \partial X_j}(X) \partial_i B(X) \partial_j B(X) W(X),
\end{aligned} \tag{2.43}$$

using the fact that the Poisson bracket is canonically invariant. In other words, the contribution of the second pairing to the short-time OTOC is again a Poisson bracket plus some other contributions, but fortunately, we will show that the latter vanishes.

2.4.3 *I term*

As previously stated, when considering both the V and Λ pairing, we are actually overcounting one situation: when all four trajectories are near one another, i.e., $\alpha \sim \beta \sim \gamma \sim \delta$. The result is expression (2.30). Therefore, we have to subtract once this contribution from the other two.

There is, however, a caveat. Whereas in the previous pairings, a double sum on the classically allowed trajectories remained, here there is only one, as only one family of paths is considered. Let us first transform the

previous expression. The Dirac δ in combination with a function f in multiple dimensions is given by

$$\delta(\mathbf{y} - f(\mathbf{x})) = \sum_i \frac{\delta(\mathbf{x} - \mathbf{x}_i)}{\left| \det \frac{df}{d\mathbf{x}}(\mathbf{x}_i) \right|}, \quad (2.44)$$

where the sum is on all $\mathbf{x}_i$ that satisfy $\mathbf{y} - f(\mathbf{x}) = 0$. To transpose it to our case that involves several variables, we simply have to choose one of the variables as being the $\mathbf{x}$ in the above expression, and the other remains constant. This can be done by choosing which integral to perform first, as the Dirac δ should be understood in this context. This yields:

$$\begin{aligned} \prod_{j=2}^3 \left| \det \frac{\partial^2 R_\alpha(\mathbf{S}_j, \mathbf{R}_j)}{\partial \mathbf{S}_j \partial \mathbf{R}_j} \right| & \delta(\Pi_j - \mathbf{p}_\alpha^i(\mathbf{S}_j, \mathbf{R}_j)) \delta(\mathbf{P}_j - \mathbf{p}_\alpha^f(\mathbf{S}_j, \mathbf{R}_j)) \\ &= \prod_{j=2}^3 \delta(\mathbf{S}_j - \mathbf{R}_t(\mathbf{R}_j, \Pi_j)) \delta(\mathbf{P}_j - \mathbf{P}_t(\mathbf{R}_j, \Pi_j)) \chi(\Pi_j) \\ &= \prod_{j=2}^3 \delta(\mathbf{S}_j - \mathbf{X}_t(\mathbf{R}_j)) \chi_\alpha(\Pi_j), \end{aligned} \quad (2.45)$$

where we switched to the symplectic formalism for the last equality. In this case, the sum in (2.44) contains only one element since there is only one zero of the argument of the Dirac delta. A part of this element cancels with one of the amplitudes of the propagator. However, there may be no trajectory such that the initial momenta Π_2 or Π_3 are within the permitted range of the considered family of trajectories. To this end, we add a characteristic function $\chi_\alpha(\Pi)$ that is equal to 1 if Π is a momentum that belongs to the permitted range, and 0 otherwise. To deal with those characteristic functions, one must recall that expression (2.45) appears within a sum. As those functions are the only remaining terms where α appears, one treat them independently and write

$$\sum_\alpha \chi_\alpha(\Pi_2) \chi_\alpha(\Pi_3) = \begin{cases} 1 & \text{for short times,} \\ 0 & \text{otherwise.} \end{cases} \quad (2.46)$$

These equalities must be understood as follows. In Figure 2.2, trajectories that are inside the blue contour belong to the same family. The initial position is represented by $\mathbf{R}_2$, and different trajectories are shown, with the corresponding initial momentum in purple. As time elapses, the range

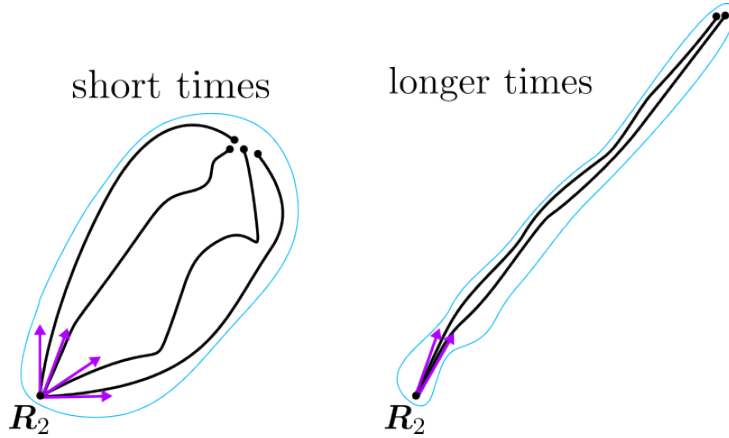


Figure 2.2: Range of permitted momentum for the I pairing. The family of trajectories is represented in a blue contour. We represent several trajectories, starting from the initial position $\mathbf{R}_2$, that belong to the family. The ends of the trajectories are some of the final positions that are reachable, depending on the initial momentum, which is represented in purple arrows. The left situation is for short times. As time passes, the range of momenta such that the resulting trajectory belongs to the family is smaller, which is shown in the right situation.

of permitted initial momenta such that the trajectories are within the same family gets narrower. Physically, this should be understood as the fact that all trajectories remaining in the vicinity of each other during the whole time evolution becomes increasingly unlikely. This can be further explained using Figure 2.3, where we show the final position of a one-degree-of-freedom system obtained from time evolving the initial condition $(q_0 = 0, p_0)$ as a function of p_0 , with the Hamiltonian specified in the caption. In the short-time situation, there is only one family of trajectories, i.e., only one set of initial conditions that yields the desired final conditions, marked here by the dotted horizontal line. At later times, the system can start from the same initial position, here $q_0 = 0$, but with several possible momenta, and end up in the desired final conditions. However, these different momenta mean that the trajectories belong to a different family, delimited by the dotted vertical lines, and thus don't contribute to the integral. This corresponds to the characteristic function being equal to zero.

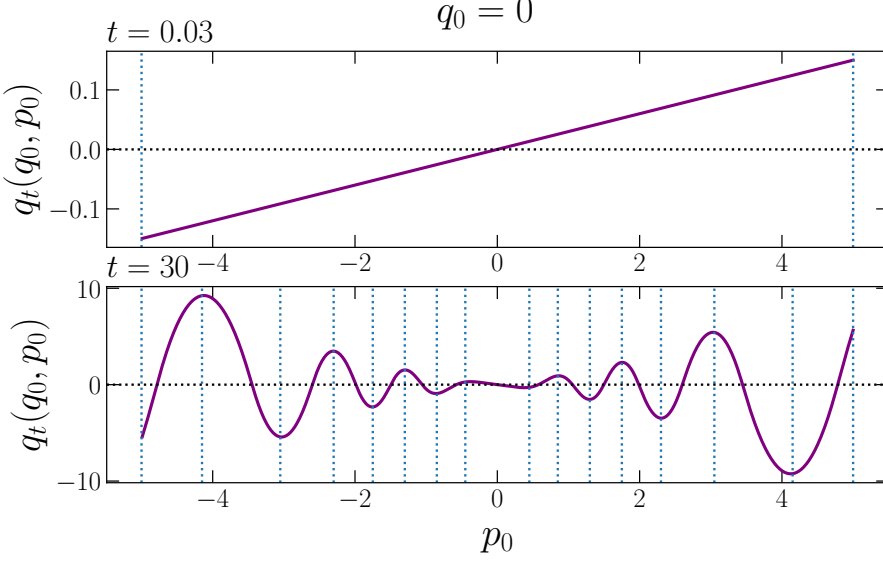


Figure 2.3: Final position as a function of initial momentum, at a fixed initial position $q_0 = 0$, for the classical one-degree-of-freedom system governed by the Hamiltonian $H(q, p) = p^2/2 + \sqrt{1 + q^2}$. The vertical dotted lines delimit the different families of trajectories departing at $q_0 = 0$ and ending near $q_t = 0$ again, after the evolution time $t = 0.03$ (resp. $t = 30$) for the top (resp. bottom) panel. In the top panel, representing the short-time situation, there is only one possible family of trajectories, i.e., meaning that inside (2.47), $\delta_{\alpha_2, \alpha_3} = 1$. The bottom panel shows a situation at a later time, where there are multiple families fulfilling the aforementioned conditions. The consequence is that in (2.47), the phase-space integrals cannot be performed independently. To obtain a non-vanishing contribution to the integral, the trajectories must belong to the same family during the whole evolution, i.e., the initial condition must be in the same region delimited by the vertical dotted lines. As time increases, this region, and thus the integration domain, becomes smaller, leading to a smaller contribution to the OTOC.

From equation (2.30), one therefore obtains

$$\begin{aligned}
C^I(t) = & \frac{1}{2^{2L}} \int \frac{dX dR_2 dR_3 dS_2 dS_3 d\Delta_1 d\Delta_2}{(2\pi)^{4L}} \delta(S_2 - X_t(R_2)) \delta(S_3 - X_t(R_3)) \\
& \times e^{i\Delta_1 \wedge (R_2 - X)} e^{i\Delta_2 \wedge (S_3 - S_2)/2} A\left(\frac{S_2 + S_3}{2} + \frac{\hbar\Delta_2}{4}\right) A\left(\frac{S_2 + S_3}{2} - \frac{\hbar\Delta_2}{4}\right) \\
& \times \left[B\left(\frac{X + R_2}{2} + \frac{\hbar\Delta_1}{4}\right) B\left(\frac{X + R_2}{2} - \frac{\hbar\Delta_1}{4}\right) \right. \\
& \left. - B(R_3) \left(B\left(\frac{X + R_2}{2} + \frac{\hbar\Delta_1}{4}\right) + B\left(\frac{X + R_2}{2} - \frac{\hbar\Delta_1}{4}\right) \right) + (\hat{B}^2)_W(R_3) \right] \\
& \times W(X) \sum_{\alpha} \chi_{\alpha}(\Pi_2) \chi_{\alpha}(\Pi_3). \tag{2.47}
\end{aligned}$$

We use the Dirac deltas of the first line, yielding

$$\begin{aligned}
C^I(t) = & \frac{1}{(2\pi)^{4L} 2^{2L}} \int dX dR_{2,3} d\Delta_{12} e^{i\Delta_1 \wedge (R_2 - X)} e^{i\Delta_2 \wedge (X_t(R_3) - X_t(R_2))/2} \\
& \times A\left(\frac{X_t(R_2) + X_t(R_3)}{2} + \frac{\hbar\Delta_2}{4}\right) A\left(\frac{X_t(R_2) + X_t(R_3)}{2} - \frac{\hbar\Delta_2}{4}\right) \\
& \times \left[B\left(\frac{X + R_2}{2} + \frac{\hbar\Delta_1}{4}\right) B\left(\frac{X + R_2}{2} - \frac{\hbar\Delta_1}{4}\right) \right. \\
& \left. - B(R_3) \left(B\left(\frac{X + R_2}{2} + \frac{\hbar\Delta_1}{4}\right) + B\left(\frac{X + R_2}{2} - \frac{\hbar\Delta_1}{4}\right) \right) + (\hat{B}^2)_W(R_3) \right] \\
& \times W(X) \sum_{\alpha} \chi_{\alpha}(\Pi_2) \chi_{\alpha}(\Pi_3). \tag{2.48}
\end{aligned}$$

Lastly, we performed a canonical change of variables from initial coordinates R_2 and R_3 to S_2 and S_3 , and then another change of variables to simplify the argument of the A symbols.

$$\begin{aligned}
C^I(t) = & \frac{1}{(2\pi)^{4L}} \int dX_1 dS_2 dS_3 d\Delta_1 d\Delta_2 e^{i\Delta_1 \wedge (X_{-t}(2S_2 - S_3) - X)} e^{i\Delta_2 \wedge (S_3 - S_2)} \\
& \times A\left(S_2 + \frac{\hbar\Delta_2}{4}\right) A\left(S_2 - \frac{\hbar\Delta_2}{4}\right) \left[B\left(X + \frac{\hbar\Delta_1}{4}\right) B\left(X - \frac{\hbar\Delta_1}{4}\right) \right. \\
& \left. - B(X_{-t}(S_3)) \left(B\left(X + \frac{\hbar\Delta_1}{4}\right) + B\left(X - \frac{\hbar\Delta_1}{4}\right) \right) + (\hat{B}^2)_W(X_{-t}(S_3)) \right] \\
& \times W(2X - X_{-t}(2S_2 - S_3)) \sum_{\alpha} \chi_{\alpha}(\Pi_2) \chi_{\alpha}(\Pi_3), \tag{2.49}
\end{aligned}$$

where we did changes of variables to simplify the arguments of the symbols. Note that the expression is now identical to (2.27), except for

the additional sum at the end. As already stated, this sum is equal to 1 for a fixed time as $\hbar \rightarrow 0$. As time gets larger, the initial conditions must be closer to each other in order to contribute, meaning that the contribution to (2.47) will get smaller, down to the point where it vanishes.

This means that for short times, we can follow exactly the same derivations as for the Λ pairing, and since (2.47) contributes with opposite sign to the OTOC, only the V pairing contributes. In other words, the short-time behaviour of the OTOC using this scheme is the same as with Wigner-Moyal. For later times, as it was stated above, only the first two pairings are expected to contribute to a quasiclassical long-time value.

2.5 LONG-TIME LIMIT

In this section, we derive a finite long-time limit of the quasiclassical OTOC. In chaotic systems, any small perturbation grows exponentially with time and becomes large. Here, we refrained from doing $\hbar$ expansion inside an evolution operator as it is incompatible with considering the system at times larger than the Ehrenfest time. Only the V pairing is considered here. Indeed, due to the strong mathematical similarities between C^V and C^Λ (which is related to the geometrical similarity between the corresponding diagrams, see figures 2.1a and 2.1b), we expect that they both yield comparable contributions to the OTOC for long times. Additionally, the I pairing, for which one considers that the four trajectories remain in the vicinity of each other at all times, is expected to give a negligible contribution in chaotic systems.

We make the hypothesis that our system is ergodic and mixing. In the case of a fully chaotic phase space, this is not a restrictive statement. We will see later how this can be generalised to a mixed phase space. One consequence is that the expression that replaces A_t will depend only on the constants of motion. Assuming K constants of motion:

$$A_t(X) \rightarrow \bar{A}(\vec{c}(X)) = \int dX' A(X') \prod_{k=1}^K \delta(c_k(X') - c_k(X)), \quad (2.50)$$

where $\bar{A}$ means the phase-space average of A_t and $c_k(X)$ is the k^{th} constant of motion evaluated at X .

To explain the average, let us consider an integral of the form

$$I(t) = \int dx f_t(x)g(x), \quad (2.51)$$

where f_t involves some time evolution and varies much more quickly than g with x . One can divide the x space into cells and compute the integral cell by cell. This would translate to

$$I \simeq \sum_{\text{cell}_i} g(\text{cell}_i) \int_{\text{cell}_i} f_t(x) dx \quad (2.52)$$

$$= \sum_{\text{cell}_i} g(\text{cell}_i) \bar{f}(\text{cell}_i), \quad (2.53)$$

where g could be taken out of the integral on a given cell as it varies slowly, and where $\bar{f}$ is the average of f_t on the whole space because of the mixing. One can then take the limit of infinitely small cells, which gives back the integration over the whole space:

$$I = \int dx \bar{f}(x) g(x). \quad (2.54)$$

Moreover, because of ergodicity, it is also equal to the time average.

Using this in (2.20) translates to

$$\begin{aligned} A_t \left(X + \frac{\hbar \Delta_2}{4} \right) &\rightarrow \bar{A} \left(\bar{c} \left(X + \frac{\hbar \Delta_2}{4} \right) \right) \\ &= \bar{A}(\bar{c}(X)) + \frac{\hbar}{4} \sum_{m=1}^K \sum_{i=1}^{2L} \Delta_{2,i} \frac{\partial \bar{A}}{\partial c_m}(\bar{c}(X)) \frac{\partial c_m}{\partial X_i}(X) \\ &\quad + \frac{\hbar^2}{16} \left(\sum_{m=1}^K \sum_{i,j=1}^{2L} \frac{\Delta_{2,i} \Delta_{2,j}}{2} \frac{\partial \bar{A}}{\partial c_m}(\bar{c}(X)) \frac{\partial^2 c_m}{\partial X_{1i} \partial X_{1j}}(X) \right. \\ &\quad \left. + \sum_{m,n=1}^K \sum_{i,j=1}^L \frac{\Delta_{2,i} \Delta_{2,j}}{2} \frac{\partial c_m}{\partial X_{1i}}(X) \frac{\partial c_n}{\partial X_{1j}}(X) \frac{\partial^2 \bar{A}(\bar{c}(X))}{\partial c_m \partial c_n} \right) \\ &\quad + \mathcal{O}(\hbar^3), \end{aligned} \quad (2.55)$$

where here, as opposed to what was derived in Section (2.4), the $\mathcal{O}(\hbar^n)$ corrections are real $\mathcal{O}(\hbar^n)$ corrections, and not initially small errors that blow up to infinity after evolution. The same development from Section 2.4 is carried out, and we obtain a Poisson bracket between 2 symbols again, this time one of them being a phase-space average:

$$C_\infty = \hbar^2 \int dX \{ \bar{A}(\bar{c}(X)), B(X) \}^2 W(X). \quad (2.57)$$

This development is also valid for mixed phase space, with some slight limitations. The phase-space average is reduced to an average over the accessible region of phase space, which again is equal to the time average, provided that the wavepacket is initially completely within the chaotic sea.

2.6 NUMERICAL SIMULATIONS

In this section, we apply our formalism to Bose-Hubbard systems, which describe ultra-cold gas of bosons [49] as well as superconducting qubits [104], and that was introduced in Section 1.4.2 with the Hamiltonian (1.126). We first focus on the trimer without driving, and then on the driven dimer. The simulations use operators that are quadratic in terms of position and momentum operators. The classical expression, i.e., the weighted integral of the Poisson bracket, is evaluated with the truncated Wigner method. As a reminder, it consists in sampling the wavepacket according to the Wigner distribution, making each sampled point evolve according to the equation (1.131), and summing the contributions to evaluate the integral [27, 61–65, 67]. We use coherent and Fock states, whose Wigner function are respectively given by (1.99) and (1.101).

In the trimer, we consider $\hat{A}$ and $\hat{B}$ to be population operators acting on two sites i and j . The corresponding classical OTOC is [26]:

$$C_{\text{cl}}(t) = \hbar^2 \int d\mathbf{n} d\boldsymbol{\theta} \left(\frac{\partial n_{i,t}}{\partial \theta_j}(\mathbf{n}, \boldsymbol{\theta}) \right)^2 W(\mathbf{n}, \boldsymbol{\theta}). \quad (2.58)$$

and the quasiclassical long-time limit is

$$C_{\infty} = \hbar^2 \int d\mathbf{n} d\boldsymbol{\theta} \left(\frac{\partial \bar{n}_{i,t}}{\partial \theta_j}(E(\mathbf{n}, \boldsymbol{\theta}), N(\mathbf{n}, \boldsymbol{\theta})) \right)^2 W(\mathbf{n}, \boldsymbol{\theta}). \quad (2.59)$$

where W will either be W_{CS} or $W_{\text{Fock,cl}}$.

In the top left part of Figure 2.4, we show a Poincaré surface of section of the phase space of the trimer with the system parameters $U = 0.02J$, a total of $N = 300$ particles at an energy of $E = 1.433J$. We represent the population of the first site n_1 on the vertical axis, and the phase difference between the first and last site, θ_1 and θ_3 modulo 2π on the horizontal axis. These sections are obtained by fixing the phase of the second site to 0 modulo 2π , and the population on the other site is fixed using the constants of motion. There are actually two solutions that fulfil these constraints, so we chose consistently the same solution. The holes in

the middle of the chaotic regions do not correspond to regular islands that were not sampled but to an absence of points satisfying the criteria to be in the Poincaré section. More details on how to obtain such a section are available in [134]. It can clearly be seen that the dynamics is strongly chaotic. We also show in arbitrary units the Wigner function of the initial states used for the plots in the right part of the figure.

In the top right part, we show the exact quantum OTOC (solid red curve) as well as the Poisson bracket (dashed blue curve) for the coherent state centred around the occupancy levels of the Fock state $|114, 140, 46\rangle$, with phases $(-3.07, 0, 0)$, and with the same system parameters as the Poincaré section. In practice, we work with number-projected coherent states for the quantum simulations. Since the experimental realisation is the framework of ultracold gas, it would correspond to Bose-Einstein condensates with a fixed number of particles, and thus those number-projected coherent states are closer to reality than regular ones. In the quantum curve, after a brief power-law increase, one can see a short exponential growth once the hyperbolic dynamics kick in, followed by a saturation after the Ehrenfest time. The classical curve matches almost perfectly the quantum one for short times. However, as it was explained in Section 2.5, obtaining the Poisson bracket was at the cost of an $\hbar$ expansion inside an evolution operator, which limits the time validity. The result is an exponential growth, exhibiting the chaotic dynamics of the system, that never stops because of the absence of quantum interferences. In addition, we plotted the long-time value as a blue horizontal dotted line. It is finite, as opposed to the Poisson bracket that grows indefinitely, but quasiclassical, i.e., without any interferences considered. The value is, however, several orders of magnitude smaller than the quantum saturation one. This shows the importance of effects beyond quasiclassical physics, such as the X pairing, as was stated in [25] and [26].

Next, we consider a Fock state. We first represent a Poincaré section of the phase space for the system parameters $U = 0.06J$ with a total population of $N = 100$ at an energy $E = 0.6NJ$ in the bottom left part of Figure 2.4. Again, the dynamics is strongly chaotic. We also show the quantum OTOC and the Poisson bracket for the Fock state $|105, 100, 100\rangle$ with the same system parameters on the right. The same observations as above can be made, i.e., an initial perfect agreement between the two curves during the power-law and the start of the exponential regime, followed by a saturation of the quantum curve, whereas the classical one continues to grow. Again, the long-time value is shown as a dotted horizontal line, and the conclusion is the same as with coherent states.

We then focus on the driven dimer. This system has the advantage of having a phase space that can be represented in 2 dimensions only. The dynamics can thus be entirely visualised using a stroboscopic section, as shown in the left part of Figure 2.5, with again the Wigner function of the initial state represented in arbitrary units. The vertical axis is the population imbalance, and the horizontal axis is the phase difference between the two sites. For this system, we used different operators. Because of the driving, the Hamiltonian is now time-dependent, and the energy is not conserved anymore. Only the number of particles is a constant of motion, which will have consequences regarding the operators we are working with. In addition, the long-time quasiclassical OTOC can be entirely computed analytically. In (2.57), one can apply the chain rule in the derivative of the Poisson bracket and show that, in general, the expression is

$$\{\bar{A}(\vec{c}(X), B(X))\} = \sum_{k=1}^K \frac{\partial \bar{A}(\vec{c}(X))}{\partial c_k} \{c_k(X), B(X)\}, \quad (2.60)$$

where here the sum contains only one contribution since there is only one constant of motion: the total number of particles. In order to obtain a nontrivial result, one has to work with operators that do not commute with the total population $\hat{N}$. We work with momentum operators in the driven dimer, $\hat{A} = \hat{p}_i^2$ and $\hat{B} = \hat{p}_j$. We compute the OTOC

$$C(t) = \langle \psi | [\hat{p}_i^2(t), \hat{p}_j(0)]^2 | \psi \rangle, \quad (2.61)$$

and its classical limit

$$C_{cl}(t) = \hbar^2 \int d\mathbf{n} d\boldsymbol{\theta} \left(\frac{\partial p_{i,t}^2}{\partial q_j}(\mathbf{n}, \boldsymbol{\theta}) \right)^2 W(\mathbf{n}, \boldsymbol{\theta}) \quad (2.62)$$

with $i = 1$ and $j = 2$. The long-time value of the driven dimer for this OTOC is given by

$$C_\infty = \hbar^2 \int d\mathbf{n} d\boldsymbol{\theta} \left(\frac{\partial \bar{p}_{i,t}^2}{\partial q_j}(N(\mathbf{n}, \boldsymbol{\theta})) \right)^2 W(\mathbf{n}, \boldsymbol{\theta}). \quad (2.63)$$

The results are shown in the right part of Figure 2.5 in the top half for coherent states, and in the bottom half for Fock states. Again, the dynamics is strongly chaotic, apart from some regular trajectories at high population imbalance. We draw the same conclusions as previously: the

initial short-time agreement is excellent, but the quasiclassical saturation value is several orders of magnitude smaller than the quantum saturation one, highlighting the importance of interference [25, 26].

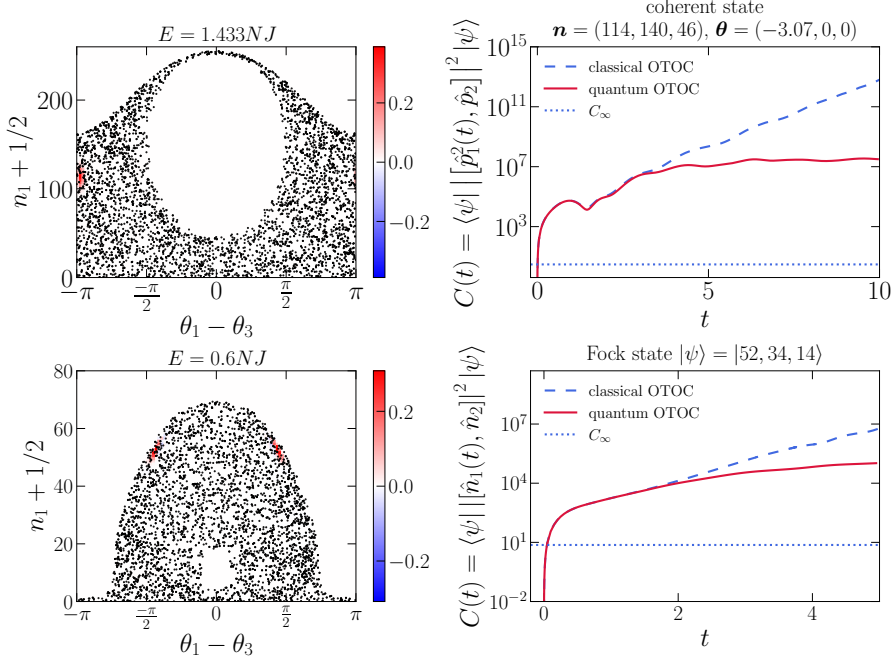


Figure 2.4: OTOC in Bose-Hubbard trimers. *Left column*: Poincaré surface of section of the Bose-Hubbard trimer for the sets of parameters $U = 0.02J$, $N = 300$, at energy $E = 1.433NJ$ (top) and $U = 0.06J$, $N = 300$, $E = 0.6NJ$ (bottom). The vertical axis represents the population of the first site n_1 and the horizontal one the difference between the phases of the first site θ_1 and the third one θ_3 . In both Poincaré surfaces of section, the Wigner function of the initial state is represented in arbitrary units.

Right column: quantum and classical OTOC (Poisson bracket) in respectively the solid red and the dashed blue curve as well as the quasiclassical saturation value C_∞ in dotted blue for (top) the coherent state centred around the occupancy levels of the Fock state $|114, 140, 46\rangle$ with phases $(-3.07, 0, 0)$, $U = 0.02J$, $C_\infty = 1.18$ and (bottom) the Fock state $|52, 34, 14\rangle$, $U = 0.06J$, $C_\infty = 10$.

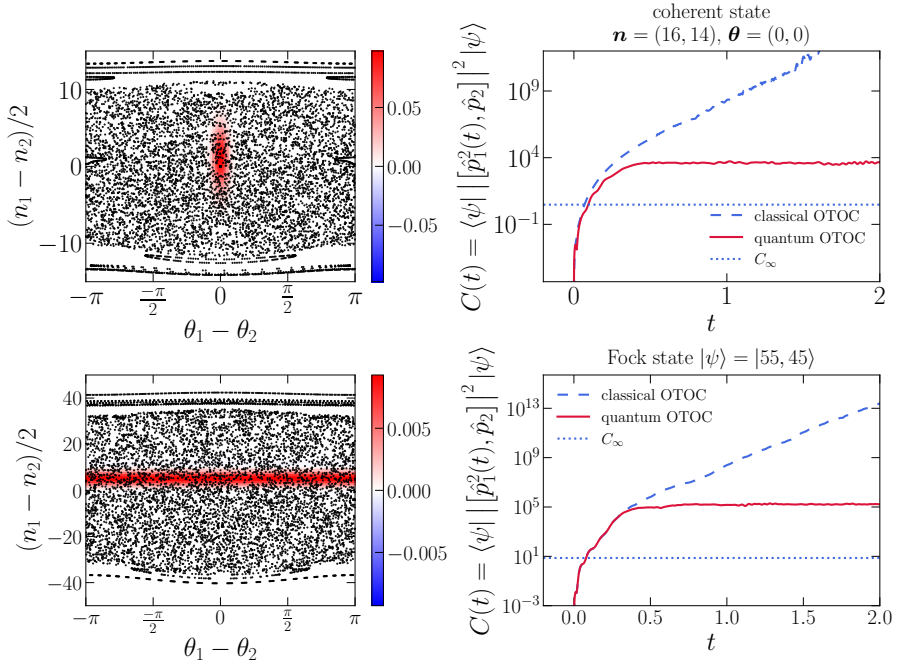


Figure 2.5: OTOC in Bose-Hubbard driven dimers. *Left column*: stroboscopic map of the Bose-Hubbard driven dimer for the sets of parameters $U = 3J$, $N = 30$, $\delta = 20J$, $\omega = 10J$ (top), and $U = 1J$, $N = 100$, $\delta = 20J$, $\omega = 10J$ (bottom). The vertical axis represents the difference between the population of the first site, n_1 , and the second one, n_2 , and the horizontal axis shows the difference between the phases of the first site, θ_1 , and the second one, θ_2 . In both stroboscopic maps, the Wigner function of the initial state is represented in arbitrary units.

Right column: quantum and classical OTOC (Poisson bracket) in respectively the solid red and the dashed blue curve as well as the quasiclassical saturation value C_∞ in dotted blue for (top) the coherent state centred around the occupancy levels of the Fock state $|16, 14\rangle$ with phases $(0, 0)$, $U = 3J$, $\delta = 20J$, $\omega = 10J$, $C_\infty = 7.375$ and (bottom) the Fock state $|55, 45\rangle$, $U = 1J$, $\delta = 20J$, $\omega = 10J$ $C_\infty = 0.2$.

3.1 INTEGRABILITY AND LOCAL HYPERBOLICITY

In the previous chapter, we established a quasiclassical theory of out-of-time-ordered correlators. The framework of this work was systems whose classical phase space is fully chaotic. Under those conditions, the OTOC is expected to grow exponentially, and this exponential growth is generally considered an indicator of chaos. However, an exponential growth of the OTOC, when being observable (i.e., if the system under consideration is not too far away from the semiclassical regime characterized by small Planck cells), is actually not a sufficient indicator to ascertain the presence of classical chaos [45, 124, 135], especially not if the state under consideration (with respect to which the OTOC expectation value is taken) is tightly localized about a specific point in phase space. If that particular point happens to be an unstable (more precisely, hyperbolic) fixed point of the classical dynamics within an integrable system, the resulting scrambling dynamics along the associated separatrix structure also results in an exponential growth of the OTOC, the growth rate being this time related to the stability exponent λ_s of the fixed point [124, 136–138]. Intricate growth regimes, with growth rates crossing over from $2\lambda_s$ to λ_s , followed by an oscillatory behaviour at long times, were reported in [127] for integrable systems, thus indicating that the latter nevertheless markedly distinguish themselves from their chaotic counterparts. Quite obviously, unstable fixed points also occur in nonintegrable systems of all possible sorts, ranging from the near-integrable to the fully chaotic regime. This raises a question of fundamental nature: if an OTOC observable is evaluated with respect to an initial state that is strongly localised about such an unstable fixed point in a chaotic system, how will the two reported OTOC growth mechanisms compete with each other? Will one of them dominate the other one (and if so, which one in which regime) or will there be some sort of “merging” of these two OTOC growth laws?

To address this question, we mainly focus here on the periodically modulated pendulum in the near-integrable limit, which can be considered as a standard model for integrability breaking in the vicinity of generic nonlinear resonances [69] and which allows for analytical investigations

using similar approaches as for the Melnikov-Arnold integral [76, 139, 140]. The scrambling observable that we consider in this context is the mean trace of the stability matrix [2], introduced in Section 1.2, which can be considered to be of a more fundamental nature than any OTOC observable (the latter always depending on the choice of individual system operators), even though it is purely classical and does not, to our knowledge, have a direct quantum counterpart. We find that, at the genesis of chaos, the trace of the stability matrix exhibits an exponential growth with a rate, which we call the *effective exponent*, that lies between the stability exponent of the unstable fixed point of the pendulum and the Lyapunov exponent characterising the tiny chaotic separatrix layer in the near-integrable regime [138]. Our analytical findings are confirmed by numerical simulations, which furthermore show the equivalence (up to a factor 2) of classical OTOC and stability matrix effective exponents, explore what happens in mixed regular-chaotic parameter regimes, and demonstrate the universality of our findings for generic driven or kicked one-degree-of-freedom systems.

This chapter is structured as follows. In Section 3.2, we provide a first numerical survey on OTOC growth behaviours associated with unstable fixed points in nonintegrable systems. In Section 3.3, we establish an approximate analytical description of the driven pendulum, which is formally valid in the limit of weak perturbations from integrability. We then show in Section 3.4 how to analytically extract an approximate expression for the effective exponent characterising the growth of the trace of the stability matrix. Section 3.5 is devoted to complementary numerical investigations, where we show how our findings are universal and can be observed in other systems as well, in particular, also using OTOCs instead of stability matrix traces. We also numerically investigate in that section what happens farther away from integrability, as well as for very long evolution times.

3.2 LOCAL AND GLOBAL INSTABILITIES

It is recently known that the OTOC can exhibit an exponential regime even in the absence of chaos [124–126]. This occurs if the initial state is located at a local instability, for instance a hyperbolic fixed point, where the exponential growth rate of the OTOC corresponds then to the stability exponent λ_s . In that case, before the saturation, the OTOC will undergo a crossover to a $\propto e^{\lambda_s t}$ regime [127].

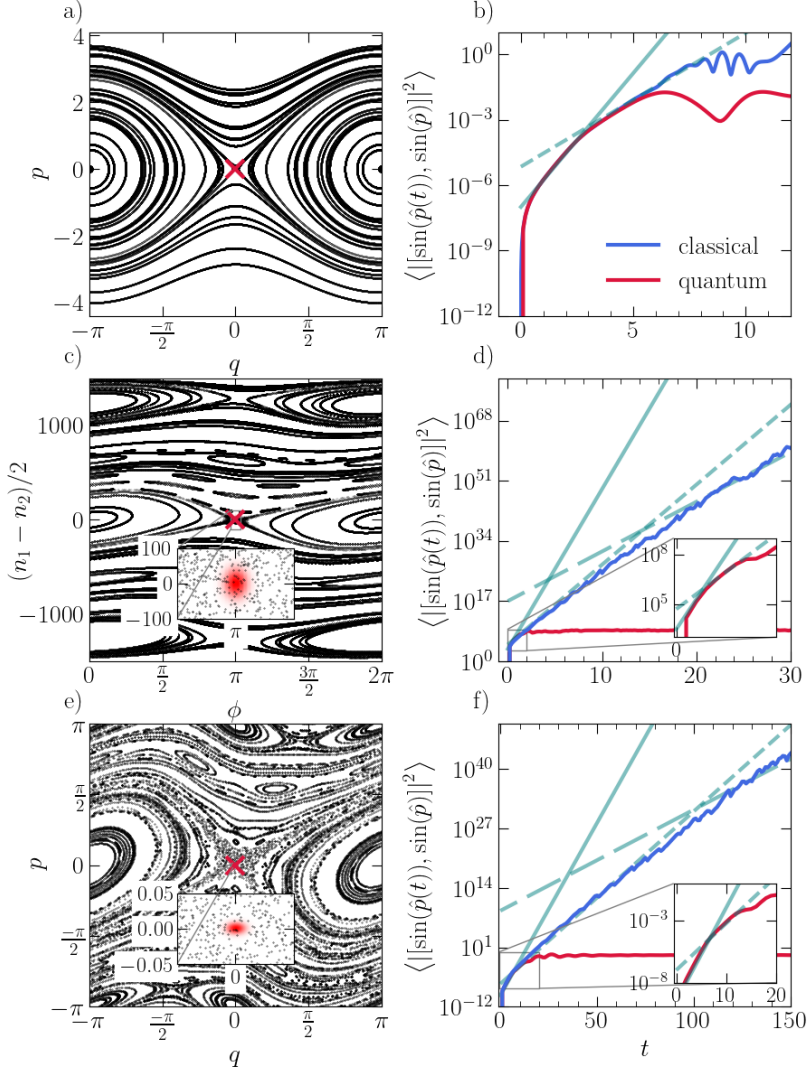


Figure 3.1: OTOC growth in integrable, near-integrable, and mixed systems.

Left column: Phase-space representations of a) the simple pendulum given by (1.137) with $\kappa = 0$, c) the kicked Bose-Hubbard dimer given by (1.133) 3000 particles, $U = 0.025J$, and the period and strength of the hopping kick $\tau = 0.2J$ and e) the kicked rotor given by (1.124) with kicking parameter $K = 0.6$. The centre of the initial coherent state is indicated by a cross and corresponds to an unstable fixed point. *Right column:* quantum (red) and classical (blue) OTOC for b) the simple pendulum with $\hbar = 2^{-11}$, d) the kicked dimer with $\hbar = 1/3000$, and f) the kicked rotor with $\hbar = 2^{-14}$. The operators used for the OTOC are shown in the label of the vertical axis. The straight lines represent exponential growth, with the rate given by $2\lambda_s$ (cyan), λ_s (dashed cyan), and $(\lambda_s + \lambda_L)/2$ (long-dashed cyan). For d) and f), an inset of the quantum OTOC is shown to highlight the first two regimes.

In this work, we will consider regimes between the integrable case and the completely chaotic one, which are all represented in Figure 3.1. We find that an effective exponent, λ_{eff} , whose value is between the stability exponent and the Lyapunov exponent, plays a role in the transition from the regular to the chaotic case. To highlight the universality of our findings, each row corresponds to a different system. The first column shows the phase-space representation of a system with a hyperbolic fixed point at the centre, while the second column shows the quantum and classical OTOC for an initial state centred on that hyperbolic fixed point (see the insets in the left column for the phase-space localisation of the wave-packet). The first row shows the integrable case for a simple pendulum. The $2\lambda_s \rightarrow \lambda_s$ transition is highlighted by representing exponentials using straight lines, the solid blue being proportional to $e^{2\lambda_s t}$ and the dashed one to $e^{\lambda_s t}$. The quantum OTOC then saturates, whereas the classical one continues to grow. The second row shows a quasi-integrable case, featuring dominantly regular dynamics with a thin chaotic layer around the hyperbolic fixed point and the homoclinic manifold linked to it. Here, there is an additional and new crossover where the exponential growth rate goes from λ_s to twice the effective exponent, which has been empirically found to be $\lambda_{\text{eff}} = (\lambda_s + \lambda_L)/4$. The long-dashed line is proportional to $e^{2\lambda_{\text{eff}} t}$. Note that this regime is only observable in the classical OTOC. Finally, the last line shows a third case with a thicker chaotic layer.

To shed more light on these findings, we investigate a different indicator, namely the trace of the stability matrix. It is a fundamental one, in the sense that it directly probes the dynamics of the system without any choice of operators which could introduce artefacts [2]. Additionally, it is invariant under canonical transformation, like the computation of the maximal Lyapunov exponent of the system. The main issue is that this probe does not have an equivalent in quantum mechanics, in which case we will resort to the OTOC. Nonetheless, both are linked as they probe the same quantity, i.e., the exponent that dictates the dynamics of the system.

3.3 DRIVEN PENDULUM

As stated in the introduction, we now focus our attention on the study of a periodically driven pendulum. Similarly to the OTOC that was central to the previous chapter, the driven pendulum is the keystone of this

chapter. We thus recall its Hamiltonian, originally introduced in Section 1.4.4:

$$H(q, p, t) = \frac{p^2}{2} + \lambda_s^2 \cos(q) + \kappa \omega \lambda_s \cos(q) \cos(\omega t + \varphi), \quad (3.1)$$

with the first two terms being the regular pendulum Hamiltonian, and where $\kappa \omega \lambda_s$ is the amplitude of the perturbation, ω its frequency, and λ_s the stability exponent associated with the hyperbolic fixed point at $(q, p) = (0, 0)$ of the Hamiltonian. The dimensionless parameter κ characterises the strength of the perturbation. We assume a weak driving amplitude with a high frequency, i.e., $\kappa \ll \lambda_s \ll \omega$ and $\kappa \omega \sim 1$. As a reminder, this Hamiltonian must be seen as a definition, as there are different ways one can choose to drive the system. Our particular choice comes from the fact that the Hamiltonian (3.1) is the one that universally describes the dynamics of a system in the vicinity of a resonance [15, 108].

The classical Hamilton equations of motion are given by

$$\ddot{q}(t) = \lambda_s^2 \sin(q(t)) + \kappa \omega \lambda_s \sin(q(t)) \cos(\omega t + \varphi), \quad (3.2)$$

which is nonintegrable. A strategy to obtain an analytical solution is, considering the initial wavepacket tightly localised on the fixed point, to separate the phase space into two regions. In the first one, labelled the *linear region*, the equations of motion can be linearised around the origin, and in the second one, the *homoclinic region*, the system only slightly deviates from the homoclinic. It is important to note that this framework is a priori valid for a wavepacket that initially is fully localised within the tiny chaotic layer around the separatrix, which is the scope of this paper, and naturally is not suited for motion within the regular phase-space regions. The crossover position between the linear and homoclinic regions is labelled q_c and must be chosen so that it satisfies both hypotheses: it must be small as compared to 1 in order to be able to linearise the dynamics around the origin, and at the same time it must be large enough so that the system only slightly deviates from the separatrix in the rest of the phase space.

3.3.1 Linear region

In the linear region, the dynamics can be linearised around the origin. Equation (3.2) is approximated by

$$\ddot{q}(t) = \lambda_s^2 q(t) + \kappa \omega \lambda_s \cos(\omega t + \varphi) q(t). \quad (3.3)$$

To solve this differential equation, we take its Laplace transform and obtain

$$\tilde{q}(z) = \frac{b(z)}{z^2 - \lambda_s^2} + \kappa\omega\lambda_s \frac{e^{i\varphi}\tilde{q}(z - i\omega) + e^{-i\varphi}\tilde{q}(z + i\omega)}{2(z^2 - \lambda_s^2)}, \quad (3.4)$$

where $b(z) = zq_0 + p_0$ was introduced for conciseness, and where q_0 and p_0 are the initial conditions when the system enters the linear region. The next step consists in injecting the expression of $\tilde{q}$ inside the terms of the right-hand side evaluated at $z \pm i\omega$. Doing so introduces corrections of order $\mathcal{O}(1/\omega^\alpha)$ with $\alpha = 1, 2$. We only consider corrections up to $\mathcal{O}(1/\omega)$ for the final answer. However, as the momentum is obtained by deriving the position with respect to time, an ω prefactor might appear, and thus we need to keep the terms $\mathcal{O}(1/\omega^2)$ until the end. Doing so leads to

$$\begin{aligned} \tilde{q}(z) = & \frac{b(z)}{z^2 - \lambda_s^2} + \frac{\kappa\omega\lambda_s e^{i\varphi}}{2(z^2 - \lambda_s^2)} \frac{b(z - i\omega)}{(z - i\omega)^2 - \lambda_s^2} \\ & + \frac{\kappa\omega\lambda_s e^{-i\varphi}}{2(z^2 - \lambda_s^2)} \frac{b(z + i\omega)}{(z + i\omega)^2 - \lambda_s^2} + \mathcal{O}\left(\frac{1}{\omega^3}\right), \end{aligned} \quad (3.5)$$

The expression of q is then obtained by taking the inverse Laplace transform of (3.5). In addition, we consider that the time is the one elapsed in the linear region, and the phase is the initial phase plus the one accumulated during the whole motion. This means doing the shifts $t \rightarrow t - t_0$ and $\varphi \rightarrow \varphi + \omega t_0$, with t_0 the time elapsed before the system entered the linear region. The position in the linear region q_{lin} in leading order in $1/\omega$ is:

$$\begin{aligned} q(t) = & q_0 \cosh(\lambda_s(t - t_0)) \\ & + \left(\frac{p_0}{\lambda_s} - \kappa \sin(\varphi + \omega t_0) q_0 \right) \sinh(\lambda_s(t - t_0)). \end{aligned} \quad (3.6)$$

The momentum in the linear region is given by

$$\begin{aligned} p_{\text{lin}}(t) = & (q_0\lambda_s + \kappa p_0 \sin(\omega t + \varphi)) \sinh(\lambda_s(t - t_0)) \\ & + (p_0 + \kappa\lambda_s q_0 (\sin(\omega t + \varphi) - \sin(\varphi + \omega t_0))) \\ & \times \cosh(\lambda_s(t - t_0)). \end{aligned} \quad (3.7)$$

This approximation is valid at least up to the crossover position $q_c \ll 1$.

The duration of the linear region can be obtained exactly by looking at

the time it takes the system to reach $\pm q_c$, where the $\pm$ indicates whether the system is propagating towards the positive or negative position:

$$t_1 = \frac{1}{\lambda_s} \log \left| \frac{q_c + \sqrt{q_c^2 - q_0^2 + \left(\frac{p_0}{\lambda_s} - \kappa q_0 \sin(\varphi)\right)^2}}{q_0 (1 - \kappa \sin(\varphi)) + \frac{p_0}{\lambda_s}} \right|. \quad (3.8)$$

After that time has elapsed, the system enters the homoclinic region.

The stability matrix in this region is given by

$$M(t) = \begin{pmatrix} \frac{\partial q_{\text{lin}}(t)}{\partial q_0} & \frac{\partial q_{\text{lin}}(t)}{\partial p_0} \\ \frac{\partial p_{\text{lin}}(t)}{\partial q_0} & \frac{\partial p_{\text{lin}}(t)}{\partial p_0} \end{pmatrix}, \quad (3.9)$$

with the derivatives of the position q_{lin} given by

$$\begin{aligned} \frac{\partial q_{\text{lin}}(t)}{\partial q_0} &= \cosh(\lambda_s(t - t_0)) \\ &\quad - \kappa \sin(\varphi + \omega t_0) \sinh(\lambda_s(t - t_0)), \end{aligned} \quad (3.10)$$

$$\frac{\partial q_{\text{lin}}(t)}{\partial p_0} = \frac{1}{\lambda_s} \sinh(\lambda_s(t - t_0)), \quad (3.11)$$

and those of the momentum p_{lin} by

$$\begin{aligned} \frac{\partial p_{\text{lin}}(t)}{\partial q_0} &= \lambda_s \sinh(\lambda_s(t - t_0)) \\ &\quad + \kappa (\sin(\omega t + \varphi) - \sin(\varphi + \omega t_0)) \lambda_s \cosh(\lambda_s(t - t_0)), \end{aligned} \quad (3.12)$$

$$\begin{aligned} \frac{\partial p_{\text{lin}}(t)}{\partial p_0} &= \cosh(\lambda_s(t - t_0)) \\ &\quad + \kappa \sin(\omega t + \varphi) \sinh(\lambda_s(t - t_0)). \end{aligned} \quad (3.13)$$

The symplectic evolution is conserved as the determinant is 1, up to some corrections in κ^2 which are neglected in this work. Details on this derivation can be found in Appendix C.

3.3.2 Homoclinic region

When a trajectory propagates sufficiently far away from the linearised region around the unstable fixed point, the trajectory stays close to the homoclinic, and its dynamics can be approximated by expanding the

trajectory in terms of the homoclinic motion. An ansatz for the solution is then given by

$$q_h(t) = q_{\text{sep}}(t) + \delta q(t), \quad (3.14)$$

with q_{sep} the position of the separatrix and δq the deviation from it such that $|\delta q| \ll q_{\text{sep}}$.

We first derive the expression of the separatrix from (3.2) with $\kappa = 0$, i.e., the unperturbed homoclinic in the absence of a driving. The solution is

$$q_{\text{sep}}(t) = 4 \arctan \left[\tan \left(\frac{q_1}{4} \right) \exp [\text{sgn}(q_1) \lambda_s (t - t_1)] \right], \quad (3.15)$$

where we define $\text{sgn}(q_1) = q_1/|q_1|$ which indicates again whether the system evolves towards the positive (outward motion) or negative positions (inward motion), $q_1 = \pm q_c$ is the position when the system enters the homoclinic region, t_1 the corresponding time, and t is the time elapsed in it. Details are found in Appendix D.

Let us now obtain an expression for the deviation from the separatrix δq by considering the presence of the driving again and assuming initial conditions (q_1, p_1) not necessarily on the separatrix. Multiplying equation (3.2) by $\dot{q}$ and integrating with respect to time yields

$$\begin{aligned} \frac{1}{2} \dot{q}^2(t) &\simeq \delta E_1 + 2\lambda_s^2 \sin^2[q(t)/2] \\ &\quad + \kappa \lambda_s \sin(\omega t + \varphi) \dot{q}(t) + O(\kappa/\omega), \end{aligned} \quad (3.16)$$

with $q_1 = q(t_1)$, $p_1 = \dot{q}(t_1)$, and

$$\begin{aligned} \delta E_1 &= \frac{p_1^2}{2} - \lambda_s^2 (1 - \cos q_1) - \kappa \lambda_s \sin(\omega t_1 + \varphi) p_1 \sin q_1 \\ &\simeq \frac{1}{2} (p_1^2 - \lambda_s^2 q_1^2) - \kappa \lambda_s \sin(\omega t_1 + \varphi) p_1 q_1 + O(q_1^3), \end{aligned} \quad (3.17)$$

the deviation, $\delta E_1 = E_1 - E_{\text{sep}}$, of the initial energy $E_1 = H(q_1, p_1, t_1)$ from the unperturbed separatrix energy $E_{\text{sep}} = \lambda_s^2$. Using the generic scalings $\kappa \ll 1$ and $\kappa \omega \sim \lambda_s$ resulting from secular perturbation theory (see Appendix B), terms of the order $\sim \kappa/\omega$ effectively scale as $\sim \kappa^2/\lambda_s \sim \lambda_s/\omega^2$ and are henceforth neglected.

Consider now that the deviation from the above separatrix solution is tiny. The energy deviation from the separatrix is small as well, and one can assume $\delta E_1 \ll \lambda_s^2 \sin^2[q(t)/2]$ for all t , provided $q(t)$ starts sufficiently

far away from the unstable fixed point and does not approach too closely the fixpoint on the other side of the separatrix arc. Taking the positive square root of equation (3.16) and performing a Taylor series expansion in $\delta E_1/\{\lambda_s^2 \sin^2[q(t)/2]\}$ yields

$$\begin{aligned} \dot{q}(t) \simeq & 2\lambda_s \sin[q(t)/2] + \kappa\lambda_s \sin(\omega t + \varphi) \sin q(t) \\ & + \frac{\delta E_1}{2\lambda_s \sin[q(t)/2]} - \frac{\delta E_1^2}{16\lambda_s^3 \sin^3[q(t)/2]}, \end{aligned} \quad (3.18)$$

where we neglect terms $\sim O(\delta E_1^3)$ that will turn out to scale quadratically either with κ or with the initial phase-space deviation from the separatrix.

Injecting our assumption (3.14), that states that the position in the homoclinic region is a small deviation from the homoclinic, yields a differential equation for δq :

$$\begin{aligned} \dot{\delta q}(t) \simeq & \left(-\lambda_s \tanh \tau(t) + \frac{\delta E_1}{8\lambda_s} \sinh[2\tau(t)] \right) \delta q(t) \\ & + \text{sgn}(q_1) \left(\frac{\delta E_1}{2\lambda_s} \cosh \tau(t) - \frac{\delta E_1^2}{16\lambda_s^3} \cosh^3 \tau(t) \right) \\ & - \kappa\lambda_s \sin(\omega t + \varphi) \left(2 \text{sgn}(q_1) \frac{\sinh \tau(t)}{\cosh^2 \tau(t)} \right. \\ & \left. - \frac{\sinh^2 \tau(t) - 1}{\cosh^2 \tau(t)} \delta q(t) \right), \end{aligned} \quad (3.19)$$

neglecting terms that scale as $O(\kappa^2)$, $O(\kappa/\omega)$, $O(\delta E_1^3)$, $O(\delta E_1^2 \delta q)$, and $O(\delta q^2)$, and where $\tau(t) = \lambda_s(t - t_1) + \log(\tan(q_1/4))$. The solution to this differential equation is given by

$$\begin{aligned} \frac{\delta q(t)}{\text{sgn}(q_1)} = & \frac{\delta E_1 \lambda_s (t - t_1)}{4\lambda_s^2 \cosh \tau(t)} \left(1 + \frac{\delta E_1}{16\lambda_s^2} [2 \cosh^2 \tau(t) - 3] \right) \\ & + \frac{\delta E_1 \{ \sinh[2\tau(t)] - \sinh[2\tau(t_1)] \}}{8\lambda_s^2 \cosh \tau(t)} \left(1 + \frac{\delta E_1}{8\lambda_s^2} [\cosh^2 \tau(t) - 2] \right) \\ & - \frac{\delta E_1^2 \{ \sinh[4\tau(t)] - \sinh[4\tau(t_1)] \}}{256\lambda_s^4 \cosh \tau(t)}. \end{aligned} \quad (3.20)$$

This approximation is valid as long as the dynamics can be linearised around the homoclinic.

Again, we can obtain the duration of the region, which we will note

t_2 . As δq contributes little to that duration, it can be safely neglected. Assuming the homoclinic region starts at q_1 and ends at q_2 , one has

$$t_2 = \frac{1}{\lambda_s} \log \left(\frac{\tan\left(\frac{q_2}{4}\right)}{\tan\left(\frac{q_1}{4}\right)} \right) \simeq \frac{1}{\lambda_s} \log \left(\frac{16}{q_c^2} \right). \quad (3.21)$$

where $q_2 = 2\pi - q_c$ or q_c depending if the system propagates towards positive or negative position respectively. It is important to note that injecting t_2 in $q_{\text{sep}} + \delta q$ will not return exactly q_2 because the deviation was not considered. This is, however, not an issue as initial conditions for the linear region will still fulfill the linearisation hypothesis and thus any deviations will be taken into account in the coming linear region.

The associated stability matrix can be calculated by evaluating the effect of a tiny initial deviation with respect to this particular reference trajectory, at fixed total propagation time t_2 :

$$M = \begin{pmatrix} \frac{\delta q_2}{\delta q_1} & \frac{\delta q_2}{\delta p_1} \\ \frac{\delta p_2}{\delta q_1} & \frac{\delta p_2}{\delta p_1} \end{pmatrix} \simeq \begin{pmatrix} 0 & (1 - \kappa_1)/\lambda_s \\ -(1 + \kappa_1)\lambda_s & \kappa_2 - \kappa_1 \end{pmatrix}, \quad (3.22)$$

with $\kappa_j = \kappa \sin(\omega t_j + \varphi)$, $j = 1, 2$. The symplectic structure is conserved as well. A more detailed derivation is shown in Appendix D.

As we split the motion such that our mathematical framework allows us to know the final position and momentum of one region using the final conditions of the previous region as initial ones, we refer to our development as a *mapping*.

3.3.3 Scaling of the crossover position with the perturbation

In this section, we analyse how q_c can be chosen while still fulfilling the conditions of validity of the linear and homoclinic regions as a function of the perturbation. The upper limit of the choice of q_c is set by the former: as the equation should be linearisable, $q_c \ll 1$. The lower limit is set by the latter. As the system evolves, the hypothesis of small deviation from the homoclinic is eventually not satisfied. Indeed, as a phase-space trajectory gets closer to the origin, its momentum remains finite, whereas the momentum of the homoclinic tends to 0. Identifying where the quasi-integrable case deviates from the integrable one enables us to know where this hypothesis breaks down, and puts a lower bound on the choice of q_c . To this end, two criteria must be investigated.

Firstly, it can be shown that a trajectory evolved with the perturbed

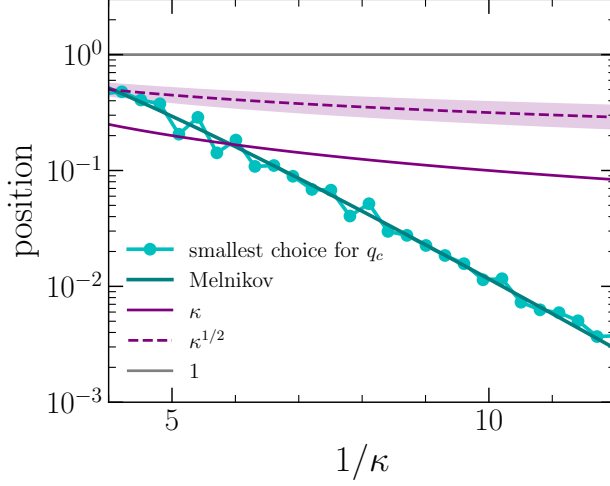


Figure 3.2: Closest position to the origin reachable before the homoclinic region formalism deviates from the numerical solution. This position is plotted as a function of the inverse perturbation parameter $1/\kappa = \omega\lambda_s/K$, obtained numerically (blue) and with the Melnikov method detailed in Appendix E (darker shade of blue). The points were obtained using $\kappa\omega = \lambda_s$, $\varphi = 0.1$. In solid purple, we show the closest position to the origin set by the linearisation condition of equation (3.18), and in dashed purple an arbitrary scaling of $q_c = \kappa^\alpha$, with $\alpha = 1/2$, that satisfies both boundaries. The shaded region corresponds to $\alpha \in [0.4, 0.6]$

Hamiltonian will remain close to one that is propagated using the unperturbed Hamiltonian for a time that increases exponentially as the perturbation decreases [141, 142]. We can use the Melnikov method [69, 76, 139, 140] to estimate the scaling of the lower bound of the crossover position. As shown in Appendix E, we obtain that the choice of q_c must satisfy

$$q_c \gg \sqrt{\frac{\sqrt{2}\pi\kappa(\omega/\lambda_s)^3}{\sinh(\pi\omega/2\lambda_s)}}, \quad (3.23)$$

letting us a generous freedom of choice for q_c . We then verify those predictions numerically. To this end, we investigate how close, from initial conditions taken near the hyperbolic fixed point, the system was able to get to the other fixed point linked to the first one by a separatrix before the exact numerical solution deviated from our analytical expression as a function of κ . We consider two solutions not to match anymore when the relative difference of momentum, estimated by $|p_1 - p_2|/(|p_1| + |p_2|)$, becomes larger than a given threshold¹. The distance between the position of deviation and the hyperbolic fixed point determines the lower bound of q_c . Those numerical verifications match perfectly with the lower bound (3.23) obtained using the Melnikov method. Nonetheless, this lower bound is not the only one to take into account.

Indeed, one must also ensure that all the steps that were followed to obtain the homoclinic region formalism are valid. The expansion that results in equation (3.18) implies

$$2\delta E_1 + 2\kappa\lambda_s \sin(\omega t + \varphi)\dot{q}(t) \ll 4\lambda_s^2 \sin^2\left(\frac{q(t)}{2}\right). \quad (3.24)$$

Using again (3.18) for the expression of $\dot{q}$ and neglecting terms of order $\mathcal{O}(\kappa^2)$, i.e., keeping only the term related to the separatrix, the inequality becomes

$$\kappa \left(q_c^2 + \sin(\omega t + \varphi) \sin\left(\frac{q(t)}{2}\right) \right) \ll \sin^2\left(\frac{q(t)}{2}\right). \quad (3.25)$$

This equation can become invalid if q_c is chosen too small, leading to a disagreement at the end of the homoclinic region between the equations before and after linearisation around the separatrix, i.e., (3.16) and (3.18).

¹ The threshold was set at 0.5, but its value is of little importance since any threshold will yield an exponential scaling.

From the equation, one infers the condition $\kappa \ll q_c$, which puts a lower bound on the scaling of the boundary position.

These results are shown in Figure 3.2, which shows the minimal value for the choice of q_c as a function of the inverse of the perturbation parameter. The numerical bound is shown in blue and is indeed exponential in the inverse of κ [141, 142]. The bound related to Nekoroshev estimates matches perfectly with the numerical one. The smaller the perturbation parameter, the closer to the origin the boundary q_c can be set. However, the bound related to the linearisation condition, in solid purple, proves to be more limiting, and is therefore the one to follow for small κ . Let us note that for a larger perturbation parameter, i.e., beyond the left border of the figure, the limiting condition would be the bound obtained using the Melnikov method, but as it is outside the scope of our work, we do not consider it here.

As a summary, as long as q_c is chosen larger than the purple line while still being smaller than 1, represented by the grey horizontal line, i.e., $\kappa \ll q_c \ll 1$, the linear-homoclinic formalism will work. A working choice is $q_c = \kappa^\alpha$, with for instance $\alpha = 1/2$, but values ranging from 0.4 to 0.6 are suitable as well, as they preserve the hierarchy. The value of α itself is of little importance.

3.4 EXPONENTIAL GROWTH RATE FROM THE STABILITY MATRIX

In Section 3.3, we developed a mathematical formalism describing the system by splitting the phase space into two regions. This means, in particular, that the trace of the stability matrix can be obtained using this mapping. Bearing in mind that when splitting the motion into different regions, the corresponding stability matrices must be multiplied, one can write

$$\text{Tr}(M(t)) = \text{Tr}(\dots M_h(t_{k+1}) M_{\text{lin}}(t_k) \dots). \quad (3.26)$$

Stroboscopic sections for a near-integrable and a mixed regime are shown on the first line of Figure 3.3. The hyperbolic fixed point is located at the origin of the axes at $(0, 0)$. On the second row of the same figure, we show the absolute value of the trace of the stability matrix obtained from the numerical solution of (3.2) for the simple pendulum (grey), for the driven pendulum numerically (purple), and using our mapping (orange) for a single point in the vicinity of the separatrix. On the last

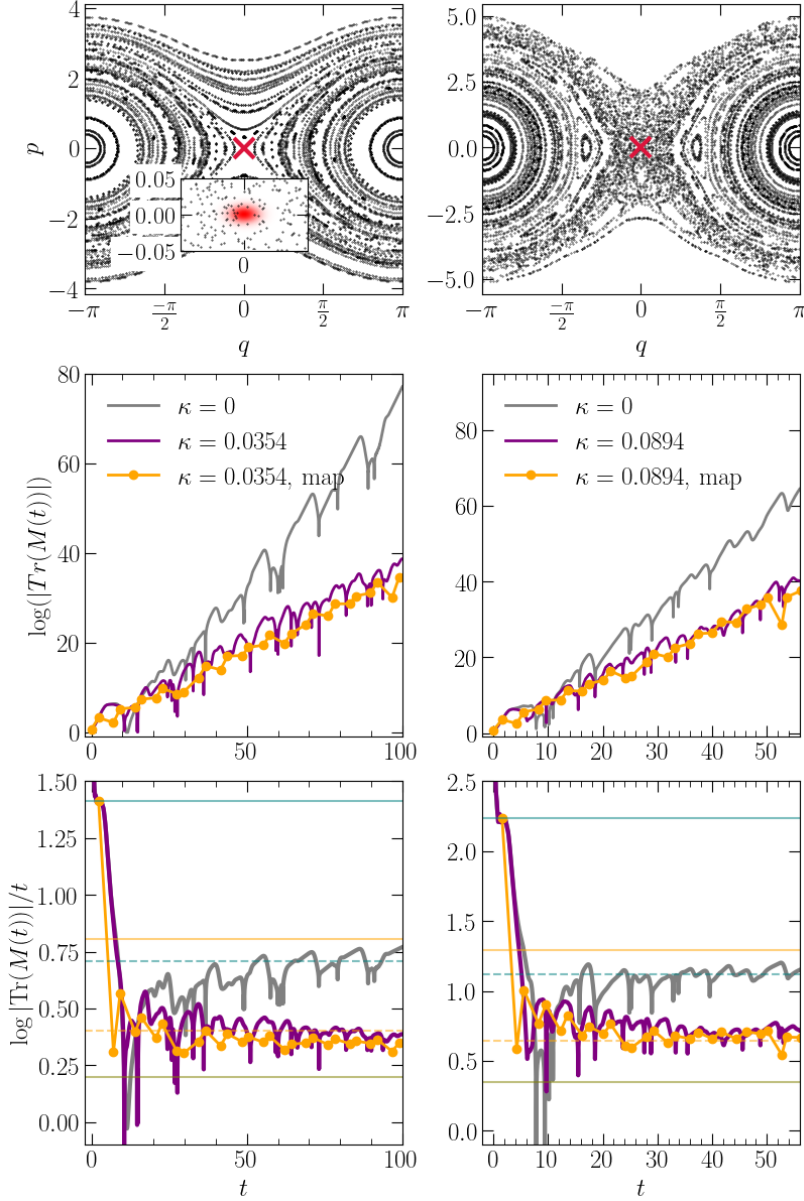


Figure 3.3: Trace of the stability matrix in the driven pendulum. *First row:* stroboscopic section of the driven pendulum. *Second row:* trace of the stability matrix for different perturbation parameters. *Third row:* Exponential growth rate extracted from the second row. Different rates are show as horizontal lines: λ_s in blue, $\lambda_s/2$ in dashed blue, $(\lambda_L + \lambda_s)/2$ in orange, and $(\lambda_L + \lambda_s)/4$ in dashed orange. The last two rows use the same colour scheme: grey for the numerical solution of the simple pendulum, purple for the driven pendulum, and orange for the driven pendulum using the mapping derived in 3.3. The first column is for $\lambda_s = \sqrt{2}$, $\omega = 10$, $\kappa = 0.0354$, and the second one for $\lambda_s = \sqrt{5}$, $\omega = 12$, $\kappa = 0.0894$.

row, we show the exponential growth rate extracted from the second row using the same colour coding as well as horizontal lines corresponding to multiples of the stability exponent, the Lyapunov exponent of the chaotic layer, and the effective exponent.

First, we notice that the trace in the absence of driving follows the same behaviour as highlighted in [127], i.e., an initial exponential growth where the rate is initially λ_s , then a crossover occurs, and the rate becomes $\lambda_s/2$. In the presence of the perturbation, the long-time behaviour is different, and the rate lies between the Lyapunov exponent and the stability exponent.

We can see that the mapping faithfully reproduces the trace of the stability matrix, even with only one trajectory. Consequently, it enables us to extract an exponent analytically. As one must propagate the system for a long time in order to obtain a reliable expression of the exponent dictating the dynamics, this means multiplying a high number of stability matrices, which, of course, becomes quickly untractable, even for one trajectory. Nonetheless, one can try to obtain a reasonably good estimate of the exponent by considering only a total of two linear regions and one homoclinic region and by taking the initial conditions at the negative-position boundary of the linear region, on the homoclinic. The reason behind this choice is the following. As the goal is to obtain an estimate of the effective exponent, a natural choice would be to consider one cycle, i.e., one linear and one homoclinic region. However, doing so results in the particular case where the trace of the stability matrix vanishes due to a sign change of the trace that occurs at that point, which implies that this particular choice will not at all yield a representative result for the average absolute value of the trace. To counter that, we considered an additional linear region for this particular evaluation. One could have made the choice to consider two homoclinic regions and one linear region. While this would have slightly modified the analytical result, the estimation would still agree with the numerical simulations.

The estimate of the trace in this region is

$$\text{Tr}(M(t_1 + t_2 + t_1)) = \text{Tr}(M_{\text{lin}}(t_1)M_{\text{h}}(t_2)M_{\text{lin}}(t_1)), \quad (3.27)$$

where $(q_0, p_0) = (-q_c, \lambda_s q_c + \delta p)$, with $\delta p \ll \lambda_s q_c$, are the initial conditions of the first linear region and correspond to the leftmost part of that region, with a slight deviation in momentum from the separatrix, (q_1, p_1) those

of the homoclinic region, and t_1 and t_2 the durations of the linear and homoclinic regions. For these initial conditions, the times are given by

$$\begin{cases} t_1 &= \frac{1}{\lambda_s} \log \left(\frac{2q_c}{\delta p + \kappa q_c \sin(\varphi)} + 1 \right) \simeq \frac{1}{\lambda_s} \log \left(\frac{2}{\kappa} + 1 \right), \\ t_2 &= \frac{1}{\lambda_s} \log \left(\frac{16}{q_c^2} \right), \end{cases} \quad (3.28)$$

where the approximation for t_1 is valid because it can be shown² that the order of magnitude of δp is $\kappa q_c \lambda_s$.

Extracting the exponent yields

$$\lambda_{\text{eff}} = \frac{1}{2t_1 + t_2} \log |\text{Tr}(M_{\text{lin}}(t_1)M_{\text{sep}}(t_2)M_{\text{lin}}(t_1))|. \quad (3.29)$$

Using the stability matrices (3.9) and (3.22), the asymptotic behaviour of the hyperbolic functions $\cosh(x) \sim \sinh(x) \sim \exp(x)/2$, as well as the durations in (3.28), the dominant contribution to the trace of the stability matrix is given by

$$\begin{aligned} & |\text{Tr}(M_{\text{lin}}(t_1)M_{\text{sep}}(t_2)M_{\text{lin}}(t_1))| \\ &= \left| \frac{8\kappa}{q_c^2} (\sin(\varphi + \omega t_2) - 2 \sin(\varphi + \omega t_1) - \sin(\varphi)) \right| + \mathcal{O}(\kappa^2) \end{aligned} \quad (3.30)$$

$$\simeq \frac{\beta \kappa}{q_c^2} + \mathcal{O}(\kappa^2), \quad (3.31)$$

with $\beta > 0$ some real coefficient and κ assumed, without loss of generality, to be positive. The combination of sine functions in the parentheses is akin to a random prefactor. Thus, one can replace it with the square root of the average of the square of all terms, which yields an estimation of $\beta = 16\sqrt{2} \simeq 20$

Taking this into account as well as the scaling of q_c as a power of κ , one obtains the following expression for the exponent dictating the dynamics of the system:

$$\lambda_{\text{eff}} = \lambda_s \frac{\log(\beta \kappa^{1-2\alpha})}{\log(16/\kappa^{2+2\alpha})}. \quad (3.32)$$

² The procedure is the following. Starting from the initial condition $(q_0, p_0) = (-q_c, \lambda_s q_c + \delta p)$, with $\delta p \ll \lambda_s q_c$, one applies the mapping for the linear region, then for the homoclinic region, which can be approximated by (D.29). The momentum deviation at the end of the homoclinic region is the initial one divided by 2, so it disappears, plus a term of the order of $\kappa q_c \lambda_s$.

A suitable (but by no means unique) choice of α that ensures the hierarchy $\kappa \ll q_c \ll 1$ is $\alpha = 1/2$, which results in the following expression for the effective exponent:

$$\lambda_{\text{eff}} = \lambda_s \frac{\log(\beta)}{\log(16/\kappa^3)}. \quad (3.33)$$

For completeness, let us also present the expression that would result from two homoclinic propagations between which one propagation in the linear region takes place. The exponent has then the form

$$\lambda_{\text{eff}} = \lambda_s \frac{\log(2/\kappa)}{\log(16^2/\kappa^{2+4\alpha})}, \quad (3.34)$$

which, using $\alpha = 1/2$, becomes

$$\lambda_{\text{eff}} = \lambda_s \frac{\log(2/\kappa)}{\log(16^2/\kappa^4)}. \quad (3.35)$$

Let us recall that, as long as the hierarchy is verified, the precise value of α is of little importance as it has a minor impact on the estimation of the effective exponent. The last two expressions must thus not be taken as an unquestionable result but as an estimation that correctly captures the dynamics.

These expressions can be compared with the numerics, as shown in Figure 3.4. In this figure, we show different exponents in unit of the stability exponent: the stability one λ_s (orange), $(\lambda_s + \lambda_L)/4$ where the two exponents have been obtained separately using the Wolf algorithm [77] (green), $(\lambda_s + \lambda_L)/4$ obtained from the evolution of the trace of the stability matrix (red), and finally the analytical expressions (3.33) (purple), using $\beta = 20$ and (3.35) (dashed purple). The predictions are consistent with what is observed numerically. We also show, using shaded areas, the range of estimation of λ_{eff} for $\alpha \in [0.4, 0.6]$. This range was chosen so that the hierarchy $\kappa \ll q_c \ll 1$ is satisfied, which ensures the validity of our formalism. Substantially higher or lower values for α are not in line with our working hypotheses and thus result in significant deviations from our numerical findings.

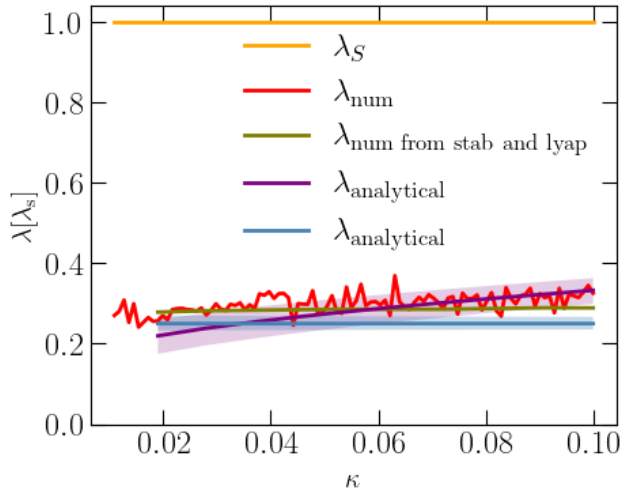


Figure 3.4: Exponential growth rates. The stability exponent λ_s is shown in orange, the effective exponent of the trace $\lambda_{\text{num}} = (\lambda_s + \lambda_L)/4$, obtained numerically is shown in red, λ_{num} but with both exponents obtained using the Wolf algorithm in green, equation (3.33), labelled $\lambda_{\text{analytical}}$ is shown in purple using $\beta = 20$, and (3.35) in dashed purple, using $q_c = \kappa^{1/2}$ for the last two. In addition, we also show in shaded areas how the estimation varies for $\alpha \in [0.4, 0.6]$.

3.5 COMPLEMENTARY NUMERICAL FINDINGS

3.5.1 *Out-of-time-ordered correlators*

The exact application of expressions (3.33) or (3.35) to other systems is not straightforward, as it implies applying secular perturbation theory. However, as the Hamiltonian of the driven pendulum is the one that universally describes any system around a resonance, the results of the previous section can be extended to any system in the near-integrable regime. We focus on the kicked rotor and the kicked Bose-Hubbard dimer. Furthermore, to link the quantum and classical dynamics, we use the OTOC as a probe.

The kicked rotator is quantally and classically described by respectively (1.124) and (1.125). In the first column of Figure 3.5, we show in the top panel a phase space representation for a kicking strength $K = 0.6$, and in the bottom panel the OTOC with the operator $\hat{A} = \hat{B} = \sin(\hat{p})$ alongside different exponentials to highlight the different regimes of exponential growth rate. First, the OTOC grows with an exponential rate of $2\lambda_s$, transitions to a $1\lambda_s$ regime as expected [127], and then reaches the $(\lambda_s + \lambda_L)/4$ regime. We thus observe the same behaviour as with the trace of the stability matrix, the only difference being the factor 2 in the growth rate due to the modulus square appearing in the OTOC definition.

The kicked Bose-Hubbard dimer is described quantally by (1.133), and classically by (1.135). Similarly to the kicked rotor, we show a stroboscopic section in the first line of the second column of Figure 3.5 for $N = 5000$ particles and $U = 0.015J$, followed by the OTOC with $\hat{A} = \hat{n}_1$, $\hat{B} = \hat{n}_2$ the population operators on site 1 and 2, and the same conclusions hold: the OTOC follows the same behaviour as the trace of the stability matrix, with a factor of 2 in the exponential growth rates.

3.5.2 *Mixed systems - exponent hierarchies*

Our formalism is built on the hypothesis of a thin chaotic layer around the homoclinic for a driven pendulum. It is nonetheless useful to see how it fares against a wider chaotic layer, i.e., well beyond the hypothesis of a small perturbation κ . The results are shown in Figure 3.6, using the trace of the stability matrix again. The phase space is represented in the first column, and the trace of the stability matrix in the second one. As the phase space becomes more chaotic, the hierarchy of the different exponents

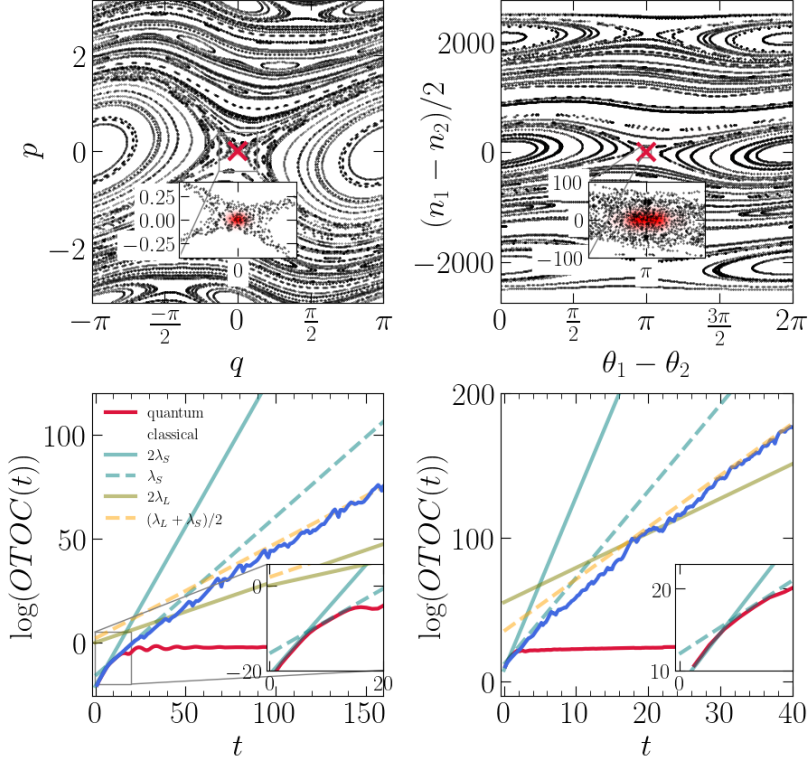


Figure 3.5: OTOC in near-integrable kicked rotor and dimer. *First column:* Standard map/kicked rotor. Top: Phase space representation of the standard map for $K = 0.6$, $\hbar_{\text{eff}} = 2^{-14}$. The centre of the initial coherent state is indicated by a cross at $(0, 0)$. Bottom: quantum (red) and classical (blue) OTOC with the operator $\hat{A} = \hat{B} = \sin(\hat{p})$. Different exponential functions are shown to highlight the different regimes. *Second column:* kicked dimer. Top: Phase space representation of the kicked dimer for $N = 5000$, $U = 0.015J$. The centre of the initial coherent state is indicated by a cross at $(\pi, 0)$. Bottom: quantum (red) and classical (blue) OTOC with the operator $\hat{A} = \hat{n}_1$, $\hat{B} = \hat{n}_2$. Different exponential functions are shown to highlight the different regimes.

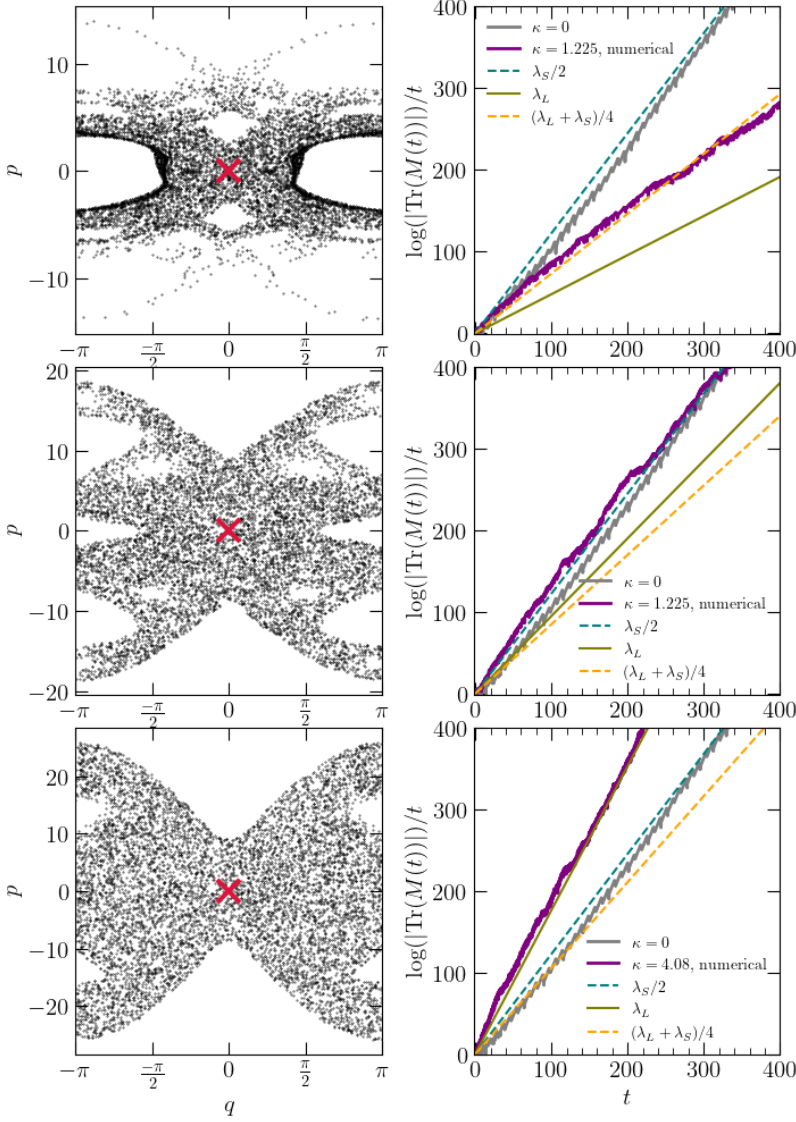


Figure 3.6: Trace of the stability matrix in strongly mixed and chaotic driven pendulums. *First column:* Phase space of the driven pendulum for $\lambda_s = \sqrt{6}$ and different perturbation parameters. *Second column:* trace of the stability matrix in the corresponding phase space for an initial coherent state centred on the fixed point (red cross in the phase space). Lines corresponding to exponentials with the rate being half the stability exponent $\lambda_s/2$, the Lyapunov exponent λ_L , or a combination of both are shown. For all: $\lambda_s = \sqrt{6}$, $\omega = 10$. First row: $\kappa = 0.245$, $\lambda_L = 0.479$. Second row: $\kappa = 1.225$, $\lambda_L = 0.951$. Third row: $\kappa = 4.08$, $\lambda_L = 1.76$.

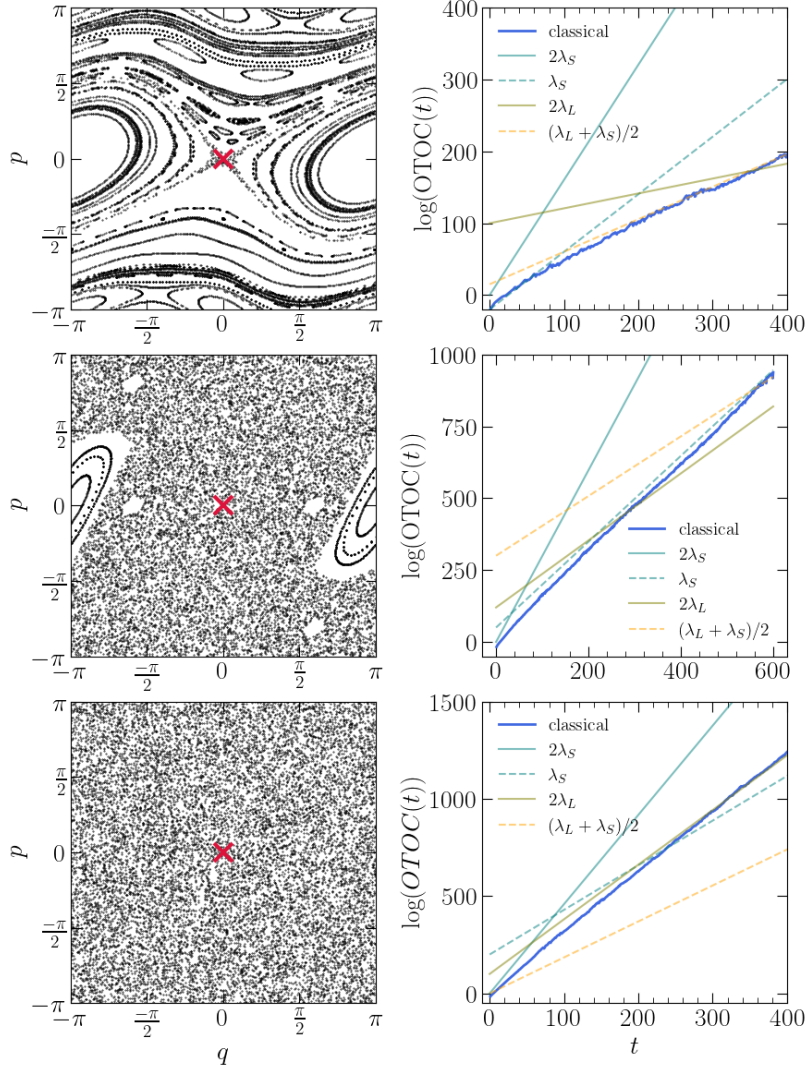


Figure 3.7: OTOC in near-integrable, strongly mixed and chaotic kicked rotors. Phase space (first column) and OTOC (right column) for different kicking parameters of the kicked rotor, for an initial coherent state centred on the fixed point at the origin (red cross in the phase space). The right plot also shows lines corresponding to exponentials with the rate being the stability exponent λ_s , the Lyapunov exponent λ_L , or a combination of both. Second row: $K = 0.676$, $\lambda_s = 0.802$, $\lambda_L = 0.104$. Second row: $K = 3.007$, $\lambda_s = 1.49$, $\lambda_L = 0.583$. Third row: $K = 8.00$, $\lambda_s = 2.29$, $\lambda_L = 1.40$. The operators for the OTOC are $\hat{A} = \hat{B} = \sin(\hat{p})$.

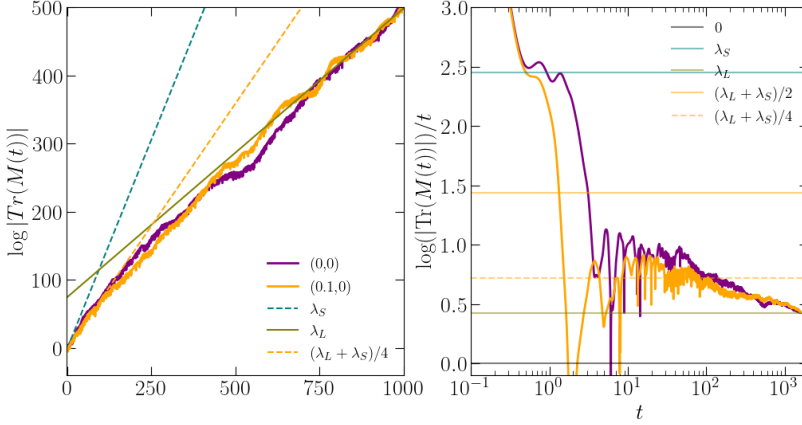


Figure 3.8: Long-time behaviour of the trace of the stability matrix. *Top*: trace of the stability matrix of the driven pendulum for $\lambda_s = \sqrt{6}$, $\kappa = 0.12$, $\hbar_{\text{eff}} = 2^{-8}$, for a coherent state centred on $(0,0)$ (purple) and $(0.2,0.2)$ (orange). *Bottom*: Exponential growth rate. Note the horizontal log scale.

changes. In the first row of the figure, it is $\lambda_L < (\lambda_s + \lambda_L)/4 < \lambda_s/2$. In the second row, the two smallest exponents are switched: $(\lambda_s + \lambda_L)/4 < \lambda_L < \lambda_s/2$. Finally, in the third row, we have $(\lambda_s + \lambda_L)/4 < \lambda_s/2 < \lambda_L$. We can notice the different behaviours depending on the hierarchy. In the first case, the long-time exponent (before going to the Lyapunov regime at very long times) is $(\lambda_s + \lambda_L)/4$. In the second one, $\lambda_s/2$ dominates, and in the last one, it is the Lyapunov exponent λ_L .

We also investigated the different hierarchies in the kicked rotor. We show, in the first column of Figure 3.7, different phase spaces of the kicked rotor corresponding to different hierarchies of λ_s , λ_L , and $(\lambda_s + \lambda_L)/4$. The systems are strongly mixed or fully chaotic. In the right column, we show out-of-time-ordered correlators for an initial coherent state centred on the hyperbolic fixed point at the origin, and we highlight the different exponential regimes with straight lines. The same conclusions as for the driven pendulum are drawn: for the first hierarchy, the effective exponent dominates, for the second hierarchy it is $\lambda_s/2$, and for the last one it is λ_L .

3.5.3 *Long-time behaviour*

Whether the system is integrable or not, the initial λ_s regime of the trace, as well as the contribution of λ_s to the later-time exponent, are purely features of the initial wavepacket being placed on the hyperbolic fixed point. One can then wonder what happens at very long times, and how the behaviour varies with the thickness of the chaotic layer. In Figure 3.8, we show the exponential growth rate of the trace of the stability matrix for an initial coherent state centred either on the hyperbolic fixed point or in the chaotic layer around the homoclinic in the driven pendulum. The trace first follows a λ_s regime. It then enters a $(\lambda_s + \lambda_L)/4$ regime, and after that the system eventually falls back to a λ_L regime. The farther from the fixed point the initial state is, the shorter the λ_s regime. However, it does not seem to have a large impact on the long-time behaviour, indicating that being on the separatrix is more important than being close to the fixed point.

Quantum mechanics is known to differ from the classical world in many aspects. For instance, as already explained, concepts like sensitivity to initial conditions only make sense in a classical scheme, due amongst other things to the uncertainty principle. Others only exist in the quantum realm, like the concept at the heart of this chapter: quantum scars. This chapter is dedicated to their study from a numerical perspective, using quantum and classical scrambling signatures.

In the previous chapter, we studied the dynamics of paradigmatic systems around unstable fixed points in near-integrable regimes. We showed that a state initially localised at those points exhibits a particular behaviour in (classical) scrambling signatures. In this chapter, we stray further from integrability and consider strongly mixed and fully chaotic systems. In those cases, unstable points, and more generally unstable periodic orbits, can be associated with a phenomenon called quantum scars.

Quantum scarring refers to an eigenstate of the Hamiltonian of a (classically) chaotic system that stays localised, and thus fails to thermalise when time-evolved, if it satisfies Heller’s criterion [18, 143]. The criterion is formulated as follows. In the classical phase space, the unstable periodic orbit on which the eigenstate is located has a stability exponent λ_s and a period T . The eigenstate is associated with a scar if the inequality

$$\lambda_s T \leq 2\pi \tag{4.1}$$

is satisfied. In other words, the considered orbit must not be too unstable and/or short enough for a scar to exist; otherwise, the state initially placed on it will simply thermalise.

While introduced initially in a single-particle context in the eighties [143, 144], they have since then been extended to many-body systems, where the scars can manifest as persistent oscillations of observables [145–149]. However, some precisions have to be brought in the many-body case. Some articles in the literature use the name of scars to refer to localisation whose origin is not always specified and thus might not be related to an underlying periodic unstable orbit [147, 150, 151]. Those “scars” are therefore not necessarily fitting Heller’s description. In this chapter, we

focus on *genuine* quantum many-body scars, meaning localisation in phase space that originates from a wavepacket initially placed on an unstable periodic orbit, exactly like the single-particle case [148, 152, 153].

Quantum scars have been experimentally realised in the context of single-particle systems with, for instance, Sinai billiard [154], stadium billiard [155], cylinder-shaped cavities [156], a hydrogen atom in a magnetic field [157], and in the many-body context using a Bose-Hubbard system made of Rubidium atoms [158].

In the continuity of the previous chapter that studied scrambling probes in the vicinity of unstable fixed points in a near-integrable regime, the goal of this one is to look at those probes in the vicinity of scars, which include unstable fixed points, but also unstable periodic orbits. We first investigate the short-time behaviour of the probes in a single-particle system. Identifying evidence of scars in a time region where the dynamics can be reproduced quasiclassically would imply that a signature of a scar can be found in the classical dynamics. In a second time, we switch to a many-body context and look at signatures of scars in the post-thermalisation regime of observables.

This chapter is structured as follows. In Section 4.1, we look at two types of resonances, the 1 : 1 and 3 : 1 resonances, of the kicked rotor, and try to find signatures of scars in the short-time behaviour of OTOCs. In Section 4.2, we study staggered dimer states in Bose-Hubbard models. More specifically, we focus on oscillations that occur beyond the saturation of two types of observables: site occupations and OTOCs.

4.1 KICKED ROTOR

The first system that we used to study quantum scars is the kicked rotor, whose Hamiltonian is given by (1.124). As always, it presents itself as a particularly useful model that exhibits universal features despite its apparent simplicity.

Let us introduce another phase-space visualisation tool: the inverse participation ratio (IPR). Consider a Hamiltonian of eigenvectors $\{|\varphi_k\rangle, k = 1, \dots, K\}$ with K the Hilbert space dimension. Our phase-space IPR is defined as

$$I(\alpha) = \sum_{k=1}^K |\langle \varphi_k | \alpha \rangle|^4, \quad (4.2)$$

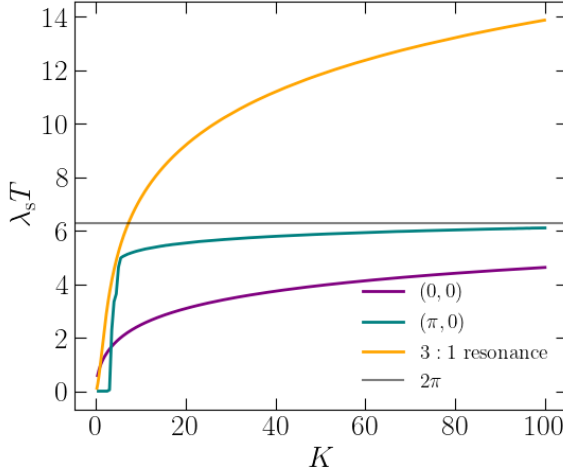


Figure 4.1: Heller’s criterion and the kicked rotor. The plot shows the product of the stability exponent λ_s and the period T associated with the fixed point at the origin (purple), $(\pi, 0)$, and the 3 : 1 resonance (orange).

with $|\alpha\rangle$ a coherent state centred on the complex number $\alpha = (q + ip)/\sqrt{2}$ with q and p the position and momentum [159, 160]. This quantity is similar to the Husimi distribution, defined in Section 1.5.4, but contains crucial differences. It is not a way to probe a state using coherent states and visualise where it lies in the phase space. Rather, it probes the Hamiltonian directly, through its eigenvectors, and gives information as to which phase-space region is associated with a localised or delocalised state. Consider, as an example, a fixed point that lies in the chaotic sea. The sum of the fourth power of the overlap of all the eigenvectors with a coherent state centred on that point is larger than for a coherent state slightly shifted. The reason is that, because that state is localised, the IPR will be large at that point due to the fourth power. Conversely, the slightly shifted coherent state will have a nonzero overlap with more eigenstates, but the components will be small, thus resulting in an overall lower IPR. The IPR thus presents itself as a phase-space probe that allows us to verify whether regions are likely to be associated with scars. However, they are not a straightforward tool, because, as will be seen, regions associated with scars might have an IPR that is much lower

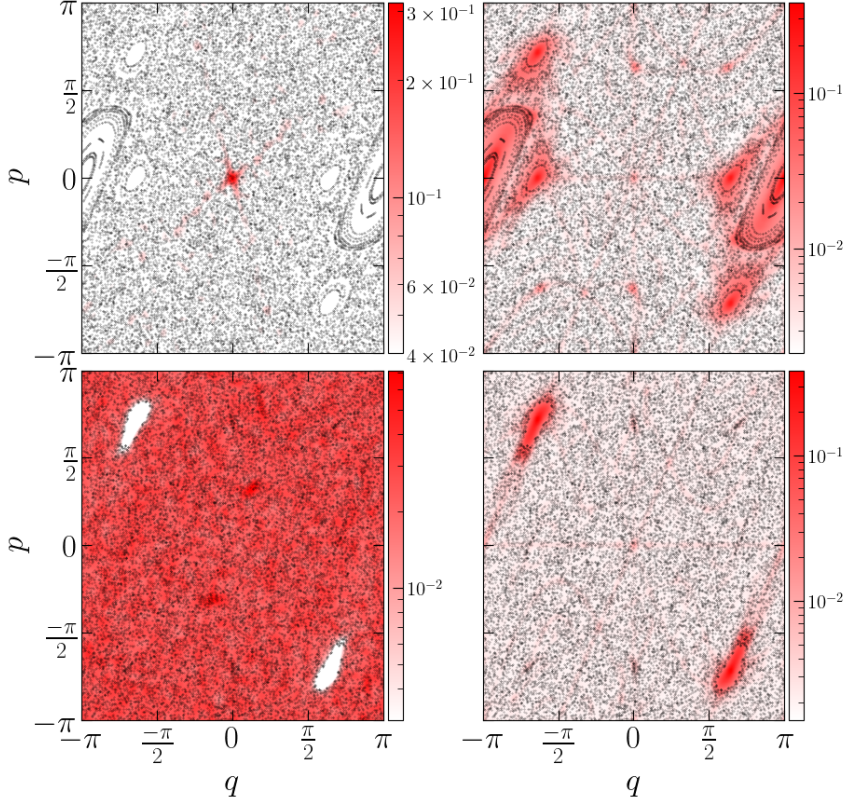


Figure 4.2: Time-averaged Husimi distributions for various evolved coherent states (left column) and inverse participation ratio (right column) of the kicked rotor, shown over the classical phase space, with $\hbar_{\text{eff}} = 2\pi/N$ and $N = 2^{10}$, and for various kicking strengths K . The first row is for $K = 2.5$, and the Husimi, averaged on 50 kicks, is computed for a coherent state centred on $(0, 0)$, the unstable fixed point, that is time-evolved for 30 kicks. The second row is for $K = 5$, and the Husimi, averaged over 50 kicks, is computed for a coherent state centred on $(0.6, 1)$, a generic point in the chaotic sea, evolved for 30 kicks. In the Husimi plots, one can notice that the state stays localised in the first row, indicating a scar, and is spread over the phase space in the second row.

that those associated with regular regions of the phase space, i.e., stable islands.

The unstable periodic orbits we will study are the following. First, the unstable fixed points, or $1 : 1$ resonances, that are found at $(0, 0)$, i.e. the origin, and at $(\pi, 0)$, the latter being unstable only for a strong enough kicking strength, and second, the $3 : 1$ resonances found on the $q = 0$ axis¹. As the goal is to look at quantum and classical scrambling signatures in the context of scars, a crucial point is comparing two kinds of situations: whether the unstable periodic orbit satisfies or not Heller's criterion. To this end, we show in Figure 4.1 the product of the stability exponent λ_s and the period T of the aforementioned orbits as a function of the kicking strength K , and a horizontal line at 2π . Concerning the unstable fixed points, for the range of K considered here, Heller's criterion is always satisfied. For the $3 : 1$ resonance, on the other hand, there is a threshold over which the criterion is not fulfilled, hence allowing us to study the influence of Heller's criterion on scrambling signatures.

The first two scar indicators that we consider are phase-space visualisations: the Husimi distribution and the IPR. We show them in Figure 4.2, using a logarithmic colour scale. All the plots are for $\hbar_{\text{eff}} = 2\pi/N$ and $N = 2^{10}$. The first and second columns contain the Husimi distributions and the IPR on top of the corresponding classical phase space, respectively. The first line is for $K = 2.5$, and the initial state used for the Husimi is a coherent state centred at the origin, i.e. the unstable fixed point. The state has been time-evolved for 30 kicks, and the Husimi distribution has been averaged over 50 kicks in order to smooth the background. One can clearly observe that the state stays localised on the fixed point, indicating the presence of a scar. The IPR shows how much a region is associated with a localised state. Obviously, the regular islands are strongly associated with localisation. One can nonetheless notice other regions where the IPR is nonzero, for instance the fixed point at the origin, as is verified with the Husimi distribution. In addition, one can also observe axes of nonzero IPR that are associated with discrete symmetries². While a state placed on it will be more localised than a state placed initially randomly in the chaotic region, the localisation must

-
- 1 The exact momentum of the latter depends on the kicking strength, and is obtained by applying the mapping three times on the initial condition $(0, p_0)$, setting the final position after the three application to be $(2\pi, p_0)$, and solving (numerically) for p_0 .
 - 2 While one could argue that they are not very well visible, they become clearly distinguishable from the background at higher kicking strength, as is the case later in Figure 4.4 for $K = 20$.

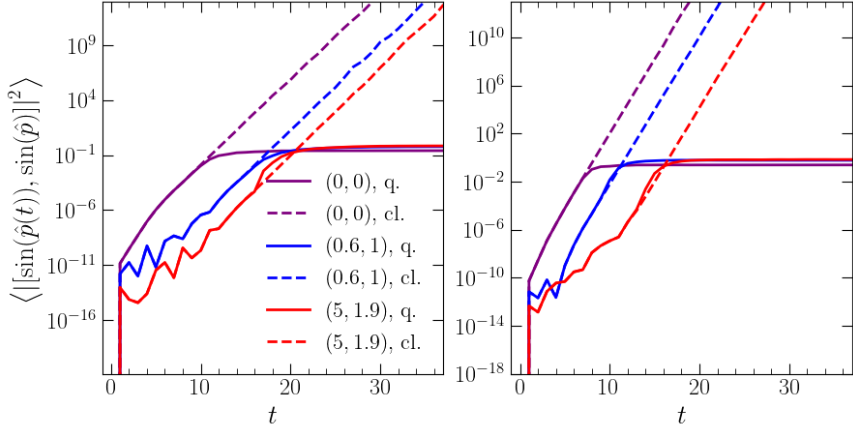


Figure 4.3: Out-of-time-ordered correlators computed in the kicked rotor for $K = 2.5$ (left) and $K = 5$ (right), with $\hbar_{\text{eff}} = 2\pi/N$ and $N = 2^{22}$. The initial states are indicated in the legend. The initial conditions of the purple curves correspond to the 1 : 1 resonance, the two others to random points in the chaotic sea. If the initial state is not on the resonance, the OTOC exhibits a temporary deviation from the exponential regime.

not be associated with a scar, as it stems from constructive interference resulting from discrete symmetries and not of unstable periodic orbits [161]. The second line of Figure 4.2 is for $K = 5$, and an initial coherent state centred on $(0.6, 1)$. To compute the Husimi, the state has been evolved for 30 kicks, and the distribution averaged over 50 kicks as well. One can notice that the state completely delocalised and is spread over the whole phase space.

Let us now, for those settings, compute out-of-time-ordered correlators. Despite quantum scars originating from quantum interferences, and thus being a beyond-Ehrenfest-time phenomenon, the goal is to see whether or not signatures are observable in indicators such as OTOCs, and in addition, if signatures before the Ehrenfest time exist. If the latter holds, this would mean that it would be possible to find a classical signature of scars. We thus show, in Figure 4.3, OTOCs computed, with $\hbar_{\text{eff}} = 2\pi/N$ and $N = 2^{22}$, for $K = 2.5$ and 5, for 3 coherent states initially centred on different points: $(0, 0)$ (purple), $(0.6, 1)$ (blue), and $(5, 1.9)$ (red). The first one corresponds, as already mentioned, to the fixed point associated with a scar, whereas the other two are random points in the chaotic sea. The quantum OTOCs are shown using solid lines, whereas the quasiclassical

ones are shown using dashed lines. As is expected in the presence of chaos, the OTOCs grow exponentially, then saturate. There is, however, a clear temporary deviation from the exponential growth in the form of a dip for the curves corresponding to initial states not centred on the $1 : 1$ resonance. In contrast, the OTOC associated with the state centred on the fixed point never deviates from the exponential regime before the saturation. This behaviour is consistent across all the tested kicking strengths and states.

While it is possible to compare probes in the cases where the initial state is placed, or not, on the $1 : 1$ resonance, it is not feasible to tell what the importance of the fulfilment of Heller's criterion is for a state placed on such an orbit. This flexibility is present with the $3 : 1$ resonance. Indeed, as can be seen in Figure 4.1, one can clearly see that the product of the stability exponent and the period quickly grows larger than 2π with K . We thus represent, in Figure 4.4, the Husimi distribution and the IPR in the first and second columns. The first row is for $K = 3.097$ and an initial coherent state centred on $(0, 1.151)$, evolved for 60 kicks. As can be seen in the Husimi distribution, that are averaged over 70 periods³, the $3 : 1$ resonance is noticeable by the two triplets of nonzero Husimi. The picture is, however, less clear in the IPR, due for instance to the IPR in the stable islands being much larger than at the scars. The second row is for $K = 20.08$ and a coherent state centred on the $3 : 1$ resonance located at $(0, 0.275)$ that is evolved for 30 kicks, and the distribution is averaged over 50 periods. For this value of the kicking strength, Heller's criterion is not satisfied, and no scar is expected. This is clearly verified in the Husimi, as it is uniformly spread on the fully chaotic phase space. The IPR highlights more clearly the symmetry axis and the $1 : 1$ resonance, but again remains a general indicator rather than a direct probe of quantum scars.

As for the unstable fixed point, we show, in Figure 4.5, OTOCs computed for the parameters of the previous paragraph. The conclusions are the same as before, no matter whether Heller's criterion is fulfilled or not. In other words, the OTOC of an initial coherent state placed on an unstable periodic orbit follows an exponential growth, whereas the OTOC of a coherent state centred on a generic point exhibits a deviation from the exponential growth. There is thus no connection to quantum scars. This brings us to the main conclusion of this section: it is not

³ For the $1 : 1$ resonance, averaging over n periods corresponds to averaging over n kicks, since the period of an unstable fixed point is 1. With the $3 : 1$ resonance, the period is 3. Thus, to take this into account, we evolve the state by multiples of 3 kicks.

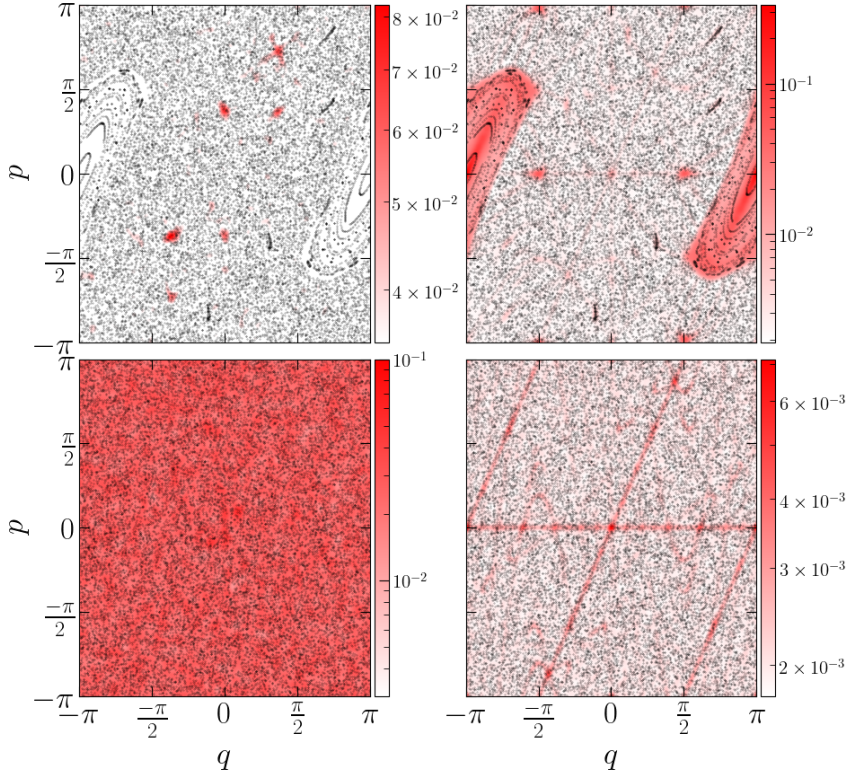


Figure 4.4: Husimi distributions for various initial coherent states (left column) and inverse participation ratio (right column) of the kicked rotor, shown in logarithmic colour scale over the classical phase space, with $\hbar_{\text{eff}} = 2\pi/N$ and $N = 2^{10}$, and for various kicking strengths K . The first row is for $K = 3.097$, and the Husimi, averaged over 70 periods of the 3 : 1 resonance, is computed for a coherent state centred on $(0, 1.151)$, the 3 : 1 resonance, that is evolved for 60 kicks. The second row is for $K = 20$, and the Husimi, averaged over 50 periods, is computed for a coherent state centred on $(0, 0.275)$, the 3 : 1 resonance for that value of K , evolved for 30 kicks. Axes of increased IPR, caused by discrete symmetry axes, can clearly be seen. In the first row, the unstable orbit satisfies Heller's criterion and yields a scar, which is not the case in the second row.

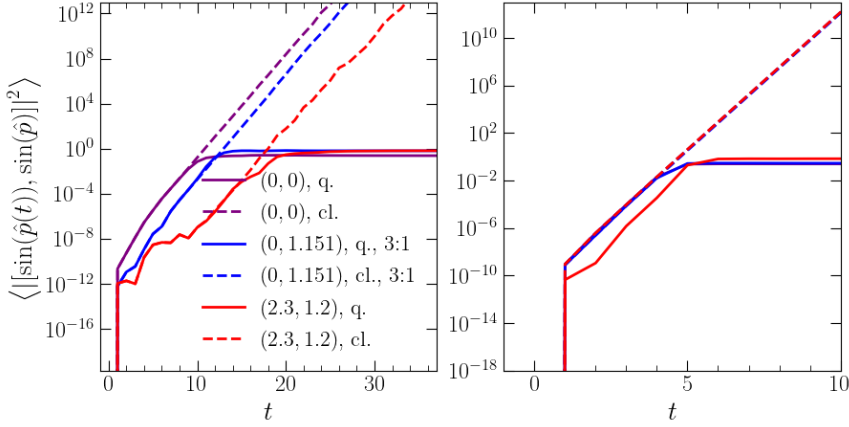


Figure 4.5: Out-of-time-ordered correlators computed in the kicked rotor for $K = 3.097$ (left) and $K = 20$ (right), with $\hbar_{\text{eff}} = 2\pi/N$ and $N = 2^{22}$. The initial states are indicated in the legend. The initial conditions of the purple curves correspond to the 1 : 1 resonance, those of the blue curves to the 3 : 1 resonance, and the red curves to a random point in the chaotic sea. If the initial state is not on an unstable periodic orbit, the OTOC exhibits a temporary deviation from the exponential regime.

possible to assess whether or not a scar is present by only using the short-time behaviour of OTOCs. Nonetheless, this behaviour is clearly different depending on whether the initial state is located on an unstable periodic orbit. This difference corresponds to the temporary deviation from the exponential growth in the short-time regime of the OTOC and is consistently present for various values of the kicking strength and initial states. As OTOCs, more specifically their short-time profile, can be recovered quasiclassically, it means that one can use that scrambling signature as a probe of unstable periodic orbits.

4.2 BOSE-HUBBARD MODELS AND STAGGERED DIMER STATES

The last part of this thesis is dedicated to the analysis of quantum scars in a many-body context. As stated in the introduction, we focus on genuine many-body quantum scars, in other words the true many-body equivalent of single-particle scars as defined by Heller [143].

As announced, the framework of our study is Bose-Hubbard models, whose Hamiltonian is given by (1.126). The system is, in general, nonintegrable, and we consider system parameters that yield a chaotic dynamics. In the following, to specify the parameters of the Bose-Hubbard models, we define a dimensionless parameter γ , similarly to [148]⁴, by

$$\gamma = \frac{UN}{JL}, \quad (4.3)$$

that characterises the competition between the interaction and hopping in the system. We will focus on states called *staggered dimer states*, which correspond to pairs of dimers whose populations is the same on the two sites of a given dimer, but with a phase difference of π . The numbers of sites L of Bose-Hubbard models in which a staggered dimer state can exist are multiples of 4. We will focus on the simplest case, i.e. $L = 4$. Such a state is defined as

$$|\psi_{\text{stag}}\rangle = |\psi_1, -\psi_1\rangle^{(1,3)} \otimes |\psi_2, -\psi_2\rangle^{(2,4)}. \quad (4.4)$$

where $|\psi_i, \psi_j\rangle^{(k,l)}$ corresponds to a coherent state centred on the complex numbers ψ_i and ψ_j on the dimer made by the sites k and l respectively. Those states, in the classical phase space, are anchored on unstable orbits [148].

⁴ Compared to the reference, we drop the $+1/2$.

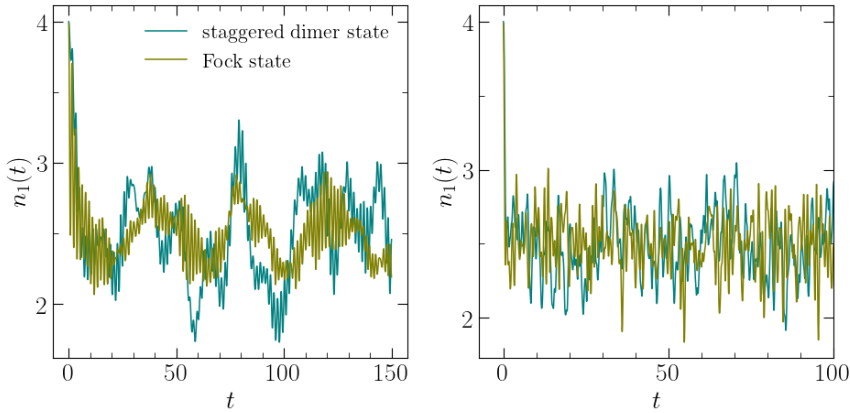


Figure 4.6: Population as a function of time: staggered dimer vs Fock states, with $N = 10$ particles. Population of site 1 as a function of time for a staggered dimer state with $\psi_1 = \sqrt{4}$ and $\psi_2 = 1$ (blue) and a Fock state $|4, 1, 4, 1\rangle$ (green), for the system parameters $U = 0.205J$, corresponding to $\gamma = 0.5$ (left) and $U = 2J$, corresponding to $\gamma = 5$ (right). Persistent oscillations are noticeable on the blue curve on the left as compared to the green curve, whereas there is no significant difference in the right plot.

4.2.1 Population

As there are too many degrees of freedom for the phase space to be easily visualised, one must resort to other ways to assess the presence of a scar. As a scar can manifest in persistent and nondecaying oscillations of observables [148, 162], we compute the population of each site for a time long enough so that a generic state with the same system parameters has reached equilibrium. In our case, the generic state in question is a Fock state possessing the same occupations as the centre of each site of the staggered dimer state. The results are shown for the first site of a 4-site Bose-Hubbard system in Figure 4.6 for $N = 10$ particles with the staggered dimer state defined by $\psi = \sqrt{4}$ and $\psi_2 = 1$, and the Fock state $|4, 1, 4, 1\rangle$, and in Figure 4.7 for $N = 30$ with $\psi_1 = \sqrt{14}$ and $\psi_2 = 1$, and the Fock state $|14, 1, 14, 1\rangle$. The left plots correspond to a lower value of γ than the right ones, the precise value being specified in the captions. The left plots contain persistent oscillations in the staggered-dimer curves, whereas the right ones do not present a significant difference between the two curves. While the presence of those oscillations, characteristic of

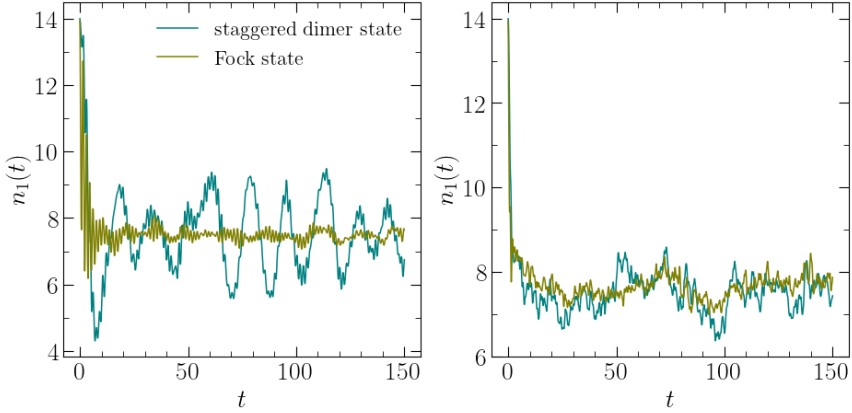


Figure 4.7: Population as a function of time: staggered dimer vs Fock states, with $N = 30$ particles. Population of site 1 as a function of time for a staggered dimer state with $\psi_1 = \sqrt{14}$ and $\psi_2 = 1$ (blue) and a Fock state $|14, 1, 14, 1\rangle$ (green), for the system parameters $U = 0.1025J$, corresponding to $\gamma = 0.768$ (left) and $U = 0.4725J$, corresponding to $\gamma = 3.54$ (right). Persistent oscillations are clearly noticeable in the blue curve in the left plot, but not in the right plot.

scars, is less obvious in the smaller population case in Figure 4.6, they are clearly noticeable in the larger population situation in Figure 4.7.

To complement these curves, we show in Figures 4.8 and 4.9 the discrete Fourier transforms of the curves of Figure 4.6 and 4.7. More specifically, we computed the transform only on the part after the Fock states have thermalised, which in our case amounts to removing⁵ everything before $t = 40$, for the two different values of N . We can see that for the lower value of γ , there is a different spectrum between the staggered dimer and Fock state curves. The former is essentially the same as the latter, with the addition of much higher values in the lower frequencies. The difference is more striking for the higher value of γ , where the spike in the lower frequencies in the left plot of Figure 4.9 is clearly defined. Thus, similarly to the occupations as a function of time, the larger-population case presents more distinct features than the other one in the presence of

⁵ Remove must be understood as deleting data for a time shorter than some cutoff value t_{cut} , and subtracting that cutoff value from the remaining times. Additionally, we also subtract the average saturation value of the population from the remaining data of the population to avoid a zero-frequency contribution in the Fourier, as is usually done in such situations.

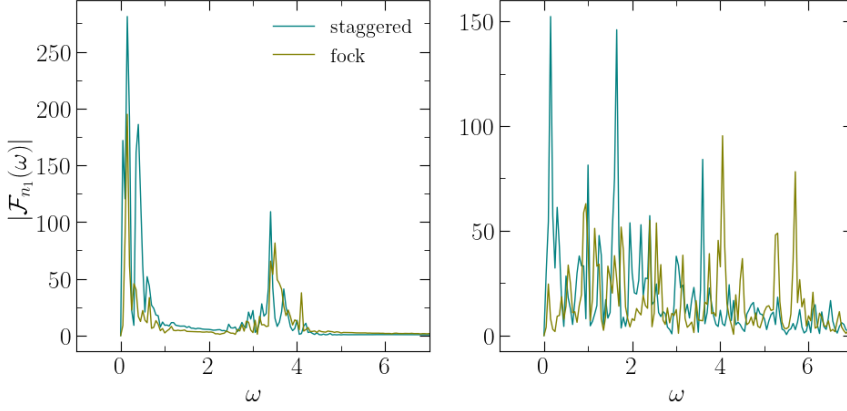


Figure 4.8: Discrete Fourier transform population of site 1 for a staggered dimer state with $\psi_1 = \sqrt{4}$ and $\psi_2 = 1$ (blue) and a Fock state $|4, 1, 4, 1\rangle$ (green), for the system parameters $U = 0.205J$, corresponding to $\gamma = 0.5$ (left) and $U = 2J$, corresponding to $\gamma = 5$ (right).

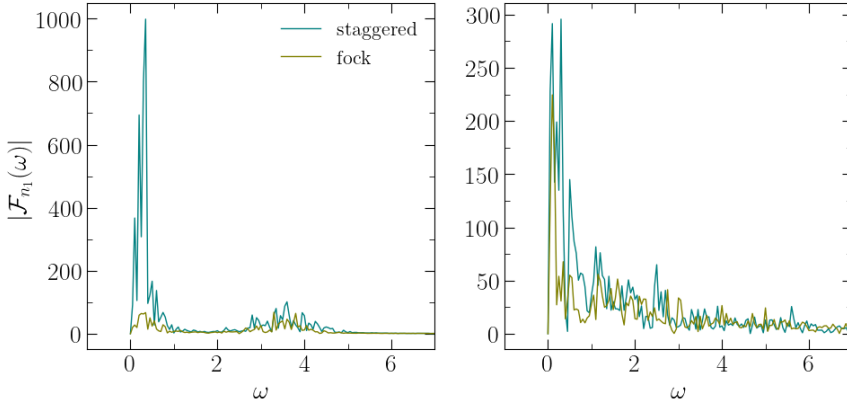


Figure 4.9: Discrete Fourier transform Population of site 1 for a staggered dimer state with $\psi_1 = \sqrt{14}$ and $\psi_2 = 1$ (blue) and a Fock state $|14, 1, 14, 1\rangle$ (green), for the system parameters $U = 0.1025J$, corresponding to $\gamma = 0.768$ (left) and $U = 0.4725J$, corresponding to $\gamma = 3.54$ (right). The larger contribution in the lower frequencies for the lower- γ curve, coming from the persistent oscillations, is clearly noticeable.

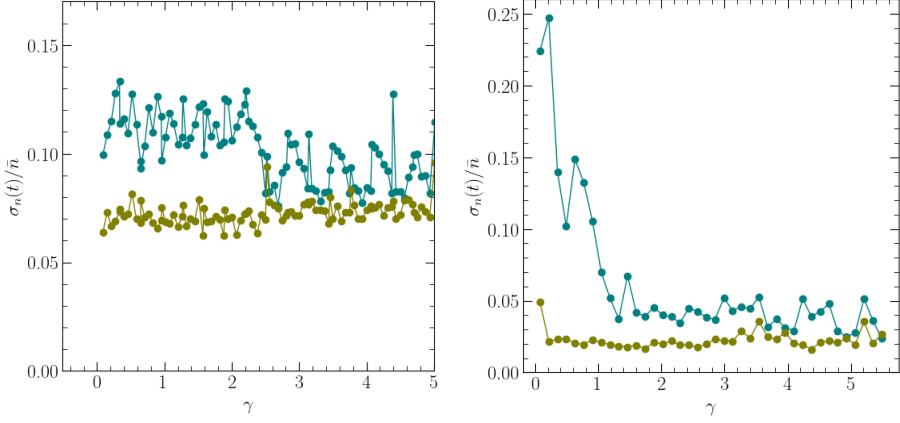


Figure 4.10: Relative standard deviation of the populations. The plot shows the standard deviation of the oscillations relative to the mean saturation value, averaged over the 4 sites of a staggered dimer state with $\psi_1 = \sqrt{4}$ and $\psi_2 = 1$ (blue, left) and with $\psi_1 = \sqrt{14}$ and $\psi_2 = 1$ (blue, right), and of a Fock state (green) as a function of γ , for the Fock states $|4, 1, 4, 1\rangle$ (left) and $|14, 1, 14, 1\rangle$ (right). The decrease of the standard deviation with γ translates the fact that scarring becomes less prevalent and thus the persistent oscillations progressively vanish.

scars. The spike at the lower frequencies is more pronounced in the lower- γ case, whereas the spectra are more similar in the higher- γ situation.

To probe more values of γ , we show in Figure 4.10 the standard deviations of the oscillations relative to the mean saturation value, averaged over the 4 sites of a staggered dimer state (blue) and a Fock state (green) as a function of γ , for the two different total populations, i.e. $N = 10$ on the left and $N = 30$ on the right. We can observe that for lower values of γ , the average relative standard deviation is noticeably larger for the staggered dimer state as compared to the Fock state. For the smaller total population, increasing γ doesn't yield significant changes until a decrease in the deviation is reached between $\gamma = 2$ and $\gamma = 3$. For the larger occupation, the tendency is much clearer: increasing γ decreases the standard deviation. As the two curves become more similar, one can conclude that while not disappearing completely, quantum scars become less prevalent at higher γ , i.e., at larger interactions.

The interested reader can find the complete set of plots, i.e. for the 4 sites of the Bose-Hubbard models, in Appendix F.

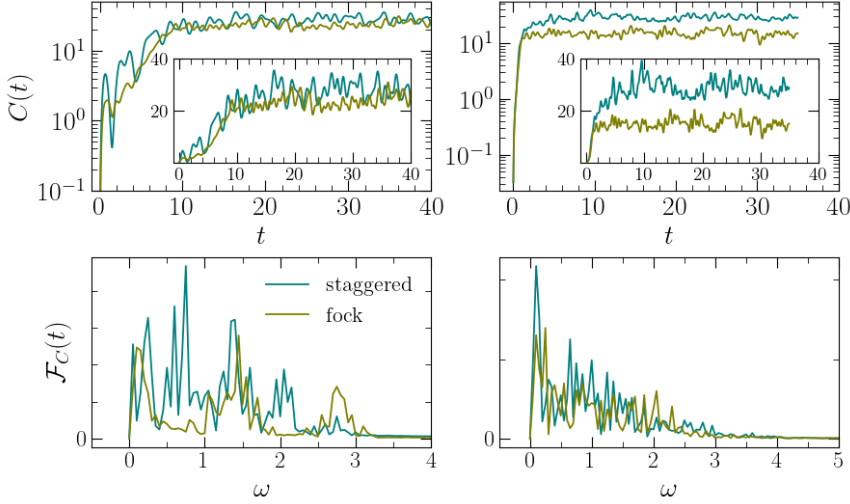


Figure 4.11: Out-of-time correlators $C(t) = \langle |[\hat{n}_1(t), \hat{n}_2]|^2 \rangle$ (first row) and their corresponding discrete Fourier transform (second row) for a staggered dimer state with $\psi_1 = \sqrt{4}$ and $\psi_2 = 1$ (blue) and the Fock state $|4, 1, 4, 1\rangle$ (green), for $U = 0.1692J$, corresponding to $\gamma = 0.423$ (first column) and $U = 2J$, corresponding to $\gamma = 5$. The insets represent the same curves as the frame in which they are, in a lin-lin scale. In the lower- γ curves, persistent oscillations are present, which translate into distinct spikes in the Fourier transform. In the higher- γ curve, scarring is not expected, and this is verified by the two OTOCs and their respective Fourier transforms having the same profile.

4.2.2 Out-of-time-ordered correlators

This last section is dedicated to the investigation of staggered dimer states using quantum OTOC. Similarly to the previous section, we computed the OTOC and the corresponding discrete Fourier transforms. First, again for $N = 10$ with the Fock state $|4, 1, 4, 1\rangle$ and the staggered dimer state with the same mean occupancies, we show in Figure 4.11 the results of our numerical simulations. The first row contains the OTOC $C(t) = \langle |[\hat{n}_1(t), \hat{n}_2]|^2 \rangle$ and the second row the corresponding discrete Fourier transform. The Fourier transform has been performed on the post-saturation section of the OTOC. To this end, we removed the data

corresponding to times shorter than $t = 12$, for all curves⁶. The first column is for $\gamma = 0.423$. As the persistent oscillations are not clearly noticeable in a log-lin scale, the usual scaling used for representing OTOC, we also show in an inset the same curves in a lin-lin scale. There, one can clearly see the larger post-saturation oscillations of the OTOC computed for the staggered dimer as compared to the Fock state. This is confirmed by the Fourier transform, which shows the same profile for the two initial states, but with additional spikes present only for the staggered dimer case. One can also notice that despite the persistent oscillations being less clearly visible in OTOCs as compared to the populations, the additional spikes in the Fourier, characteristic of scars, are much more defined. Increasing γ to 5, we can notice that the post-saturation oscillations either vanish or become clearly negligible, indicating the disappearance or shrinking of scars. This is shown in the Fourier as well, where both curves can be assimilated to noise.

Finally, we show in Figure 4.12 the same curves, this time for $N = 30$ and the Fock $|14, 1, 14, 1\rangle$. The left column is for $\gamma = 0.768$ while the right is for $\gamma = 3.54$. The same conclusions as for the lower total population, and by extension as for the populations, hold. Namely, a lower value of γ is associated with post-saturation persistent oscillations, indicating a scar. The signature is very clear in the discrete Fourier transform of the saturating section of the OTOC. For a larger value of γ , the amplitude of the oscillations decreases, indicating the disappearance of the scar. The discrete Fourier transform confirms this by showing a quasi identical spectra between the curve associated with a staggered dimer state and the one associated with a Fock state.

⁶ In addition, we proceeded similarly as above to analyse only the fluctuations: we subtracted the cutoff time $t_{\text{cut}} = 12$ from all the times so the new sample started at $t = 0$, and subtracted the average saturation value of the OTOC from the remaining OTOC data.

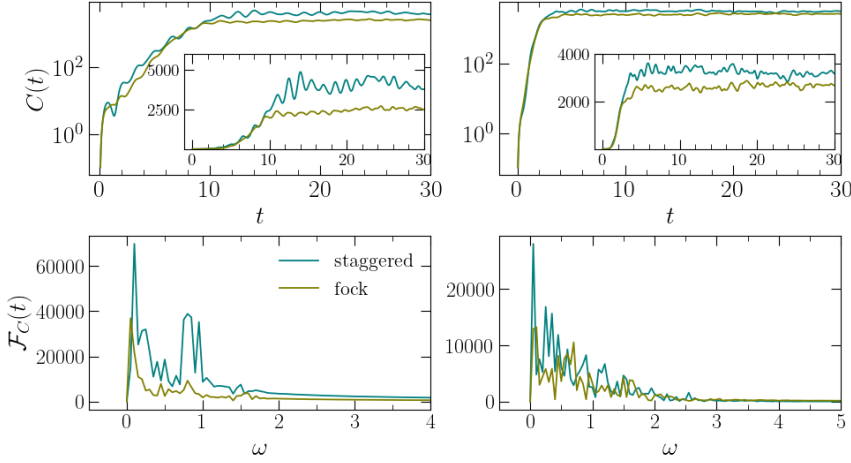


Figure 4.12: Out-of-time correlators $C(t) = \langle |[\hat{n}_1(t), \hat{n}_2]|^2 \rangle$ (first row) and their corresponding discrete Fourier transform (second row) for a staggered dimer state (blue) with $\psi_1 = \sqrt{4}$ and $\psi_2 = 1$ (left) and with $\psi_1 = \sqrt{14}$ and $\psi_2 = 1$ (right) and the Fock state $|14, 1, 14, 1\rangle$ (green), for $U = 0.1025$, corresponding to $\gamma = 0.768$ (first column) and $U = 0.4725$, corresponding to $\gamma = 3.54$. The insets represent the same curves as the frame in which they are, in a lin-lin scale. In the lower- γ curves, persistent oscillations are present, which translate into distinct spikes in the Fourier transform. In the higher- γ curve, scarring is not expected, and this is verified by the two OTOCs and their respective Fourier transforms having the same profile.

CONCLUSION

In this manuscript, we studied scrambling in near-integrable and chaotic systems. We focused on scrambling signatures such as out-of-time-ordered correlators, which have enabled us to link quantum chaos with its classical counterpart. More specifically, we have established a quasiclassical description of OTOCs in strongly mixed and fully chaotic systems, which sets a robust justification for the textbook Wigner-Moyal approach of the OTOC. Then, we focused on systems with a small presence of chaos: near-integrable systems. We have formulated an analytical description of the dynamics inside the thin chaotic layer present around an unstable fixed point, and provided an estimation of the exponent that dictates the evolution: a combination of the stability exponent of the unstable fixed point and the Lyapunov exponent of the chaotic layer. Finally, in the last chapter, we continued the study of those unstable fixed points, and added to our scope unstable periodic orbits: we went back to fully chaotic systems and focused on scars. More specifically, we looked at quasiclassical signatures of scars in scrambling probes. While those were not found yet, we still managed to show that those probes can be used as unstable-periodic-orbit indicators. We then showed that post-saturation oscillations of observables can be an indicator of scars. Let us emphasise the key points of each chapter in more detail.

In Chapter 2, we developed a full-fledged semiclassical framework for the calculation of Out-of-Time-Ordered Correlators in chaotic systems via the van Vleck-Gutzwiller propagator. By means of a diagonal approximation, this framework allowed us to yield a proper quasiclassical expression for the OTOC. In the strict classical limit $\hbar \rightarrow 0$, the result of the Wigner-Moyal approach is recovered, corresponding effectively to a replacement of the quantum commutator by the classical Poisson bracket multiplied by $i\hbar$, and consequently amounting to an exponential increase $\propto e^{2\lambda t}$ of the OTOC governed by the system's Lyapunov exponent λ .

The quasiclassical expression that we derived also allowed us to obtain a prediction for an asymptotic long-time threshold value of the OTOC. However, comparisons with numerical results that were obtained within unperturbed and periodically driven low-dimensional Bose-Hubbard sys-

tems reveal that this threshold value grossly underestimates the actual saturation value of the quantum OTOC. This strongly supports the conjecture that nondiagonal contributions, where quantum interferences have to be taken into account, dominantly determine the OTOC value for long evolution times [25].

In Chapter 3, we focused on the regular-to-chaotic transition of exponential growth laws of scrambling signatures associated with unstable fixed points. While in the purely integrable and fully chaotic cases the growth laws of OTOCs and related observables are exclusively governed by the (local) instability and (global) Lyapunov exponents, λ_s and λ_L respectively, with characteristic crossovers $2\lambda_s \rightarrow \lambda_s$ occurring in the integrable case [127], effective exponents interpolating between these two limiting cases emerge in generic near-integrable and mixed regular-chaotic systems. In the near-integrable regime in particular, a crossover to an OTOC growth law with the exponent $(\lambda_s + \lambda_L)/2$ is found for long evolution times in the deep semiclassical limit. This finding is corroborated by an analytical study of a more elementary (classical) scrambling signature, namely the mean trace of the stability matrix, in the framework of the rapidly driven pendulum system, which can be seen as a standard model describing the emergence of chaos near nonlinear resonances. Scaling estimates of the effective exponent with the perturbation from integrability can thus be yielded, in good agreement with numerical simulations.

In Chapter 4, the centre of attention was quantum scarring. We continued the study of unstable fixed points, this time in fully chaotic systems, while also adding to our scope unstable periodic orbits. More specifically, we focused on unstable periodic orbits of a fully chaotic system that can be associated with quantum scars, a type of phase-space localisation [18, 143].

Using a single-particle system, the kicked rotor, we showed that the OTOC can be used as a probe for unstable periodic orbits. The initial localisation of a state on such an orbit induces a temporary deviation from the exponential regime typically observed for an OTOC in a chaotic regime. In addition, we showed that the OTOC behaviour is not sensitive to the presence of quantum scars, in other words to the fulfilment of Heller's criterion.

Finally, we investigated genuine many-body quantum scars using staggered dimer states in Bose-Hubbard models [148]. We verified that those states, that are initially localised on an unstable periodic orbit in the

classical phase space, are associated with scars. The scarring is manifested in persistent oscillations of different indicators [145–149] that remain after a reference state, here a Fock state centred on the same occupations, has thermalised. The indicators that we used are the occupations of the different sites of the system as well as out-of-time-ordered correlators. As the interaction strength becomes stronger, the scarring phenomenon is expected to be less prevalent, which is verified numerically. To complete our findings, we looked at the discrete Fourier transforms of the different indicators, which show additional frequencies in the spectrum if scars are present as compared to a reference state, here a Fock state.

PERSPECTIVES

Quantum chaos is a very rich field of physics, where a plethora of interesting phenomena take place. As with all research work, this manuscript is of course not the end of the road. There are many directions that can be investigated.

Regarding the quasiclassical formalism of OTOC that we established, though exemplified only within low-dimensional Bose-Hubbard systems, it is universally valid for all types of quantum single-, few- and many-body systems that exhibit a well-defined classical counterpart, and thus can be applied to those types of systems. Moreover, we expect that it will also provide a valuable starting point for spin chains [163–165] or fermionic systems [166, 167] for which the validity of the semiclassical approximation cannot be straightforwardly justified. This will open perspectives to properly refine the notion of chaos in such systems.

Then, concerning the dynamics inside the thin chaotic layer of a near-integrable system, most of the results that were shown, including those related to OTOC growth behaviours, are essentially classical. One can thus wonder to what extent the intricate growth crossovers that we found for near-integrable dynamics are actually observable in quantum systems, given the smallness of the Planck cell that would be required in order to avoid saturation before reaching the crossover time scale. In addition, considering higher-dimensional systems would allow one to investigate Arnold diffusion [140].

Regarding quantum scars, there are several things to mention. One could pursue studies through the lens of OTOCs, where, for instance, the saturation value of OTOC seems to be related to the presence of

scars [162]. Particular attention can be brought to many-body systems, where the definition is not always rigorous. Some articles in the literature claim to study quantum scars, while in practice they focus on localisation whose origin is not always specified and thus might not be related to an underlying periodic unstable orbit [147, 150, 151]. In addition, one could follow similar steps to the quasiclassical formalism of OTOC developed in Chapter 2 in order to find beyond-diagonal contribution of the semiclassical Green's function that could yield quasiclassical contribution to scars.

Then, similarly to what was done with the kicked rotor, a natural continuation of the work is to look at the quasiclassical limit of staggered dimer states in Bose-Hubbard models in order to see if signatures of scars can be extracted in the short-time dynamics.

One can resort to quantum computing to study the lifetime of a scarred state [168] or the stability of a scar at finite temperature [169]. To this end, a protocol to prepare quantum many-body scar states on quantum computers was presented in [168]. In addition, as there is a strong interest in open systems, a perspective is to study quantum scars in this context [170]. It is, to our knowledge, a new and largely unexplored field with a strong and growing focus [171–174].

Besides quantum scarring, there exist different mechanisms that result in phase-space localisation. It would be fruitful to study how OTOCs are sensitive to localisation in the broad sense, for instance in situations where the localisation originates from many-body localisation (MBL). Works that investigate signatures in the short-time [175, 176] or the long-time regime, i.e. the saturation value [177], exist, but are only numerical studies, and a rigorous and general mathematical framework is still lacking. In parallel, using semiclassical methods to study MBL proves to be useful, as was done in [178], meaning that a study of MBL through the lens of OTOC and semiclassics is a promising path.

Finally, everything mentioned above would gain from advancements in the field of quantum simulators [179–181], which would allow one to run faster simulations, but also access parameter regimes that would be intractable using classical computers. Quantum computers offer the same advantages, but they also require to be more universal. Quantum simulators, on the other hand, have a more specialised scope, meaning that they are also more easily realisable [181].

APPENDIX

WEYL SYMBOL OF A SQUARED OPERATOR

The expression of the symbol of a squared operator as well as its expansion in $\hbar$ is detailed in this appendix.

Applying the definition of a Weyl symbol (1.95) for a squared operator reads

$$\begin{aligned}
 (\hat{A}^2)_W(\mathbf{q}, \mathbf{p}) &= \int d\boldsymbol{\xi} \left\langle \mathbf{q} + \frac{\boldsymbol{\xi}}{2} \left| \hat{A}^2 \right| \mathbf{q} - \frac{\boldsymbol{\xi}}{2} \right\rangle e^{-i\mathbf{p} \cdot \boldsymbol{\xi} / \hbar} \\
 &= \int d\boldsymbol{\xi} d\boldsymbol{\chi} \left\langle \mathbf{q} + \frac{\boldsymbol{\xi}}{2} \left| \hat{A} \right| \boldsymbol{\chi} \right\rangle \left\langle \boldsymbol{\chi} \left| \hat{A} \right| \mathbf{q} - \frac{\boldsymbol{\xi}}{2} \right\rangle e^{-i\mathbf{p} \cdot \boldsymbol{\xi} / \hbar} \\
 &= \frac{1}{(2\pi\hbar)^{2L}} \int d\boldsymbol{\xi} d\boldsymbol{\chi} d\mathbf{p}_1 d\mathbf{p}_2 A\left(\frac{\mathbf{q} + \boldsymbol{\chi}}{2} + \frac{\boldsymbol{\xi}}{4}, \mathbf{p}_1\right) A\left(\frac{\mathbf{q} + \boldsymbol{\chi}}{2} - \frac{\boldsymbol{\xi}}{4}, \mathbf{p}_2\right) \\
 &\quad \times \exp\left[\frac{i}{\hbar} \left(\mathbf{p}_1 \cdot \left(\mathbf{q} + \frac{\boldsymbol{\xi}}{2} - \boldsymbol{\chi} \right) + \mathbf{p}_2 \cdot \left(\boldsymbol{\chi} - \mathbf{q} + \frac{\boldsymbol{\xi}}{2} \right) - \mathbf{p} \cdot \boldsymbol{\xi} \right)\right].
 \end{aligned} \tag{A.1}$$

We then perform a change of variables to go to centre-of-mass and relative coordinates, and we obtain

$$\begin{aligned}
 (\hat{A}^2)_W(\mathbf{q}, \mathbf{p}) &= \int \frac{d\mathbf{y} d\mathbf{z} d\boldsymbol{\Pi} d\boldsymbol{\omega}}{(2\pi)^{2L}} A\left(\mathbf{y} + \frac{\hbar\mathbf{z}}{4}, \boldsymbol{\Pi} + \frac{\hbar\boldsymbol{\omega}}{4}\right) A\left(\mathbf{y} - \frac{\hbar\mathbf{z}}{4}, \boldsymbol{\Pi} - \frac{\hbar\boldsymbol{\omega}}{4}\right) \\
 &\quad \times \exp[i((\mathbf{q} - \mathbf{y}) \cdot \boldsymbol{\omega} + \mathbf{z} \cdot (\boldsymbol{\Pi} - \mathbf{p}))].
 \end{aligned} \tag{A.2}$$

This expression can easily be rewritten in symplectic formalism, using $Y = (\mathbf{y}, \boldsymbol{\Pi})$, $X = (\mathbf{q}, \mathbf{p})$ and $\Delta = (\mathbf{z}, \boldsymbol{\omega})$:

$$(\hat{A}^2)_W(X) = \frac{1}{(2\pi)^{2L}} \int dY d\Delta e^{i\Delta \wedge (Y - X)} A\left(Y + \frac{\hbar\Delta}{4}\right) A\left(Y - \frac{\hbar\Delta}{4}\right). \tag{A.3}$$

Then, we do an expansion in the perturbation variables and this leads us to

$$\begin{aligned}
 (\hat{A}^2)_W(X) &= \int \frac{dY d\Delta}{(2\pi)^{2L}} e^{i\Delta \wedge (Y-X)} \\
 &\times \left[A^2(Y) + \frac{\hbar^2}{16} \sum_{k,l=1}^{2L} \Delta_k \Delta_l (A(Y) \partial_{kl}^2 A(Y) - \partial_k A(Y) \partial_l A(Y)) \right] + \mathcal{O}(\hbar^3) \\
 &= A^2(X) + \frac{\hbar^2}{16} \int \frac{dY d\Delta}{(2\pi)^{2L}} e^{i\Delta \wedge (Y-X)} \\
 &\times \sum_{k,l=1}^{2L} [\Delta_k \Delta_l (A(Y) \partial_{kl}^2 A(Y) - \partial_k A(Y) \partial_l A(Y))] + \mathcal{O}(\hbar^3),
 \end{aligned} \tag{A.4}$$

using $\int dY d\Delta e^{i\Delta \wedge (Y-X)} = (2\pi)^{2L} \delta(Y-X)$, where $\partial_k A(Y) = \partial A(Y)/\partial Y_k$ and $\partial_{kl}^2 A(Y) = \partial^2 A(Y)/\partial Y_k \partial Y_l$. The next step consists in turning the Δ_k 's of the second term into derivative operators acting on the exponential:

$$\Delta_k \exp[i\Delta \wedge (Y-X)] = -\frac{\sigma_{\bar{k}}}{i} \frac{\partial}{X_{\bar{k}}} \exp[i\Delta \wedge (Y-X)]. \tag{A.5}$$

As neither the rest of the integrand or the integration bounds depend on X , the derivation operators can be taken outside of the integral entirely, which eventually gives

$$(\hat{A}^2)_W(X) = A^2(X) - \frac{\hbar^2}{8} \sum_{k,l=1}^{2L} \sigma_k \sigma_l \partial_{kl}^2 A(X) \partial_{\bar{k}\bar{l}}^2 A(X). \tag{A.6}$$

Here we use the property:

$$\sum_{k=1}^{2L} \sigma_k \frac{\partial f}{\partial Y_k Y_{\bar{k}}}(Y) = \sum_{k=1}^L \left[\frac{\partial f}{\partial y_k \partial \Pi_k}(\mathbf{y}, \mathbf{\Pi}) - \frac{\partial f}{\partial \Pi_k \partial y_k}(\mathbf{y}, \mathbf{\Pi}) \right] = 0, \tag{A.7}$$

for an arbitrary twice-differentiable function f of a symplectic vector $Y = (\mathbf{y}, \mathbf{\Pi})$, where we have switched from the symplectic to the regular formalism at the first equality. This can also straightforwardly be shown in the symplectic formalism using $\sum_{k=1}^{2L} \sigma_k \partial_k A(Y) = -\sum_{k=1}^{2L} \sigma_{\bar{k}} \partial_{\bar{k}} A(Y)$ since $\sigma_k = -\sigma_{\bar{k}}$.

In this development, we assumed that the observable A vanishes at the integration boundaries so that all the expressions that appear are integrable. While this is technically not the case for the standard population operator $A(Y) = (Y_k^2 + Y_{\bar{k}}^2)/2$, we consider this operator to be amended, *e.g.* $A(Y) = \exp\left(-\varepsilon \sum_{k=1}^{2L} Y_k^2\right)(Y_k^2 + Y_{\bar{k}}^2)/2$ for sufficiently small ε . This reflects the experimental limitations for the detection of such an observable.

SECULAR PERTURBATION THEORY

In this appendix, we review the basic calculation steps of secular classical perturbation theory, with the aim of motivating the choice of the driven pendulum Hamiltonian (3.1). More details on this perturbative approach to solve the classical equations of motion near a resonance can be found in the standard literature on nonlinear Hamiltonian dynamics [69].

Consider a two-degrees-of-freedom (2-dof) system described by two approximate action variables I_1, I_2 and the associated angle variables θ_1, θ_2 . Near integrability, the Hamiltonian describing this system is written as

$$H(I_1, I_2, \theta_1, \theta_2) = H_0(I_1, I_2) + H_1(I_1, I_2, \theta_1, \theta_2) \quad (\text{B.1})$$

with H_0 the unperturbed part and H_1 a weak perturbation. The latter can be represented as a 2π -periodic function in the angle variables,

$$H_1(I_1, I_2, \theta_1, \theta_2) = \sum_{k_1, k_2 = -\infty}^{\infty} V_{k_1, k_2}(I_1, I_2) e^{i(k_1 \theta_1 + k_2 \theta_2)}, \quad (\text{B.2})$$

with the Fourier coefficients $V_{k_1, k_2} = V_{-k_1, -k_2}^*$. While no specific assumption is made for the former, we shall be particularly interested in using this 2-dof autonomous system in order to emulate a 1-dof system under perturbative periodic driving, described by the Hamiltonian $H_0^{(1)}(I_1) + H_1(I_1, \theta_1, \omega t)$ with ω the driving frequency. For this purpose, one can choose

$$H_0(I_1, I_2) = H_0^{(1)}(I_1) + \omega I_2 \quad (\text{B.3})$$

and identify ωI_2 with the negative (time-dependent) energy of the driven 1-dof system, through considering the submanifold of vanishing total energy $H = 0$ within the 2-dof system's phase space.

For a sufficiently weak deviation from integrability, the angle variable dependence of the Hamiltonian H can be eliminated through canonical perturbation theory [69], provided the system is sufficiently far away from important resonances of its unperturbed dynamics. This is the essence of the Kolmogorov-Arnold-Moser (KAM) theorem. Classical motion thus

continues to evolve along invariant tori in phase space, as in the strictly integrable case. Near a resonance, however, the canonical perturbative approach fails to converge and the invariant tori break up. New substructures, reminiscent of pendulum dynamics, emerge at their place in the phase space, as predicted by the Poincaré-Birkhoff theorem.

Consider the occurrence of such a $r:s$ resonance in action space, where $r \in \mathbb{N}$ full cycles of the angle variable θ_2 are exactly matched by $s \in \mathbb{N}$ full cycles of θ_1 . At the corresponding action variables $I_1 = I_1^{r:s}$ and $I_2 = I_2^{r:s}$ we thus have

$$r\Omega_1(I_1^{r:s}, I_2^{r:s}) = s\Omega_2(I_1^{r:s}, I_2^{r:s}), \quad (\text{B.4})$$

with

$$\Omega_j(I_1, I_2) = \frac{\partial H_0}{\partial I_j}(I_1, I_2) \quad (\text{B.5})$$

the unperturbed angular frequencies associated with the degrees of freedom $j = 1, 2$. To describe the motion in the vicinity of this resonance, we first perform a canonical transformation to a frame that corotates with one of the degrees of freedom. This transformation introduces new pairs of canonically conjugated phase-space variables (J, ϑ) and (p, q) ,

$$(I_1, \theta_1, I_2, \theta_2) \xrightarrow{F} (J, \vartheta, p, q), \quad (\text{B.6})$$

and is defined via the generating function

$$F(J, p, \theta_1, \theta_2) = (I_1^{r:s} + p)\theta_1 + \left(I_2^{r:s} + \frac{1}{r}(J - sp) \right) \theta_2 \quad (\text{B.7})$$

that depends on the new (approximate) action variables J, p and the old (approximate) angle variables θ_1, θ_2 . The old (approximate) action and new (approximate) angle variables are then obtained according to

$$I_1 = \frac{\partial F}{\partial \theta_1} = I_1^{r:s} + p, \quad (\text{B.8})$$

$$I_2 = \frac{\partial F}{\partial \theta_2} = I_2^{r:s} + \frac{1}{r}(J - sp), \quad (\text{B.9})$$

$$q = \frac{\partial F}{\partial p} = \theta_1 - \frac{s}{r}\theta_2, \quad (\text{B.10})$$

$$\vartheta = \frac{\partial F}{\partial J} = \frac{1}{r}\theta_2. \quad (\text{B.11})$$

The classical Hamiltonian (B.1) is then (exactly) rewritten in terms of these phase-space variables as

$$H(I_1, I_2, \theta_1, \theta_2) = \tilde{H}_0(J, p) + \tilde{H}_1(J, p, \vartheta, q) \quad (\text{B.12})$$

with

$$\tilde{H}_0(J, p) = H_0[I_1^{r:s} + p, I_2^{r:s} + (J - sp)/r], \quad (\text{B.13})$$

$$\begin{aligned} \tilde{H}_1(J, p, \vartheta, q) &= H_1[I_1^{r:s} + p, I_2^{r:s} + (J - sp)/r, \\ &\quad q + s\vartheta, r\vartheta]. \end{aligned} \quad (\text{B.14})$$

The transformation to this corotating frame is particularly meaningful in the vicinity of the $r:s$ resonance where one of the new angle variables, namely q , will evolve much more slowly with time than the other one. This can be seen from Taylor expanding $\tilde{H}_0$ in the vicinity of the resonance, given by $J = p = 0$. Owing to the resonance condition (B.4) one has $\partial\tilde{H}_0/\partial p|_{J=p=0} = 0$ whereas the complementary derivative $\partial\tilde{H}_0/\partial J|_{J=p=0} = \Omega_2(I_1^{r:s}, I_2^{r:s})/r$ yields a finite frequency. Our interests are the deviations of the action variables in leading order from the resonance, thus we obtain

$$\tilde{H}_0(J, p) \simeq E_{r:s} + \omega_{r:s}J + \frac{p^2}{2m_{r:s}} + O(J^2, Jp, p^3) \quad (\text{B.15})$$

for the unperturbed Hamiltonian, with the resonance parameters

$$E_{r:s} = H_0(I_1^{r:s}, I_2^{r:s}), \quad (\text{B.16})$$

$$\omega_{r:s} = \frac{1}{r}\Omega_2(I_1^{r:s}, I_2^{r:s}), \quad (\text{B.17})$$

$$\frac{1}{m_{r:s}} = \left(\frac{\partial\Omega_1}{\partial I_1} - 2\frac{s}{r}\frac{\partial\Omega_1}{\partial I_2} + \frac{s^2}{r^2}\frac{\partial\Omega_2}{\partial I_2} \right) (I_1^{r:s}, I_2^{r:s}) \quad (\text{B.18})$$

(noting that $\partial\Omega_1/\partial I_2 = \partial\Omega_2/\partial I_1$ for a twice continuously differentiable H_0). Note that we deliberately neglect cross-terms $\propto Jp$ in the above expression (B.15), to simplify the discussion. These cross-terms translate the fact that the resonance condition (B.4), which traces a curve in action space, generally shifts with varying J . For the particularly interesting case of a periodically driven system, for which we would have the unperturbed Hamiltonian (B.3), those cross-terms vanish and the expression (B.15) is exact up to corrections scaling as $O(p^3)$.

Employing the Fourier series representation (B.2), the perturbation term (B.14) is in leading order written as

$$\begin{aligned} V_{r:s}(q, \vartheta) &= H_1(I_1^{r:s}, I_2^{r:s}, q + s\vartheta, r\vartheta) \\ &= \sum_{k_1, k_2=-\infty}^{\infty} V_{k_1, k_2}^{r:s} e^{ik_1 q} e^{i(sk_1 + rk_2)\vartheta} \end{aligned} \quad (\text{B.19})$$

with $V_{k_1, k_2}^{r:s} = V_{k_1, k_2}(I_1^{r:s}, I_2^{r:s})$. The resulting total Hamiltonian $\tilde{H}_0(J, p) + V_{r:s}(q, \vartheta)$ generates a trivial time evolution for ϑ , through the associated Hamilton equation $\dot{\vartheta} = \partial \tilde{H}_0 / \partial J = \omega_{r:s}$. This entitles us to make the substitution $\vartheta = \vartheta_0 + \omega_{r:s}t$ in equation (B.19) and thus describe the system in terms of the equivalent driven 1-dof Hamiltonian

$$H_{r:s}(p, q, t) = \frac{p^2}{2m_{r:s}} + V_{r:s}(q, \omega_{r:s}t). \quad (\text{B.20})$$

Adiabatic perturbation theory [69], a variant of canonical perturbation theory, allows one to eliminate the dependence on the rapidly evolving angle variable ϑ through an infinitesimal canonical transformation of the phase-space coordinates, thus yielding an integrable system. In practice, this procedure amounts to replacing the perturbation term (B.19) by its ϑ -average over one period,

$$\bar{V}_{r:s}(q) = \frac{1}{2\pi} \int_0^{2\pi} V_{r:s}(q, \vartheta) d\vartheta = \sum_{l=-\infty}^{\infty} V_{lr, -ls}^{r:s} e^{ilrq}. \quad (\text{B.21})$$

Neglecting the constant $V_{0,0}^{r:s}$ and using the fact that low-order Fourier coefficients generally dominate over high-order components, we can limit the above sum to the terms $l = \pm 1$. With $\bar{V}^{r:s} \equiv |V_{r,-s}^{r:s}| = |V_{-r,s}^{r:s}|$ this yields the effective pendulum Hamiltonian

$$\bar{H}_{r:s}(p, q) = \frac{p^2}{2m_{r:s}} + 2\bar{V}^{r:s} \cos[r(q - q_0)] \quad (\text{B.22})$$

for some offset angle q_0 , featuring r elliptic and r hyperbolic fixpoints as requested by the Poincaré-Birkhoff theorem.

Going beyond the adiabatic approximation, equation (B.20) in combination with equation (B.19) provides a meaningful setting to investigate universal characteristics related to the emergence of chaos near the hyperbolic fixpoints of the above pendulum Hamiltonian (B.22). To simplify things as much as possible, let us specifically focus on the most elementary

case of a 1:1 resonance, $r = s = 1$. Restricting ourselves to the most dominant nontrivial Fourier coefficients $V_{\pm 1,0}^{1:1}$ in the expansion of $V_{1:1}$ allows us to rewrite equation (B.20) in leading order as

$$\begin{aligned} H_{1:1}(p, q, t) \simeq & \frac{p^2}{2m_{1:1}} + 2\bar{V}^{1:1} \cos(q - q_0) \\ & + 2|V_{1,0}^{1:1}| \cos(q + \omega_{r:s}t + \varphi) \end{aligned} \quad (\text{B.23})$$

for some other offset angle φ . Setting $q_0 = 0$ without loss of generality, the above expression is rewritten as

$$\begin{aligned} H_{1:1}(p, q, t) \simeq & \frac{p^2}{2m_{1:1}} + 2\bar{V}^{1:1} \cos(q) \\ & + 2|V_{1,0}^{1:1}| \cos(q) \cos(\omega_{r:s}t + \varphi) \\ & - 2|V_{1,0}^{1:1}| \sin(q) \sin(\omega_{r:s}t + \varphi). \end{aligned} \quad (\text{B.24})$$

This is essentially equivalent to the Hamiltonian (3.1) that we focus on in our study, with the only difference that the parity-breaking term $\propto \sin q$ is omitted in the latter.

SOLUTION IN THE LINEAR REGION OF THE DRIVEN PENDULUM

Let us obtain the equations of motion of the system in the linear region. The starting point is (3.3), written again here for convenience:

$$\ddot{q}(t) = \lambda_s^2 q(t) + \kappa \omega \lambda_s \cos(\omega t + \varphi) q(t) \quad (\text{C.1})$$

The first step consists in taking the Laplace transform of the equation in order to remove the time derivatives and only deal with an algebraic equation.

The Laplace transform of a function f is given by

$$\tilde{f}(z) \equiv \mathcal{L}(f)(z) = \int_0^{+\infty} f(t) e^{-zt} dt \quad (\text{C.2})$$

where both notations were introduced, as one might prefer over the other depending on the length of the term. While the Laplace transforms of most terms are standard cases, the one containing the driving is slightly different and is given by

$$\begin{aligned} & \mathcal{L}(\kappa \lambda_s \omega \cos(\omega t + \varphi) q(t))(z) \\ &= \frac{\kappa \lambda_s \omega}{2} \left(e^{i\varphi} \tilde{q}(z - i\omega) + \frac{\kappa \lambda_s \omega}{2} e^{-i\varphi} \tilde{q}(z + i\omega) \right). \end{aligned} \quad (\text{C.3})$$

Isolating in the new equation the Laplace transform of the position, $\tilde{q}$, one obtains

$$\tilde{q}(z) = \frac{b(z)}{z^2 - \lambda_s^2} + \kappa \omega \lambda_s \frac{e^{i\varphi} \tilde{q}(z - i\omega) + e^{-i\varphi} \tilde{q}(z + i\omega)}{2(z^2 - \lambda_s^2)} \quad (\text{C.4})$$

where $b(z) = zq_0 + p_0$ was introduced for conciseness and where q_0 and p_0 are the initial conditions when the system enters the linear region.

This equation is not directly exactly solvable. To obtain a solution, we inject the expression of $\tilde{q}$ evaluated at $z \pm i\omega$:

$$\begin{aligned} \tilde{q}(z) = & \frac{b(z)}{z^2 - \lambda_s^2} \\ & + \kappa\omega\lambda_s e^{i\varphi} \frac{b(z - i\omega) + \frac{\kappa\omega\lambda_s}{2} (e^{i\varphi}\tilde{q}(z - 2i\omega) + e^{-i\varphi}\tilde{q}(z))}{2(z^2 - \lambda_s^2)((z - i\omega)^2 - \lambda_s^2)} \\ & + \kappa\omega\lambda_s e^{-i\varphi} \frac{b(z + i\omega) + \frac{\kappa\omega\lambda_s}{2} (e^{i\varphi}\tilde{q}(z) + e^{-i\varphi}\tilde{q}(z + 2i\omega))}{2(z^2 - \lambda_s^2)((z + i\omega)^2 - \lambda_s^2)} \end{aligned} \quad (\text{C.5})$$

One could go on indefinitely by injecting again the expression of $\tilde{q}$ evaluated at $z \pm 2i\omega$. However, one can notice that the dominating term is the first one, which scales as the inverse of the argument. This means that $\tilde{q}(z + \alpha\omega) = \mathcal{O}((z + \alpha\omega)^{-1})$ since $b(z) \propto z$. The terms with the argument $z \pm 2i\omega$ can thus be safely neglected as we restrict our development to $\mathcal{O}(1/\omega^2)$ included for now¹, using the fact that $\omega \gg \lambda_s$ with $\kappa\omega \sim \lambda_s$. We thus obtain

$$\tilde{q}(z) = \tilde{q}_I(z) + \tilde{q}_{II}(z) + \tilde{q}_{III}(z) + \mathcal{O}\left(\frac{1}{\omega^3}\right) \quad (\text{C.6})$$

with

$$\tilde{q}_I(z) = \frac{b(z)}{z^2 - \lambda_s^2} \quad (\text{C.7})$$

$$\tilde{q}_{II}(z) = \frac{\kappa\omega\lambda_s}{2(z^2 - \lambda_s^2)} \left(\frac{e^{i\varphi}b(z - i\omega)}{(z - i\omega)^2 - \lambda_s^2} + \frac{e^{-i\varphi}b(z + i\omega)}{(z + i\omega)^2 - \lambda_s^2} \right) \quad (\text{C.8})$$

$$\tilde{q}_{III}(z) = \frac{\kappa^2\omega^2\lambda_s^2 b(z)}{4(z^2 - \lambda_s^2)^2} \left(\frac{1}{(z - i\omega)^2 - \lambda_s^2} + \frac{1}{(z + i\omega)^2 - \lambda_s^2} \right) \quad (\text{C.9})$$

To obtain the position q , one must perform the inverse Laplace transform of (C.6), which is given by

$$q(t) = \frac{1}{2\pi i} \int_{\Gamma} \tilde{q}(z) e^{zt} dz \quad (\text{C.10})$$

with $\Gamma : [-R, R] \rightarrow \mathbb{C}, x \mapsto \gamma + ix$ in the limit $R \rightarrow \infty$, with $\text{Re}(\gamma) > \gamma_0$, with γ_0 the real part of the singularity of $\tilde{q}$ with the highest real part. As

¹ We will only keep the first order for the position and the momentum, but as obtaining the latter is done by time-derivating the former, this introduces some ω prefactor. To be consistent in our approximation, we must keep the $\mathcal{O}(1/\omega^2)$ and neglect them only after the derivation.

usual, we use the residue theorem to compute this integral. The closed path we use is $\Gamma_o = \Gamma \circ \Gamma_R$, with $\Gamma_R : [\pi/2, 3\pi/2] \rightarrow \mathbb{C}, \theta \mapsto Re^{i\theta}$. In the limit $R \rightarrow \infty$, all the singularities of $\tilde{q}$ are encompassed by Γ_o by construction, once and counterclockwise. We can thus apply the residue theorem, which in this case reads

$$\frac{1}{2\pi i} \int_{\Gamma} \tilde{q}(z) e^{zt} dz = \sum_{z_i} \text{Res}(z_i) \quad (\text{C.11})$$

with the sum being on all the singularities z_i of the integrand of the left-hand side, $\text{Res}(z_i)$ the residue of the integrand in $z = z_i$, and where only the integral along Γ remains in the limit $R \rightarrow \infty$, the one along Γ_R tends to zero.

As the Laplace transform and its inverse are linear, let us consider the inverse transform of $\tilde{q}_I$, $\tilde{q}_{II}$ and $\tilde{q}_{III}$ separately. The inverse transform $\tilde{q}_I$, labelled q_I , is given by

$$q_I(t) = \cosh(\lambda_s t) + \frac{p_0}{\lambda_s} \sinh(\lambda_s t) \quad (\text{C.12})$$

and corresponds to the hyperbolic behaviour that the system would have even in the absence of driving.

The inverse Laplace transform of $\tilde{q}_{II}$, labelled q_{II} , is

$$\begin{aligned} q_{II}(t) = \frac{\kappa}{4\lambda_s^2 + \omega^2} & \left[\lambda_s \cosh(\lambda_s t) \left(2p_0 \sin(\omega t + \varphi) \right. \right. \\ & \left. \left. - q_0 \omega \cos(\omega t + \varphi) + \lambda_s (q_0 \omega \cos(\varphi) - 2p_0 \sin(\varphi)) \right) \right. \\ & + \sinh(\lambda_s t) \left(2\lambda_s^2 q_0 \sin(\omega t + \varphi) - p_0 \omega \cos(\omega t + \varphi) \right. \\ & \left. \left. - 2 \sin(\varphi) \lambda_s^2 q_0 - \omega (p_0 \cos(\varphi) + q_0 \omega \sin(\varphi)) \right) \right]. \end{aligned} \quad (\text{C.13})$$

As $\kappa \ll \lambda_s \ll \omega$ and $\kappa \omega \sim \lambda_s$, only the very last term is of order $1/\omega$. However, the terms with the time dependence in trigonometric functions have to be kept for the momentum, as taking the time derivative introduces an additional ω prefactor, thus rendering the term of order $1/\omega$. Those can safely be neglected for the position, though.

Finally, inverse Laplace transform of $\tilde{q}_{III}$ can be neglected. The singularities are the same as for $\tilde{q}_{II}$. For the singularities that do not depend on ω , the associated residue is of order $1/\omega^2$ and no ω prefactor will appear

when taking the time derivative. For the singularities that do depend on ω , such a prefactor would appear, but as the residue is of the order $1/\omega^6$, it will not contribute either.

We then consider that the time is the one elapsed in the linear region and the phase is the initial phase plus the one accumulated during the whole motion. This means doing the shifts $t \rightarrow t - t_0$ and $\varphi \rightarrow \varphi + \omega t_0$, with t_0 the time elapsed before the system entered the linear region. Combining all this in (C.11) and renaming the position in the linear region q_{lin} for clarity yield the solution in leading order in $1/\omega$:

$$q_{\text{lin}}(t) = q_0 \cosh(\lambda_s(t - t_0)) + \left(\frac{p_0}{\lambda_s} - \kappa \sin(\varphi + \omega t_0) q_0 \right) \sinh(\lambda_s(t - t_0)). \quad (\text{C.14})$$

The momentum in the linear region is given by

$$p_{\text{lin}}(t) = (q_0 \lambda_s + \kappa p_0 \sin(\omega t + \varphi)) \sinh(\lambda_s(t - t_0)) + (p_0 + \kappa \lambda_s q_0 (\sin(\omega t + \varphi) - \sin(\varphi + \omega t_0))) \times \cosh(\lambda_s(t - t_0)). \quad (\text{C.15})$$

The corresponding stability matrix is given by

$$M(t) = \begin{pmatrix} \frac{\partial q_{\text{lin}}(t)}{\partial q_0} & \frac{\partial q_{\text{lin}}(t)}{\partial p_0} \\ \frac{\partial p_{\text{lin}}(t)}{\partial q_0} & \frac{\partial p_{\text{lin}}(t)}{\partial p_0} \end{pmatrix} \quad (\text{C.16})$$

with

$$\frac{\partial q_{\text{lin}}(t)}{\partial q_0} = \cosh(\lambda_s(t - t_0)) - \kappa \sin(\varphi + \omega t_0) \sinh(\lambda_s(t - t_0)), \quad (\text{C.17})$$

$$\frac{\partial q_{\text{lin}}(t)}{\partial p_0} = \frac{1}{\lambda_s} \sinh(\lambda_s(t - t_0)), \quad (\text{C.18})$$

$$\frac{\partial p_{\text{lin}}(t)}{\partial q_0} = \lambda_s \sinh(\lambda_s(t - t_0)) + \kappa (\sin(\omega t + \varphi) - \sin(\varphi + \omega t_0)) \lambda_s \cosh(\lambda_s(t - t_0)), \quad (\text{C.19})$$

$$\frac{\partial p_{\text{lin}}(t)}{\partial p_0} = \cosh(\lambda_s(t - t_0)) + \kappa \sin(\omega t + \varphi) \sinh(\lambda_s(t - t_0)). \quad (\text{C.20})$$

SOLUTION IN THE HOMOCLINIC REGION OF THE DRIVEN PENDULUM

In this appendix, we show how to approximately solve the evolution equation (3.2) of the driven pendulum in the homoclinic region and calculate the associated stability matrix.

The starting point is equation(3.2), rewritten here,

$$\ddot{q}(t) = \lambda_s^2 \sin q(t) + \kappa\omega\lambda_s \sin q(t) \cos(\omega t + \varphi), \quad (\text{D.1})$$

for the sake of convenience. A first integral yields

$$\begin{aligned} \frac{1}{2}\dot{q}^2(t) &= \frac{p_1^2}{2} + \lambda_s^2 \cos q_1 - \lambda_s^2 \cos q(t) \\ &\quad + \kappa\omega\lambda_s \int_{t_1}^t \sin q(t') \cos(\omega t' + \varphi) \dot{q}(t') dt' \\ &\simeq \delta E_1 + 2\lambda_s^2 \sin^2[q(t)/2] \\ &\quad + \kappa\lambda_s \sin(\omega t + \varphi) \dot{q}(t) + O(\kappa/\omega) \end{aligned} \quad (\text{D.2})$$

with $q_1 = q(t_1)$, $p_1 = \dot{q}(t_1)$, and

$$\begin{aligned} \delta E_1 &= \frac{p_1^2}{2} - \lambda_s^2(1 - \cos q_1) - \kappa\lambda_s \sin(\omega t_1 + \varphi) p_1 \sin q_1 \\ &\simeq \frac{1}{2}(p_1^2 - \lambda_s^2 q_1^2) - \kappa\lambda_s \sin(\omega t_1 + \varphi) p_1 q_1 + O(q_1^3) \end{aligned} \quad (\text{D.3})$$

the deviation, $\delta E_1 = E_1 - E_{\text{sep}}$, of the initial energy $E_1 = H(q_1, p_1, t_1)$ from the unperturbed separatrix energy $E_{\text{sep}} = \lambda_s^2$. Using the generic scalings $\kappa \ll 1$ and $\kappa\omega \sim \lambda_s$ resulting from secular perturbation theory (see Appendix B), terms of the order $\sim \kappa/\omega$ effectively scale as $\sim \kappa^2/\lambda_s \sim \lambda_s/\omega^2$ and are henceforth neglected.

Right on the separatrix and in the absence of the driving, i.e., for $\delta E_1 = \kappa = 0$, equation(3.2) — and hence also equation(D.2) — is equivalent to

$$\dot{q}(t) = \pm 2\lambda_s \sin[q(t)/2], \quad (\text{D.4})$$

where the sign denotes the initial direction of motion near the unstable fixpoint at the origin, i.e., outwards from (+) or inwards to (−) the fixpoint. This equation is exactly solved as

$$q(t) = 4 \arctan \left(\tan(q_1/4) e^{\pm \lambda_s(t-t_1)} \right). \quad (\text{D.5})$$

Focusing on outward motion and neglecting terms scaling as $\sim q_1^3$, the unperturbed separatrix solution is thus written as

$$q_{\text{sep}}(t) = 4 \arctan \left[\text{sgn}(q_1) e^{\tau(t)} \right] \quad (\text{D.6})$$

where we define $\text{sgn}(q_1) = q_1/|q_1|$ and

$$\tau(t) = \lambda_s(t - t_1) - \log(4/|q_1|). \quad (\text{D.7})$$

Consider now a tiny deviation from the above separatrix solution. We thus also have a tiny value for the energy deviation from the separatrix and can safely assume $\delta E_1 \ll \lambda_s^2 \sin^2[q(t)/2]$ for all t , provided $q(t)$ starts sufficiently far away from the unstable fixed point and does not approach too closely the fixpoint on the other side of the separatrix arc. Taking the positive square root of equation (D.2) and performing a Taylor series expansion in $\delta E_1 / \{\lambda_s^2 \sin^2[q(t)/2]\}$ yields

$$\begin{aligned} \dot{q}(t) \simeq & 2\lambda_s \sin[q(t)/2] + \kappa \lambda_s \sin(\omega t + \varphi) \sin q(t) \\ & + \frac{\delta E_1}{2\lambda_s \sin[q(t)/2]} - \frac{\delta E_1^2}{16\lambda_s^3 \sin^3[q(t)/2]}, \end{aligned} \quad (\text{D.8})$$

where we neglect terms $\sim O(\delta E_1^3)$ that will turn out to scale quadractically either with κ or with the initial phase-space deviation from the separatrix. Making the ansatz

$$q(t) = q_{\text{sep}}(t) + \delta q(t) \quad (\text{D.9})$$

and using the linearising expansions

$$\sin[q(t)/2] \simeq \sin[q_{\text{sep}}(t)/2] + \cos[q_{\text{sep}}(t)/2] \frac{\delta q(t)}{2}, \quad (\text{D.10})$$

$$\sin[q(t)] \simeq \sin[q_{\text{sep}}(t)] + \cos[q_{\text{sep}}(t)] \delta q(t) \quad (\text{D.11})$$

together with the relations

$$\sin[q_{\text{sep}}(t)/2] = \frac{\text{sgn}(q_1)}{\cosh \tau(t)}, \quad (\text{D.12})$$

$$\cos[q_{\text{sep}}(t)/2] = -\tanh \tau(t) \quad (\text{D.13})$$

that result from equations (D.6) and (D.7), one obtains from equation (D.8)

$$\begin{aligned} \delta \dot{q}(t) \simeq & \left(-\lambda_s \tanh \tau(t) + \frac{\delta E_1}{8\lambda_s} \sinh[2\tau(t)] \right) \delta q(t) \\ & + \text{sgn}(q_1) \left(\frac{\delta E_1}{2\lambda_s} \cosh \tau(t) - \frac{\delta E_1^2}{16\lambda_s^3} \cosh^3 \tau(t) \right) \\ & - \kappa \lambda_s \sin(\omega t + \varphi) \left(2 \text{sgn}(q_1) \frac{\sinh \tau(t)}{\cosh^2 \tau(t)} \right. \\ & \left. - \frac{\sinh^2 \tau(t) - 1}{\cosh^2 \tau(t)} \delta q(t) \right), \end{aligned} \quad (\text{D.14})$$

neglecting terms that scale as $O(\kappa^2)$, $O(\kappa/\omega)$, $O(\delta E_1^3)$, $O(\delta E_1^2 \delta q)$, and $O(\delta q^2)$.

Upon integration by parts, the term oscillating as $\kappa \sin(\omega t + \varphi)$ will give rise to another contribution scaling as $\sim \kappa/\omega$ that can be neglected for the determination of $\delta q(t)$. The solution of the above equation for $\delta q(t_1) = 0$ is then given by

$$\begin{aligned} \delta q(t) = & \text{sgn}(q_1) \int_{t_1}^t dt' \frac{\exp \left(-\frac{\delta E_1}{8\lambda_s^2} \cosh^2 \tau(t') \right)}{\exp \left(-\frac{\delta E_1}{8\lambda_s^2} \cosh^2 \tau(t) \right)} \\ & \times \left(\frac{\delta E_1 \cosh^2 \tau(t')}{2\lambda_s \cosh \tau(t)} - \frac{\delta E_1^2 \cosh^4 \tau(t')}{16\lambda_s^3 \cosh \tau(t)} \right) \end{aligned} \quad (\text{D.15})$$

and can be further simplified by neglecting terms scaling as $O(\delta E_1^4)$ upon expansion of the exponential functions. This yields

$$\begin{aligned} \frac{\delta q(t)}{\text{sgn}(q_1)} = & \frac{\delta E_1 \lambda_s (t - t_1)}{4\lambda_s^2 \cosh \tau(t)} \left(1 + \frac{\delta E_1}{16\lambda_s^2} [2 \cosh^2 \tau(t) - 3] \right) \\ & + \frac{\delta E_1 \{ \sinh[2\tau(t)] - \sinh[2\tau(t_1)] \}}{8\lambda_s^2 \cosh \tau(t)} \\ & \times \left(1 + \frac{\delta E_1}{8\lambda_s^2} [\cosh^2 \tau(t) - 2] \right) \\ & - \frac{\delta E_1^2 \{ \sinh[4\tau(t)] - \sinh[4\tau(t_1)] \}}{256\lambda_s^4 \cosh \tau(t)}. \end{aligned} \quad (\text{D.16})$$

The propagation within the homoclinic region is considered to be accomplished as soon as the opposite end of the separatrix arc is reached. We thus define the homoclinic propagation time T such that $q_{\text{sep}}(t_1 + T) =$

$2\pi \operatorname{sgn}(q_1) - q_1$. With equations (D.6) and (D.7) one has $\lambda T = 2 \log(4/|q_1|)$ and hence $\tau(t_1 + T) = -\tau(t_1) = \log(4/|q_1|)$, from which one obtains

$$\cosh \tau(t_1 + T) \simeq \sinh \tau(t_1 + T) \simeq 2/|q_1| + O(q_1) \quad (\text{D.17})$$

in leading order in q_1 . Inserting this into equation (D.16) and keeping only terms in leading order in q_1 yields the rather simple expression

$$\delta q(t_2) \simeq \frac{\delta E_1}{\lambda_s^2 q_1} (1 + O(q_1^2)) \quad (\text{D.18})$$

for the position deviation from the separatrix solution at final time $t_2 = t_1 + T$. The corresponding final momentum deviation, given by equation (D.14) evaluated at $t_2 = t_1 + T$, is

$$\delta \dot{q}(t_2) \simeq -\frac{\delta E_1}{\lambda_s q_1} - \kappa \lambda_s q_1 \sin(\omega t_2 + \varphi) \quad (\text{D.19})$$

in leading order, neglecting terms that scale as δE_1^2 . The above two expressions further simplify if we neglect the deviation of the initial phase-space point from the separatrix and hence consider $q_1 = \pm q_c$ and $p_1 = \pm 2\lambda_s \sin(q_c/2) \simeq \pm \lambda_s q_c$, with q_c the crossover scale separating the linear from the homoclinic region. We then have $\delta E_1 \simeq -\kappa \lambda_s^2 \sin(\omega t_1 + \varphi) q_c^2$ and thus

$$\delta q(t_2) \simeq \mp \kappa q_c \sin(\omega t_1 + \varphi), \quad (\text{D.20})$$

$$\delta \dot{q}(t_2) \simeq \mp \kappa \lambda_s q_c \sin(\omega t_2 + \varphi). \quad (\text{D.21})$$

The associated stability matrix can be calculated by evaluating the effect of a tiny initial deviation with respect to this particular reference trajectory, at fixed total propagation time $T = 2 \log(4/q_c)/\lambda_s$. Setting $q_1 = q_c + \delta q_1$ and $p_1 = \lambda_s q_c + \delta p_1$ (we henceforth restrict the discussion to the case $q_1 > 0$ without loss of generality), the separatrix solution (D.6) is advanced by

$$\delta q_{\text{sep}}(t_2) = q_{\text{sep}}(t_2) - (2\pi - q_c) \simeq \delta q_1 \quad (\text{D.22})$$

at the end of the propagation. With equation (D.4), the corresponding advancement of the time derivative of the separatrix solution is obtained as

$$\begin{aligned} \delta \dot{q}_{\text{sep}}(t_2) &= 2\lambda_s \sin[q_{\text{sep}}(t_2)/2] - 2\lambda_s \sin(q_c/2) \\ &\simeq -\lambda_s \delta q_1. \end{aligned} \quad (\text{D.23})$$

Additional shifts of the final position and momentum variables result from equations (D.14) and (D.16). Using

$$\cosh \tau(t_1) \simeq -\sinh \tau(t_1) \simeq \frac{2}{q_c} \left(1 - \frac{\delta q_1}{q_c} \right), \quad (\text{D.24})$$

$$\cosh \tau(t_2) \simeq \sinh \tau(t_2) \simeq \frac{2}{q_c} \left(1 + \frac{\delta q_1}{q_c} \right), \quad (\text{D.25})$$

and

$$\begin{aligned} \delta E_1 &\simeq \lambda_s q_c (\delta p_1 - \lambda_s \delta q_1) - \kappa \lambda_s q_c \sin(\omega t_1 + \varphi) \\ &\quad \times [\lambda_s (q_c + \delta q_1) + \delta p_1], \end{aligned} \quad (\text{D.26})$$

all expanded in linear order in $\delta q_1, \delta p_1$, one obtains from equation (D.16)

$$\delta q(t_2) \simeq \frac{\delta p_1}{\lambda_s} - \delta q_1 - \kappa \sin(\omega t_1 + \varphi) \left(q_c + \frac{\delta p_1}{\lambda_s} \right) \quad (\text{D.27})$$

in leading order in q_c (more precisely, up to terms that scale as $\sim q_c^2 \log q_c$). Inserting this expression into equation (D.14) yields the corresponding final momentum shift

$$\begin{aligned} \delta \dot{q}(t_2) &\simeq -\kappa \sin(\omega t_1 + \varphi) (\delta p_1 + \lambda_s \delta q_1) \\ &\quad - \kappa \sin(\omega t_2 + \varphi) (\lambda_s q_c - \delta p_1), \end{aligned} \quad (\text{D.28})$$

again in leading order in q_c .

The final position and momentum deviations from the reference expressions (D.20) and (D.21) are then obtained as

$$\begin{aligned} \delta q_2 &= \delta q_{\text{sep}}(t_2) + \delta q(t_2) - \delta q(t_2)|_{\delta q_1=\delta p_1=0} \\ &\simeq [1 - \kappa \sin(\omega t_1 + \varphi)] \frac{\delta p_1}{\lambda_s}, \end{aligned} \quad (\text{D.29})$$

$$\begin{aligned} \delta p_2 &= \delta \dot{q}_{\text{sep}}(t_2) + \delta \dot{q}(t_2) - \delta \dot{q}(t_2)|_{\delta q_1=\delta p_1=0} \\ &\simeq -[1 + \kappa \sin(\omega t_1 + \varphi)] \lambda_s \delta q_1 \\ &\quad + \kappa [\sin(\omega t_2 + \varphi) - \sin(\omega t_1 + \varphi)] \delta p_1 \end{aligned} \quad (\text{D.30})$$

in leading order in q_c . This yields the stability matrix

$$M = \begin{pmatrix} \frac{\delta q_2}{\delta q_1} & \frac{\delta q_2}{\delta p_1} \\ \frac{\delta p_2}{\delta q_1} & \frac{\delta p_2}{\delta p_1} \end{pmatrix} \simeq \begin{pmatrix} 0 & (1 - \kappa_1)/\lambda_s \\ -(1 + \kappa_1)\lambda_s & \kappa_2 - \kappa_1 \end{pmatrix} \quad (\text{D.31})$$

where we use the abbreviations $\kappa_j = \kappa \sin(\omega t_j + \varphi)$ for $j = 1, 2$.

CROSSOVER BETWEEN THE LINEAR AND THE HOMOCLINIC REGION OF THE DRIVEN PENDULUM

In this appendix, we use the Melnikov-Arnold integral [69, 76, 139, 140] to derive a lower bound for the crossover position scale q_c that formally separates the linear from the homoclinic region in our analytical treatment of the driven pendulum problem. We calculate, for this purpose, the energy gain ΔH of a trajectory that closely follows the broken separatrix structure in the presence of a weak perturbation from integrability. This energy gain is given by

$$\begin{aligned}\Delta H &= \int_{t_1}^{t_2} \frac{d}{dt} H[q(t), p(t), t] dt \\ &= -\kappa\omega^2\lambda_s \int_{t_1}^{t_2} \cos[q(t)] \sin(\omega t + \varphi) dt, \quad (\text{E.1})\end{aligned}$$

using $\frac{d}{dt} H[q(t), p(t), t] = \frac{\partial}{\partial t} H[q(t), p(t), t]$ with H given by equation(3.1).

In leading order in the perturbation from integrability, $q(t)$ in the above expression (E.1) can be approximately substituted by the unperturbed separatrix solution $q_{\text{sep}}(t)$ given by equation(D.6) (where we use, without loss of generality, $\text{sgn}(q_1) = 1$). The latter is rewritten as

$$q_{\text{sep}}(t) = 4 \arctan e^{\lambda_s(t-t_\pi)} \quad (\text{E.2})$$

where t_π is the evolution time at which $q_{\text{sep}}(t_\pi) = \pi$. Considering the limits $t_1 - t_\pi \rightarrow -\infty$ and $t_2 - t_\pi \rightarrow \infty$, equation(E.1) is then approximately evaluated as

$$\begin{aligned}\Delta H &\simeq -\kappa\omega^2\lambda_s \int_{-\infty}^{\infty} \cos\left(4 \arctan e^{\lambda_s t'}\right) \\ &\quad \times \sin[\omega(t_\pi + t') + \varphi] dt' \\ &= -\frac{\kappa\omega^2}{4i} \left\{ [A(\omega/\lambda_s) + A^*(-\omega/\lambda_s)] e^{i(\omega t_\pi + \varphi)} \right. \\ &\quad \left. - [A^*(\omega/\lambda_s) + A(-\omega/\lambda_s)] e^{-i(\omega t_\pi + \varphi)} \right\}, \quad (\text{E.3})\end{aligned}$$

where we introduce by

$$A(\Omega) = \int_{-\infty}^{\infty} \exp[i(4 \arctan e^t + \Omega t)] dt \quad (\text{E.4})$$

the Melnikov-Arnold integral [76, 139, 140]. Using

$$\exp(4i \arctan e^t) = \left(\frac{1 + ie^t}{1 - ie^t} \right)^2 \quad (\text{E.5})$$

and applying residue calculus, one obtains

$$A(\Omega) = -\frac{4\pi\Omega}{\sinh \pi\Omega} e^{-\pi\Omega/2}. \quad (\text{E.6})$$

This yields the expression

$$\Delta H \simeq \frac{2\pi\kappa\omega^3 \sin(\omega t_\pi + \varphi)}{\lambda_s \sinh(\pi\omega/2\lambda_s)} \quad (\text{E.7})$$

for the asymptotic energy gain along the broken separatrix structure.

Using $\omega \gg \lambda_s$ and performing an average over the specific driving phase $\omega t_\pi + \varphi$ arising at $t = t_\pi$, the mean scale for the energy deviation along the separatrix is yielded as

$$\overline{\Delta H} = \left(\overline{\Delta H^2} \right)^{1/2} \simeq \frac{\sqrt{2}\pi\kappa\omega^3}{\lambda_s \sinh(\pi\omega/2\lambda_s)}. \quad (\text{E.8})$$

This energy gain or loss can be approximately translated into a mean momentum deviation from the unperturbed separatrix trajectory, $\delta p(t_2) = \dot{q}(t_2) - \dot{q}_{\text{sep}}(t_2)$, evaluated for $q(t_2) = 2\pi - q_c$ at the end of the homoclinic region. Using $\Delta H \simeq [\dot{q}^2(t_2) - \dot{q}_{\text{sep}}^2(t_2)]/2$ with $\dot{q}_{\text{sep}} \simeq \lambda_s q_c$, one obtains $\Delta H \simeq \lambda_s q_c \delta p(t_2)$ in leading order in δp . The requirement $|\delta p(t)| \ll \lambda_s q_c$, which translates closeness to the separatrix structure in the homoclinic region, then yields the inequality $|\Delta H| \ll (\lambda_s q_c)^2$, from which follows, with equation (E.8),

$$q_c^2 \gg \frac{\overline{\Delta H}}{\lambda^2} = \frac{\sqrt{2}\pi\kappa(\omega/\lambda_s)^3}{\sinh(\pi\omega/2\lambda_s)}. \quad (\text{E.9})$$

This latter inequality constitutes a lower bound for the crossover position scale q_c .

BOSE-HUBBARD STAGGERED DIMER STATES – CATALOGUE OF PLOTS

In Chapter 4, Section 4.2, we only presented the minimal amount of figures to ensure that our findings are correctly transmitted. To ensure completeness, we use this appendix to give the interested reader a complete overview of our results.

First, we show in Figures F.1 and F.2 the populations of the 4 sites as a function of time, for $\gamma = 0.5$ and $\gamma = 5$, respectively, for the Fock state $|4, 1, 4, 1\rangle$ and a staggered dimer state whose mean occupancies are those of the Fock state. We then show in Figures F.3 and F.4 the corresponding Discrete Fourier transforms. The points before the thermalisation of the Fock states have been removed to focus on late-time oscillations

We then present in Figures F.5 and F.6 the same observables for this time the Fock state $|14, 1, 14, 1\rangle$ and the staggered dimer state centred on the same occupations, and the corresponding Discrete Fourier transform in Figures F.7 and F.8. Once again, the pre-thermalisation regime has been removed to consider only the late-time fluctuations.

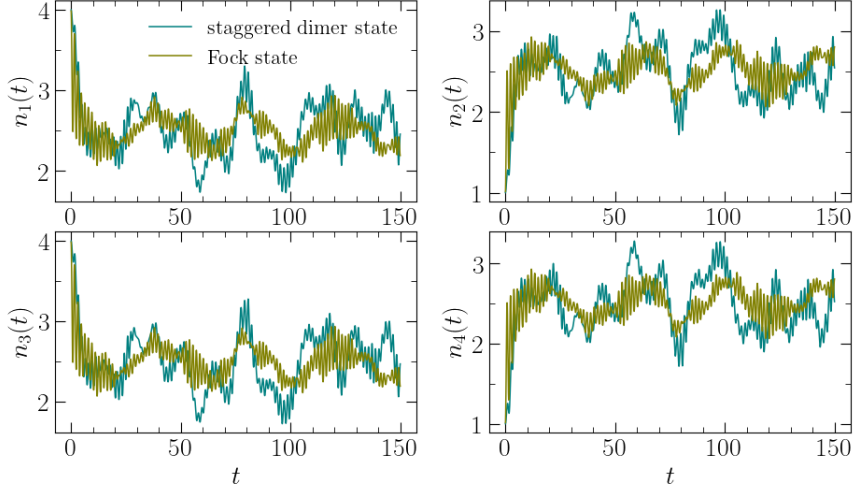


Figure F.1: Population as a function of time for a staggered dimer state (blue) and a Fock state $|4, 1, 4, 1\rangle$ (green), for each site, for $\gamma = 0.5$. The mean site occupancies of the staggered dimer state are the same as the occupations of the Fock state.

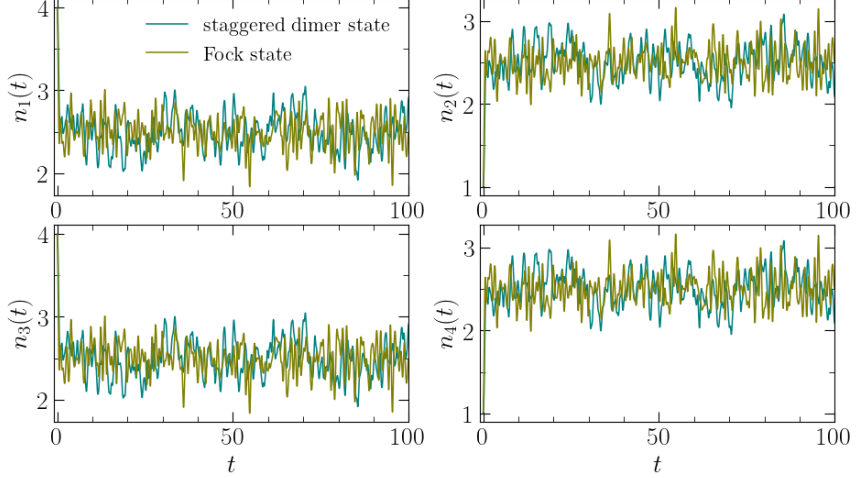


Figure F.2: Population as a function of time for a staggered dimer state (blue) and a Fock state $|4, 1, 4, 1\rangle$ (green), for each site, for $\gamma = 5$. The mean site occupancies of the staggered dimer state are the same as the occupations of the Fock state.

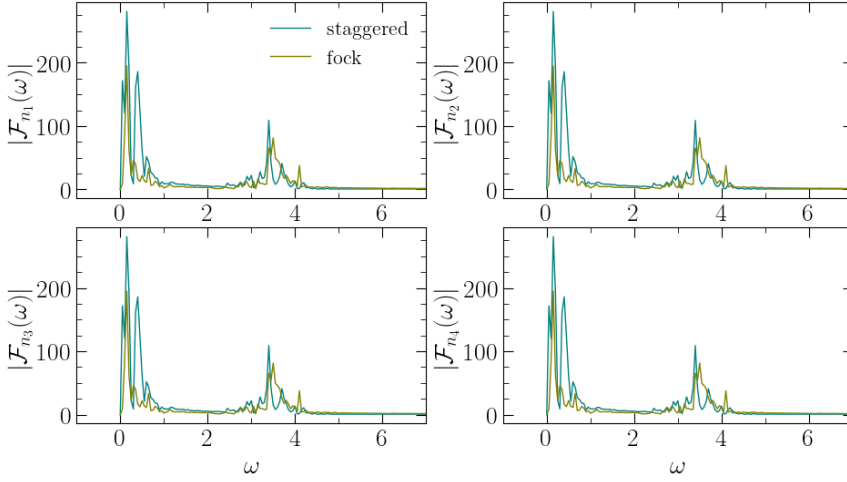


Figure F.3: Discrete Fourier transform of the population as a function of time for a staggered dimer state (blue) and a Fock state $|4, 1, 4, 1\rangle$ (green), for each site, for $\gamma = 0.5$. The mean site occupancies of the staggered dimer state are the same as the occupancies of the Fock state.

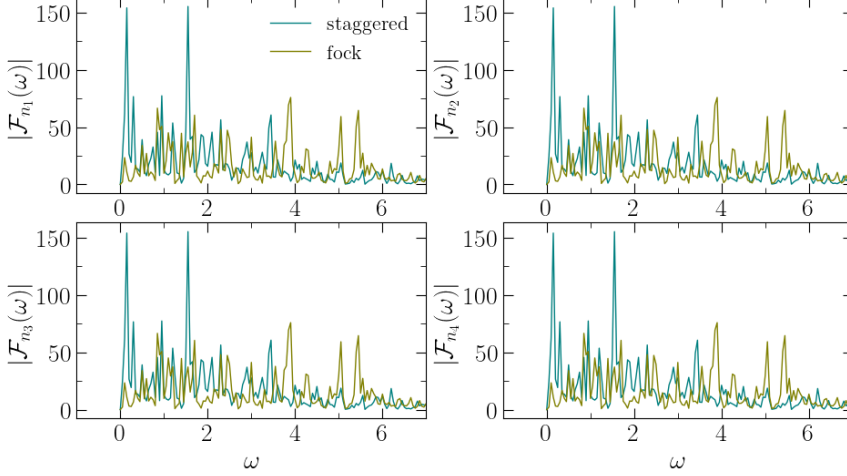


Figure F.4: Discrete Fourier transform of the population as a function of time for a staggered dimer state (blue) and a Fock state $|4, 1, 4, 1\rangle$ (green), for each site, for $\gamma = 5$. The mean site occupancies of the staggered dimer state are the same as the occupancies of the Fock state.

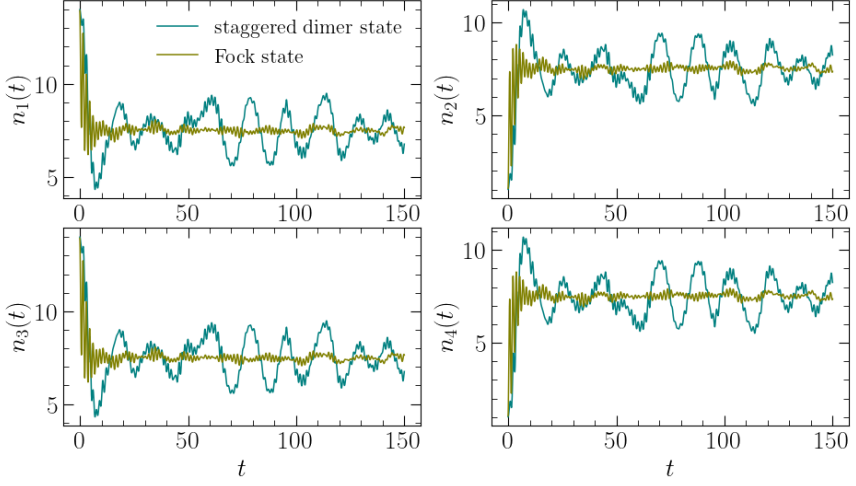


Figure F.5: Population as a function of time for a staggered dimer state (blue) and a Fock state $|14, 1, 14, 1\rangle$ (green), for each site, for $\gamma = 0.765$. The mean site occupancies of the staggered dimer state are the same as the occupations of the Fock state.

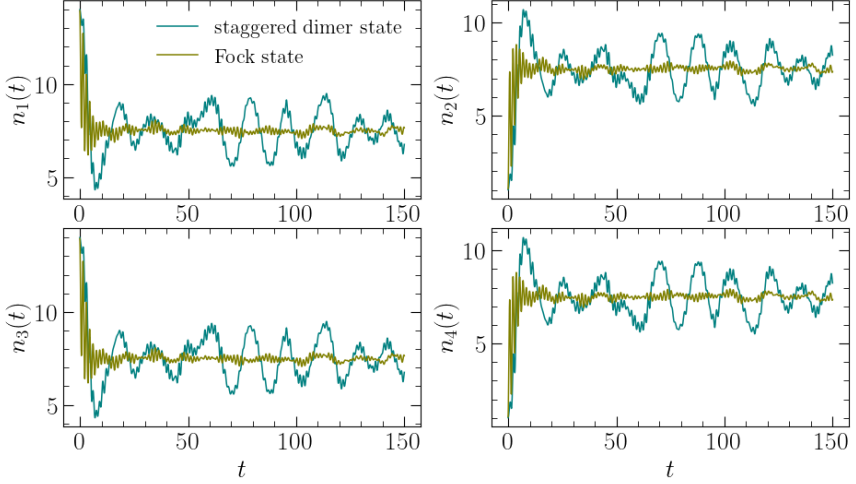


Figure F.6: Population as a function of time for a staggered dimer state (blue) and a Fock state $|14, 1, 14, 1\rangle$ (green), for each site, for $\gamma = 3.54$. The mean site occupancies of the staggered dimer state are the same as the occupations of the Fock state.

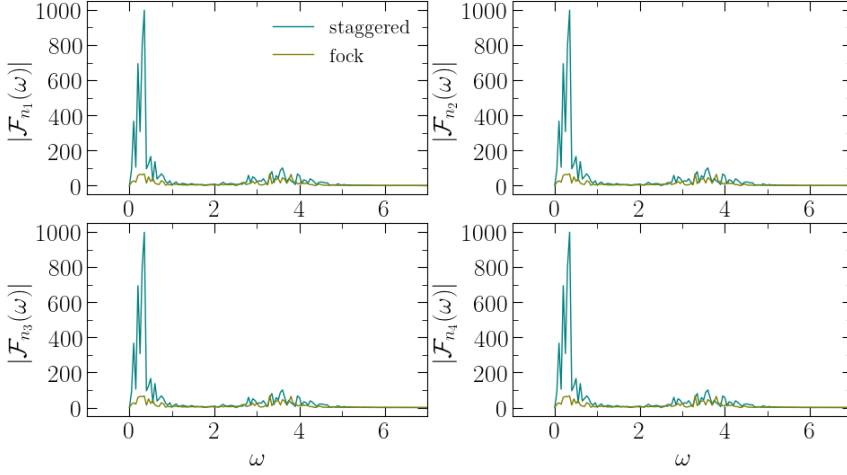


Figure F.7: Discrete Fourier transform of the population as a function of time for a staggered dimer state (blue) and a Fock state $|14, 1, 14, 1\rangle$ (green), for each site, for $\gamma = 0.765$. The mean site occupancies of the staggered dimer state are the same as the occupations of the Fock state.

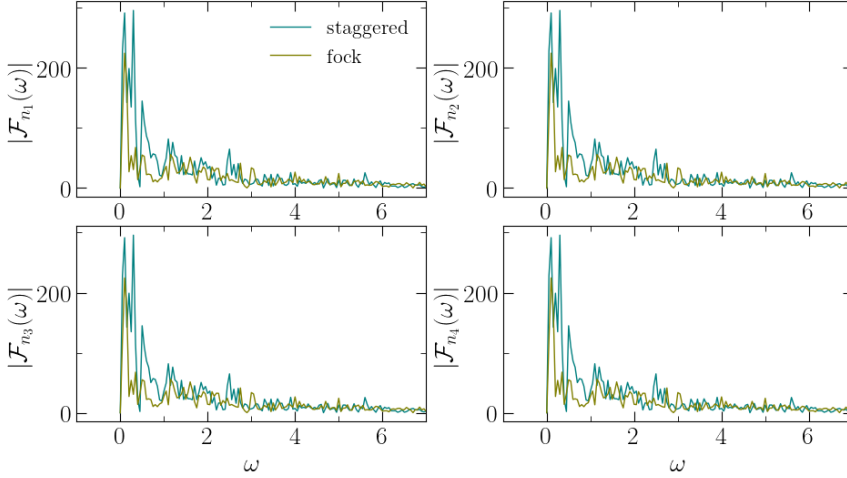


Figure F.8: Discrete Fourier transform of the population as a function of time for a staggered dimer state (blue) and a Fock state $|14, 1, 14, 1\rangle$ (green), for each site, for $\gamma = 3.54$. The mean site occupancies of the staggered dimer state are the same as the occupations of the Fock state.

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