Quantum-Chaotic Evolution Reproduced from Effective Integrable Trajectories

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Classically integrable approximants are here constructed for a family of predominantly chaotic periodic systems by means of the Baker-Hausdorff-Campbell formula. We compare the evolving wave density for the corresponding exact quantum systems using semiclassical approximations based alternatively on the chaotic and on the integrable trajectories. It is found that the latter reproduce the quantum oscillations and provide superior approximations even when the initial coherent state is placed in a broad chaotic region. Time regimes are then accessed in which the propagation based on the system’s exact chaotic trajectories breaks down.

\textit{Introduction} – A fundamental dichotomy between the quantum and the classical theories in physics is that, while the first is governed by a linear equation, the latter allows for much more dynamic complexity due to its general non-linearity. Such non-linearities are a requisite for chaos in Hamiltonian mechanics, and their absence in the quantum world indicates that chaos must be somewhat filtered out in a microscopic description of nature. Research carried out in the second half of the 20th century has subsequently shown that even if Schrödinger’s equation forchaos, the quantum mechanics corresponding to classically chaotic systems can be considered as a field on its own – even though, strictly speaking, “there is no quantum chaos, only quantum chaology” \cite{1}.

An important branch of quantum chaos is dedicated to reproducing quantum dynamics using solely the input extractable from the trajectories of its classical counterpart. This is most often achieved by picking one from a plethora of methods that relate trajectories to quantum objects such as the density of states \cite{2}, the autocorrelation function \cite{3}, the Wigner distribution \cite{4}, or the wavefunction \cite{5,6}. These \textit{semiclassical} approximations are usually obtained from asymptotic methods that explore the smallness of \(\hbar\) with respect to the typical classical action, so it is expected that \(\hbar\) limits the size of the semiclassically relevant phase-space structure. Quantum mechanics should then be immune to the intertwining of classical trajectories, a characteristic of chaotic evolution, in regions with area less than \(\hbar\) \cite{3,7}.

There is strong evidence, however, that quantum mechanics can be accurately reproduced by employing classical trajectories even when they are chaotic, despite the “\(\hbar\)-area rule” \cite{3,8,9}. We here shift direction by investigating the extent to which the trajectories of a specifically tailored integrable system supply a semiclassical approximation for the exact quantum evolution corresponding to a chaotic system – and for how long. The subject is further enriched by comparing the semiclassical results obtained from the effective (integrable) trajectories with the exact (chaotic) ones. Although the idea of substituting chaotic objects by integrable approximations is not new (\textit{e.g.} in chaos assisted tunneling \cite{10,11}), its employment in time-evolution was not previously investigated.

We apply our methods to the propagation of an initial coherent state under the dynamics of the recently introduced “coserf map” \cite{9}, which is exactly quantizable. The short, long and very long time-regimes are examined for a kicking strength that renders the system strongly chaotic. The effective integrable system is devised using the Baker-Hausdorff-Campbell formula and its trajectories are obtained using a recently proposed numerical algorithm able to deal with Hamiltonians that are not sums of kinetic and potential terms \cite{12}. The semiclassical approximations are calculated using the Herman-Kluk propagator, which is very accurate and easily modified to deal with discrete systems \cite{9,13,14}.

\textit{Discrete dynamical systems} – Hamiltonians with time-dependence of the form

\[
H(q,p,t) = \frac{p^2}{2} + TV(q) \sum_k \delta(t-Tk), \quad k \in \mathbb{N},
\]

where \(q\) is the position, \(p\) is the momentum and \(V\) is a position-dependent potential, present exact solutions to Hamilton’s equations and are extensively studied in the context of quantum chaos. The reason for their repeated use is that the corresponding equations of motion are expressed as a discrete map, which can be chaotic even for a single degree of freedom. Here, the sum of delta functions expresses the fact that the potential energy is turned on at times \(T\), multiples of the \textit{kicking strength} \(T\), outside of which the system evolves with constant momentum \(p\). The corresponding equations of motion generate stroboscopic maps, \textit{e.g.} the standard map \cite{15}, that split propagation into purely kinetic and purely potential steps. By writing Hamilton’s equations for a phase-space point \(z = (q,p)\) using Poisson brackets as \(dz/dt = \{z,H\}\) we can express the orbits of \(\{H\}\) for a single kick as composition of two shears generated by two separate Hamiltonians \cite{9}:

\[
\begin{align*}
\{H_1(p) = p^2/2\} & \quad \Rightarrow \quad U_1^T(\cdot) = \exp(-T \{\cdot, H_1\}) \\
\{H_2(q)= V(q)\} & \quad \Rightarrow \quad U_2^T(\cdot) = \exp(-T \{\cdot, H_2\})
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\end{align*}
\]
Using the group property of the solutions above, the final point at \( \tau = NT \) for \( N \) steps is

\[
   z_{\tau} = U_{T}^{N}(z_0) = (U_{T}^{2} U_{\frac{T}{2}})^{N}(z_0).
\]

(3)

Since the flow can be decomposed as successive mappings of the integrable steps in \([3]\), which are exactly quantizable, the corresponding quantum propagation is exact. We shall focus on an initial coherent state centered at \( z_0 = (q_0, p_0) \), taken as

\[
   \langle q|z_0\rangle = (\pi \hbar)^{-\frac{1}{2}} \exp \left\{ - (q - q_0)^2 / 2\hbar + ip_0(q - q_0) / \hbar \right\},
\]

for which the exact quantum evolution in position representation after \( N \) kicks reads

\[
   \langle q|z_0, \tau\rangle = \langle q|U_{T}^{N}|z_0\rangle = \langle q|(U_{T}^{2} U_{\frac{T}{2}})^{N}|z_0\rangle.
\]

(4)

Quantization for each Hamiltonian evolution in \([3]\) is then straightforwardly given by \( q \mapsto \hat{q}, p \mapsto \hat{p} \), and \( \{\}, \{\} \mapsto i\hbar[\cdot,\cdot] \), so that \( U_{T}^{2} \mapsto \hat{U}_{T}^{2}, j = 1, 2 \), without the need of any ordering considerations.

Effective Hamiltonians – Using the Baker-Hausdorff-Campbell formula \([10]\) we can approximate the two steps in \([3]\) by an effective one:

\[
   e^{-T\{\cdot, H_{1}\}} e^{-T\{\cdot, H_{2}\}} \approx e^{-T\{\cdot, \mathcal{H}\}},
\]

(6)

where

\[
   \mathcal{H} = H_{1} + H_{2} + (T/2)\{H_{1}, H_{2}\}
   + (T^2 / 6) \{H_{1} + H_{2}, \{H_{2}, H_{1}\}\} + O(T^3).
\]

(7)

The effective Hamiltonian \( \mathcal{H} \) above is time-independent, so its solutions for a period \( T \) can be considered as perturbations of the original system for both the classical and quantum cases. Note also that \( \mathcal{H} \) cannot be generally expressed as a sum of potential and kinetic energies due to terms proportional to \( \{H_{1}, H_{2}\} \) not vanishing – a Hamiltonian of this type is known as non-separable (even though the system itself is integrable). This implies that solving the equations of motion associated to \( \mathcal{H} \), namely

\[
   dz/dt = \{z, \mathcal{H}\},
\]

(8)

requires the use of special numerical integrators that both preserve the invariants of classical mechanics (such as energy) and can be applied to non-separable functions. These integrators are called non-separable symplectic integrators, and until very recently were limited to algorithms given in terms of computationally expensive implicit functions, being only accurate for short times. Here, however, we are interested in classical propagation for very long times – enough for chaotic behavior to set in and dominate phase space. We then implement the explicit algorithm recently proposed by M. Tao \([12]\), which consists of injecting the system in a larger phase space where its equations of motion are separable, solving them, and projecting the solutions back. We refer to the original article \([12]\) for error estimates and a very accessible exposition of the method.

In Fig. 1 we display some discrete orbits of \([3]\) for the coserf system, defined by

\[
   V_{\text{coserf}}(q) = q^2 / 2 - 2 \cos(q) - \sqrt{\pi} \text{erf}(q)/2,
\]

(9)

and their integrable approximations, obtained by applying Tao’s method to the effective Hamiltonian \( \mathcal{H} \) truncated at \( O(T^4) \). All algorithms to integrate Hamilton’s equations are discrete, meaning that they have a small integration step, and the step \( \delta \) we used to numerically solve \([8]\) is small enough for the solutions to look continuous when compared to the discrete dynamics of \([3]\). Notice that even though both \( T \) and \( \delta \) represent distances between iteration steps, they are very different in nature: The kicking strength \( T \) is seen as a true parameter that we vary in order to achieve chaos in \([3]\); \( \delta \), on the other hand, is just a numerical integration step that we take as small in order to obtain good accuracy in solving \([8]\).

We use the simplest version of Tao’s algorithm, for which the trajectories obtained from \([8]\) have errors of \( O(\delta^4) \).

The trajectories are functions of position and momentum, so it is worthwhile to look at how an initial phase-space distribution evolves under both the chaotic and the effective trajectories in order to have a clear picture of their contrast. The obvious choice is the phase-space Gaussian

\[
   W(q, p) = \exp \{- [(q - q_0)^2 + (p - p_0)^2] / \hbar \} / \pi \hbar,
\]

(10)

which can be identified with the quantum Wigner function for the coherent state \([4]\) \([17]\). Then the classical
evolution of this distribution by the classical trajectories under either the chaotic map or the effective Hamiltonian corresponds to the approximation of the Wigner evolution to lowest order in $\hbar$ [15–20]. The results of both classical evolutions are depicted in Fig. 2, where it is seen that the initial distribution deforms into a filament as if they were smooth and structureless (see Fig. 1). The quantum coserf map, however, has an effective approximant, that the semiclassical propagator employing the exact dynamics. We see here, quite contrary to intuition, that the semiclassical propagator employing the effective trajectories is at least as accurate as its chaotic twin: An analysis of Fig. 3 actually shows it to be better than the one employing the classical map’s exact dynamics, allowing for the exploration of time regimes in which the original distribution has deformed into a stain (see Fig. 2(d)). It is expected that for small $T$ we have good agreement between both semiclassical schemes, since in

\begin{equation}
R(z) = \sqrt{\frac{1}{2} \left( \frac{\partial p}{\partial q} + \frac{\partial q}{\partial p} + i \frac{\partial q}{\partial \tau} \right)} (13)
\end{equation}

\begin{equation}
S(z) = \sum \Delta \tau L(q, p, \tau) (14)
\end{equation}

where $L$ is the system’s discretized Lagrangian [9, 21]. The square root in (13) can and usually does change branch in the complex plane throughout evolution, and it is fundamental to keep track of these changes in order to match the final phases (a procedure known as Maslov tracking [22]). The semiclassical approximation for the propagation of a coherent state by the Herman-Kluk method is, therefore,

\begin{equation}
\langle Q|z, \tau \rangle \approx \int dQ' k_r(Q', Q)\langle Q'|z_0 \rangle (15)
\end{equation}

When implementing this formula for the map [3], we take $\tau = TN$, where $T$ is the kicking strength and $N$ is the number of kicks. For the effective trajectories that solve (5), we use $\tau = \delta M$ in Tao’s algorithm, where $M$ is chosen such that the final propagation times are the same for both the chaotic and the effective orbits, i.e., $TN = \delta M \Rightarrow M = N(T/\delta)$. These propagation times were already used in Fig. 2. The semiclassical wave densities $|\langle q|z_0, \tau \rangle|^2$ for both propagation schemes are plotted against the exact quantum result in Fig. 3 for the same time values as in Fig. 2.

As is usual in the field, the semiclassical wave densities in Fig. 3 are also renormalized in order to have $\int dq |\langle q|z_0, \tau \rangle|^2 = 1$, since it is well-known that the wavefunctions obtained via the Herman-Kluk propagator might lose normalization due to the effect of rapidly separating chaotic orbits in the pre-factor (13) [23]. The wavefunction obtained using effective trajectories, however, comes out entirely normalized, since the obstruction to full normalization is due exclusively to chaos.

**Discussion** – As we can see in Fig. 2 the chaotic propagation is markedly different from its integrable approximation, which interpolates the chaotic orbits in phase space as if they were smooth and structureless (see Fig. 1). The quantum coserf map, however, has an exact classical counterpart, so that it is expected that replacing its true classically chaotic orbits by integrable ones should result in at least some degree of loss with respect to the exact dynamics. We see here, quite contrary to intuition, that the semiclassical propagator employing the effective trajectories is at least as accurate as its chaotic twin: An analysis of Fig. 3 actually shows it to be better than the one employing the classical map’s exact dynamics, allowing for the exploration of time regimes in which the original distribution has deformed into a stain (see Fig. 2(d)). It is expected that for small $T$ we have good agreement between both semiclassical schemes, since in
FIG. 3: Wave densities for the time-evolution of the coherent state (4) obtained via the Herman-Kluk propagation (15) and the exact quantum map (5) for $T = 0.6$. The exact quantum result is displayed as a solid green line, while the semiclassical propagations using chaotic and effective trajectories are shown as black and red dashed lines, respectively. The number of kicks for the first three panels is the same as in Fig. 2, namely (a) $N = 9$, (b) $N = 18$ and (c) $N = 49$, but in (d) we have $N = 70$. We take $\hbar = 1$ and, as in the other figures, the numerical integration step for the effective trajectories is $\delta = 10^{-2}$.

this case the classical map (3) is not yet chaotic. It is the very large kicking strength we choose here that shows that quantum-chaotic evolution can be reproduced without the use of chaotic orbits.

A time threshold also exists in which the effective and the chaotic semiclassical approximations are expected to match quite closely: This is known in the field as the Ehrenfest time $\tau_E$, defined as the moment at which the classical and quantum autocorrelation functions start to deviate due to characteristic quantum oscillations [8, 24].

We expect the semiclassical schemes to be equivalent in this regime because chaos has not yet impacted classical propagation very strongly – this can be directly observed in Fig. 2(b), which is taken near the Ehrenfest time for this system, and the closely matching wave densities in Fig. 3(a). The panels (b) and (c) of Fig. 3 already correspond to Ehrenfest-time multiples, namely $5\tau_E$ and $7\tau_E$, regimes usually referred to as long times – here, we expected to see no resemblance between effective and chaotic semiclassical propagations, since they are obtained from quite different systems which possess incompatible dynamics (see Fig. 2). In Fig. 3(d) we are beyond $10\tau_E$ and within $O(\tau_H)$, where $\tau_H$ is the Heisenberg time at which individual energy levels are resolved: Here, only the effective trajectories are able to approximate the quantum result and the chaotic propagation breaks down.

The fact that quantum-chaotic evolution could be better reproduced from an integrable Hamiltonian indicates that the latter’s quantization lies very close to the exact quantum map, since the Herman-Kluk propagator has been shown to be remarkably accurate for integrable systems [3]. It is then expected that more aspects regarding the quantization of a classically chaotic system can also be obtained from chaos-free methods.

Although we have used a stroboscopic map due to its visual appeal and exact quantum evolution to compare semiclassical results, we remark that there is no obstruction to employing the formalism described to continuous chaotic systems in higher-dimensional phase spaces. The effective integrable trajectories could be then obtained from e.g. normal forms [25, 26] or other approximation method.

**Conclusion** – We have shown that the quantum mechanical propagation of a coherent state with chaotic classical analogue can be semiclassically approximated very accurately by substituting the original chaotic trajectories with effective integrable ones. Besides suggesting that chaos might not be fundamental to quantum evolution, the resulting effective semiclassical approximation was seen to be even more accurate than the original one for very long times, presenting itself as a useful tool to access deeply chaotic regimes.

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