Quantum chaos and effective thermalization

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We demonstrate effective equilibration for unitary quantum dynamics under conditions of classical chaos. Focusing on the paradigmatic example of the Dicke model, we show how a constructive description of the thermalization process is facilitated by the Glauber $Q$ or Husimi function, for which the evolution equation turns out to be of Fokker-Planck type. The equation describes a competition of classical drift and quantum diffusion in contractive and expansive directions. By this mechanism the system follows a ‘quantum smoothened’ approach to equilibrium, which avoids the notorious singularities inherent to classical chaotic flows.

How do thermally isolated many particle quantum systems relax towards stationary states? Along with the recent advances in quantum optics and cold atom experimentation, this fundamental question of theoretical physics presents itself under new perspectives. The interacting, and in many instances thermally decoupled many particle states realizable in cold atom devices show novel forms of relaxation which can be monitored at hitherto unimaginable degrees of resolution. Examples of unconventional relaxation phenomena include the formation of negative temperature states$^1$, the buildup of textures in Brillouin zones by an interplay of interaction and single particle kinematics$^2$, or the relaxation into ergodic and other types of ‘non-thermal’ distributions$^3$$^5$. While computationally efficient, this scheme does not reveal the physical processes leading to thermalization.

In this letter we approach the phenomenon from a more dynamical perspective. We present our case for the paradigmatic example of the Dicke model$^6$ which describes the coupling of a (large) spin and an oscillator. At a critical coupling strength, the model undergoes a quantum phase transition into a ‘superradiant’ phase, characterized by a nonvanishing mean oscillator amplitude and chaotic dynamics$^7$. In view of the recent experimental observation of that phase transition$^8$, the issue of thermalization has become concrete.

Our approach hinges on a manageable description of the impact of quantum fluctuations on the semiclassical dynamics. A representation of the quantum density operator, by Glauber’s $Q$-function (aka Husimi function), turns out to be the key. Von Neumann’s equation for the density operator assumes the form of a Fokker Planck equation for $Q$. The equilibration processes can be then understood by appreciating the competition of classical drift and quantum diffusion in expansive and contractive directions of the ’flow’ supporting $Q$. We augment the general discussion by an exact solution of a toy model which arguably reflects the essence of the full problem.

In the end we will indicate that our methodology is applicable to a whole class of chaotic dynamics. Even certain periodically kicked systems qualify.

Dicke Model $\rightarrow$. We write the Dicke Hamiltonian as

$$\hat{H} = \hbar \left\{ \omega_0 \hat{J}_z + \omega a^\dagger a + g \sqrt{\frac{2}{J}} (a + a^\dagger) \hat{J}_z \right\}. \quad (1)$$

Here, $\hat{J}_a = x, y, z$ are spin operators acting in a spin-$j$ representation, and $a/a^\dagger$ are photon annihilation/creation operators. The first two terms in (1) respectively describe spin precession about the $J_z$-axis with frequency $\omega_0$ and harmonic oscillation with frequency $\omega$. The last term describes the coupling of spin and oscillator with coupling constant $g$. Crucially, the interaction contains the so called antiresonant terms $J_x a^\dagger + J_y a$ where $J_x = J_z \pm 1$ are the familiar raising and lowering operators. This fact makes the model distinct from an integrable variant where these terms are neglected (rotating wave approximation). At a critical value of the coupling strength, $g_c \equiv \sqrt{\omega_0/\omega}$, the non-integrable model$^1$ undergoes a quantum phase transition into a ‘superradiant phase’. For values $g > g_c$, the photon ‘amplitude’ $a$ builds up a nonvanishing excitation value, and the dynamics becomes globally chaotic.

Coherent state representation $\rightarrow$. In view of the large-ness of the spin, $j \gg 1$, we find it convenient to represent the theory in terms of coherent states$^9$$^11$.

$$|z\rangle \equiv \frac{1}{(1 + |z|^2)^{j/2}} e^{-\frac{1}{2} J_z} |j, j\rangle, \quad (2)$$

where $z \in \mathbb{C}$ and $|j, j\rangle$ is a ‘maximum-weight’ eigenstate of $J_z$, i.e. $J_z |j, j\rangle = j |j, j\rangle$. The states $|z\rangle$ are unit normalized, $\langle z|z\rangle = 1$. They entail the expectation values $\langle z| J_a |z\rangle = J_a$, where $J_x,y,z$ are the three components of a unit vector $\mathbf{1} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)^T$, whose angular orientation is defined through $z = e^{i \phi} \tan(\theta/2)$. Each $|z\rangle$ has minimum angular uncertainty, characterized by the solid angle $4 \pi/(2j + 1)$ which defines a Planck cell on the unit sphere. The overcomplete set $\{ |z\rangle \}$ provides a resolution of unity as $\mathbf{1} = \sum_{z} |z\rangle \langle z|$.
Similarly, oscillator coherent states are defined as \[ |\alpha\rangle = e^{-a^a/2} e^{aa} |0\rangle, \]
where \( \alpha \in \mathbb{C} \) and \( |0\rangle \) is the vacuum, \( a|0\rangle = 0 \). The states \( |\alpha\rangle \) assign a minimal uncertainty product to displacement and momentum such that these quantities are 'confined' to a single Planck cell located at \( x \propto (\alpha + \alpha^*) \sqrt{\hbar} \), \( p \propto i(\alpha - \alpha^*) \sqrt{\hbar} \) within the classical phase space. The completeness relation here reads \( \mathbb{I} = \frac{1}{\pi} \int da \langle \alpha | \alpha \rangle \).

We next represent the system’s time dependent density operator \( \hat{\rho}(t) \) in terms of a coherent state based quasiprobability density. Among the many possible choices the Glauber \( Q \)-function,

\[
Q(\alpha, z) = \frac{2j + 1}{\pi(1 + z^2)} \langle \alpha, z | \rho | \alpha, z \rangle,
\]
turns out to be the most convenient one by far, for our purposes. We here denote by \( |\alpha, z\rangle = |\alpha\rangle \otimes |z\rangle \) the overall coherent state for spin and oscillator. Using the completeness relations given above one sees that \( Q \) is normalized as \( \int dz Q(\alpha, z) = 1 \) and yields expectation values of (anti-normal ordered) operators as \( \langle a^m | \alpha \rangle = \int dz a^m Q(\alpha, z) \). By its definition, \( Q \) exists and is non-negative, \( Q(\alpha, z) \geq 0 \), for any density operator \( \rho \). The latter property allows \( Q \) to converge to the classical phase space density as \( \hbar \to 0 \). As the most rewarding property we shall presently find that \( Q \) enables us to map the quantum evolution equation \( i\hbar \partial_t \hat{\rho} = [\hat{H}, \hat{\rho}] \) onto a differential equation of the Fokker-Planck type, optimally suited to describe the dissipation-free equilibration.

Quantum dynamics —. Using identities such as \( \hat{J}_x |z\rangle \langle z| = ((1 - z^2) \partial_z + 2j z (1 + |z|^2)) |z\rangle \langle z| \) and \( a^1 |\alpha\rangle \langle \alpha| = (\partial_\alpha + \alpha^*) |\alpha\rangle \langle \alpha| \), it is straightforward to show that the evolution equation of the distribution function \( Q \) assumes the Fokker-Planck form

\[
\dot{Q} = (\mathcal{L} + \mathcal{L}_{\text{diff}}) Q
\]

\[
\mathcal{L} = i \partial_\alpha \left( \omega_0 + g \sqrt{2j} \frac{z + z^*}{1 + |z|^2} \right) + i \partial_z \left( -\omega_0 z + \frac{g}{\sqrt{2j}} (1 - z^2)(\alpha + \alpha^*) \right) + \text{c.c.}, \quad \mathcal{L}_{\text{diff}} = \frac{ig}{\sqrt{2j}} \partial_\alpha \partial_z (1 - z^2) + \text{c.c.}
\]

Most remarkably, derivatives terminate at second order. Less prudent, derivatives of a quasiprobability might have brought the plague of higher derivatives.

To understand the meaning of the first order, or drift term, it is convenient to introduce canonically conjugate action angle variables \( (I, \psi) \) as \( \alpha = \sqrt{J} \exp(i \psi) \) for the oscillator and the canonical pair \( (\cos \theta, \phi) \) for the spin. It is then a straightforward (if tedious) matter to show that the drift operator becomes the classical Liouville operator, \( \mathcal{L} Q = \{ h, Q \} \), where the effective Hamilton function

\[
h = \omega_0 \cos \theta + \omega I + g \sqrt{I} \cos \psi \sin \theta \cos \phi,
\]

obtains from the operator \( \hat{J} \) by substituting \( \hat{J} \to J, a \to \sqrt{J} \exp(i \psi) \) and dividing out \( \hbar j = L \). The operator \( \mathcal{L} \) thus describes the drift of the quasi-probability along the classical trajectories of the Hamiltonian flow.

The distinctive feature of the classical dynamics is global chaos in the superradiant regime, \( g > g_c \). Referring for an in-depth discussion to [14], we here merely note that for \( g > g_c \) and for excitations energies only slightly above the ground state bound \( E_0 \simeq -j \omega_0 \left( \frac{g}{2} \right)^2 \) ergodic dynamics is observed. This is illustrated in the Poincaré sections of Fig. 1 where the top/bottom row are for low \( (\Delta E/|E_0| \approx 0.20)/\text{high} (\Delta E/|E_0| \approx 30) \) excitation. Both sections \( (c) \) reflect dominance of chaos and indicate equilibration. In particular, the low-excitation portrait \( (e) \) reveals chaos as dominant, even though the energy shell includes but a small part of the Bloch sphere.

Quantum diffusion —. How does quantum mechanics interfere with the classical drift? Quantum mechanics enters the Fokker-Planck equation \( \mathcal{L} Q = \{ h, Q \} \) through the diffusion operator \( \mathcal{L}_{\text{diff}} \). A key feature of the diffusion operator is the absence of second order derivatives w.r.t. only oscillator \( (x_{1,2} = I, \psi) \) or spin \( (x_{3,4} = \cos \theta, \phi) \), phase space variables. The ‘diffusion matrix’ \( D \) defining the operator \( \mathcal{L}_{\text{diff}} = \sum_{ij} \partial_{x_i} \partial_{x_j} D_{ij}(x) \) thus possesses a block off-diagonal chiral structure, \( D = \left( \begin{array}{cc} 0 & d \end{array} \right) \). While there will be no need to spell out the explicit dependence of the chiral block \( d \) on the variables \( x = (I, \psi, \cos \theta, \phi) \), we emphasize its smallness in \( j^{-1} \). The ‘chiral’ block structure of \( D \) entails a secular equation for the eigenvalues of the form \( \lambda^4 - \lambda^2 \text{ tr } dd^\dagger + \text{det } dd^\dagger = 0 \). The four eigenvalues of \( D \) thus come in two pairs \( \pm \sqrt{a}, \pm \sqrt{b} \) where \( a, b \) are the eigenvalues of the non-negative \( 2 \times 2 \) matrix \( dd^\dagger \). Each eigenvalue is associated with an eigenvector corresponding to diffusive spreading (+) or ‘anti-diffusive’ shrinking (−). These four ‘quantum’ directions form a Cartesian frame wherein the four directions distinguished by the chaotic drift lie askew — one expansive (unstable), one contractive (stable), and two neutral (along the flow and transverse to the energy shell).

Since \( Q \) is guaranteed existence and positivity, quantum diffusion (along the eigenvectors of \( D \) with positive eigenvalues) must oppose the contraction along the clas-
sically stable manifold, thus preventing the buildup of singular phase space structures. Deterministic contraction and quantum diffusion balance at quantum scales $1/\sqrt{\hbar} \sim \sqrt{\hbar}$. At shorter ‘length’ scales (which can be brought into play by initial states squeezed along the classically stable direction), the second order differential diffusion operator becomes dominant (as can be seen by straightforward scaling estimates); it prevents further contraction and smooths the distribution. By contrast, at the large scales generated in the classically unstable direction, the quantum (anti-)diffusive correction is of no significance. Rather, expansion continues uninhibited, accompanied by the chaotic ‘folding’ necessitated by the compactness of the energy shell.

Toy model —. It is instructive to illustrate the interplay of classical drift and quantum diffusion on an analytically solvable toy model, provided by the Fokker-Planck equation $\dot{P} = (\partial^2_p - \partial^2_x x + D(\partial^2_p - \partial^2_p^2))P$; the diffusion constant must be imagined small, $0 < D \ll 1$ and of quantum origin, $D \propto \hbar$. Anti-diffusive contraction and deterministic stretching are carried by $x$ according to $\text{var}_t(x) = (\text{var}_0(x) - D)e^{2t} + D$, where the variance is calculated using an averaging prescription $\langle f(x,p) \rangle = \int dx dp f(x,p)P(x,p)$. We infer that the minimum allowable ‘quantum’ scale of $x$ is $\sqrt{D}$. If $\text{var}_t(x)$ is of the order but larger than $D$, the characteristic scale for (the variance of) $x$ will grow to (‘macroscopic’) order unity within the Ehrenfest time $\sim \ln(1/D)$. On the other hand, diffusive expansion and deterministic contraction are carried by $p$ as $\text{var}_t(p) = (\text{var}_0(p) - D)e^{-2t} + D$. The balancing scale for $p$ is $\sqrt{D}$. If the initial variance of $p$ is much larger than $D$ (say, of the ‘macroscopic’ order unity), the exponential decrease to the order of $D$ takes a time of the order $\ln(1/D)$, again the ‘Ehrenfest time’.

Generalizing the toy model one may choose the axes of classical contraction and expansion skew to the principal axes of quantum (anti)diffusion. Positivity of all variances then restricts the relative orientations: clearly, the classically stable direction must not coincide with the axis of antidiffusion, or else the respective variance would go negative within a finite time. Referring for a detailed discussion of the ensuing correlations in the Dicke system to [14], we here merely note that its guaranteed existence protects the $Q$-function from such type of alignment, save for exceptional regions in phase space.

Thermalization —. Turning back to the full problem, we conclude that the interplay of deterministic expansion/contraction, quantum diffusion, and chaotic folding (the latter of course absent in the toy model) will spread out any initial distribution over the compact energy shell. Location, $E$, and width, $\Delta E$ of the shell are determined by the initial state, with $\Delta E \sim j^{-1/2}$ a minimal value for coherent state initial distributions. Given any fixed phase space resolution, $\Delta x$, and a characteristic width $x_0 \gg \Delta x$ of the initial distribution, the quantum and a purely classical description of the flow, resp., both predict full coverage of the energy shell for time scales $t > \tau \ln(\Delta x_0/\Delta x)$, where $\tau$ is the Lyapunov time. However, important differences occur in the dynamical buildup of the equilibrated state: while the classical approach describes equilibration in terms of the formation of an infinitely filigree structure of alternating high and vanishing phase space density, — the result of continued stretching and folding of the initial distribution —, the quantum distribution remains smooth (on scales $\sim j^{-1/2}$) all the way along. This hallmark of

FIG. 1. Poincaré sections generated by monitoring the projection $(l_y, l_y)$ of $l$ in the southern hemisphere at fixed values of the phase $\psi$. For each parameter value $\Delta g/g_c$, nine trajectories of different on-shell initial conditions are sampled. Upper row: energy $\Delta \epsilon \simeq 0.2|\epsilon_0|$ above the ground state and values $g/g_c$: a) 0.2, b) 0.7, c) 0.9, d) 1.01, e) 1.5. Lower row: energy $\Delta \epsilon \simeq 20|\epsilon_0|$.
quantum chaotic propagation should be experimentally visible by current spectroscopic techniques \[15\]. Finally, let us remark on the universality of the above picture with regard to variations in the initial conditions. Coherent states, being isotropically ‘supported’ by a single Planck cell, come closest to the classical fiction of a single phase space point. They naturally qualify as initial states for the equilibration described above. Equally well suited are squeezed minimum uncertainty states, even if squeezed along the classically stable direction; the diffusion then smears the pertinent uncertainty to the characteristic quantum scale mentioned. Yet broader states succumb to equilibration even more willingly.

Beyond the Dicke model —. While the relevance of ‘quantum diffusion’ operators to the description of the long time dynamics in chaotic quantum systems has been noted before, previous work \[16\] has added these contributions by hand. Our present analysis exemplifies how quantum diffusion emerges naturally. Evolution equations with derivatives terminating at second order are not an exclusive privilege of the Dicke model. Rather, whenever a chaotic dynamical system has a Hamiltonian of the form of a second-order polynomial in the pertinent observables and allows for a coherent-state-based $Q$-function, we expect a Fokker-Planck equation to govern the time evolution of $Q$ and everything to go through in much the same way as above. Examples are autonomous $SU(3)$ dynamics \[17\] whose Hamiltonians contain terms of first and second order in the $SU(3)$ generators. Certain kicked systems qualify as well. Most notable among those is the kicked top \[18\] whose near classical quantum behavior has recently been observed experimentally \[15\]. Genuine many-body systems also have Fokker-Planck equations for $Q$, provided the Hamiltonians are quartic in creation and annihilation operators but contain no antiresonant terms. Examples of much current interest are Bose-Hubbard systems \[19, 20\]. Finally, chaotic dynamics where the evolution equations of $Q$ contains higher-order derivatives can allow for reasonable Fokker-Planck approximations, if good arguments are available for neglecting third and higher derivatives. We shall cover such extensions of our work in a separate publication \[14\].

Summarizing, we have discussed the principles whereby the probability flux of a classically chaotic quantum systems covers its shell of conserved energy. The dynamics crucially hinges on effectively diffusive quantum propagation interfering with the deterministic exponential contraction inherent to classically chaotic flows. (In the expansive directions of the flow, quantum corrections are negligible.) The net effect of this competition is the smoothing of a flow which in a classical system would soon turn into a singular structure. We discussed these phenomena on the example of the Dicke model where the Husimi representation of the quantum flow equation assumes the particularly handy form of a Fokker-Planck equation. While the Fokker-Planck representation pertains to other quantum systems, it is far from generic. In general, one will meet higher-order, differential equations. However, power counting arguments \[14\] suggest that at the microscopic length scales $\sim \hbar^{1/2}$ where quantum diffusion becomes effective, higher terms in the expansion will be sub-dominant. It thus stands to reason that the smoothing of the classical flow by mechanisms similar to those discussed above is a general effect.

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