Kolmogorov-Arnol'd-Moser Barriers in the Quantum Dynamics of Chaotic Systems

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(Received 18 August 1986)

Classical Kolmogorov-Arnol'd-Moser tori and cantori are found to act as barriers in the quantum dynamics of a kicked rotator. In their vicinity the asymptotic distribution decays exponentially. The penetration depth of a Kolmogorov-Arnol'd-Moser torus scales as $\hbar^{0.66}$ and the penetration probability as $\hbar^{2.5}$. Cantori can inhibit the diffusive growth of mean square displacements and thus act as barriers more drastically than in classical systems.

PACS numbers: 05.45.+b, 03.65.-w

For a long time there has not been much interest in the quantum mechanics of nonintegrable Hamiltonian systems. Paradoxically, about half a century after the formulation of quantum mechanics, important advances in the understanding of classical mechanics [e.g., the Kolmogorov-Arnol'd-Moser (KAM) theorem] posed new questions for quantum mechanics, in particular for its limit $\hbar \to 0$. The correspondence principle requires that quantum mechanics recover classical mechanics, e.g., in the limit $\hbar \to 0$. The two theories exhibit strongly contrasting properties, however, because classical equations of motion may be nonlinear, whereas the Schrödinger equation is a linear differential equation: In quantum mechanics the large-scale chaotic motions (diffusion) occurring in classical systems are suppressed, and the so-called sensitive dependence on initial conditions is absent. Thus quantum mechanics (for $\hbar \neq 0$) does not show certain phenomena that must exist in its classical limit ($\hbar = 0$). We therefore ask how quantum mechanics manages such an amazing transition for $\hbar \to 0$.

In particular, on the basis of the Kolmogorov-Arnol'd-Moser theorem we now understand that classical chaos may be confined to certain regions of phase space. Invariant KAM tori can act as impenetrable barriers to the probability flow. In quantum mechanics, however, we expect the spreading of wave packets in contrast to the confinement in the classical case. In the present work we have asked how quantum mechanics reconciles these opposing properties in the limit $\hbar \to 0$. We have found that even in quantum systems the classical KAM tori and cantori (broken tori) play a role as dynamical barriers. There is only a small transition probability into states that are classically inaccessible (as a result of a KAM torus); it scales as $\hbar^{2.5}$. The asymptotic probability distribution decays exponentially near KAM tori and cantori; the penetration depth scales as $\hbar^{0.66}$. One may interpret this as a (KAM) localization mechanism in quantum systems; its origins are the classical KAM tori and cantori, as opposed to quantum interferences (Anderson localization) discussed previously. Amazingly, (classical) cantori appear to act as barriers even more drastically than in the classical case: e.g., they can entirely inhibit the diffusive growth of mean square displacements, whereas classically their presence only slows down the growth. This means that a cantorus virtually prevents the quantum system from exploring regions of phase space that are eventually explored by its classical analog. These results were obtained for the model of a kicked quantum rotator, where a single confining KAM torus can be isolated. We expect, however, that they are also characteristic of the permeability of KAM tori and cantori and not of a particular model. Thus, they may also be relevant, e.g., in laser chemistry for multiphonon dissociation of molecules, where the regions of phase space relating to bound and dissociated states can be separated by KAM tori or cantori. Their permeability, as studied, here, then determines the dissociation rate. As a matter of fact, in a recent numerical study of multiphonon dissociation, Brown and Wyatt have observed that dissociation can indeed be inhibited considerably by the presence of cantori.

An appropriate model for the investigation of the above problems is the kicked planar rotator, defined by the Hamiltonian

$$\hat{H} = \hat{p}^2/2I + k \cos \hat{\theta} \sum_{n=-\infty}^{\infty} \delta(t-nT),$$

(1)

where $\hat{\theta}$ and $\hat{p}$ are angle and angular momentum operators, $I$ is the moment of inertia, and the kicking strength $k$ determines the degree of nonlinearity. Classically the equation of motion following from Eq. (1) is Chirikov's standard map (we assume $I = T = 1$)

$$p_{t+1} = p_t + k \sin \theta_{t+1},$$

$$\theta_{t+1} = \theta_t + p_t,$$

(2)

where $p_t$ and $\theta_t$ denote the coordinates immediately after the kick at time $t$. Its classical phase space (Fig. 1) according to the Poincaré-Birkhoff theorem and KAM theory typically exhibits elliptic and hyperbolic fixed points and KAM tori (here as circles). The KAM tori are invariant sets and thus cannot be penetrated by the chaotic orbits that develop near hyperbolic fixed points.

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With increasing nonlinearity $k$, the KAM tori break up into cantori\textsuperscript{11,12} (invariant Cantor sets) and become partially penetrable. There is a critical nonlinearity $k = k_c = 0.9716$ with universal scaling properties,\textsuperscript{16} where the last KAM tori divide the phase space into cells along the $p$ axis. This is the situation shown in Fig. 1. It follows that the asymptotic distribution

$$\rho(\theta,p) = \lim_{N \to \infty} \frac{1}{N} \sum_{i=0}^{N-1} \rho_i(\theta,p)$$

remains confined to a momentum interval $(p_c^-, p_c^+)$ = (2.015, 4.269), e.g., if an initial distribution $\rho_0(\theta,p) = (1/2\pi)\delta(p - p_0)$ with $p_0 = 3.2$ is chosen. Above $k_c$ these KAM tori are broken, giving rise to a diffusive motion along the $p$ axis\textsuperscript{15} similar to that in dissipative systems.\textsuperscript{17}

The quantum dynamics can be expressed in terms of the time evolution operator $\hat{U}$,

$$|\psi_{t+1}\rangle = \hat{U} |\psi_t\rangle,$$

where $|\psi_t\rangle$ denotes the quantum state immediately after the kick at time $t$, and for Eq. (1) $\hat{U}$ follows as

$$\hat{U} = \exp \left[ \frac{-i}{\hbar} k \cos \theta \right] \exp \left[ \frac{-i T}{\hbar} \hat{p}^2 \right].$$

With $\hat{p} = -i \hbar \partial / \partial \theta$ it is clear that quantum effects depend on the ratio $\hbar T / I$. In practice, the classical limit can be approached by variation of $I$ or $T$. Equivalently we may consider $\hbar T / I$ as an effective Planck’s constant that can be varied. Without loss of generality we will henceforth assume that $I = T = 1$ and vary $\hbar$ instead (i.e., measure $\hbar$ in units of $I / T$). Iteration of the time evolution operator yields

$$|\psi_I\rangle = \hat{U}^I |\psi_0\rangle.$$

As an initial state we use a momentum eigenstate $|\psi_0\rangle = |p_0\rangle$ with $\hat{p} |p_0\rangle = p_0 |p_0\rangle$ and $p_0 = 3.2$. This is the analog of the initial distribution $\rho_0(\theta,p)$ discussed in the classical case above. We define the asymptotic distribution of angular momenta as a time average

$$P(p | p_0) = \lim_{N \to \infty} \frac{1}{N} \sum_{i=0}^{N-1} |\langle p | \psi_i \rangle|^2,$$  

its existence and convergence were verified numerically by variation of $N$. With Eq. (7) $P$ can be written as

$$P(p | p_0) = \lim_{N \to \infty} \frac{1}{N} \sum_{i=0}^{N-1} |\langle p | \hat{U}^i | p_0 \rangle|^2.$$

The operator $\hat{U}$ can, in principle, be represented in the momentum basis and iterated. Analytically $|\langle p | \hat{U}^i | p' \rangle|^2$ can be expressed in terms of Bessel functions ($\rho = m \hbar$),

$$\langle m \hbar | \hat{U}^i | m' \hbar \rangle = \left( \frac{m - m' / \hbar}{\sqrt{\hbar}} \right) e^{-i m' \hbar / \sqrt{\hbar}} J_m(k / \hbar).$$

For numerical purposes, however, it is more convenient to iterate $\hat{U}$ by use of forward and backward fast Fourier transforms.\textsuperscript{5}

We have calculated the asymptotic momentum distribution $P(p | p_0)$ for various values of $k$ and $\hbar$.\textsuperscript{18} This quantity is the analog of the classical distribution $\beta(\theta,p)$ [Eq. (4)] projected onto the momentum axis. Figure 2(a) shows for $k = k_c$ that most of the time-averaged probability remains confined to the classically accessible interval $(p_c^-, p_c^+)$. This demonstrates the role of KAM tori as barriers in quantum systems. The logarithmic display in Fig. 2(b) shows in more detail how the probability leaks through the torus. It decays exponentially into the classically inaccessible region,

$$P(p | p_0) \propto e^{-k |p - p_c|},$$

FIG. 1. Classical phase space for $k = k_c = 0.9716$ showing 5000 iterates of 13 initial points $(\omega_0, p_0)$ according to Eqs. (2) and (3). Orbits starting between the two KAM tori remain confined to the momentum interval $(p_c^-, p_c^+)$.  

FIG. 2. Asymptotic momentum distribution Eq. (8) (a) on a linear and (b) on a logarithmic scale. Borders of classical confinement due to KAM tori (dot-dashed lines) and cantori (dashed lines) are indicated. The initial momentum $p_0$ was in the interval $(p_c^-, p_c^+)$.  

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where $p_e = p_c^{\pm}$. Moreover the figure shows that there is also an exponential decay near cantori, as indicated by the dashed lines. The same is observed for $k = 1.1 > k_c$ where the tori near $p_e^{\pm}$ have turned into cantori. We can understand the exponential decays in terms of Wigner functions corresponding to quasienergy states $|j\rangle$ (eigenfunctions of $\hat{U}$). $P(p | p_0)$ can be expressed as

$$P(p | p_0) = \sum_j |\langle p | j \rangle|^2 |\langle p_0 | j \rangle|^2,$$

(12)

where $|\langle p | j \rangle|^2$ is the projection of the Wigner function $W_j(\theta, p)$ belonging to $|j\rangle$. It is known that Wigner functions that are located on tori in the semiclassical limit decay exponentially. From this simple argument one would expect that $\lambda \sim h^{-1}$ for $h \to 0$. The same behavior would be found for penetration of a potential step due to tunneling. What we observe, however, is an algebraic dependence of $\lambda$ as $h^{-0.66}$ (Fig. 3); we attribute it to the complexity of phase space near the KAM torus. Penetration of a torus is obviously more complicated than tunneling through a potential barrier. The exponent $-0.66$ might be related to critical exponents at the stochastic transition, where in the semiclassical limit $h$ acts as a relevant variable. As the argument following Eq. (12) cannot be made rigorous, Ref. 19 might also suggest other forms of decay, e.g., $P(p | p_0) \sim \exp(-|p-p_e^{\pm}|^{1.2}/h)$ instead of Eq. (11). This possibility, however, can be ruled out from a detailed inspection of our results. We have observed exponential decays that followed Eq. (11) in some cases up to eight orders of magnitude of $P$.

The quantum permeability of a KAM torus can be characterized best by the asymptotic transition probability $\overline{W}$ into classically inaccessible regions, i.e., the total probability outside the dot-dashed lines in Fig. 2,

$$\overline{W} = \sum_{p < p_c^-} P(p | p_0) + \sum_{p > p_c^+} P(p | p_0).$$

(13)

Figure 4(a) shows that this transition probability decreases considerably when $k_e$ is approached from above, i.e., when a KAM torus builds up. The suppression of $\overline{W}$ between $k_e$ and 1.1 shows that cantori can act as barriers as well. At the critical nonlinearity $k_e$ [Fig. 4(b)] the permeability due to quantization exhibits a power-law dependence $h^{-3.5}$. If we choose $p_0$ in the much larger cells around integer resonances, we find that the exponent is changed. This appears to be due to partial localization before the wave function reaches the torus.

We quote some results on time-dependent quantities, which will be reported in more detail elsewhere. Where tori and cantori act as barriers, the transition probability increases algebraically in time before turning into quasiperiodic behavior. The same is true for the mean square displacement of momentum, but only for larger $k$ ($k > 1.2$). For smaller $k$ ($k_c < k < 1.2$, $10^{-4} < h < 10^{-1}$) it remains bounded within the cantori ($\langle \Delta p_t^2 \rangle < 10^{-1}$) and does not show any diffusive growth. This should be contrasted with the classical case, where it grows to infinity. The role of classical cantori as barriers in quantum systems thus is even more drastic than in classical mechanics. This property represents a striking difference in the performance of classical chaotic systems and their quantum analogs and can be used as a test in experiments on quantum chaos. Classically, probability can flow constantly across a cantorus such that after a sufficiently long time the system has essentially penetrated it. Most of the quantum mechanical probability, however, remains confined asymptotically (see also Fig. 4(a)) for $k_c < k < 1.1$. The classical and the quantum systems can be found in different states after a sufficiently long time. This phenomenon should be observable in experiments where a cantorus separates two qualitatively different states, as is the case for multiphonon dissociation of diatomic molecules. It might even
explain why diatomic molecules show little dissociation in comparison, e.g., to SiF₄, where cantori do not act as barriers because of a higher-dimensional phase space.

We acknowledge financial support by the Deutsche Forschungsgemeinschaft. One of us (T.G.) acknowledges receipt of a Heisenberg fellowship.

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18T. Geisel, G. Radons, and J. Rubner, to be published.

