Quantum Breaking Time near Classical Equilibrium Points

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In the evolution of distributions localized around classical equilibrium points, the quantum-classical correspondence breaks down at a time, the so-called quantum breaking, or Ehrenfest time, which is related to the minimal separation of the quantum levels in proximity of the classical equilibrium energy. By studying one-dimensional systems with single- and double-well polynomial potentials, we find that the Ehrenfest time diverges logarithmically with the inverse of the Planck constant whenever the equilibrium point is exponentially unstable. In all the other cases, we have a power law divergence with the exponent determined by the degree of the potential near the equilibrium point.

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The question of estimating how long classical and quantum evolutions stay close is one of the main problems of semiclassical analysis. The evolution of a quantum observable can follow that of the corresponding classical one up to a finite time, the so-called quantum breaking, or Ehrenfest time. As initially conjectured in [1–3] and rigorously proven in [4–6], whenever the classical flow is chaotic, the Ehrenfest time diverges logarithmically in $\hbar$. This result is easily understood. Starting from an initial value $\Delta(\hbar) \sim \hbar/I$, where I is a characteristic action of the system, the difference between a classical flow, with Lyapunov exponent $\lambda > 0$, and the corresponding quasiperiodic quantum flow increases as $\Delta(\hbar)\exp(\lambda t)$. The two flows depart at $t \sim \lambda^{-1}\log(I/\hbar)$. The situation is different for a regular classical flow. In this case, starting from the work [7], it was suggested in [8] that the Ehrenfest time grows algebraically as $\hbar^{-\delta}$. The determination of the value of δ and its possible universal nature is still an open problem. See [9] and references therein for recent results.

The study of the quantum-classical correspondence is particularly important in proximity of classical equilibrium points where classical trajectories spend most of the time. An example is given by the ubiquitous double-well system defined by the Hamiltonian $H(p,q) = p^2/2 - q^2/2 + q^4/4$. Associated to the unstable equilibrium point $(p_0, q_0) = (0,0)$ there is an isolated exponentially unstable periodic orbit with positive Lyapunov exponent $\lambda = 1$. For this system, different rigorous results are available which allow us to conclude that in proximity of this point the Ehrenfest time diverges logarithmically with the inverse of the Planck constant. In [4] it is shown that a coherent state, initially located around (p_0, q_0), spreads exponentially as $\exp(2\lambda t)$ for times not larger than $\lambda^{-1}\log(1/\hbar)$. From a complementary point of view, in [10–13] a semiclassical analysis of the stationary Schrödinger problem has pointed out the presence of an $\hbar$-logarithmically anomalous density of the levels around the energy of the equilibrium point.

The usual definition of the Ehrenfest time is based on the comparison of the evolution of classical observables with the quantum expectation value of the corresponding operators, either in the coherent state representation [4] or in the framework of Weyl quantization [5]. A coherent state represents a natural choice for the initial condition; however, the results obtained in this way can be generalized to arbitrary initial conditions [14]. For the purpose of studying the Ehrenfest time which characterizes the evolution of distributions localized around classical equilibrium points, we propose a simpler approach based on the analysis of the quantum spectrum. We know that on going towards a classical equilibrium point (p_0, q_0) the period of motion diverges, so that the classical evolution of a phase-space distribution function localized around this point must show a continuous frequency distribution around $\nu = 0$. In the quantum case, due to the discrete nature of the spectrum, the frequency distribution is characterized by a gap between zero and a minimal frequency. We call this minimal frequency the Ehrenfest frequency, ν_E. In fact, its inverse, ν_E^{-1}, is an upper bound to the time at which the quantum-classical correspondence of the evolution of any observable breaks down, independently of the choice of the initial state. We define the Ehrenfest time as ν_E^{-1}.

By using numerical and semiclassical methods, we study the behavior of ν_E around classical equilibrium points, both stable and unstable, for several autonomous one-dimensional systems. We find that ν_E^{-1} diverges logarithmically for $\hbar \to 0$ whenever the equilibrium point is exponentially unstable. In all the other cases, the Ehrenfest time follows a power law with an exponent related to the degree of the potential near the equilibrium point.

In the following, we consider systems described by the Hamiltonians,

$$H(p,q) = \frac{p^2}{2m} + A\,\frac{q^{2\alpha}}{2\alpha} + B\,\frac{q^{2\beta}}{2\beta}, \qquad (1)$$

with $A \le 0$, $B > 0$, and $\beta > \alpha \ge 1$. By properly rescaling position, momentum, and time, we can always reduce

to the case $B = 1$, $m = 1$ and either $A = 0$ or $A = -1$. For $A = 0$, we have single-well systems with a stable classical equilibrium point $(p_0, q_0) = (0, 0)$ at energy $\varepsilon = 0$. For $A = -1$, the systems are double-well oscillators and the classical equilibrium point $(p_0, q_0) = (0, 0)$ at energy $\varepsilon = 0$ is unstable. In the particular case $\alpha = 1$, the equilibrium point is also exponentially unstable. In both cases, $A = 0$ or $A = -1$, the periodic orbits near the equilibrium point at $\varepsilon = 0$ have a period which diverges for $\varepsilon \to 0$.

On the quantum mechanical side, we are interested in the evolution of a phase-space distribution $W(p, q; t)$ initially centered around the point (p_0, q_0) and with the property that $\lim_{\hbar \to 0} W(p, q; 0) = \delta(p - p_0)\delta(q - q_0)$. As an example, we can consider the Wigner function,

$$W(p, q; 0) = \frac{1}{\pi\hbar} \exp\left[-\frac{(p - p_0)^2 + (q - q_0)^2}{\hbar} \right], \tag{2}$$

associated to the initial wave function,

$$\langle q|\psi(0)\rangle = \frac{1}{(\pi\hbar)^{1/4}} \exp\left[-\frac{(q - q_0)^2}{2\hbar} + i\,\frac{p_0 q}{\hbar} \right]. \tag{3}$$

In the above expressions, $\hbar$ is the dimensionless rescaled Planck constant which vanishes when, for instance, the mass m of the system is taken larger and larger.

Instead of studying the evolution of a specific observable, consider the simpler survival probability,

$$\mathcal{P}(t) = |\langle\psi(0)|\psi(t)\rangle|^2, \tag{4}$$

which contains the same gross dynamical information. On the basis of the eigenstates of the Hamiltonian,

$$H|\phi_n\rangle = \varepsilon_n|\phi_n\rangle, \qquad n = 0, 1, 2, \ldots, \tag{5}$$

the survival probability $\mathcal{P}(t)$ can be written as

$$\mathcal{P}(t) = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} |c_n|^2 |c_m|^2 \exp(i\nu_{nm} t), \tag{6}$$

where $c_n = \langle\psi(0)|\phi_n\rangle$ and $\nu_{nm} = (\varepsilon_n - \varepsilon_m)/2\pi\hbar$. Note that, if $\psi(0)$ is chosen as in (3) with $(p_0, q_0) = (0, 0)$, $c_n = 0$ for n odd, due to the symmetry of the system and of the initial wave function. By using semiclassical and numerical techniques, we now show that the Fourier transform of the survival probability,

$$\tilde{\mathcal{P}}(\nu) = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} |c_n|^2 |c_m|^2 \delta(\nu - \nu_{nm}), \tag{7}$$

for sufficiently small values of $\hbar$ is characterized by a gap, large with respect to the typical level spacing, between $\nu = 0$ and the Ehrenfest frequency,

$$\nu_E = \min_{\substack{n>m \\ |c_n|^2|c_m|^2 \neq 0}} \nu_{nm}. \tag{8}$$

The inverse of this frequency gives the largest period in the evolution of a quantum observable. Since the evolution of the corresponding classical observable in the proximity of an equilibrium point displays arbitrary large periods, ν_E^{-1} represents an upper bound to the time at which the quantum-classical correspondence breaks down. The estimate of the Ehrenfest time as ν_E^{-1} is independent of the choice of the initial wave function and of the monitored observable.

In the simple case $A = 0$, by using standard WKB approximations, we have

$$\varepsilon_n = \left[\left(n + \frac{1}{2} \right) \hbar\, \delta(\beta) \right]^{2\beta/(\beta+1)}, \tag{9}$$

with

$$\delta(\beta) = \frac{\sqrt{\pi/2}\,\Gamma(\frac{3}{2} + \frac{1}{2\beta})}{\Gamma(1 + \frac{1}{2\beta})\,(2\beta)^{1/2\beta}}. \tag{10}$$

For the coherent state (3) with $(p_0, q_0) = (0, 0)$, we get

$$|c_n|^2 = \frac{2\sqrt{\pi}(2\beta)^{-1/2\beta} \hbar^{1/2} \varepsilon_n^{-1/2\beta} e^{-2\varepsilon_n/\hbar}}{\frac{\Gamma(\frac{1}{2}+\frac{1}{2\beta})}{\Gamma(\frac{1}{2})\Gamma(1+\frac{1}{2\beta})} + \frac{\sin[\sigma(\varepsilon_n, \hbar; \beta)]}{\sigma(\varepsilon_n, \hbar; \beta)}}, \tag{11}$$

with $\sigma(\varepsilon, \hbar; \beta) = 2\sqrt{2}(2\beta)^{1/2\beta} \hbar^{-1} \varepsilon^{(\beta+1)/2\beta}$. The behavior of $\tilde{\mathcal{P}}(\nu)$ obtained by using these expressions for ε_n and $|c_n|^2$ is shown in Fig. 1 in the case $\beta = 2$. We see that for $\hbar \to 0$ the frequency distribution $\tilde{\mathcal{P}}(\nu)$ approaches a continuous limit given by

$$\tilde{\mathcal{P}}_0(\nu) = \lim_{\hbar \to 0} \int d\varepsilon\, d\eta\, p(\varepsilon) p(\eta)\, \delta\left(\nu - \frac{\varepsilon - \eta}{2\pi\hbar} \right), \tag{12}$$

where $p(\varepsilon) = |c_{n(\varepsilon)}|^2 dn(\varepsilon)/d\varepsilon$ and $n(\varepsilon)$ is obtained by inverting $\varepsilon = \varepsilon_n$. By using (9) and (11), we find

$$\tilde{\mathcal{P}}_0(\nu) = 4K_0(4\pi|\nu|), \tag{13}$$

where K_0 is the Bessel function of zeroth order. Figure 1 also shows the presence of the gap at $\nu = 0$ and its shrinking as $\hbar \to 0$. Since the level spacing $\varepsilon_{n+1} - \varepsilon_n$ increases by increasing n, the Ehrenfest frequency (8) turns out to be $\nu_E = (\varepsilon_2 - \varepsilon_0)/2\pi\hbar$. According to (9), its inverse diverges as

$$\nu_E^{-1} \sim \hbar^{(1-\beta)/(1+\beta)}. \tag{14}$$

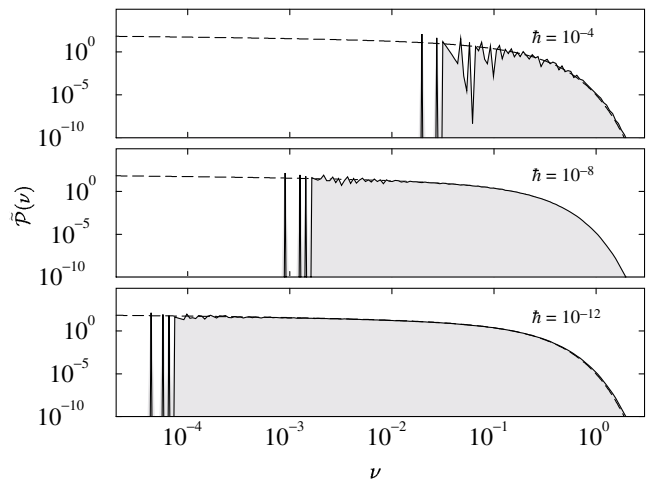

FIG. 1. Histogram of the Fourier transform of the survival probability $\tilde{\mathcal{P}}(\nu)$ for different values of $\hbar$ in the single-well case $\beta = 2$. The dashed line is the $\hbar \to 0$ limit distribution given by Eq. (13). Histogram bins are chosen according to the law $\log\nu_i = -5 + i7/240$, $i = 1, \ldots, 240$.

We now consider double-well systems obtained in the case $A = -1$. For these systems, the standard first-order WKB approximation fails near the unstable equilibrium point at energy $\varepsilon = 0$, and one has to resort to a more accurate semiclassical analysis [10–13,15]. Only in the case of a quadratic barrier embedded in a quartic well, i.e., for $\alpha = 1$, $\beta = 2$, the quantization condition for the energy levels has been written explicitly and, up to terms of order $\hbar$, reads [16]

$$\frac{1}{\sqrt{1 + \exp(2\pi\varepsilon/\hbar)}} = \cos[\phi(\varepsilon, \hbar)], \qquad (15)$$

where

$$\phi(\varepsilon, \hbar) = \frac{4}{3\hbar} - \frac{\varepsilon}{\hbar}\log\frac{\hbar}{16} - \arg\Gamma\left(\frac{1}{2} + i\,\frac{\varepsilon}{\hbar}\right) - \pi\,. \qquad (16)$$

We determine the eigenvalues and the eigenfunctions of a generic double-well system by solving numerically the stationary Schrödinger equation. Our results are exact, in the sense that for all the evaluated quantities the estimated relative errors are not greater than 10^{-4} independently of the $\hbar$ value used.

The evaluation of the spectrum of a double-well system at energy close to the barrier top represents, for $\hbar$ small, an unsurmountable task with standard numerical techniques. In fact, the relevant eigenstates have a quantum number n which diverges quickly for $\hbar \to 0$. We bypass the problem by using the algorithm [17] which allows one to evaluate selected eigenstates having a very large number of nodes. As an example, in Fig. 2 we show the couple of even eigenfunctions with energy closest to $\varepsilon = 0$ evaluated for $\hbar = 10^{-2}$ in the double-well case $\alpha = 1$, $\beta = 2$. Note that, already for this still relatively large value of $\hbar$, the corresponding quantum number is $n \sim 40$. In our numerical calculations we go beyond $n \sim 10^4$.

In Fig. 3 we show the superposition coefficients relative to different double-well systems evaluated for the coherent state (3) and $\hbar = 10^{-3}$. We see that $|c_n|^2$ decreases exponentially departing from $\varepsilon = 0$. For smaller values of $\hbar$, the superposition coefficients $|c_n|^2$ follow approximately the same exponential behavior as a function of $|\varepsilon_n|/\hbar$ and become denser and denser.

In Fig. 4 we show the Fourier transform of the survival probability (7) obtained in the case $\alpha = 1$, $\beta = 2$ by using the eigenvalues and the superposition coefficients determined numerically as described above. As in the single-well case, at $\nu = 0$ we have a gap whose width shrinks for $\hbar \to 0$. The width of this gap, namely, the Ehrenfest frequency, is yielded by a couple of eigenvalues, close to the energy $\varepsilon = 0$ of the classical equilibrium point. This can be understood roughly in the following way. Consider the number of states, $\mathcal{N}_\varepsilon$, in the energy range $[\varepsilon - \hbar, \varepsilon + \hbar]$. The frequencies associated to the eigenvalues in this energy range are $\nu \sim \mathcal{N}_\varepsilon^{-1}$, so that,

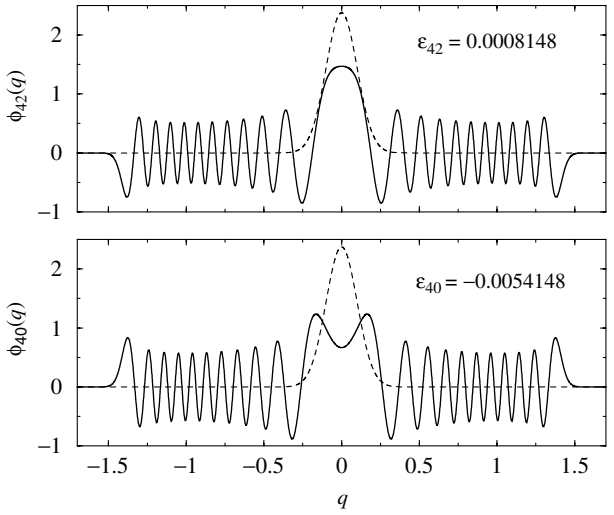

FIG. 2. Eigenfunctions ϕ_{40} and ϕ_{42} corresponding to the minimal frequency ν_E in the double-well case $\alpha = 1$, $\beta = 2$ for $\hbar = 10^{-2}$. The dashed curve is the initial wave function (3) with $(p_0, q_0) = (0, 0)$.

in the limit $\hbar \to 0$, ν vanishes if $\mathcal{N}_\varepsilon$ diverges. According to the Weyl formula, $\mathcal{N}_\varepsilon$ is proportional to the classical phase-space volume bounded by the energy shells $H(p, q) = \varepsilon \pm \hbar$. This volume can be evaluated exactly in terms of simple functions in the single-well case and in terms of special functions for double-well systems. In all cases, we have that $\mathcal{N}_\varepsilon$ diverges when $\hbar \to 0$ only for $\varepsilon = 0$. If the initial state is even as in the case of the coherent state (3) with $(p_0, q_0) = (0, 0)$, the couple of closest eigenvalues determining ν_E is even. For a double well with $\alpha = 1$, $\beta = 2$, these eigenvalues have energies of opposite sign, as shown in Fig. 2, while for $\alpha > 1$ they are both positive if $\hbar$ is sufficiently small.

The scaling of ν_E^{-1} with $\hbar$ is shown in Fig. 5 for different double-well systems. The plotted points are calculated using the numerically determined spectrum while the solid line represents the inverse of the Ehrenfest frequency

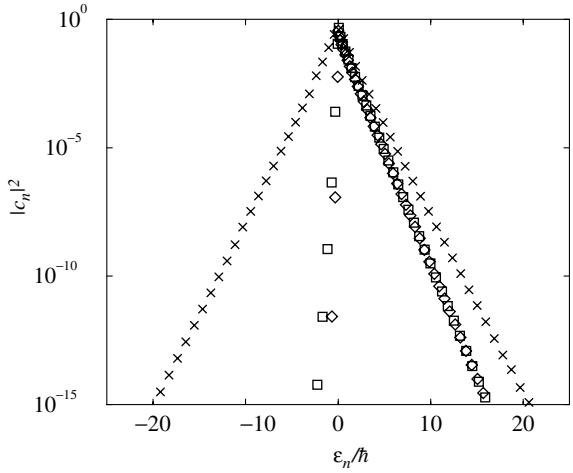

FIG. 3. Superposition coefficients $|c_n|^2$ as a function of $\varepsilon_n/\hbar$ for $\hbar = 10^{-3}$ in the double-well cases $\alpha = 1$, $\beta = 2$ ($\times$), $\alpha = 2$, $\beta = 4$ ($\square$), and $\alpha = 3$, $\beta = 6$ ($\diamond$).

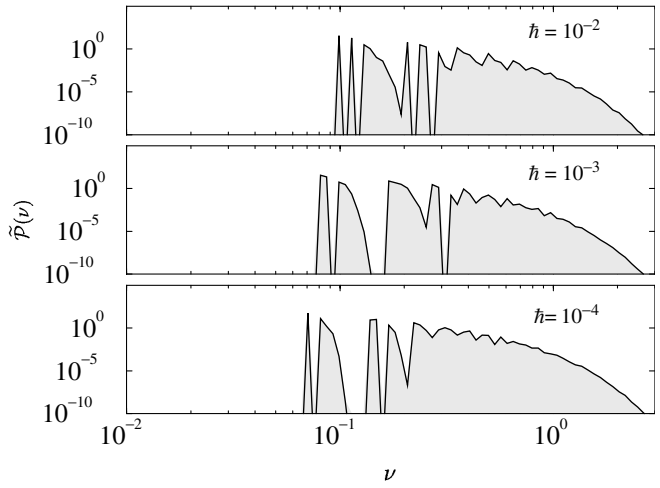

FIG. 4. As in Fig. 1 in the double-well case $\alpha = 1$, $\beta = 2$.

evaluated by using the semiclassical quantization (15) and (16). The Ehrenfest time increases logarithmically with $\hbar^{-1}$ only in the case $\alpha = 1$, $\beta = 2$, i.e., when the equilibrium point is exponentially unstable. In all the other cases $\alpha > 1$, a numerical fit suggests that

$$\nu_E^{-1} \sim \hbar^{(1-\alpha)/(1+\alpha)}. \tag{17}$$

This is the same scaling law which we would obtain, as described by Eq. (14), in the case of a single-well potential $V(q) = q^{2\alpha}/2\alpha$. This can be understood with the following rough semiclassical arguments which we have checked numerically. For $\hbar \to 0$, the spacings of the eigenvalues of the double well above $\varepsilon = 0$ correspond to the spacings between the maxima of the transmission coefficient of the barrier $-q^{2\alpha}/2\alpha$. These resonances of the continuous spectrum are linked, in turn, to the energies of the bound states of the corresponding inverted potential $q^{2\alpha}/2\alpha$.

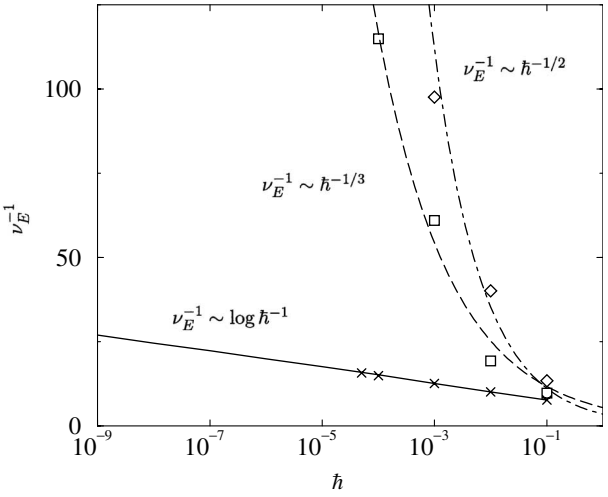

FIG. 5. Inverse of the Ehrenfest frequency, ν_E^{-1}, as a function of $\hbar$ in the double-well cases $\alpha = 1$, $\beta = 2$ ($\times$), $\alpha = 2$, $\beta = 4$ ($\square$), and $\alpha = 3$, $\beta = 6$ ($\diamond$). The solid line is the regularized WKB prediction based on (15) and (16), while the dashed line and the dot-dashed line are numerical fits.

In conclusion, the quantum breaking time near a classical equilibrium point scales logarithmically or with a power law in $\hbar^{-1}$ according to the exponential instability of the associated orbit. This feature may be relevant in all mesoscopic systems which are modeled by one-dimensional multiwell Hamiltonians [18,19]. In these systems, the Ehrenfest time behavior is related to experimentally detectable properties as the classical to quantum crossover of the shot noise [20].

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