Statistics of Chaotic Tunneling

Stephen C. Creagh
Division of Theoretical Mechanics, School of Mathematical Sciences, University of Nottingham, Nottingham NG7 2RD, United Kingdom

Niall D. Whelan
Department of Physics and Astronomy, McMaster University, Hamilton, Ontario, Canada L8S 4M1
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The distribution of tunneling rates in the presence of classical chaos is derived. We use classical information about tunneling trajectories plus random matrix theory arguments about wave function overlaps. The distribution depends on the stability of a specific tunneling orbit and is not universal, though it does reduce to the universal Porter-Thomas form when the orbit is very unstable. For some situations there may be systematic deviations due to scarring of real periodic orbits. The theory is tested in a model problem and possible experimental realizations are discussed.

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Tunneling is crucial in describing many physical phenomena, from chemical and nuclear reactions to conductances in mesoscopic devices and ionization rates in atomic systems. When such systems are complex, it is natural to model tunneling effects using random matrix theory (RMT) [1]. We show here that when the underlying system is one of clean chaotic dynamics, successful statistical modeling requires explicit incorporation of nonuniversal, but simple, dynamical information. We derive a distribution for the tunneling rate which depends on a single parameter, calculated from the stability properties of the dominant tunneling orbit.

The signatures of chaos in tunneling have recently received much attention [2–8], two important regimes having been considered. The first is that the quantum state is initially localized in a region where the dynamics is largely nonchaotic and one wants to understand the tunneling rate through chaotic regions of phase space [2–6]. The second, and the one we focus on, is that virtually all of the energetically accessible phase space is chaotic [7,8] so that the quantum state is initially localized in a chaotic region of phase space. These two situations are different in many important ways. In particular, the statistical distribution of the tunneling rates in the first regime has power law decays [3] whereas we show that the distribution in the second regime has exponential decay. The result is a generalization of the Porter-Thomas distribution [9] used to model neutron and proton resonances [9–11] and conductance peak heights in quantum dots [12,13].

It is shown in Ref. [7] that the average tunneling rate is determined by a complex orbit we call the instanton. To characterize fluctuations about this average we define a rescaled tunneling rate as follows. In the case of metastable wells the absolute tunneling rate of a given state labeled by n is measured by the resonance width, or inverse lifetime Γ_n. The corresponding normalized tunneling rate is defined to be

$$y_n = \Gamma_n/\overline{\Gamma}, \qquad (1)$$

where $\overline{\Gamma}(E,\hbar) = \langle \Gamma_n \rangle$ is a local average computed for a given set of physical parameters. $\overline{\Gamma}(E,\hbar)$ is a smooth, monotonic function of its arguments and is given by an explicit formula in terms of the (purely imaginary) action and stability of the instanton [7]. A similar definition holds for splittings in double wells and in either case $\langle y_n \rangle = 1$ by construction.

Fluctuations in y_n are calculated using a *tunneling operator* $\mathcal{T}$ which is constructed from the semiclassical Green's function and can be interpreted as transporting the wave function across the barrier. Specifically,

$$y_n \propto \langle n|\mathcal{T}|n\rangle, \qquad (2)$$

where $|n\rangle$ is the wave function represented in a Hilbert space which quantizes a surface of section. This matrix element is interpreted physically as measuring the size of the wave function in a small region (in which the kernel of $\mathcal{T}$ is not small) surrounding a unique real orbit. This orbit connects to the instanton and is referred to as its real extension. Details can be found in [8], but in this Letter it will be enough to know the spectrum of $\mathcal{T}$. For a two-dimensional system this is approximately $\{\lambda^k|\lambda|^{1/2}, k = 0, 1, \ldots\}$, where λ is the inverse of the stability of the instanton orbit, which is always less than unity in magnitude and can easily be found using real dynamics in the inverted potential. (The discussion is readily generalized to a higher dimension but we refrain from doing so for clarity.) To derive distributions for y_n we make statistical assumptions about the state $|n\rangle$, but not about the operator $\mathcal{T}$.

We express $\mathcal{T}$ in its own eigenbasis $\sum_k \lambda^k|\lambda|^{1/2}|k\rangle\langle k|$ and find

$$y_n = a\sum_{k=0}^{\infty} \lambda^k |\langle k \mid n\rangle^2 = a\sum_{k=0}^{\infty} \lambda^k |x_k|^2, \qquad (3)$$

where we denote $x_k = \langle k \mid n\rangle$ and the prefactor $a = 1 - \lambda$ ensures that $\langle y \rangle = 1$. The states $|n\rangle$ are normalized so

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that on average $|x_k|^2$ is unity. We now assume that the x_k's can be treated as Gaussian random variables, as is appropriate for classically chaotic dynamics.

We simplify the derivation by assuming Gaussian orthogonal ensemble (GOE) statistics, i.e., that the x_k are statistically independent and given by the joint distribution $P(\mathbf{x})d\mathbf{x} = \prod_k [\exp(-x_k^2/2)/\sqrt{2\pi}]\, dx_k$ where $\mathbf{x} = \{x_k\}$, so that

$$P(y;\lambda) = \int d\mathbf{x}\, P(\mathbf{x})\ \delta\Big(y - a \sum_{k=0}^{\infty} \lambda^k x_k^2\Big). \tag{4}$$

We use $\delta(z) = \int dt \exp(itz)/2\pi$ and observe that each x_k involves a simple Gaussian integral. The final result [and generalizing to the Gaussian unitary ensemble (GUE) case] is

$$P(y;\lambda) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dt\, e^{ity} \prod_{k=0}^{\infty} \Big(1 + \frac{2i}{\beta} a \lambda^k t\Big)^{-\beta/2}, \tag{5}$$

where $\beta = 1$ and 2 for GOE and GUE, respectively. The product converges rapidly if λ is not too close to unity so (5) can easily be used to calculate $P(y;\lambda)$ in practice. We remark that in Ref. [14] the authors derive a distribution which can be understood to be a special case of (5) in the case that the resonance energy is close (in a classical sense) to that of the potential saddle through which the tunneling is taking place. They applied their results to the data of [15] on the D_2CO molecule.

An extensive formalism exists for the application of random matrix theory to scattering from chaotic systems (see [16] for a review and [17] for developments relevant to scattering resonances, and references therein). Tunneling problems necessarily involve weak coupling to the continuum, and it is then better to compare our results to those of [18]. If we interpret each state $|k\rangle$ of $\mathcal{T}$ as labeling a distinct and statistically independent channel, then Eq. (5) corresponds to a situation with an infinite number of distinctly weighted channels [19]; the average partial width of each is proportional to λ^k. This exponential decrease of the coupling to the higher channels means that effectively only a finite number of channels are active. It is the power of the present method to ascribe the weight of each channel uniquely in terms of classical dynamics (specifically the instanton stability) so that there are no free parameters.

Recall that $\langle y \rangle = 1$; the second moment is

$$\langle y^2 \rangle = 1 + \frac{2}{\beta} \frac{1-\lambda}{1+\lambda}. \tag{6}$$

The channel interpretation helps in understanding this distribution as we vary λ. For small λ, only the $k = 0$ channel is significant and the distribution is of the Porter-Thomas form: $\exp(-y/2)/\sqrt{2\pi y}$ and $\exp(-y)$ for $\beta = 1$ and 2, respectively. This can be understood from (5) by a branch-point/residue analysis around the singularity at $t = i\beta/2a$. This distribution is commonly used to model point tunneling contacts [12,18]. It is often very accurate but its validity is not universal, as we discuss. For λ close to unity, many channels contribute significantly, the fluctuations around the mean are reduced, and the distribution approaches a Gaussian with variance $\sigma^2 \approx a/\beta$ (approaching a delta function for small a).

For $\lambda > 0$ and $y \le 0$ we close the contour of (5) in the lower half plane; since the integrand has no singularities there, the result is simply zero. This is consistent with the fact that $\mathcal{T}$ is a positive definite operator so that Eq. (3) does not admit negative y. Similarly, any derivative of $p(y)$ is also zero for $y \le 0$, implying that $p(y)$ goes to zero faster than any power of y for y small and positive. In the limit $y \gg \lambda$ we expand around the first singularity to obtain

$$\begin{aligned} P(y;\lambda)_{\rm GOE} &\approx \frac{\exp(-y/2a)}{\sqrt{2\pi a y}}, \\ P(y;\lambda)_{\rm GUE} &\approx \frac{\exp(-y/a)}{a}. \end{aligned} \tag{7}$$

This falls off exponentially with y and not with a power law as observed in the chaos-assisted regime [3].

In metastable wells or in double wells whose symmetry is reflection through an axis, λ is always positive. In double wells whose symmetry is inversion through a point, however, λ is negative and $\mathcal{T}$ is nondefinite [8]. In that case negative splittings (for which the odd member of a doublet has a lower energy than the even member) can arise. Equations (3), (5), and (6) remain valid in this case and produce a distribution which allows negative as well as positive values of y. It decays exponentially for $|y| \gg \lambda$ as in Eq. (7) but with different exponents for $y > 0$ and $y < 0$. Note in particular that the distribution allows for zero splittings (which we might induce for a particular doublet by tuning a system parameter). This means that we can construct states which remain localized in either well for all time, as in the one-dimensional time-dependent system considered in [20].

Since it is a simpler numerical task to calculate many splittings in a double well than to calculate many resonance widths in a metastable well, we use the former to test our predictions and note that any conclusions apply identically to the latter. Consider the potential

$$V(x,y) = (x^2 - 1)^4 + x^2 y^2 + \mu y^2 + \nu y + \sigma x^2 y. \tag{8}$$

There is a reflection symmetry in x and if the energy is less than $1 - \nu^2/4\mu$ the motion is classically confined either to $x < 0$ or to $x > 0$. It is convenient to work at fixed energy in order to keep λ constant and we do this by quantizing $q = 1/\hbar$ [8], that is, by finding those values of $\hbar$ which are consistent with a specified choice of parameters and energy. This is effectively what happens, for example, in scaling problems such as a hydrogen atom in a magnetic and an electric field [21]. In the physically more common case of energy spectra, the shape of the distribution would change with energy (since λ does) and we should either superimpose distributions or restrict the ensemble to a classically small energy window.

In Fig. 1 we show histograms constructed from the q spectra for two choices of parameters such that the classical dynamics is almost fully chaotic. We also show the distribution (5) with $\beta = 1$ and using the corresponding values of λ. Clearly, the numerically computed histograms are well captured by the theoretical distribution. We show, for comparison, the Porter-Thomas distribution which clearly fails to model the numerical data correctly. We remark that this sort of agreement was observed for most parameter values as long as the dynamics was fully chaotic.

In Fig. 2 we show an exception to the general agreement, for which the histogram is intermediate between the distribution (5) and the Porter-Thomas form. We attribute this to the effects of scarring [22,23], as follows. The instanton has real turning points where the momentum vanishes and the position is real. At these points we can integrate in imaginary time, in which case the instanton retraces itself, or in real time, in which case we get a real trajectory. We refer to this real trajectory as the real extension of the instanton.

There is no reason why the real extension should itself be periodic. Typically it is not. However, the parameters of Fig. 2 have been tuned so that the real extension is in fact periodic. We find in this case that the overlaps $x_k = \langle k | n \rangle$ are no longer distributed according to the Gaussian $P(x_k) = \exp(-x_k^2/2)/\sqrt{2\pi}$ as assumed in our derivation—there are relatively more large overlaps and more small overlaps. This effect can be explained using a recent theory of scarring [23] which describes how the overlaps between a wave packet placed on a periodic orbit and the chaotic eigenstates deviate from random matrix theory. In our problem the eigenvectors $|k\rangle$ behave like wave packets of this type when the real extension is periodic. The effect of this deviation from random matrix theory is to give more large splittings and more small splittings than (5) predicts and, therefore, to push the distribution in the direction of the Porter-Thomas form. We remark that for $\nu = \sigma = 0$, the real extension is always a periodic orbit [7] and we see anomalous statistics for that situation as well.

In the final case we discuss, the term $\nu y + \sigma x^2 y$ in (8) is replaced by τxy. Now the potential is symmetric under $(x, y) \to (-x, -y)$ rather than under $(x, y) \to (-x, y)$. In this case $\lambda < 0$ [8] and negative splittings can occur. Results are shown in Fig. 3. Again, the theoretical distribution agrees with the histogram.

Our results are relevant to situations in which particles tunnel out of or between chaotic regions separated by an energetic barrier. Applications include hydrogen atoms in parallel electric and magnetic fields where the competition between the imposed fields and the Coulomb force causes chaotic motion while the presence of the electric field causes tunneling [21]. Dissociative decays of excited nuclei and molecules may also fall into this regime and a possible application is to the D_2CO molecule [15] whose dissociation widths have a distribution which is very different from the χ^2 distribution which one would have from a theory with a finite number of equivalently weighted channels.

Another application is to conductances of quantum dots. In the Coulomb blockade regime electrons must tunnel into and out of dots which are thought to be chaotic. Such experiments have been done [13] leading to results which are consistent with the Porter-Thomas distribution for the tunneling widths. We contend that the reason is that the instanton path in all cases is very unstable, leading to a small value of λ. For energies near the saddle

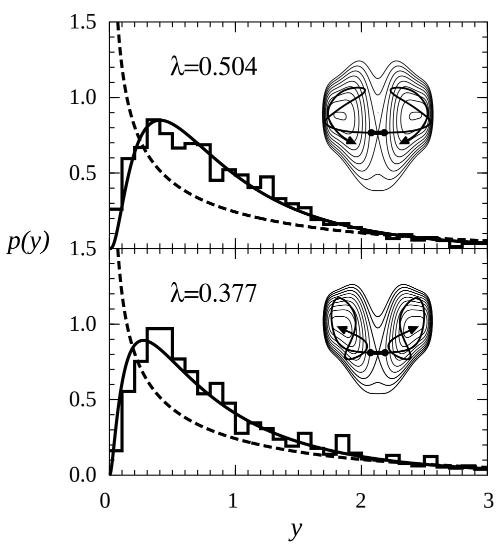

FIG. 1. Results for two typical potentials, with $(\mu, \nu, \sigma) = (0.15, 0.17, 0.00)$ above and $(0.25, 0.50, 0.00)$ below. In both cases the energy is lower than saddle maximum by an amount 0.1. The continuous curves are the theoretical distributions calculated using the appropriate values of λ (shown). The dashed curves show the Porter-Thomas distribution for comparison. The insets show the corresponding instanton orbits and their real extensions.

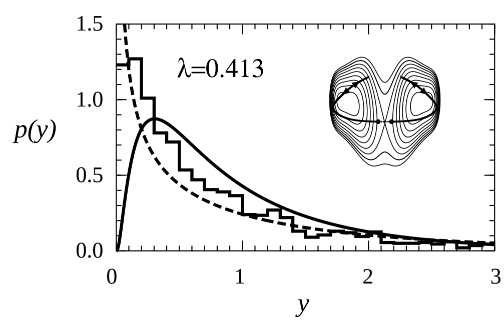

FIG. 2. As in Fig. 1 but for parameter values $(\mu, \nu, \sigma) = (0.25, 0.40, 0.254)$ for which the real extension of the instanton orbit is periodic and the resulting distribution is significantly different from the RMT prediction.

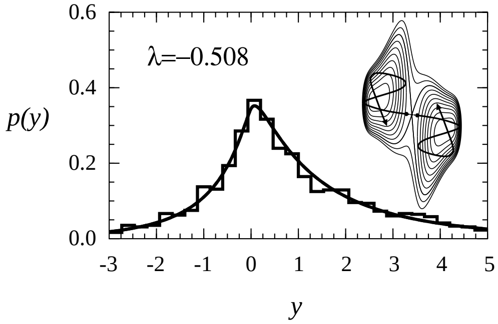

FIG. 3. Results for the inversion-symmetric potential with $(\mu, \tau) = (0.1, 1.0)$ which possesses nonpositive splittings.

$\lambda \approx \exp(-2\pi\omega_y/\omega_x)$ [24], where ω_x and ω_y are the curvatures of the potential saddle along and transverse to the instanton, respectively. This is often small, but by making the saddle flat in the transverse direction or sharp in the instanton direction, it is possible to have λ be of order unity. It is an interesting issue whether this can be arranged for the quantum dots. One feature which helps in this regard is that we predict a distribution which vanishes for small y, whereas the Porter-Thomas distribution diverges as $1/\sqrt{y}$. This difference could be discernible even for rather small values of λ.

Another possibility for nonuniversal statistics would be a situation analogous to Fig. 2, where the tunneling route is directly connected to a real periodic orbit. This geometry could be engineered into quantum dots and is present in the hydrogen atom problem [21]. In this case we predict deviation from random matrix theory results. This would be similar in spirit to the work of Narimanov *et al.* [25] who look for dynamical effects in conductance peaks of quantum dots.

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