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Delay times in chaotic quantum systems

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Abstract. Based on recent results of the joint moments of proper delay times of open chaotic systems with ideal coupling, a new insight to obtain the partial delay times distribution, for an arbitrary number of channels and symmetry, is given. This distribution is completely verified for all symmetry classes by means of random matrix theory simulations of ballistic chaotic cavities. In addition, the normalization constant of the Laguerre ensemble is obtained.

1 Introduction

The delay experienced by a quantum particle due to interactions with a scattering region has been the subject of intense investigation for more than thirty years in several areas of physics that include nuclear and condensed matter physics [1–7]. The interest in this subject has resurged due to the recent appearance of theoretical investigations in chaotic systems [8–14] and atomic physics [15–18]; the later motivated by experiments of interaction of light with matter during a mean time with attosecond precision [19].

The delay time first introduced by Wigner for the one channel case [1] and its multichannel generalization by Smith [2], in the so-called Wigner-Smith time delay matrix, is written in terms of the scattering matrix S and its derivative with respect to the energy ε. In units of the Heisenberg time τ_{H}, it is given by

$$Q_{\mathrm{W}} = -\mathrm{i}\frac{\hbar}{\tau_{\mathrm{H}}} S^{-1} \frac{\partial S}{\partial \varepsilon}. \tag{1}$$

The eigenvalues of Q_{W} represent the delay time on each channel and the Wigner time delay is the average of these proper delay times. In the context of mesoscopic systems the electrochemical capacitance of a mesoscopic capacitor is described by the Wigner time delay [20–22]. Some other transport observables that depend on the proper delay times are the thermopower [23], the derivative of the conductance with respect to the Fermi energy [24], the DC pumped current at zero bias [25], among

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others (see for instance Ref. [26] and references therein). For ballistic systems with chaotic classical dynamics, these physical observables fluctuate with respect to small variations of external parameters, like an applied magnetic field, the Fermi energy or the system shape [26–28]. The proper delay times are of interest in the characterization of those fluctuations, which only depend on the symmetry present in the problem. The distribution of the proper delay times is given in terms of the joint distribution of their reciprocals, known as the Laguerre ensemble [26,28]. An interesting feature of this ensemble is the presence of repulsion between the proper times, as occurs in the spectral statistics.

Alternatively, the partial delay times defined as the energy derivative of the phase shifts are also useful in the characterization of chaotic scattering [27]. Although the partial times are correlated, this correlation is of different nature than that of between the proper delay times; they do not show the level repulsion [29]. In the one channel situation the proper and partial delay times are identical to the Wigner time delay whose distribution is known for all symmetry classes [27,30,31]: $\beta = 1$ (4) in the presence of time reversal and presence (absence) of spin-rotation symmetry and $\beta = 2$ in the absence of time reversal symmetry. For the general case of arbitrary number of channels the distribution of the partial times is known for any β, except by a normalization constant [29]. With a suitable normalization this result encompasses a previous one for $\beta = 2$ [27,32]. Numerical simulations for $\beta = 1$ and 2 have been given in reference [33], but only the $\beta = 2$ case was successfully compared with the appropriate theoretical result. The $\beta = 4$ symmetry is seldom discussed.

In the present paper, an alternative approach to verify the general expression for the properly normalized probability distribution of the partial delay times is obtained. This was done by extracting the essence that comes from the level repulsion in the joint distribution of proper delay times that transcends to the kth moment of a proper delay time [34]. This procedure leads to the distribution of partial times in the equivalent channels situation, that we test by means of random matrix theory simulations, for all symmetry classes and several number of channels. In addition, this method also allows us to obtain the normalization constant of the Laguerre distribution.

In the next section we establish the theoretical framework of the proper and partial delay times; we review the known results for the kth moment of the proper delay times, from which we obtain the general expression of the probability distribution of the partial times, for all symmetry classes and any number of channels. Also, it is in this section where we present our findings of the normalization constant of the Laguerre distribution. In Section 3 we compare this general distribution with the numerical predictions from random matrix theory. We conclude in Section 4.

2 Distributions of proper and partial delay times

2.1 Scattering approach

Single-electron scattering by a ballistic cavity attached ideally to two leads which support N_1 and N_2 propagating modes (channels), respectively, can be described by an $N \times N$ scattering matrix S, where $N = N_1 + N_2$. When the dynamics of the cavity is classically chaotic, the scattering matrix belongs to one of the three circular ensembles from random matrix theory (RMT) [35,36]. The Circular Unitary Ensemble (CUE) is obtained when flux conservation is the only restriction in the problem, such that $S^\dagger S = 1_N$, where 1_N denotes the unit matrix of dimension N. In the Dyson scheme this case is labeled by $\beta = 2$. Additionally, in the presence of time reversal invariance (TRI) and integral spin or TRI, half-integral spin, and rotation symmetry,

S is a symmetric matrix, $S = S^T$ (the upper script T means transpose). This case is denoted by $\beta = 1$ and the corresponding ensemble is the Circular Orthogonal Ensemble (COE). In the presence of TRI, half-integral spin, and no rotation symmetry, S is self-dual and the ensemble is the Circular Symplectic Ensemble (CSE), labeled by $\beta = 4$.

In the diagonal form, the S matrix can be written as

$$S = UEU^{\dagger}, \tag{2}$$

where U is an $N \times N$ unitary matrix, the matrix of eigenvectors, and E is the diagonal matrix of eigenphases,

$$E_{ij} = \mathrm{e}^{\mathrm{i}\theta_i}\, \delta_{ij}, \tag{3}$$

with δ_{ij} the Kronecker delta.

2.2 Proper delay times

A symmetrized form of the Wigner-Smith time delay matrix can be written in dimensionless units as [26,28]

$$Q = -\mathrm{i}\frac{\hbar}{\tau_{\mathrm{H}}}\, S^{-1/2}\frac{\partial S}{\partial \varepsilon} S^{-1/2}, \tag{4}$$

where ε is the energy and τ_{H} is the Heisenberg time ($\tau_{\mathrm{H}} = 2\pi\hbar/\Delta$, with Δ the mean level spacing). The matrix Q is Hermitian for $\beta = 2$, real symmetric for $\beta = 1$, and quaternion self-dual for $\beta = 4$. Its eigenvalues, q_i's ($i = 1, \ldots, N$), are the proper delay times measured in units of τ_{H}. The distribution of the q_i's is given by the Laguerre ensemble in terms of their reciprocals $x_i = 1/q_i$ [28], namely

$$p_\beta(\{x_i\}) = C_N^{(\beta)} \prod_{a<b}^{N} |x_b - x_a|^\beta \prod_{c=1}^{N} x_c^{\beta N/2}\, \mathrm{e}^{-\beta x_c/2}, \tag{5}$$

where $C_N^{(\beta)}$ is a normalization constant. It is worth mentioning that the repulsion between the proper delay times is inherited from the level repulsion of the Hamiltonian eigenvalues. The normalization constant for the energy level distribution is well known [37], but the constant $C_N^{(\beta)}$ in equation (5) has not been given yet, although the Laguerre distribution has been widely used.

Here, we follow an inductive method to obtain a general expression for $C_N^{(\beta)}$. A summary of the results for this normalization constant previously reported in reference [34], as well as new others, is shown in Table 1. We notice that the results for $\beta = 2$ suggest a general dependence on N, namely

$$C_N^{(2)} = \frac{1}{N!} \prod_{n=0}^{2N-1} \frac{1}{n!}\,, \tag{6}$$

that gives an indication for the other two symmetry classes. For example, for $\beta = 4$ the normalization constant can be written as

$$C_N^{(4)} = \frac{2^{(2N)^2}}{(2N)!} \prod_{n=0}^{2N-1} \frac{1}{(2n)!}\,. \tag{7}$$

Table 1. Summary of the results for the normalization constant $C_N^{(\beta)}$ of the Laguerre distribution for each symmetry class. For $\beta = 1$ and 4, the cases $N = 1$ and 2, and for $\beta = 2$, the ones for $N = 1$, 2, 3, and 4, were reported in reference [34]. The remaining values were obtained numerically for the purpose of this paper.

N	1	2	3	4	5
$C_N^{(1)}$	$\frac{(1/2)^{3/2}}{(1/2)!}$	$\frac{1}{48}$	$\frac{(1/2)^{3/2}}{(1/2)! \cdot 180 \cdot 48}$	$\frac{1}{53760 \cdot 180 \cdot 48}$	$\cdots$
$C_N^{(2)}$	$\frac{1}{1!(1!)}$	$\frac{1}{2!(3! \cdot 2! \cdot 1!)}$	$\frac{1}{3!(5! \cdot 4! \cdot 3! \cdot 2! \cdot 1!)}$	$\frac{1}{4!(7! \cdot 6! \cdot 5! \cdot 4! \cdot 3! \cdot 2! \cdot 1!)}$	$\frac{1}{5!(9! \cdots 3! \cdot 2! \cdot 1!)}$
$C_N^{(4)}$	$\frac{2^4}{2!(2! \cdot 0!)}$	$\frac{2^{16}}{4!(6! \cdot 4! \cdot 2! \cdot 0!)}$	$\frac{2^{36}}{6!(10! \cdot 8! \cdot 6! \cdot 4! \cdot 2! \cdot 0!)}$	$\frac{2^{64}}{8!(14! \cdot 12! \cdot 10! \cdot 8! \cdot 6! \cdot 4! \cdot 2! \cdot 0!)}$	$\frac{2^{100}}{10!(18! \cdots 2! \cdot 0!)}$

The dependence on N of the normalization constant for $\beta = 1$ is more complicated than the corresponding one for $\beta = 2$ and 4, but it can be obtained in a similar manner with the result

$$C_N^{(1)} = \frac{\left[\left(\frac{1}{2}\right)!\right]^N}{2^{N(N+1/2)}\left(\frac{N}{2}\right)!}\prod_{n=0}^{2N-1}\frac{1}{\left(\frac{n}{2}\right)!}\,. \tag{8}$$

From the last three expressions it is straightforward to arrive at the general result for $C_N^{(\beta)}$; that is

$$C_N^{(\beta)} = \frac{\left[\left(\frac{\beta}{2}\right)^{\beta(N-1/2)+1}\left(\frac{\beta}{2}\right)!\right]^N}{\left(\frac{\beta N}{2}\right)!}\prod_{n=0}^{2N-1}\frac{1}{\left(\frac{\beta n}{2}\right)!}\,. \tag{9}$$

What is very interesting of this result is its similarity with the normalization constant of the joint probability density of the eigenvalues of the Hamiltonian for the Gaussian ensembles [37].

In addition, let us note that the kth moment of a proper delay time, valid for any symmetry and an arbitrary number of channels, given by [34]

$$\left\langle q_i^k\right\rangle^{(\beta)} = \left(\frac{\beta}{2}\right)^k\frac{\left(\frac{\beta N}{2}-k\right)!}{\left(\frac{\beta N}{2}\right)!}\,K_N^{(\beta)}(k,0,\ldots,0), \tag{10}$$

with $0 \leq k < 1 + \beta N/2$, shows the underlying part that comes from the repulsion in equation (5) through the factor $K_N^{(\beta)}(k,0,\ldots,0)$.

2.3 Partial delay times

The partial delay times, defined as the energy derivative of the diagonal form of the scattering matrix as in equation (1), are given, in dimensionless units, by [27,33]

$$\hat{\tau} = -\mathrm{i}\frac{\hbar}{\tau_{\mathrm{H}}}E^{-1}\frac{\partial E}{\partial \varepsilon}. \tag{11}$$

This is an $N \times N$ diagonal matrix whose elements are

$$\tau_s = \frac{\hbar}{\tau_{\mathrm{H}}}\frac{\partial \theta_s}{\partial \varepsilon}. \tag{12}$$

Once the inherent part of the repulsion in the kth moment of the proper times has been identified, it is straightforward to arrive at the expression of the kth moment of the partial times since they do not show that repulsion; for equivalent channels it is [34]

$$\left\langle \tau_s^k\right\rangle^{(\beta)} = \left(\frac{\beta}{2}\right)^k\frac{\left(\frac{\beta N}{2}-k\right)!}{\left(\frac{\beta N}{2}\right)!}. \tag{13}$$

This expression is in agreement with the results that can be obtained directly from the distribution for $N = 1$ in reference [30]. Also, equation (13) includes the known results for $\beta = 2$ and arbitrary N [27,32] and it is consistent with the distribution

$$P_\beta(\tau_s) = \frac{2/\beta}{\left(\frac{\beta N}{2}\right)!}\left(\frac{\beta}{2\tau_s}\right)^{2+\beta N/2}\mathrm{e}^{-\beta/2\tau_s}. \tag{14}$$

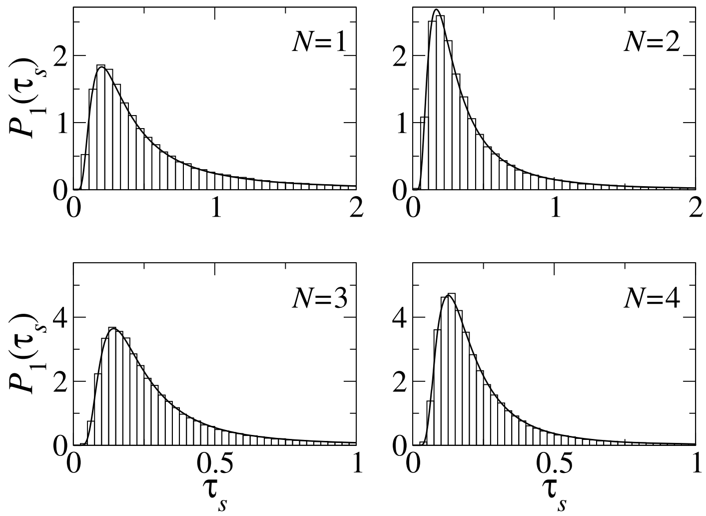

Fig. 1. Comparison between the numerical simulations (histograms) and theory (continuous lines), equation (14), for the distribution of τ_s (we take $s = 1$) in the $\beta = 1$ case.

Our expression, equation (14), encompasses the existing results in the literature for $\beta = 2$ [27,30–33] and agrees with the distribution of partial times previously obtained in reference [29][1].

In what follows we verify our findings with random matrix theory simulations.

3 Numerical calculations

The Hamiltonian approach, also known as the Heidelberg approach, is the best suited for the calculation of the energy derivative of the scattering matrix since it is written explicitly in terms of the energy, namely [37–39]

$$S(\varepsilon) = 1_N - 2\mathrm{i}\pi W^\dagger \frac{1}{\varepsilon 1_M - H + \mathrm{i}\pi W W^\dagger} W, \tag{15}$$

where H is an M-dimensional Hamiltonian matrix that describes the chaotic dynamics of the system, with M resonant single-particle states, and W is an $M \times N$ matrix, independent of the energy, which couples these resonant states to the N propagating modes in the leads; 1_n stands for the unit matrix of dimension n. For ideal coupling of uncorrelated equivalent channels, $W_{\mu n} = \sqrt{M\Delta}/\pi$ ($\mu = 1, \ldots, M$ and $n = 1, \ldots, N$) for the matrix elements of W [39].

For chaotic systems, H is a random matrix chosen from one of the Gaussian ensembles: orthogonal ($\beta = 1$), unitary ($\beta = 2$) or symplectic ($\beta = 4$). The matrix elements of H are uncorrelated random variables with a Gaussian probability distribution with zero mean and variance $\lambda^2/\beta M$; the later determines the mean level spacing at the center of the band, $\Delta = \pi\lambda/M$ [37]. An ensemble of Hamiltonian matrices leads to an ensemble of S-matrices, which represents the several realizations of systems for which the statistical analysis is performed. To implement the simulations we follow the same method as in reference [40] for $\beta = 1$ and 2, while for $\beta = 4$ the subroutine given in reference [41] was used to generate the random Hamiltonian.

[1] A misprint appears in the normalization constant in equation (11) of reference [29].

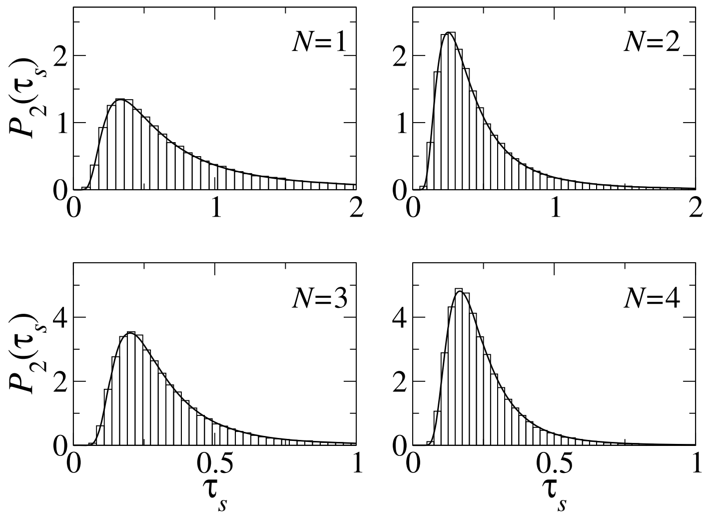

Fig. 2. The same as in Fig. 1, but for $\beta = 2$.

For each realization we diagonalize the matrix S to determine its eigenvalues. We are only interested in one of them, $E_s(\varepsilon) = \exp[\mathrm{i}\theta_s(\varepsilon)]$ let say, but evaluated at three energies in order to calculate the energy derivative. That is,

$$\tau_s = -\frac{\mathrm{i}}{2\pi\epsilon}\,\frac{E_s(\epsilon/2) - E_s(-\epsilon/2)}{E_s(0)}, \tag{16}$$

where $\epsilon = \varepsilon/\Delta$.

In Figure 1 we compare the theoretical distribution of equation (14), for $\beta = 1$, with the numerical results obtained from the random matrix simulations with 10^5 realizations of τ_s, calculated as in equation (16) for $M = 100$ and $\epsilon = 0.001$. We observe a good agreement for the several cases of N presented. This result is an important one since it had not been verified numerically before. Figure 2 shows the corresponding comparison for $\beta = 2$, which is in agreement with those of reference [33]. For $\beta = 4$ the theoretical result fits well with the numerical simulation as can be seen in Figure 3. Let us note that this is the first time that the distribution of the partial times is verified for $\beta = 4$.

4 Conclusions

Based on known results of the joint moments of proper delay times, we obtained the distribution of the partial delay times, for an arbitrary number of channels and any symmetry, in the equivalent channels situation. This was done following an inductive method by extracting the underlying part coming from the level repulsion that trascends to the kth moment of the proper delay times. This distribution was tested by random matrix theory simulations of ballistic chaotic cavities with ideal coupling, extending its numerical verification to all symmetry classes. This result reproduces the existing expressions for the distribution of partial delay times previously obtained in the literature when properly normalized. Also, we were able to provide the normalization constant for the joint distribution of the proper delay times.

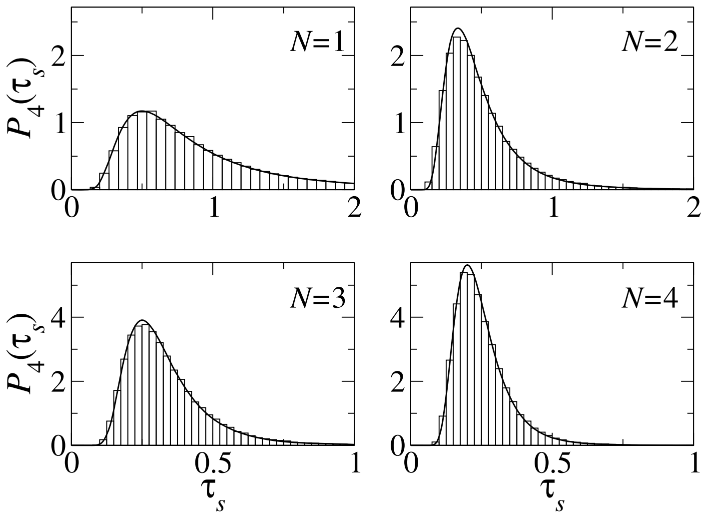

Fig. 3. The same as in Figure 1, but for $\beta = 4$.

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