Quantum Mechanical Time-Delay Matrix in Chaotic Scattering

P. W. Brouwer, K. M. Frahm,* and C. W. J. Beenakker
Instituut-Lorentz, Leiden University, P.O. Box 9506, 2300 RA Leiden, The Netherlands
(Received 21 March 1997)

We calculate the probability distribution of the matrix $Q = -i\hbar S^{-1}\partial S/\partial E$ for a chaotic system with scattering matrix S at energy E. The eigenvalues τ_j of Q are the so-called proper delay times, introduced by Wigner and Smith to describe the time dependence of a scattering process. The distribution of the inverse delay times turns out to be given by the Laguerre ensemble from random matrix theory. [S0031-9007(97)03411-X]

PACS numbers: 05.45.+b, 03.65.Nk, 42.25.Bs, 73.23.-b

Eisenbud [1] and Wigner [2] introduced the notion of time delay in a quantum mechanical scattering problem. Wigner's one-dimensional analysis was generalized to an $N \times N$ scattering matrix S by Smith [3], who studied the Hermitian energy derivative $Q = -i\hbar S^{-1}\partial S/\partial E$ and interpreted its diagonal elements as the delay time for a wave packet incident in one of the N scattering channels. The matrix Q is called the Wigner-Smith time-delay matrix and its eigenvalues $\tau_1, \tau_2, \ldots, \tau_N$ are called proper delay times.

Recently, interest in the time-delay problem was revived in the context of chaotic scattering [4]. There is considerable theoretical [4–7] and experimental [8–10] evidence that an ensemble of chaotic billiards containing a small opening (through which N modes can propagate at energy E) has a uniform distribution of S in the group of $N \times N$ unitary matrices—restricted only by fundamental symmetries. This universal distribution is the circular ensemble of random-matrix theory [11], introduced by Dyson for its mathematical simplicity [12]. The eigenvalues $e^{i\phi}$ of S in the circular ensemble are distributed according to

$$P(\phi_1, \phi_2, \ldots, \phi_N) \propto \prod_{n<m} |e^{i\phi_n} - e^{i\phi_m}|^{\beta}, \qquad (1)$$

with the Dyson index $\beta = 1, 2, 4$ depending on the presence or absence of time-reversal and spin-rotation symmetry.

No formula of such generality is known for the time-delay matrix, although many authors have worked on this problem [6,13–23]. An early result, $\langle \mathrm{tr}\, Q\rangle = \tau_H$, is due to Lyuboshits [13], who equated the ensemble average of the sum of the delay times $\mathrm{tr}\, Q = \sum_{n=1}^{N} \tau_n$ to the Heisenberg time $\tau_H = 2\pi\hbar/\Delta$ (with Δ the mean level spacing of the closed system). The second moment of $\mathrm{tr}\, Q$ was computed by Lehmann *et al.* [18] and by Fyodorov and Sommers [19]. The distribution of Q itself is not known, except for $N = 1$ [19,21]. The trace of Q determines the density of states [24], and is therefore sufficient for most thermodynamic applications [21]. For applications to quantum transport, however, the distribution of all individual eigenvalues τ_n of Q is needed, as well as the distribution of the eigenvectors [25].

The solution of this 40 year old problem is presented here. We have found that the eigenvalues of Q are independent of S [26]. The distribution of the inverse delay times $\gamma_n = 1/\tau_n$ turns out to be the Laguerre ensemble of random-matrix theory,

$$P(\gamma_1, \ldots, \gamma_N) \propto \prod_{i<j} |\gamma_i - \gamma_j|^{\beta} \prod_k \gamma_k^{\beta N/2} e^{-\beta\tau_H\gamma_k/2}, \qquad (2)$$

but with an unusual N-dependent exponent. (The function P is zero if any one of the τ_n's is negative.) The correlation functions of the τ_n's consist of series over (generalized) Laguerre polynomials [27], hence the name "Laguerre ensemble." The eigenvectors of Q are not independent of S, unless $\beta = 2$ (which is the case of broken time-reversal symmetry). However, for any β the correlations can be transformed away if we replace Q by the symmetrized matrix

$$Q_E = -i\hbar S^{-1/2} \frac{\partial S}{\partial E} S^{-1/2}, \qquad (3)$$

which has the same eigenvalues as Q. The matrix of eigenvectors U which diagonalizes $Q_E = U \times \mathrm{diag}(\tau_1, \ldots, \tau_N)U^{\dagger}$ is independent of S and the τ_n's, and uniformly distributed in the orthogonal, unitary, or symplectic group (for $\beta = 1, 2,$ or 4, respectively). The distribution (2) confirms the conjecture by Fyodorov and Sommers [19] that the distribution of $\mathrm{tr}\, Q$ has an algebraic tail $\propto (\mathrm{tr}\, Q)^{-2-\beta N/2}$.

Although the time-delay matrix was interpreted by Smith as a representation of the "time operator," this interpretation is ambiguous [19]. The ambiguity arises because a wave packet has no well-defined energy. There is no ambiguity in the application of Q to transport problems where the incoming wave can be regarded monochromatic, like the low-frequency response of a chaotic cavity [21,22,28] or the Fermi-energy dependence of the conductance [25]. In the first problem, time delay is described by complex reflection (or transmission) coefficients $R_{mn}(\omega)$,

$$R_{mn}(\omega) = R_{mn}(0)[1 + i\omega\tau_{mn} + \mathcal{O}(\omega^2)], \qquad (4a)$$

$$R_{mn}(0) = |S_{mn}|^2, \qquad \tau_{mn} = \mathrm{Im}\, \hbar S_{mn}^{-1} \partial S_{mn}/\partial E. \qquad (4b)$$

The delay time τ_{mn} determines the phase shift of the ac signal and goes back to Eisenbud [1]. With respect to a suitably chosen basis, we may require that both the matrices $R_{mn}(0)$ and τ_{mn} are diagonal. Then we have

$$R_{mn}(\omega) = \delta_{mn}[1 + i\omega\tau_m + \mathcal{O}(\omega^2)], \tag{5}$$

where the τ_m ($m = 1,\ldots,N$) are the proper delay times (eigenvalues of the Wigner-Smith time-delay matrix Q). For electronic systems, the $\mathcal{O}(\omega)$ term of $R_{mn}(\omega)$ is the capacitance. Hence, in this context, the proper delay times have the physical interpretation of "capacitance eigenvalues" [29].

We now describe the derivation of our results. We start with some general considerations about the invariance properties of the ensemble of energy-dependent scattering matrices $S(E)$, following Wigner [30], and Gopar, Mello, and Büttiker [21]. The $N \times N$ matrix S is unitary for $\beta = 2$ (broken time-reversal symmetry), unitary symmetric for $\beta = 1$ (unbroken time-reversal and spin-rotation symmetry), and unitary self-dual for $\beta = 4$ (unbroken time-reversal and broken spin-rotation symmetry). The distribution functional $P[S(E)]$ of a chaotic system is assumed to be invariant under a transformation

$$S(E) \rightarrow VS(E)V', \tag{6}$$

where V and V' are arbitrary unitary matrices which do not depend on E ($V' = V^{\mathrm{T}}$ for $\beta = 1$, $V' = V^{\mathrm{R}}$ for $\beta = 4$, where T denotes the transpose and R the dual of a matrix). This invariance property is manifest in the random-matrix model for the E dependence of the scattering matrix given in Ref. [22]. A microscopic justification starting from the Hamiltonian approach to chaotic scattering [31] is given in Ref. [32]. Equation (6) implies with $V = V' = iS^{-1/2}$ that

$$P(S, Q_E) = P(-\mathbb{1}, Q_E). \tag{7}$$

Here $P(S, Q_E)$ is the joint distribution of S and Q_E, defined with respect to the standard (flat) measure dQ_E for the Hermitian matrix Q_E and the invariant measure dS for the unitary matrix S. From Eq. (7) we conclude that S and Q_E are statistically uncorrelated; their distribution is completely determined by its form at the special point $S = -\mathbb{1}$.

The distribution of S and Q_E at $S = -\mathbb{1}$ is computed using established methods of random-matrix theory [11,31]. The $N \times N$ scattering matrix S is expressed in terms of the eigenvalues E_α and the eigenfunctions $\psi_{n\alpha}$ of the $M \times M$ Hamiltonian matrix $\mathcal{H}$ of the closed chaotic cavity [6],

$$S = \frac{1 - iK}{1 + iK}, \qquad K_{mn} = \frac{\Delta M}{\pi} \sum_{\alpha=1}^{M} \frac{\psi_{m\alpha}\psi_{n\alpha}^*}{E - E_\alpha}. \tag{8}$$

The Hermitian matrix $\mathcal{H}$ is taken from the Gaussian orthogonal (unitary, symplectic) ensemble [11], $P(\mathcal{H}) \propto \exp(-\beta\pi^2 \operatorname{tr} \mathcal{H}^2/4\Delta^2 M)$. This implies that the eigenvector elements $\psi_{j\alpha}$ are Gaussian distributed real (complex, quaternion) numbers for $\beta = 1$ (2, 4), with zero mean and with variance M^{-1}, and that the eigenvalues E_α have distribution

$$P(\{E_\alpha\}) \propto \prod_{\mu<\nu} |E_\mu - E_\nu|^\beta \prod_\mu e^{-\beta\pi^2 E_\mu^2/4\Delta^2 M}. \tag{9}$$

The limit $M \rightarrow \infty$ is taken at the end of the calculation.

The probability $P(-\mathbb{1}, Q_E)$ is found by inspection of Eq. (8) near $S = -\mathbb{1}$. The case $S = -\mathbb{1}$ is special, because S equals $-\mathbb{1}$ only if the energy E is an (at least) N-fold degenerate eigenvalue of $\mathcal{H}$. For matrices S in a small neighborhood of $-\mathbb{1}$, we may restrict the summation in Eq. (8) to those N energy levels E_α, $\alpha = 1,\ldots,N$, that are (almost) degenerate with E (i.e., $|E - E_\alpha| \ll \Delta$). The remaining $M - N$ eigenvalues of $\mathcal{H}$ do not contribute to the scattering matrix. This enormous reduction of the number of energy levels involved provides the simplification that allows us to compute the complete distribution of the matrix Q_E.

We arrange the eigenvector elements $\psi_{n\alpha}$ into an $N \times N$ matrix $\Psi_{j\alpha} = \psi_{j\alpha}M^{1/2}$. Its distribution $P(\Psi) \propto \exp(-\beta \operatorname{tr} \Psi\Psi^\dagger/2)$ is invariant under a transformation $\Psi \rightarrow \Psi O$, where O is an orthogonal (unitary, symplectic) matrix. We use this freedom to replace Ψ by the product ΨO, and choose a uniform distribution for O. We finally define the $N \times N$ Hermitian matrix $H_{ij} = \sum_{\alpha=1}^{N} O_{i\alpha}(E_\alpha - E)O_{j\alpha}^*$. Since the distribution of the energy levels E_α close to E is given by $\prod_{\mu<\nu} |E_\mu - E_\nu|^\beta$ [cf. Eq. (9)], it follows that the matrix H has a uniform distribution near $H = 0$. We then find

$$S = -\mathbb{1} + (i\tau_H/\hbar)\Psi^{\dagger-1}H\Psi^{-1}, \tag{10a}$$

$$Q_E = \tau_H\Psi^{\dagger-1}\Psi^{-1}. \tag{10b}$$

Hence the joint distribution of S and Q_E at $S = -\mathbb{1}$ is given by

$$P(-\mathbb{1}, Q_E) \propto \int d\Psi\, dH\, e^{-\beta \operatorname{tr}\Psi\Psi^\dagger/2} \delta(\Psi^{\dagger-1}H\Psi^{-1})\delta(Q_E - \tau_H\Psi^{\dagger-1}\Psi^{-1}),$$

$$= \int d\Psi\, e^{-\beta \operatorname{tr}\Psi\Psi^\dagger/2}(\det \Psi\Psi^\dagger)^{(\beta N+2-\beta)/2}\delta(Q_E - \tau_H\Psi^{\dagger-1}\Psi^{-1}). \tag{11}$$

The remaining integral depends entirely on the positive-definite Hermitian matrix $\Gamma = \Psi\Psi^\dagger$. In Refs. [27] and [33] it is shown that

$$\int d\Psi f(\Psi\Psi^\dagger) = \int d\Gamma (\det\Gamma)^{(\beta-2)/2} f(\Gamma)\Theta(\Gamma), \tag{12}$$

where $\Theta(\Gamma) = 1$ if all eigenvalues of Γ are positive and 0 otherwise, and f is an arbitrary function of $\Gamma = \Psi\Psi^\dagger$. Integration of Eq. (11) with the help of Eq. (12) finally yields the distribution (2) for the inverse delay times and the uniform distribution of the eigenvectors, as advertised.

In addition to the energy derivative of the scattering matrix, one may also consider the derivative with respect to an external parameter X, such as the shape of the system, or the magnetic field [19,20]. In random-matrix theory, the parameter dependence of energy levels and wave functions is described through a parameter dependent $M \times M$ Hermitian matrix ensemble,

$$\mathcal{H}(X) = \mathcal{H} + M^{-1/2} X \mathcal{H}', \tag{13}$$

where $\mathcal{H}$ and $\mathcal{H}'$ are taken from the same Gaussian ensemble. We characterize $\partial S/\partial X$ through the symmetrized derivative

$$Q_X = -iS^{-1/2} \frac{\partial S}{\partial X} S^{-1/2}, \tag{14}$$

by analogy with the symmetrized time-delay matrix Q_E in Eq. (3). To calculate the distribution of Q_X, we assume that the invariance (6) also holds for the X-dependent ensemble of scattering matrices. (A random-matrix model with this invariance property is given in Ref. [34].) Then it is sufficient to consider the special point $S = -\mathbb{1}$. From Eqs. (10b) and (13) we find

$$Q_X = \Psi^{\dagger -1} H' \Psi^{-1}, \qquad P(H') \propto \exp(-\beta \operatorname{tr} H'^2/16), \tag{15}$$

where $H'_{\mu\nu} = -(\tau_H/\hbar) M^{-1/2} \sum_{i,j} \psi^*_{i\mu} \mathcal{H}'_{ij} \psi_{j\nu}$. A calculation similar to that of the distribution of the time-delay matrix shows that the distribution of Q_X is a Gaussian, with a width set by Q_E,

$$P(S, Q_E, Q_X) \propto (\det Q_E)^{-2\beta N - 3 + 3\beta/2} \times \exp\left[-\frac{\beta}{2} \operatorname{tr}\left(\tau_H Q_E^{-1} + \frac{1}{8} \times (\tau_H Q_E^{-1} Q_X)^2\right)\right] \tag{16}$$

The fact that delay times set the scale for the sensitivity to an external perturbation in an open system is well understood in terms of classical trajectories [35], in the semiclassical limit $N \to \infty$. Equation (16) makes this precise in the fully quantum-mechanical regime of a finite number of channels N. Correlations between parameter dependence and delay time were also obtained in Refs. [19,20], for the phase shift derivatives $\partial\phi_j/\partial X$.

In summary, we have calculated the distribution of the Wigner-Smith time-delay matrix for the chaotic scattering. This is relevant for experiments on frequency and parameter-dependent transmission through chaotic microwave cavities [9,10] or semiconductor quantum dots with ballistic point contacts [36]. The distribution (1) has been known since Dyson's 1962 paper as the circular ensemble [12]. It is remarkable that the Laguerre ensemble (2) for the (inverse) delay times was not discovered earlier.

We acknowledge support by the Dutch Science Foundation NWO/FOM.

*Present address: Laboratoire de Physique Quantique, UMR 5626 du CNRS, Université Paul Sabatier, 31062 Toulouse Cedex 4, France.

[1] L. Eisenbud, Ph.D. thesis, Princeton, 1948.
[2] E. P. Wigner, Phys. Rev. **98**, 145 (1955).
[3] F. T. Smith, Phys. Rev. **118**, 349 (1960).
[4] U. Smilansky, in *Chaos and Quantum Physics,* edited by M.-J. Giannoni, A. Voros, and J. Zinn-Justin (North-Holland, Amsterdam, 1991).
[5] R. Blümel and U. Smilansky, Phys. Rev. Lett. **60**, 477 (1988); **64**, 241 (1990).
[6] C. H. Lewenkopf and H. A. Weidenmüller, Ann. Phys. (N.Y.) **212**, 53 (1991).
[7] P. W. Brouwer, Phys. Rev. B **51**, 16 878 (1995).
[8] E. Doron, U. Smilansky, and A. Frenkel, Phys. Rev. Lett. **65**, 3072 (1990).
[9] J. Stein, H.-J. Stöckmann, and U. Stoffregen, Phys. Rev. Lett. **75**, 53 (1995).
[10] A. Kudrolli, V. Kidambi, and S. Sridhar, Phys. Rev. Lett. **75**, 822 (1995).
[11] M. L. Mehta, *Random Matrices* (Academic, New York, 1991).
[12] F. J. Dyson, J. Math. Phys. (N.Y.) **3**, 140 (1962).
[13] V. L. Lyuboshits, Phys. Lett. **72B**, 41 (1977); Yad. Fiz. **27**, 948 (1978) [Sov. J. Nucl. Phys. **27**, 502 (1978)]; Yad. Fiz. **37**, 292 (1983), [Sov. J. Nucl. Phys. **37**, 174 (1983)].
[14] M. Bauer, P. A. Mello, and K. W. McVoy, Z. Phys. A **293**, 151 (1979).
[15] H. L. Harney, F. M. Dittes, and A. Müller, Ann. Phys. (N.Y.) **220**, 159 (1992).
[16] B. Eckhardt, Chaos **3**, 613 (1993).
[17] F. Izrailev, D. Saher, and V. V. Sokolov, Phys. Rev. E **49**, 130 (1994).
[18] N. Lehmann, D. V. Savin, V. V. Sokolov, and H.-J. Sommers, Physica (Amsterdam) **86D**, 572 (1995).
[19] Y. V. Fyodorov and H.-J. Sommers, Phys. Rev. Lett. **76**, 4709 (1996); J. Math. Phys. **38**, 1918 (1997); Y. V. Fyodorov, D. V. Savin, and H.-J. Sommers, Phys. Rev. E **55**, 4857 (1997).
[20] P. Šeba, K. Zyczkowski, and J. Zakrewski, Phys. Rev. E **54**, 2438 (1996).
[21] V. A. Gopar, P. A. Mello, and M. Büttiker, Phys. Rev. Lett. **77**, 3005 (1996).
[22] P. W. Brouwer and M. Büttiker, Europhys. Lett. **37**, 441 (1997).
[23] E. R. Mucciolo, R. A. Jalabert, and J. L. Pichard, J. Phys. (France) I (to be published).
[24] E. Akkermans, A. Auerbach, J. E. Avron, and B. Shapiro, Phys. Rev. Lett. **66**, 76 (1991).
[25] P. W. Brouwer, S. A. van Langen, K. M. Frahm, M. Büttiker, and C. W. J. Beenakker, Phys. Rev. Lett. (to be published).

[26] The absence of correlations between the τ_n's and the ϕ_n's is a special property of the proper delay times In contrast, the derivatives $\partial\phi_n/\partial E$ considered in Refs [19,20] are correlated with the ϕ_n's
[27] K Slevin and T Nagao, Phys Rev B **50**, 2380 (1994), T Nagao and K Slevin, J Math Phys (N Y) **34**, 2075 (1993), T Nagao and P J Forrester, Nucl Phys **B435**, 401 (1995)
[28] M Buttiker, A Prêtre, and H Thomas, Phys Rev Lett **70**, 4114 (1993)
[29] For an electronic system (with capacitance C), Coulomb interactions need to be taken into account self-consistently, see, e g , Refs [21,28] The result is $R_{mn}(\omega) = \delta_{mn}(1 + i\omega\tau_m) - [i\omega\tau_m\tau_n/(hC/2e^2 + \sum_j \tau_j)] + \mathcal{O}(\omega^2)$
[30] E P Wigner, Ann Math **53**, 36 (1951), Proc Cambridge Philos Soc **47**, 790 (1951), Ann Math **55**, 7 (1952)
[31] J J M Verbaarschot, H A Weidenmuller, and M R Zirnbauer, Phys Rep **129**, 367 (1985)
[32] P W Brouwer, Ph D thesis, Leiden University, 1997
[33] E Brézin, S Hikami, and A Zee, Nucl Phys B **464**, 411 (1996)
[34] P W Brouwer and C W J Beenakker, Phys Rev B **54**, 12705 (1996)
[35] R A Jalabert, H U Baranger, and A D Stone, Phys Rev Lett **65**, 2442 (1990)
[36] R M Westervelt, in *Nano-Science and Technology,* edited by G Timp (American Institute of Physics, New York, 1997)