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Exact Results and Microwave Experiments

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Scattering experiments are indispensable for the study of classical and quantum systems. In the Heidelberg approach, universal features are addressed by assuming that the reaction zone is fully quantum chaotic. Although it stems from nuclear physics, it later on turned out to be applicable to a large variety of systems on different scales, including classical wave systems. For a long time, the distribution of the off-diagonal scattering-matrix elements resisted analytical treatment. I review two recent studies in which my collaborators and I fully solved this problem. We also carried out a comparison with data from microwave experiments.

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1. Introduction

Most of what we know about quantum systems comes from scattering experiments [1]. Applications range from nuclear, atomic and molecular physics, over mesoscopic ballistic devices all the way classical to wave systems such as microwave and elastomechanical billiards, as well as to wireless communication [2-31]. We begin with briefly sketching the general theoretical modeling of the scattering process. As illustrated in Fig. 1, waves propagate in real or fictitious channels and are scattered at a target, here also referred to as interaction zone. The scattering matrix S connects ingoing and outgoing waves. If there are M channels, the scattering matrix S is an $M \times M$ matrix. Flux conservation requires unitarity, $SS^{\dagger} = \mathbb{1}_M = S^{\dagger}S$. If direct reactions between any two channels are not observed, the energy average \bar{S} may be assumed to be diagonal. Important observables are the transmission coefficients $T_a = 1 - |\bar{S}_{aa}|^2$.



Fig. 1. Schematic drawing of the scattering process: interaction zone and channels.

Often, the scattering process is in a broad sense chaotic due to the complexity of the interactions, allowing us to use statistical approaches. In the present context, there are two different ansatzes, which are both based on random matrices [32], referred to as the Mexico and the Heidelberg approaches to stochastic scattering. In the Mexico approach [7], S itself is modeled as a stochastic quantity, and a minimum information principle yields the probability measure

$$P(S) d\mu(S) \sim \frac{d\mu(S)}{|\det^{\beta(M-1)+2}(\mathbb{1}_M - S\langle S \rangle^{\dagger})|}, \qquad (1)$$

where the following symmetries on S are imposed:

- no invariance under time-reversal: S is unitary, $\beta = 2$;
- invariance under time-reversal:
 - spin-rotation symmetry: S is unitary symmetric, $\beta = 1$;
 - no spin-rotation symmetry: S is unitary self-dual, $\beta = 4$.

The input is the ensemble average $\langle S \rangle$, assumed to be equal to the energy average, $\langle S \rangle = \bar{S}$. In spite of its beauty and power in various applications [33], this approach suffers from some shortcomings. In particular, energy and parameter dependences are not clear, e.g., when transitions between different symmetries and invariances are considered.

The Heidelberg approach [11, 34] is rooted in the microscopic description of the scattering process displayed in Fig. 1. The total Hamiltonian reads

$$\mathcal{H} = \sum_{n,m=1}^{N} |n\rangle H_{nm} \langle m| + \sum_{a=1}^{M} \int dE |a, E\rangle E \langle a, E|$$
$$+ \sum_{n,a} \left(|n\rangle \int dE W_{na} \langle a, E| + \text{c.c.} \right), \qquad (2)$$

where H stands for the bound states Hamiltonian of the interaction zone. The number N of these bound states $|n\rangle$ has to be very large to apply statistical modeling. The M channel states are denoted $|a, E\rangle$, their couplings to the bound states W_{na} . The elements of the scattering matrix are then given by

$$S_{ab}(E) = \delta_{ab} - i2\pi W_a^{\dagger} G(E) W_b, \qquad (3)$$

where W_a is the N component vector of the couplings to channel a. The matrix resolvent

(4)

$$G(E) = \frac{\mathbb{1}_N}{E\mathbb{1}_N - H + i\pi \sum_{c=1}^M W_c W_c^{\dagger}}$$

generalizes the Lorentz–Cauchy resonance to matrices. As in one dimension, the imaginary part in the denominator will yield the width of the resonances. In the absence of direct reactions, we may impose the orthogonality relation

$$W_a^{\dagger} W_b = \frac{\gamma_a}{\pi} \delta_{ab}.$$
 (5)

One now assumes that the chaoticity renders the Hamiltonian H of the interaction zone random. One replaces it by a random matrix chosen from non-compact versions of the above symmetric spaces,

- no invariance under time-reversal: H is Hermitian, $\beta = 2$;
- invariance under time-reversal:
 - spin-rotation symmetry:
 - H is real symmetric, $\beta = 1$;
 - no spin-rotation symmetry:
 - H is Hermitian self-dual, $\beta = 4$.

The probability distribution is Gaussian, as is justified by universality [5]. In the Heidelberg approach one can also employ random matrices H which model transitions between symmetries and invariances in such a way that the parameters have a well-defined physics meaning.

2. A new variant of the supersymmetry method

The supersymmetry method, put forward by Efetov for disordered mesoscopic systems [35], drastically reduces the number of integration variables for certain statistical models involving ensemble averages. It was first applied to the Heidelberg approach by Verbaarschot et al. [9], who calculated the two-point correlator $\langle S_{ab}(E_1)S_{cd}(E_2)\rangle$, and a series of further applications followed, for reviews see Refs. [5, 36]. Particularly important in the present context are the calculations of some higher order correlators with and without time-reversal invariance breaking [10]. The much desired distribution of the scattering matrix elements, however, seemed to be out of reach. Fyodorov et al. [17] eventually managed to compute the distribution $P(S_{aa}(E))$ of the diagonal elements $S_{aa}(E)$. All these calculations use a representation of the observable in terms of determinants, such as

$$G_{nm}(E) = \frac{\partial}{\partial J_{nm}} \frac{\det(G^{-1}(E) - J)}{\det(G^{-1}(E) + J)} \bigg|_{J=0}$$
(6)

for the elements of the matrix resolvent (4). In these determinants the random matrix H to be averaged over must appear linearly, such that the random matrix Hcan be moved into the exponent with the help of integrals over commuting and anticommuting variables. For the common Gaussian distributions, the ensemble average is then simply a Fourier transform in matrix space and yields again a Gaussian-type of function which has a twofold interpretation, in the original ordinary as well as in a much smaller space of supermatrices, see the review in Ref. [36].

Unfortunately, the requirement to start from determinants outruled a calculation of the distribution $P(S_{ab}(E))$ for the off-diagonal scattering matrix elements S_{ab} with $a \neq b$ along the above mentioned lines. In Refs. [37, 38] we finally solved this long-standing problem by developing a variant of the supersymmetry method which is partly based on determinants and partly on bilinear forms in the exponent. We wish to calculate the distribution of the real and imaginary parts

$$\wp_s(S_{ab}) = \pi \left((-i)^s W_a^{\dagger} G W_b + i^s W_b^{\dagger} G^{\dagger} W_a \right)$$
(7) of the scattering matrix, where

$$x_1 = \wp_1(S_{ab}) = \operatorname{Re} S_{ab}(E)$$

and

$$x_2 = \wp_2(S_{ab}) = \operatorname{Im} S_{ab}(E).$$
(8)

The distribution is given as the filter integral

$$P_s(x_s) = \int d[H] \exp(-\text{Tr}H^2) \delta(x_s - \wp_s(S_{ab})),$$

$$s = 1, 2, \tag{9}$$

but easier to handle is its characteristic function

$$R_s(k) = \int d[H] \exp(-\mathrm{Tr}H^2) \exp(-ik\wp_s(S_{ab})), \quad (10)$$

which yields the distribution via Fourier backtransform. Inserting the definition of the scattering matrix, we have

$$R_s(k) = \int d[H] \exp(-\mathrm{Tr}H^2) \exp(-\mathrm{i}k\pi W^{\dagger} A_s W)$$
(11)

with

$$W = \begin{bmatrix} W_a \\ W_b \end{bmatrix} \quad \text{and} \quad A_s = \begin{bmatrix} 0 & (-\mathbf{i})^s G \\ \mathbf{i}^s G^{\dagger} & 0 \end{bmatrix}.$$
(12)

The Hermitian matrix A_s contains the inverse of H, making the standard procedure for ensemble averaging impossible. Thus, we have to invert A_s to find a form in which we can do the average over H. A Fourier transform in W space does the job for us,

$$\exp(-ik\pi W^{\dagger}A_{s}W) \sim \int d[z] \exp\left(\frac{i}{2}(W^{\dagger}z+z^{\dagger}W)\right) \\ \times \det^{\beta/2}A_{s}^{-1} \exp\left(\frac{i}{4\pi k}z^{\dagger}A_{s}^{-1}z\right),$$
(13)

where z is an 2N component vector. However, the price we pay is the occurrence of the determinant that ensures the proper normalization. However, using a N component vector ζ of anticommuting variables,

$$\det^{\beta/2} A_s^{-1} \sim \int d[\zeta] \exp\left(\frac{\mathrm{i}}{4\pi k} \zeta^{\dagger} A_s^{-1} \zeta\right), \qquad (14)$$

we achieve that H is fully moved into the exponent and appears there only linearly. Hence, the ensemble average can be done as the usual Fourier transform in matrix space, and supersymmetry becomes applicable. We notice the different rôle of commuting and anticommuting variables. While the former are here used to rewrite a bilinear form, the latter occur as usual for reexpressing a determinant. We perform the Hubbard–Stratonovitch transformation and find

$$R_{s}(k) = \int d[\sigma]$$

$$\times \exp\left(-\frac{4\beta\pi^{2}k^{2}N}{v^{2}}\operatorname{str} \sigma^{2} - \frac{\beta}{2}\operatorname{str} \ln \boldsymbol{\Sigma} - \frac{\mathrm{i}}{4}F_{s}\right)$$
(15)

with a $8/\beta \times 8/\beta$, i.e., 8×8 or 4×4 supermatrix σ for $\beta = 1, 2$, respectively, and with

$$\boldsymbol{\varSigma} = \left(\sigma - \frac{E}{4\pi k} \mathbb{1}_{8/\beta}\right) \otimes \mathbb{1}_N + \frac{\mathrm{i}}{4k} L \otimes \sum_{c=1}^M W_c W_c^{\dagger}, \quad (16)$$

where the matrix L is some superspace metrik indicating compact and non-compact degrees of freedom. The Fourier variable k occurs at three places, v^2 is the variance of the Gaussian ensemble. The structure of the supermatrix model (15) is very similar to the standard ones for the generating functions of correlators [9], but it crucially differs in the way how supersymmetry is broken. While commuting and anticommuting variables, i.e. bosons and fermions, appear on equal footing in the generating functions of correlators, this is not so in the present case. The term F_s in the exponent is apart from details a bilinear form in which only the bosonboson block of Σ^{-1} is projected out by the vector W.

The unfolding procedure involving the limit $N \to \infty$ is done by the usual saddlepoint approximation. The massive modes are integrated out and we eventually arrive at the integral

$$R_s(k) = \int d\mu(\sigma_G) \exp\left(-\frac{i}{4}F_s\right)$$
(17)

$$\times \prod_{c=1}^{M} \operatorname{sdet}^{-\beta/2} \left(\mathbb{1}_{8/\beta} + \frac{\mathrm{i}\gamma_{c}}{4\pi k} \left(\sigma_{G} - \frac{E}{4\pi k} \mathbb{1}_{8/\beta} \right)^{-1} L \right)$$

over the Goldstone modes σ_G . They describe the massless rotations about the saddlepoints and are given as a coset manifold in superspace. We integrate out all remaining anticommuting variables and are left with ordinary integrals only, two for $\beta = 2$ and four for $\beta = 1$. The integrals are structurally similar to the ones for the correlators [9]. As they are quite bulky, we refer the reader to Refs. [37, 38].

3. Analytical results versus numerical simulations and experiment

To begin with, we compare our analytical results for the case $\beta = 2$ with numerical simulations. It is a special feature of the case $\beta = 2$ that the characteristic functions and thus also the distributions for real and imaginary parts, corresponding to s = 1, 2, are the same. As Fig. 2 shows, there is a very good agreement. All energies have to be normalized to the local mean level spacing D. In sufficiently flat microwave cavities, the electromagnetic Helmholtz equation formally coincides with the two-dimensional stationary Schrödinger equation. The experiments are of the scattering type as sketched in Fig. 1, because microwave cables act as channels for the ingoing and outgoing waves. A series of measurements carried out by the the Darmstadt group [24–26] is ideally suited for testing our analytical results. We first look into the regime of isolated resonances, in which the average resonance width Γ is smaller than the mean level spacing D. This corresponds to a frequency range between about 10 and 12 GHz.



Fig. 2. Comparison of the analytical calculation for $\beta = 2$ with numerical simulations. Characteristic function (left) and distribution (right) for M = 3 channels, normalized energy E/D = 0.08 and normalized width parameters $\gamma_1/D = 0.25$, $\gamma_2/D = 0.32$, $\gamma_3/D = 0.38$.



Fig. 3. Comparison of the analytical calculation for $\beta = 1$ with numerical simulations and experimental data in the regime of isolated resonances. Characteristic function of the real (left) and the imaginary (right) parts for M = 3 channels and $\Gamma/D = 0.234$.

In Fig. 3 we compare the characteristic functions for the analytical result, the numerical simulation and the experimental data. The agreement is very good. We then turn to the regime of overlapping resonances, referred to as Ericson regime, in which Γ is larger than D. The frequency range considered is between about 24 and 25 GHz.

The distributions for the analytical result and the experimental data are displayed in Fig. 4. Once more, the agreement is very good. In the Ericson regime, one can come up with rather general arguments that the distributions should become Gaussian. Indeed, while the distributions in Fig. 4 are already very close to Gaussian shape, the characteristic functions in Fig. 3 are different and imply heavier tails for the distributions.



Fig. 4. Comparison of the analytical calculation for $\beta = 1$ with numerical simulations and experimental data in the regime of overlapping resonances. Distribution of the real (left) and the imaginary (right) parts for M = 3 channels and $\Gamma/D = 1.21$.

4. Conclusions

With our analytical results for the distribution of the off-diagonal scattering matrix elements, we solved a long-standing problem in the Heidelberg approach. To make the calculation feasible, we developed a new variant of the supersymmetry method, which applies if the observable can (partly) be written as a bilinear form in the exponent. A certain Fourier transform in a vector space is then needed to perform the ensemble average, which is a Fourier transform in matrix space. Combining these ingredients, we put forward a method for the direct calculation of distributions. As our method yields the characteristic function of the desired distribution, we also have, as a side result, the generating function of all moments. Here, an important comment is in order. In the regime of isolated resonances, the distribution has heavy tails, and it is very well possible that higher moments do not exist. In such a situation, the construction of the distribution from it moments by resummation is bound to fail. Our approach that yields the characteristic function directly and the distribution by its Fourier transform does not suffer from such a shortcoming. For further physics applications, it is important that our results yield a full analytical understanding of the transition form the regime of isolated resonances to the Ericson regime. Brouwer [39] gave an equivalence proof of the Heidelberg and the Mexico approaches. As the latter leads to highly cumbersome integrals even for small channel numbers M, our results also give an explicit handle on the Mexico approach for arbitrary channel number.

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