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Induced vs spontaneous breakdown of S-matrix unitarity: probability of no return in quantum chaotic and disordered systems

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We investigate systematically sample-to sample fluctuations of the probability τ of no return into a given entrance channel for wave scattering from disordered systems. For zero-dimensional ("quantum chaotic") and quasi one-dimensional systems with broken time-reversal invariance we derive explicit formulas for the distribution of τ, and investigate particular cases. Finally, relating τ to violation of S-matrix unitarity induced by internal dissipation, we use the same quantity to identify the Anderson delocalisation transition as the phenomenon of spontaneous breakdown of S-matrix unitarity.

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Various aspects of chaotic wave scattering in the presence of absorption or internal losses attracted a considerable attention in recent years [1 – 10]. In the general case a convenient framework for extracting universal properties of the corresponding S-matrix is provided by the method of effective non-Hermitian Hamiltonian

$$\mathcal{H} = H - i\pi \sum_{a=1}^{M} W_a \otimes W_a^\dagger,$$

in terms of which the energy-dependent element S_{ab} of the $M \times M$ scattering matrix $\hat{S}$ is expressed as:

$$S_{ab} = \delta_{ab} - 2i\pi W_a^\dagger \frac{1}{\mathcal{E} - \mathcal{H}} W_b, \tag{1}$$

see [11, 12] and references therein. Here H stands for a self-adjoint Hamiltonian describing the closed counterpart of the disordered or chaotic system under consideration, $\mathcal{E}$ stands for the energy of incoming waves and the (energy-independent) vectors $W_a,\ a = 1, 2, ..., M$, contain matrix elements coupling the internal motion to one of open M channels. As is easy to verify such a construction ensures the unitarity of the scattering matrix: $S^\dagger S = \mathbf{1}_M$, provided the energy $\mathcal{E}$ takes only real values. When one allows for energy parameter to have nonzero imaginary part $\epsilon = \mathrm{Im}\mathcal{E} > 0$, the S-matrix unitarity is immediately lost: $S^\dagger S < \mathbf{1}_M$. Physically the parameter ϵ stands for a uniform damping inside the system, and is responsible for the fact of losses of the outgoing flux of the particles as compared to the incoming flux. The balance between the two fluxes is precisely the physical mechanism standing behind the S-matrix unitarity.

In the present paper we concentrate on the "probability of no return" (PNR), which is defined as the quantum-mechanical probability for a particle entering the system via a given channel a never exit through the same channel. This quantity is well-defined for a given realization of disorder and will show sample-to-sample fluctuations whose statistics we are going to study. In the case of no internal dissipation PNR is the same as the probability to exit via any of the remaining channels, known as the transmission probability $\sum_{b\neq a} |S_{ab}|^2 \equiv 1 - |S_{aa}|^2$. For a system with absorption the last equality is violated, and we keep the notation $\tau_a = 1 - |S_{aa}|^2$ for the PNR related to the reflection probability R_a in the same channel as $\tau_a = 1 - R_a$. In particular, if only a single open channel is attached to our disordered system and the boundaries are purely reflecting, then neglecting dissipation trivially results in $\tau \equiv 0$. The nontrivial statistics of τ then arises solely due to an absorption, and for small absorption the PNR value $\tau \simeq 2\epsilon\tau_W$ [2, 3, 7], where τ_W is the so-called Wigner delay time intensively studied in recent years, see [3, 4, 11, 13 – 15] and references therein.

It is convenient to write explicitly the normalisation of the channel vectors as $W_a^\dagger W_a = \gamma_a/\pi$, and assume that different channel vectors are orthogonal: $W_a^\dagger W_b = 0$ for $a \neq b$. In fact, one should remember that the effective strength of every open channel is more appropriately characterised by the so-called "transmission coefficients" [12] (also known as the "sticking probabilities"): $T_a = 1 - |\langle S_{aa}\rangle|^2$, related to bare couplings γ_a by

$$\frac{1}{T_a} = \frac{1}{2}\left(1 + g_a\right), \quad g_a = \frac{1}{2\pi\nu}(\gamma_a + \gamma_a^{-1}), \tag{2}$$

where ν stands for the mean spectral density. Here and afterwards the angular brackets stand for the disorder-averaged value of the quantities. Two limiting cases

$T_a = 1$ and $T_a = 0$ correspond to situations of perfectly coupled and decoupled (closed) channel a, respectively.

The starting point of our analysis is based on the following convenient representation for the diagonal elements of the scattering matrix:

$$S_{aa} = \frac{1 - iG_a}{1 + iG_a} \quad , \quad G_a = \pi W_a^\dagger \frac{1}{\mathcal{E} - \mathcal{H}_a} W_a, \tag{3}$$

where

$$\mathcal{H}_a = H - i\pi \sum_{b \neq a}^{M} W_b \otimes W_b^\dagger.$$

In this way we reduce our problem to investigating statistics of the diagonal entries of the resolvent G_a of the "reduced-rank" non-Hermitian operator $\mathcal{H}_a$ independent of the vector W_a. In particular, for the single-channel case $M = 1$ the operator $\mathcal{H}_a$ will not contain the channel vector W at all, and will be therefore a self-adjoint one: $\mathcal{H} = H$.

The statistics of the diagonal entries of the resolvent of a random self-adjoint Hamiltonian H describing the motion of a quantum particle in a static disorder was discussed in much detail by Mirlin and Fyodorov [16] in the framework of the supermatrix nonlinear $\sigma-$ model [17]. In particular, for the case of systems with broken time reversal invariance they were able to find a very compact representation for the joint probability density $\mathcal{P}(u, v)$ of the real $u = \mathrm{Re}G_a$ and imaginary $v = \mathrm{Im}G_a$ parts of the quantity G_a, assuming normalisation $W_a^\dagger W_a = 1/\pi$. Physically the variable v is the most important and being the local density of states enjoyed thorough investigations, see [18, 19] and references therein.

In fact, it is quite straightforward to incorporate non-Hermitian part of the Hamiltonian $\mathcal{H}_a$ into the method, as was already partly done in [20] where statistics of $\mathrm{Im}G_a$ was addressed as describing fluctuations of the photodissociation cross-section.

According to [16] the function $\mathcal{P}(u, v)$ is given, for the centre of spectrum $\mathrm{Re}\mathcal{E} = 0$, by

$$\mathcal{P}(u, v) = \frac{1}{4\pi v^2} P(x),$$

where x stands for the combination $x = (u^2 + v^2 + 1)/2v$, and the function $P(x)$ is given by

$$P(x) = \hat{\mathbf{L}} F(x), \quad F(x) = \int_{-1}^{1} \frac{d\lambda}{x - \lambda} \mathcal{F}(x, \lambda), \tag{4}$$

where we introduced the (Legendre) operator

$$\hat{\mathbf{L}} = \frac{d}{dx}(x^2 - 1)\frac{d}{dx}.$$

The particular form of the function $\mathcal{F}(x, \lambda)$ depends crucially on the effective spatial dimension of the underlying disordered system, and is, for example, quite different for zero-dimensional systems ("quantum chaos") and for "diffusive" extended quasi-one dimensional, or higher dimensional systems. We will give explicit analysis of several physical possibilities later on in the paper.

Having at our disposal the expression for $\mathcal{P}(u, v)$ we can relate the PNR distribution $\mathcal{P}(\tau_a)$ to the function $P(x)$. After a set of algebraic transformations we find the following attractively simple formula:

$$\mathcal{P}(\tau_a) = \frac{1}{\pi \tau_a^2} \int_0^\pi P[x(\tau_a, \theta)] d\theta, \tag{5}$$

$$x(\tau_a, \theta) = \left(\frac{2}{\tau_a} - 1\right)\left(\frac{2}{T_a} - 1\right) +$$

$$+ 4\cos\theta \frac{\sqrt{(1 - \tau_a)(1 - T_a)}}{\tau_a T_a}.$$

Now we proceed with a separate analysis of a few physical situations possible in disordered systems. In all cases we assume time reversal symmetry to be broken.

1. *"Zero-dimensional" quantum chaotic system.* We assume that the disordered region is coupled to M scattering channels characterized by effective coupling constants $g_1, ..., g_M$, see eq.(2), with g_1 corresponding to the chosen entrance channel. The strength of uniform damping will be characterized by the parameter $\eta = 2\pi\epsilon/\Delta$, where Δ stands for the mean level spacing generated by the Hermitian Hamiltonian H. According to the standard argumentation, H can be effectively replaced by a large $N \times N$ random Hermitian matrix taken from the Gaussian Unitary Ensemble, see e.g.[11, 12]. Then in the limit of large enough $N \gg M$ the function $\mathcal{F}(x, \lambda)$ depends on the remaining $M - 1$ coupling constants, as well as on the effective damping η as [20]:

$$\mathcal{F}(x, \lambda) = \prod_{a=2}^{M} \frac{g_a + \lambda}{g_a + x} e^{-\eta(x - \lambda)}. \tag{6}$$

The function $F(x)$ in Eq.(4) can be found in a closed form for any M as one gets, in fact, a simple recursion relating $F_M(x)$ to $F_{M-1}(x)$. Here we restrict ourself mainly to the cases of one and two open channels $M = 1, 2$:

$$F_1(x) = \int_{x-1}^{x+1} \frac{du}{u} e^{-\eta u}, \; F_2(x) = F_1(x) - 2\frac{e^{-\eta x}}{g_2 + x} \frac{\sinh \eta}{\eta}. \tag{7}$$

The distribution $\mathcal{P}(\tau)$ for $M = 1$ is then equal to (cf. [4])

$$\mathcal{P}(\tau)=\frac{2}{\tau^2}e^{-\eta A}\left\{I_0(\eta B)\left[\sinh\eta(\eta A-1)+\eta\cosh\eta\right]-\right.$$
$$\left.-\ \eta B\sinh\eta I_1(\eta B)\right\},\ A=\left(\tfrac{2}{\tau}-1\right)\left(\tfrac{2}{T_1}-1\right),\qquad (8)$$
$$B=4\frac{\sqrt{(1-\tau)(1-T_1)}}{\tau T_1},$$

where $I_0(z), I_1(z)$ stand for the modified Bessel functions of the respective order. For particular case of perfectly coupled channel $T_1=1$ Eq.(8) reduces to the formula

$$\mathcal{P}_1(\tau)=\frac{1}{\tau^3}e^{-2\eta/\tau}\left[\tau\left(1+2\eta-e^{2\eta}\right)+2\eta\left(e^{2\eta}-1\right)\right] \qquad (9)$$

derived earlier [2] with a very different method.

The function $\mathcal{P}(\tau)$ for $M=2$ can be obtained straightforwardly, but the general formula is too long, and we restrict our discussion by a few particular cases. First of all, when dissipation is absent ($\eta=0$) we recover the exact distribution of the transmission probability found earlier in [21, 22] by rather different methods. Next case to be considered is that of a lossy system coupled to two perfectly open channels $g_1=g_2=1$:

$$\mathcal{P}_2(\tau)=\mathcal{P}_1(\tau)+\frac{1-e^{-2\eta/\tau}}{\eta}\left[\frac{1}{2}+\frac{\eta}{\tau}+\frac{2\eta^2}{\tau^2}-\frac{2\eta^2}{\tau^3}\right] \qquad (10)$$

where $\mathcal{P}_1(\tau)$ is given in Eq.(9). In fact, it is not difficult to find a similar recursive formula relating $\mathcal{P}(\tau)$ for M perfectly coupled channels to the same function for $M-1$ perfect channels. We do not give that formula, apart from the simplest case of no dissipation:

$$\mathcal{P}_M(\tau)=\mathcal{P}_{M-1}(\tau)+\left[(M-1)\tau^{M-2}-(M-2)\tau^{M-3}\right],$$

which immediately yields $\mathcal{P}_M(\tau)=(M-1)\tau^{M-2}$, $M\ge$ ≥ 1. This formula (as well as its counterpart $\mathcal{P}(\tau)\propto\tau^{\frac{M-3}{2}}$ for *preserved* time reversal invariance), in fact, follows from the known distribution of 1×1 subunitary block of random unitary scattering matrices, see [23].

2. *Quasi-1D systems.* Consider a single channel attached to one edge of a piece of quasi one-dimensional disordered metal of length L, with the opposite edge being in contact with perfectly conducting lead of very many channels. When the internal dissipation is absent, the function $F(x)$ was found by Mirlin [24]:

$$F(x)=\ln\frac{x+1}{x-1}- \qquad (11)$$
$$-\ 2\int_0^\infty\frac{dkk}{1+k^2}\tanh\left(\frac{\pi k}{2}\right)P_{-\frac{1}{2}+\frac{ik}{2}}(x)e^{-t(k^2+1)/4},$$

where the dimensionless parameter $t=L/\xi$ is the sample length L measured in units of the localisation lengths ξ. The (real) functions $P_\nu(x)$, $\nu=-1/2+ik/2$ are known as conical functions, and represent a special case of Legendre functions. As such they satisfy: $\hat{\mathbf{L}}P_\nu(x)=\nu(\nu+1)P_\nu(x)$. This observation immediately yields the following expression for the PNR distribution:

$$\mathcal{P}(\tau)=\frac{1}{2\tau^2}I\left(t;\frac{2}{\tau}-1\right), \qquad (12)$$

$$I(t;x)=\int_0^\infty dkk\tanh\left(\frac{\pi k}{2}\right)P_{-\frac{1}{2}+\frac{ik}{2}}(x)e^{-t(k^2+1)/4}, \qquad (13)$$

where we assumed, for simplicity, that the selected single channel is perfectly coupled to the scattering medium. Surprisingly, this distribution is practically the same as the distribution of the reflection coefficient from a piece of strictly one-dimensional medium obtained long ago in the framework of the Berezinskii technique [25]. In particular, for any value of the parameter t the distribution displays a log-normal far tail corresponding to very small PNR values $\tau\to 0$. To find it for $t\ll 1$ one needs an asymptotic of the conical functions for large arguments $x\gg 1$ which we borrow from Eq.(50) of the paper [24]. A calculation very similar to that presented in [24] yields:

$$\mathcal{P}(\tau\ll 1)\simeq\frac{1}{2\sqrt{2t}}\frac{\sqrt{-\ln\tau}}{\tau}\exp\left\{-\frac{1}{4t}\ln^2\tau\right\},\ t\ll|\ln\tau|. \qquad (14)$$

This log-normal tail is related to the presence of the anomalously localised states [26]. In the opposite case of very long samples $t\gg 1$ the PNR values are exponentially small due to localisation phenomenon and the distribution is purely log-normal:

$$\mathcal{P}(\tau)\simeq\frac{1}{2\tau}\frac{1}{\sqrt{\pi t}}\exp\left\{-\frac{1}{4t}(t+\ln\tau)^2\right\}.\quad t\sim|\ln\tau|\gg 1 \qquad (15)$$

Let us turn our attention now to the case of a quasi-1D disordered sample with a nonvanishing internal dissipation $\epsilon>0$, assuming second edge of the sample to be impenetrable for waves. The scaling physical parameter controlling the role of dissipation is then given by [18] $\delta=\pi\rho\epsilon\xi$, with ρ standing for the mean spectral density. This is just the dissipation ϵ measured in units of the mean level spacing for a sample whose length is ξ. The most interesting regime is that of small $\delta\ll 1$. In that limit the function $\mathcal{F}(x,\lambda)$ turned out to be independent of λ, whereas the x-dependence persists in a form of the scaling combination $y=2\delta x$, i.e. $\mathcal{F}(x,\lambda)\to\tilde{F}(2\delta x)$. This implies that the relevant values of parameters are $2/\tau\simeq x\sim\delta^{-1}\gg 1$. The latter condition immediately results in the formula $F(x) \to 4\delta\tilde{F}(y)/y$, and also converts the Legendre operator $\hat{\mathbf{L}}$ to

$$\hat{\mathbf{L}}_y = \frac{d}{dy}y^2\frac{d}{dy}.$$

Let us note that the emerging PNR distribution yields, in fact, the distribution of the Wigner delay time via the relation $\tau_W = 2\pi\rho\xi/y$.

The expression for the function $\tilde{F}(y)$ is known explicitly [27]: $\tilde{F}(y) = \tilde{F}_\infty(y) + \tilde{F}_t(y)$, where

$$\tilde{F}_t(y) = \frac{4}{\pi}y^{\frac{1}{2}}\int_0^\infty \frac{dkk}{1+k^2}\sinh\frac{\pi k}{2}K_{ik}\left(2y^{\frac{1}{2}}\right)e^{-t(k^2+1)/4} \quad (16)$$

and $\tilde{F}_\infty(y) = 2y^{\frac{1}{2}}K_1\left(2y^{\frac{1}{2}}\right)$, with $K_\nu(u)$ standing for the Macdonald function.

For the case of very short ($t \ll 1$) sample the function $\tilde{F}(y)$ is known to be approximated by $\exp-(ty)$ [27]. A simple calculation then yields the distribution $\mathcal{P}(\tau) = \left[(4t\delta)^2/\tau^3\right]\exp\{-4t\delta/\tau\}$. Realising that $2t\delta \equiv \eta$ we see that the distribution coincides with the weak absorption limit of Eq.(9). As expected, the same distribution follows from that of the Wigner delay time [11].

In the opposite limit of very long samples $t \to \infty$ only first term survives, and by noticing that $\hat{\mathbf{L}}_y\left[\tilde{F}_\infty(y)/y\right] = \tilde{F}_\infty(y)$, we find the corresponding PNR distribution:

$$\mathcal{P}(\tau) = \frac{16}{\delta}\left(\frac{\delta}{\tau}\right)^{5/2}K_1\left(4\sqrt{\delta/\tau}\right). \quad (17)$$

Although the typical value of τ is of the order of δ, the moments $\langle\tau^m\rangle$ do not exist for $m \geq 1$ because of the powerlaw tail $\mathcal{P}(\tau \gg \delta) \propto \tau^{-2}$. A similar tail was found in the distribution of the total reflection coefficient from multichannel long disordered 1D sample in [9], and is also typical for the Wigner delay time distribution in purely 1D system [15]. Negative moments of τ are equal to $\langle\tau^{-k}\rangle = (4\delta)^{-k}k!(k+1)!$. Note that they differ from the corresponding moments in purely 1D system [15] by extra factorial factor $(k+1)!$, reminiscent of similar relations between other quantities in 1D and quasi 1D [18].

Finally, in the case of strong absorption $\delta \gg 1$ in a long wire $t \to \infty$ the function $\mathcal{F}(x,\lambda) = \exp\{-\sqrt{\delta}(x-\lambda)\}$ [17] and the resulting distribution $\mathcal{P}(\tau)$ coincides with that given by Eq.(9), with η replaced by $\sqrt{\delta}$.

3. *Behaviour at the Anderson transition.* Lets us shortly discuss a possible qualitative behaviour of the PNR τ in a scattering system formed by a single perfect channel attached to a $d-$ dimensional disordered sample at the vicinity of the point of the Anderson delocalisation transition α_c (the mobility edge). Here we denote by α an effective parameter which controls the transition in the infinite sample, with states being localised (extended) for $\alpha > \alpha_c$ (respectively, $\alpha < \alpha_c$).

Our arguments are based on a picture of the transition as described in terms of a functional order parameter developed in detail in [16], see also earlier results in [17] and [28]. For a sample of finite size L the PNR is a function of three parameters: ϵ, L, α. According to the suggested scenario, the behaviour of the function $\mathcal{F}(x,\lambda)$ in the insulating phase in the weak absorption limit $\delta \propto \epsilon\xi^d \to 0$ is expected to be reminiscent of that described above for the one-dimensional case, i.e. $\mathcal{F}(x,\lambda) \to \tilde{F}(2\delta x)$, and the function $\tilde{F}(y)$ decays to zero for $y \gg 1$. Then it is natural to expect that all negative PNR moments in the infinite volume limit $L \to \infty$ are to scale as $\langle\tau^{-k}\rangle \sim \epsilon^{-k}\xi^{-dk}$, where ξ is the localisation length diverging in the vicinity of the mobility edge.

In contrast, in the delocalized phase the function $\mathcal{F}(x,\lambda)$ is expected to remain a non-trivial function of both x and λ even when $\epsilon \to 0$, provided the latter limit is taken *after* the infinite volume limit $L \to \infty$. This should immediately result in a finite-width distribution $\mathcal{P}(\tau)$ of the PNR. From this point of view the Anderson transition acquires a natural interpretation as the phenomenon of *spontaneous* breakdown of S-matrix unitarity. As long as $\alpha \to \alpha_c$, the widths of the distribution and properly defined (negative) PNR moments should vanish, with some set of critical exponents.

If, however, we take limit $\epsilon \to 0$ first, then for $\alpha < \alpha_c$ PNR in large but finite sample should scale with the system size L as $\langle\tau^{-k}\rangle \sim C(\alpha)\epsilon^{-k}L^{-dk}$, where $C(\alpha)$ is expected to diverge when $\alpha \to \alpha_c$. In some sense the behaviour of the negative moments of the Wigner delay time defined as $\tau_W = \lim_{\epsilon\to 0}\tau(\epsilon, L, \alpha)/2\epsilon$ is reminiscent of that for the inverse participation ratio [26]. This analogy suggests a possibility for anomalous scaling $\langle\tau_W^{-k}\rangle \sim L^{-dr_k}$ with $r_k \neq k$ at the mobility edge $\alpha = \alpha_c$, which would then reflect the underlying multifractality of the wavefunctions.

It will be very interesting to perform a detailed numerical analysis of PNR and Wigner delay times for realistic and well-controlled models of scattering from disordered systems, e.g. quantum graphs [29] or models used in [13] and to verify the suggested picture qualitatively and quantitatively in various regimes. The statistics of PNR should be also of experimental accessibility in microwave resonators type of experiments, see e.g [6, 7] and references therein.

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