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Reaction matrix for Dirichlet billiards with attached waveguides

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Abstract

The reaction matrix of a cavity with attached waveguides connects scattering properties to properties of a corresponding closed billiard for which the waveguides are cut off by straight walls. On the one hand, this matrix is directly related to the *S*-matrix, on the other hand it can be expressed by a spectral sum over all eigenfunctions of the closed system. However, in the physically relevant situation where these eigenfunctions vanish on the impenetrable boundaries of the closed billiard, the spectral sum for the reaction matrix, as it was used before, fails to converge and does not reliably reproduce the scattering properties. We derive here a convergent representation of the reaction matrix in terms of eigenmodes satisfying Dirichlet boundary conditions and demonstrate its validity in the rectangular and the Sinai billiards.

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Recently, there has been some interest in the application of the reaction-matrix theory of Wigner and Eisenbud [1] and the projection-operator formalism of Feshbach [2], originally developed for the description of nuclear collisions, to chaotic cavities with attached scattering channels [3–7]. Such models are frequently used as paradigms of chaotic scattering [8–11] and found important experimental realizations by electron transport through open quantum dots [12,13], lasing optical micro-cavities [14–16] and scattering of microwaves in resonators with attached waveguides [6,17]. It is known that the quantum scattering in the open system shows signatures of the classical dynamics in the closed system. For example, conductance fluctuations of open quantum dots are different for systems whose closed counterparts have integrable, fully chaotic or mixed phase space [12,13]. In fact, many statistical results for quantum chaotic scattering rely on this connection as for their derivation an ad hoc formulation of the scattering problem in terms of an effective non-Hermitian Hamiltonian is used [2,21], which describes the dynamics inside a closed system and an additional coupling of the corresponding eigenstates to some scattering channels. Classical chaos enters via the random-matrix assumption for the Hermitian part of this Hamiltonian [18–20]. However, while the effective Hamiltonian appears naturally within the formalism from nuclear physics, it is not a priori clear when this formalism applies to some given billiard system and how the parameters of the two different models are related.

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Therefore, it is important and interesting to develop a thorough understanding of the connection between the scattering properties of billiards, in particular the S-matrix, and the properties of the corresponding closed system, i.e. spectrum and eigenfunctions. For example, today it is well known that the spectrum can be found from a secular equation involving the S-matrix [8–10]. For scattering from the outside of convex billiards in $\mathscr{R}^2$ this scattering approach to quantization allows even for a mathematically rigorous formulation [22].

Unfortunately, the opposite direction is less profoundly understood. Here, the unitary S-matrix is related to a Hermitian reaction matrix, and this can in turn be expressed as a sum over the internal spectrum with coefficients reflecting the behavior of the internal wave function at the boundary separating billiard and waveguide. From the physical point of view, and in particular for the aforementioned applications [12–17], the most natural situation is a wave function which vanishes outside the billiard and on the boundary (Dirichlet b.c.): electrons in a quantum dot are depleted from the boundary by a high negative gate voltage, the radiation field is restricted to the optical cavity by total internal reflection or additional mirrors, and in microwave resonators the metallic walls do not admit the electrical field. However, for this choice of boundary conditions the representation of the reaction matrix as a spectral sum has a problem: we derived a formal expression [3,4] but found both numerically and from semiclassical estimates that it fails to converge.

It is certainly possible to circumvent this problem: in principle all boundary conditions providing a self-adjoint Hamiltonian are admissible for defining the closed system, see Ref. [7] for a nice explanation of this point. In particular, Neumann b.c. with finite wave function but zero derivative at the interface were considered previously [3–7]. In this case the spectral sum converges, and the resulting reaction matrix successfully reproduces numerical or experimental scattering data. Nevertheless, it would be very unsatisfying, could the formulation of a proper reaction-matrix theory for billiards not be based on the physically relevant boundary conditions.

It was recently pointed out [7] that the divergence encountered for Dirichlet b.c. is related to the δ-function singularity of the second derivative of the Green function at coinciding arguments. As in other problems, where this type of singularity is present, a renormalization should be possible by subtracting a second divergent series which removes the δ-function. However, for our purpose this approach is less suitable because it does not provide renormalized coupling constants which are needed for the formulation of an effective Hamiltonian of the scattering problem and for making contact with the formalism of Refs. [1,2,21].

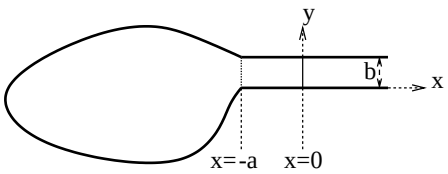

Fig. 1. A scattering system consisting of a cavity and an attached waveguide of width b is shown with bold lines. The coordinate system is chosen such that x is the parallel and y the transversal coordinate with respect to the waveguide.

To remedy this situation, we establish in the present note a convergent expansion of the reaction matrix for Dirichlet billiards with attached waveguides. Our main result is Eq. (15) below, where the renormalized coupling constants entering this series are given. Before we get to this equation, we recall some results from previous work. After stating the result, Eq. (15), we give a derivation of this formula, discuss some interesting aspects related to it and show with two examples how it works.

We consider the same "frying-pan" setup as in Refs. [4,9], i.e. a cavity with an attached waveguide as shown in Fig. 1. The wave function must vanish on the boundary of the system. To obtain the corresponding closed system, Dirichlet boundary conditions are imposed also on the line $x = 0$. It is assumed that this point of separation is well inside the waveguide such that for $-a < x < \infty$ the wave function can be expanded in transversal modes

$$\phi_\lambda(y) = \sqrt{2/b}\,\sin(\lambda\pi y/b). \tag{1}$$

A condition on the minimum value of a will be given later.

Energy eigenfunctions in a billiard satisfy the Helmholtz equation $(\Delta + k^2)\psi(\mathbf{r}) = 0$ with $k = \sqrt{2mE/\hbar^2}$ and $\mathbf{r} = \{x, y\}$. In particular, the scattering

states ψ_λ are in the channel region given in terms of the S-matrix as

$$\psi_\lambda(\mathbf{r},k)=\sum_{\lambda'}\frac{\phi_{\lambda'}(y)}{\sqrt{k_{\lambda'}}}(\delta_{\lambda',\lambda}\mathrm{e}^{-\mathrm{i}k_{\lambda'}x}+S_{\lambda',\lambda}\mathrm{e}^{+\mathrm{i}k_{\lambda'}x}), \quad (2)$$

where $k_\lambda=\sqrt{k^2-(\lambda\pi/b)^2}$ is the longitudinal momentum. There is a finite number $\Lambda=[kb/\pi]$ of open modes with real k_λ. All other modes are evanescent and give contributions to the scattering states which decay exponentially into the waveguide. It is known that their influence is negligible unless the energy nearly coincides with a threshold for the opening of a new channel [10,5]. For simplicity we will disregard evanescent modes here. Then the $\Lambda\times\Lambda$ S-matrix is unitary and, therefore, it is related to a Hermitian *reaction matrix* [1] K by

$$K=-\mathrm{i}(I+S)^{-1}(I-S), \quad (3)$$

$$S=(I+\mathrm{i}K)^{-1}(I-\mathrm{i}K). \quad (4)$$

As billiards are invariant under time-reversal, S and K are symmetric matrices.

On the other hand, we consider the eigenfunctions of the closed billiard which vanish at $x=0$ and can, therefore, be represented as

$$\Psi_n(\mathbf{r})=\sum_\lambda u_{n,\lambda}\phi_\lambda(y)\sin(k_{n,\lambda}x)/k_{n,\lambda}$$
$$(-a\leqslant x<0). \quad (5)$$

The corresponding eigenvalue is k_n, and $k_{n,\lambda}$ follows in analogy to k_λ. Again because of time-reversal symmetry the coefficients $u_{n,\lambda}$ can be chosen real. These coefficients are obtained by projecting the normal derivative of the eigenfunction at the interface on the transversal modes

$$u_{n,\lambda}=\int_0^b \mathrm{d}y\,\phi_\lambda(y)[\mathrm{d}/\mathrm{d}x\,\Psi_n(\mathbf{r})]_{x=0}. \quad (6)$$

It is our goal to represent at arbitrary wave number k the reaction matrix K (and thus via Eq. (3) also the S-matrix) in terms of the discrete set $\{k_n,u_{n,\lambda}\}$. For this purpose, we consider the Green's function for the closed billiard which is defined by $(\Delta+k^2)G(\mathbf{r};\mathbf{r}',k)=\delta(\mathbf{r}-\mathbf{r}')$, as this quantity can at the same time be represented in terms of the S-matrix and by a spectral sum. Indeed we have [4]

$$G(\mathbf{r};\mathbf{r}';k)=\sum_{n=1}^\infty\frac{\Psi_n(\mathbf{r}')\Psi_n(\mathbf{r})}{k^2-k_n^2} \quad (7)$$
$$=\sum_{\lambda,\lambda'}\mathrm{s}_\lambda(\mathbf{r},k)g_{\lambda\lambda'}(k)\psi_{\lambda'}(\mathbf{r}',k)$$
$$(-a\leqslant x'\leqslant x<0) \quad (8)$$

with

$$\mathrm{s}_\lambda(\mathbf{r},k)=\phi_\lambda(y)\sin(k_\lambda x)/\sqrt{k_\lambda} \quad (9)$$

and

$$g(k)=(I+S(k))^{-1}. \quad (10)$$

The S-matrix of the scattering system is implicitly contained in Eq. (8), both in the scattering states ψ_λ and in the matrix $g(k)$. We can extract this information from the normal derivative of Green's function at the interface, projected to transversal modes. After inserting Eqs. (2) and (9) into Eq. (8) we have

$$\lim_{x'\to-0}\lim_{x\to-0}\frac{\partial^2}{\partial_x\partial_{x'}}G_{\lambda,\lambda'}(x,x')$$
$$=\mathrm{i}\sqrt{k_\lambda k_{\lambda'}}\sum_{\lambda''}g_{\lambda\lambda''}(-\delta_{\lambda'',\lambda'}+S_{\lambda'',\lambda'}). \quad (11)$$

Using Eqs. (10) and (3) we see that the r.h.s. reduces essentially to an element of the reaction matrix

$$K_{\lambda\lambda'}=\frac{1}{\sqrt{k_\lambda k_{\lambda'}}}\lim_{x'\to-0}\lim_{x\to-0}\frac{\partial^2}{\partial_x\partial_{x'}}G_{\lambda,\lambda'}(x,x'). \quad (12)$$

Because of the symmetry of Green's function with respect to its spatial arguments the result does not depend on the order of limits, just the singularity occurring for $x=x'$ must be avoided. Comparing Eq. (12) with the spectral decomposition of Green's function (Eq. (7)), one naively expects that the reaction matrix has a spectral representation in the form

$$K_{\lambda\lambda'}=\pi\sum_{n=1}^\infty\frac{W_{n,\lambda}W_{n,\lambda'}}{k^2-k_n^2} \quad (13)$$

with coupling constants

$$\tilde{W}_{n,\lambda}=u_{n,\lambda}/\sqrt{\pi k_\lambda}. \quad (14)$$

[1] Despite some minor differences in the definition we use this term here because of the strong analogy to Ref. [1].

However, this is not the case, as it was found in Refs. [4,7] that with Eq. (14) the sum (13) fails to converge. Convergence is lost because the second derivative of the (absolutely convergent) series for the Green function, Eq. (7), produces a δ-function at coinciding spatial arguments [7].

We will show in the following that Eq. (13) is still valid, albeit with modified coupling constants

$$W_{n,\lambda} = \sqrt{\frac{k_\lambda}{\pi}}\,\frac{\sin((k_{n,\lambda}/k_\lambda)\pi/2)}{k_{n,\lambda}}\,u_{n,\lambda}. \tag{15}$$

To derive this result we will represent the second derivative of Green's function in Eq. (12) by the *value* of Green's function at some shifted point in space in order to avoid the singularity spoiling Eq. (14). We return to Eq. (11) and bring it by some formal manipulations into the shape of Eq. (8), projected onto the transversal modes. Then we get a representation of the reaction matrix which is equivalent to Eq. (12) but does not require differentiation, namely

$$\begin{aligned} K_{\lambda\lambda'} &= \mathrm{i}\sum_{\lambda''} g_{\lambda\lambda''}(-\delta_{\lambda'',\lambda'} + S_{\lambda'',\lambda'}) \\ &= \sqrt{k_\lambda k_{\lambda'}}\sum_{\lambda''}\frac{\sin(-\pi/2)}{\sqrt{k_{\lambda'}}}\,g_{\lambda\lambda''} \\ &\quad\times\frac{1}{\sqrt{k_{\lambda''}}}(\delta_{\lambda'',\lambda'}\mathrm{e}^{+\mathrm{i}\pi/2} + S_{\lambda'',\lambda'}\mathrm{e}^{-\mathrm{i}\pi/2}) \\ &= \sqrt{k_\lambda k_{\lambda'}}\,G_{\lambda,\lambda'}(-\pi/2k_\lambda, -\pi/2k_{\lambda'}). \end{aligned} \tag{16}$$

Now we can safely use the spectral decomposition of Green's function (Eq. (7)) together with Eq. (5) to obtain

$$\begin{aligned} K_{\lambda\lambda'} &= \sqrt{k_\lambda k_{\lambda'}}\sum_n \frac{1}{k^2 - k_n^2}\sin\left(\frac{k_{n,\lambda}}{k_\lambda}\,\frac{\pi}{2}\right) \\ &\quad\times\frac{u_{n,\lambda}}{k_{n,\lambda}}\sin\left(\frac{k_{n,\lambda'}}{k_{\lambda'}}\,\frac{\pi}{2}\right)\frac{u_{n,\lambda'}}{k_{n,\lambda'}}. \end{aligned} \tag{17}$$

This is indeed equivalent to Eq. (13) with the coupling constants given in Eq. (15).

Some comments are in order at this stage. The point $x_\lambda = -\pi/2k_\lambda$ in Eq. (16) corresponds to the first maximum of the partial wave λ. Although no differentiation was involved, the normal derivatives of the wave functions $u_{n,\lambda}$ appear in Eq. (17) because they determine the amplitudes of the partial waves at these maxima according to Eq. (5). However, the full reaction matrix K can be obtained by the outlined procedure only, if the points x_λ are inside the waveguide for all $\lambda = 1,\ldots,\Lambda$. Otherwise Eq. (16) breaks down. This implies a restriction which is at its strongest for the minimum of k_λ at $\lambda = \Lambda$. We can represent the wave number as $k = (\Lambda + \kappa)\pi/b$ with $0 \leqslant \kappa < 1$ and find $k_\Lambda = \sqrt{2\Lambda\kappa + \kappa^2}\pi/b$. Hence, our expression for the reaction matrix will be valid provided that

$$b/2a \leqslant \sqrt{2\Lambda\kappa + \kappa^2}. \tag{18}$$

This condition will always be violated at the threshold energies for the opening of new scattering channels where $\kappa = 0$. On the other hand, if we avoid these singular points by fixing κ to some positive value, the condition will always be satisfied in the semiclassical limit $\Lambda \to \infty$. In some sense, these restrictions on the validity of our approach are similar to those allowing to neglect evanescent modes [5,8,10]. From Eq. (18) we conclude that the situation which is most favourable for reaction-matrix theory in Dirichlet billiards is a closed billiard which extends very far into the waveguide $b \ll a$. Intuitively this should be clear, because then the shape of the billiard resembles a scattering system.

A second comment concerns the uniqueness of the suggested procedure. According to Eq. (8), and because of the special geometry we consider, any point $-a \leqslant x \leqslant \infty$ inside the waveguide region can be used to extract information about the S-matrix, while we have selected only those points where some partial wave λ has maximum amplitude. This may appear like an arbitrary choice. Indeed, if we sample Green's function at sufficiently many points, arbitrarily placed inside the waveguide, it is in principle possible to compute the S-matrix or the reaction matrix. However, the resulting expression will not have the canonical form of Eq. (13) and no coupling constants for individual levels can be defined in this case. Therefore, the connection to the formalism of Refs. [1,2,21] would be lost within such an approach and, consequently, it would not be very useful. As pointed out in the introduction, the same applies to an apparently more straightforward renormalization of Eq. (12) by subtraction of a δ-function. In other words, the main accomplishment of our approach is not the mere possibility to compute the S-matrix from data obtained in the closed billiard, rather it is the fact that the resulting expression is still of the form of Eq. (13).

Eq. (15) and also the S-matrix computed from these coupling constants do depend on the choice of the closed billiard and, in particular, also on the location of the point where the waveguide is cut off by the wall. This may surprise on first sight, because the dynamics inside the frying pan of Fig. 1 are clearly independent of any auxiliary closed system. Nevertheless, there is no contradiction. It was convenient to fix the origin of coordinates, $x = 0$, to the wall of the auxiliary closed billiard. Changing the position of the wall corresponds, therefore, to a basis transformation and accordingly the S-matrix is subjected to a unitary transformation which is automatically accounted for by the modified coupling constants. If one prefers to use other coordinates, say to fix $x = 0$ to the point where the waveguide is connected to the cavity, it is still possible to use any position of the auxiliary wall for computing the S-matrix because the unitary matrix U accounting for the basis transformation $\tilde{S} = USU^{\dagger}$ contains only trivial phase factors $U_{mn} = \delta_{mn} e^{ik_n a}$.

The deeper reason for this dependence of the S-matrix on the auxiliary closed system is that a single Hamiltonian, as the one given by the frying-pan geometry in Fig. 1, is never enough to define a scattering matrix. For this purpose, one must compare the dynamics generated by two different Hamiltonians which are asymptotically equivalent, see e.g. Ref. [23]. In the conventional formulation of reaction-matrix theory this second Hamiltonian describes the uncoupled continuum, cf. Ref. [7]. In our approach, we do not need any explicit reference to the form of these continuum states. Nevertheless, the information about them is implicitly contained in Eq. (2) and can be extracted from this equation by setting $S = I$. In this way, we obtain the eigenstates of a particle inside the waveguide which is closed at $x = 0$ with *Neumann b.c.* Equally well we could have chosen a different form for Eq. (2) and then all the following calculations and, in particular, also the coupling constants would change. For example, a minus sign in front of S would yield continuum states obeying Dirichlet b.c. and the modified coupling constants would in this case contain an extra factor i.

We note further that the coupling constants in Eq. (15) reduce to the naively anticipated Eq. (14) for states n which are close to the energy shell of scattering, i.e. $W_{n,l} \sim u_{n,l}/\sqrt{k_\lambda \pi}$ for $k_n \sim k$. This explains why Eq. (14) provides the correct result for the mean coupling strength in the semiclassical regime [4]: The approximation $k_n \sim k$ was always made from the outset. In general, this approximation is not justified and Eq. (14) breaks down.

The crucial difference between Eqs. (14) and (15) is their behavior for $n \to \infty$ which decides the issue of convergence. To discuss this question, we need the semiclassical estimate for the average behavior of the boundary functions $\langle |u_{n,\lambda}|^2 \rangle / k_{n,\lambda} \sim 4/A$ which we derived in Eqs. (34) and (38) of Ref. [4] for chaotic billiards (see Ref. [24] for more general and accurate estimates of this type). A denotes here the area of the billiard. Substitution into Eq. (15) leads to

$$\frac{|W_{n,\lambda} W_{n,\lambda'}|}{k^2 - k_n^2} \sim k_n^{-3} \sim n^{-3/2} \quad (n \to \infty), \tag{19}$$

i.e. Eq. (13) is indeed absolutely convergent.

We find it illuminating to apply presented theory to a simple toy model, where all relevant quantities are known in closed form. Consider a rectangular billiard with side lengths a and b which yields a half-infinite empty waveguide of width b if one of the walls is removed. This is an integrable system since the transversal modes of the waveguide are decoupled. Therefore, we can restrict attention to some particular mode λ. The corresponding diagonal element of the S-matrix is found to be

$$S_\lambda = -e^{2ik_\lambda a}. \tag{20}$$

This is to be reproduced by the spectral sum equation (13). The normalized eigenfunctions of the closed billiard are

$$\Psi_{\mu,\lambda}(x, y) = 2/\sqrt{ab} \sin(\mu \pi x/a) \sin(\lambda \pi y/b) \tag{21}$$

and, therefore, we have the longitudinal momentum $k_{\mu,\lambda} = \mu\pi/a$, the boundary function $u_{\mu,\lambda} = \sqrt{2/a} k_\mu$ and the coupling constants

$$W_{\mu,\lambda} = \sqrt{\frac{2k_\lambda}{a\pi}} \sin\left(\frac{\pi^2}{2a} \frac{\mu}{k_\lambda}\right). \tag{22}$$

Substitution into Eq. (13) yields after some straightforward transformations

$$K_\lambda = \frac{a k_\lambda}{\pi^2} \sum_{\mu=1}^{\infty} \frac{1 - \cos((\pi^2/a)(\mu/k_\lambda))}{(ak_\lambda/\pi)^2 - \mu^2}. \tag{23}$$

According to the two terms in the numerator we split this expression into two series which can separately

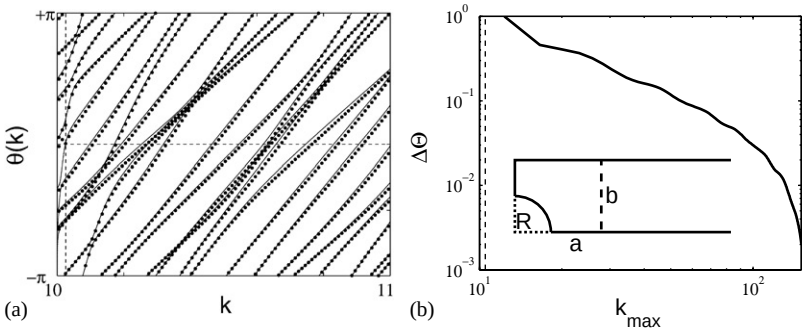

Fig. 2. In the energy interval with 10 open modes the numerically exact S-matrix is compared to the result of Eq. (13) for the quarter Sinai billiard shown in the inset ($b=\pi$, $R=\pi/2$, $R+a=5\pi/4$). (a) Shown are the eigenphases $\theta_\lambda(k)$ ($\lambda=1,\ldots,10$) as a function of the wave number k. Full line: exact result. Dots: approximation based on all 1000 eigenfunctions up to $k_{\max}=36.27$. Vertical line: Range of validity of Eq. (13) as given by Eq. (18). (b) Shown is the deviation of the total phase $\Theta=\sum_\lambda \theta_\lambda$ from the exact result for some fixed wave number $k=10.50$ (vertical line) but with varying cutoff $k_{\max}$ for the included billiard eigenfunctions.

be evaluated with the help of Eq. (1.445.6) from Ref. [25]. Upon recombination of the two results we have

$$K_\lambda = \cot k_\lambda a, \tag{24}$$

which is precisely the reaction matrix corresponding to the S-matrix equation (20) via Eq. (3).

Now we test the outcome of Eq. (13) in the Sinai billiard. S-matrix and eigenstates were computed with the methods described in Ref. [10]. For Fig. 2 we have chosen a large number of open modes, $\Lambda=10$, and a geometry which does not allow for narrow resonances. This is a very demanding regime, as a high number of states is expected to contribute. Nevertheless, in Fig. 2a we show that a reasonable agreement can already be obtained from the 1000 lowest internal modes. The agreement improves as we increase the number of states (Fig. 2b). For $k_{\max}=150$, corresponding to 15,575 modes, hardly any deviation is visible on the scale of Fig. 2a (not shown). In contrast, from Eq. (14) we get garbage irrespective of $k_{\max}$ (also not shown). Note that the error in an individual eigenphase θ_λ of the S-matrix is at its largest when $\theta_\lambda=0$. These are the eigenvalues for a billiard with identical geometry but Neumann b.c. at $x=0$, while at $\theta_\lambda=\pm\pi$ the Dirichlet billiard is quantized and we get perfect agreement. Had we chosen Neumann b.c. as starting point for the evaluation of the reaction matrix, the result would show relatively large deviations close to $\theta_\lambda=\pm\pi$. In this sense the different boundary conditions are complementary. Finally, we remark that from Eq. (18) we cannot expect agreement in the interval $10\leqslant k\leqslant 10.025$ in Fig. 2a. Indeed, we observe in this region a few points which are very far off the exact result.

Summarizing we have shown how and under what circumstances the reaction matrix of a cavity with attached waveguides can be represented as a spectral sum of a closed billiard with the physically relevant Dirichlet boundary conditions.

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