

The role of orbital dynamics in spin relaxation and weak antilocalization in quantum dots

Oleg Zaitsev,^{1,*} Diego Frustaglia,² and Klaus Richter¹

¹*Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany*

²*Scuola Normale Superiore, Piazza dei Cavalieri 7, 56126 Pisa, Italy*

We develop a semiclassical theory for spin-dependent quantum transport to describe weak (anti)localization in quantum dots with spin-orbit coupling. This allows us to distinguish different types of spin relaxation in systems with chaotic, regular, and diffusive orbital classical dynamics. We find, in particular, that, for typical Rashba spin-orbit coupling strengths, integrable ballistic systems can exhibit weak localization, while corresponding chaotic systems show weak antilocalization. We further calculate the magneto-conductance and analyze how the weak antilocalization is suppressed with decreasing quantum dot size and increasing additional in-plane magnetic field.

PACS numbers: 03.65.Sq, 71.70.Ej, 73.23.-b

Weak localization (WL) and antilocalization (AL) are important examples for quantum interference and spin-orbit interaction effects on the conductance (for a review see [1, 2]). Recently, progress has been made in treating these phenomena for *clean* ballistic quantum dots (elastic mean free path larger than the size of the system) within random-matrix theory (RMT) [3, 4]. However, the RMT results are still dependent on geometric parameters that have not yet been computed for such systems. Alternatively, in this case it would be natural to employ semiclassical methods relying on the classical trajectories. In this paper we combine the semiclassical theory of WL [5, 6] and the spin-orbit semiclassics [7, 8, 9] to derive a semiclassical Landauer formula with spin and the AL correction to the conductance in a two-dimensional cavity. We determine the effect of an in-plane magnetic field and of the system size on AL. In addition, we find significant qualitative differences in average spin relaxation in chaotic, integrable, and open diffusive systems.

Our study is based on the semiclassical Landauer formula [5, 6] that we generalize here for systems with spin-orbit interaction. To this end we consider a Hamiltonian linear in the spin-operator vector $\hat{\mathbf{s}}$,

$$\hat{H} = \hat{H}_0(\hat{\mathbf{q}}, \hat{\mathbf{p}}) + \hbar \hat{\mathbf{s}} \cdot \hat{\mathbf{C}}(\hat{\mathbf{q}}, \hat{\mathbf{p}}), \quad (1)$$

where $\hat{\mathbf{C}}(\hat{\mathbf{q}}, \hat{\mathbf{p}})$ is a vector function of the coordinate and momentum operators $\hat{\mathbf{q}}, \hat{\mathbf{p}}$ (it may include an external magnetic field). In a large number of systems of interest the spin-orbit interaction can be considered sufficiently weak, i.e. $\hbar s C \ll H_0$, where s is the particle's spin, $C \equiv |\mathbf{C}(\mathbf{q}, \mathbf{p})|$, and the phase-space functions without hat denote the classical counterparts (Wigner-Weyl symbols) of the respective operators. Formally this “weak-coupling” limit¹ (assumed throughout this paper) can be realized by taking $\hbar \rightarrow 0$, while keeping all the other

quantities finite. This asymptotics already implies that the orbital subsystem H_0 is in the *semiclassical* regime, i.e. the typical classical action $\mathcal{S} \gg \hbar$.

The weak spin-orbit coupling was first incorporated into the semiclassical trace formula in Ref. [7] for spin $s = 1/2$. The theory was then extended (Sec. 4.1 of [8]) to arbitrary spin using path integrals in orbital and spin variables. As a consequence of weak coupling, the influence of spin on the orbital motion can be neglected. Thus the Hamiltonian H_0 determines the classical trajectories $\gamma = (\mathbf{q}(t), \mathbf{p}(t))$, $0 \leq t \leq T_\gamma$. They, in turn, generate an effective time-dependent magnetic field $\mathbf{C}_\gamma(t) = \mathbf{C}(\mathbf{q}(t), \mathbf{p}(t))$ that acts on spin via the Hamiltonian $\hat{H}_\gamma(t) = \hbar \hat{\mathbf{s}} \cdot \mathbf{C}_\gamma(t)$. Hence the spin dynamics can be treated *quantum-mechanically* and described, for example, by a propagator $\hat{K}_\gamma(t)$.

The Landauer formula relates the conductance G of a sample with two ideal leads to its transmission coefficient \mathcal{T} as $G = (e^2/h)\mathcal{T}$ [10]. We will assume that the leads of width w and w' support N and N' open orbital channels, respectively, and that there is no spin-orbit interaction or external magnetic field in the leads. Then in each channel we can distinguish $2s + 1$ spin polarizations that will be labeled by $\sigma = -s, \dots, s$. The transmission and reflection (for one of the leads) can be expressed as double sums

$$\begin{aligned} \mathcal{T} &= \sum_{n=1}^{N'} \sum_{m=1}^N \sum_{\sigma, \sigma'=-s}^s |t_{n\sigma', m\sigma}|^2, \\ \mathcal{R} &= \sum_{n=1}^N \sum_{m=1}^N \sum_{\sigma, \sigma'=-s}^s |r_{n\sigma', m\sigma}|^2, \end{aligned} \quad (2)$$

where $t_{n\sigma', m\sigma}$ is the transition amplitude between the incoming channel $|m, \sigma\rangle$ and outgoing channel $|n, \sigma'\rangle$ belonging to different leads and $r_{n\sigma', m\sigma}$ is defined for the channels of the same lead. The transmission and reflection satisfy the normalization condition $\mathcal{T} + \mathcal{R} = (2s + 1)N$ that follows from the unitarity of the scattering matrix.

¹ Still, the spin-precession length can be of the order of the system size.

From now on we will be dealing with a two-dimensional cavity with hard-wall leads. In the semiclassical limit the transition amplitudes are given by a sum over classical paths at fixed energy (see [5] for spinless case)

$$t_{n\sigma',m\sigma} = \sum_{\gamma(\bar{n},\bar{m})} (\hat{K}_\gamma)_{\sigma'\sigma} \mathcal{A}_\gamma \exp\left(\frac{1}{\hbar} \mathcal{S}_\gamma\right),$$

$$\bar{n} = \pm n, \quad \bar{m} = \pm m, \quad (3)$$

and similar for $r_{n\sigma',m\sigma}$ [11]. Here $\gamma(\bar{n},\bar{m})$ is any classical trajectory that enters (exits) the cavity at a certain angle $\Theta_{\bar{m}}$ ($\Theta_{\bar{n}}$) measured from the normal at the lead cross section. The angles are determined by the transverse momentum in the leads: $\sin \Theta_{\bar{m}} = \bar{m}\pi/kw_{\text{en}}$ and $\sin \Theta_{\bar{n}} = \bar{n}\pi/kw_{\text{ex}}$, where k is the wavenumber and $w_{\text{en}}, w_{\text{ex}}$ are the widths of the entrance and exit leads. \mathcal{S}_γ is the action along the path γ . The prefactor \mathcal{A}_γ is given in [5]. According to the discussion above, $\gamma, \mathcal{A}_\gamma, \mathcal{S}_\gamma$ are determined by the orbital Hamiltonian H_0 , when the spin-orbit coupling is weak. The entire spin effect is contained in the matrix elements of the spin propagator $(\hat{K}_\gamma)_{\sigma'\sigma}$ between the initial and final spin polarizations [$\hat{K}_\gamma \equiv \hat{K}_\gamma(T_\gamma)$].

Inserting the expressions of type (3) in Eq. (2) we obtain the semiclassical Landauer formula with spin-orbit interaction

$$(\mathcal{T}, \mathcal{R}) = \sum_{nm} \sum_{\gamma(\bar{n},\bar{m})} \sum_{\gamma'(\bar{n},\bar{m})} \mathcal{M}_{\gamma,\gamma'} \mathcal{A}_\gamma \mathcal{A}_{\gamma'}^* \times \exp\left[\frac{1}{\hbar} (\mathcal{S}_\gamma - \mathcal{S}_{\gamma'})\right], \quad (4)$$

where in the case of transmission (reflection) the paths γ, γ' connect different leads (return to the same lead). The orbital contribution of each pair of paths is multiplied by the *modulation factor*

$$\mathcal{M}_{\gamma,\gamma'} = \text{Tr}(\hat{K}_\gamma \hat{K}_{\gamma'}^\dagger). \quad (5)$$

The Gutzwiller trace formula for weak spin-orbit coupling [8] has a similar structure.

Let us now identify the leading contributions to (4) in the semiclassical limit for a chaotic cavity *with* time-reversal symmetry. (i) The *classical* part consists of the terms with $\gamma' = \gamma$ [12], for which the fast-varying phase in the exponent of Eq. (4) disappears. In this case the modulation factor $\mathcal{M}_{\gamma,\gamma} = \text{Tr}(\hat{K}_\gamma \hat{K}_\gamma^\dagger) = 2s+1$ is independent of spin-orbit interaction and reduces to the trivial spin degeneracy. (ii) The *diagonal* quantum correction is defined for the reflection only. It contains the terms with $n = m$ and $\gamma' = \gamma^{-1}$, where γ^{-1} is the time-reversal of γ [5].² Again the phase cancellation takes place. The

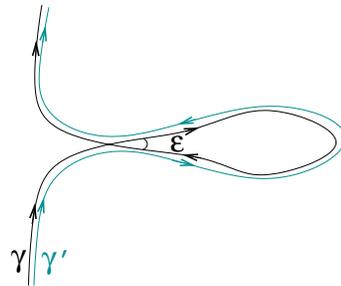


FIG. 1: Pair of orbits with a loop.

modulation factor is $\mathcal{M}_{\gamma,\gamma^{-1}} = \text{Tr}(\hat{K}_\gamma^2)$. (iii) The *loop* contribution is produced by pairs of long orbits that stay close to each other in the configuration space. One orbit of the pair has a self-crossing with a small crossing angle ε , thus forming a loop, its counterpart has an anticrossing. Away from the crossing region the orbits are located exponentially close to each other: they are related by the time-reversal along the loop and coincide along the tails [6, 13] (Fig. 1). The action difference for these orbits is of second order in ε . We compute the modulation factor for γ and γ' neglecting the crossing region. It is $\mathcal{M}_{\gamma,\gamma'} = \text{Tr}(\hat{K}_l^2)$, where l is the loop part of γ . If the time-reversal symmetry is broken, e.g. by a magnetic field, $\mathcal{M}_{\gamma,\gamma'}$ should be calculated directly from Eq. (5).

In Ref. [6] the classical transmission and reflection, as well as the quantum corrections, were expressed in terms of N and N' for a spinless particle in a chaotic cavity with hyperbolic dynamics. In the limit $N = N' \gg 1$ they are $\mathcal{T}_{\text{cl}}^{(0)} = \mathcal{R}_{\text{cl}}^{(0)} = N/2$, $\delta\mathcal{R}_{\text{diag}}^{(0)} = 1/2$, $\delta\mathcal{T}_{\text{loop}}^{(0)} = \delta\mathcal{R}_{\text{loop}}^{(0)} = -1/4$ in agreement with the RMT. Here the superscript refers to zero spin and zero magnetic field and the subscripts denote the classical, diagonal, and loop contributions. The magnetic-field dependence was derived in [5, 6]. Below we extend this derivation to include the effect of spin-orbit interaction as well.

Let us consider a constant uniform arbitrarily directed magnetic field \mathbf{B} . We will neglect the bending of the trajectories by the Lorentz force implying that the cyclotron radius $R_c \gg L_b$, where L_b is the average distance between two consecutive bounces. The diagonal and loop terms in Eq. (4) acquire an Aharonov-Bohm (AB) phase factor $\varphi = \exp(i4\pi\mathbf{A}_\gamma B_z/\Phi_0)$ due to the field component B_z perpendicular to the cavity. Here \mathbf{A}_γ is the loop area for the loop contribution and the effective “area” $\mathbf{A}_\gamma \equiv \int_\gamma \mathbf{A} \cdot d\mathbf{l}/B_z$ for the diagonal contribution, $\Phi_0 = hc/e$ is the flux quantum. The generalized modulation factor $\mathcal{M}_\varphi \equiv \mathcal{M}\varphi$ is distributed according to a function $P(\mathcal{M}_\varphi; L, \mathbf{B})$, where L is the length of the trajectory (loop) in the diagonal (loop) contribution. The \mathbf{B} -dependence comes from φ , as well as from the Zeeman interaction. Thus we can define an average modulation

² In [6] the diagonal contribution is defined differently and includes the classical part.

factor

$$\overline{\mathcal{M}}_\varphi(L; \mathbf{B}) = \int d\mathcal{M} P(\mathcal{M}_\varphi; L, \mathbf{B}) \mathcal{M}_\varphi. \quad (6)$$

The distribution of orbit lengths in a chaotic system is given by $\exp(-L/L_{\text{esc}})$ [5]. The escape length $L_{\text{esc}} = \pi \mathbf{A}_c / (w + w') \gg L_b$ is the average length the particle traverses before leaving the cavity, \mathbf{A}_c is the area of the cavity. It can be shown [6, 14] that the relevant distribution of loop lengths is determined by the same exponent. According to the theories of [5, 6], the product of the AB and modulation factors in Eq. (4) can be eventually substituted by its average $\langle \overline{\mathcal{M}}_\varphi \rangle$ and pulled out of the sum. Thereby we obtain the relative quantum corrections to the transmission and reflection

$$\begin{aligned} \delta\mathcal{R}_{\text{diag}}/\delta\mathcal{R}_{\text{diag}}^{(0)} &= \delta\mathcal{R}_{\text{loop}}/\delta\mathcal{R}_{\text{loop}}^{(0)} = \delta\mathcal{T}_{\text{loop}}/\delta\mathcal{T}_{\text{loop}}^{(0)} \\ &= \langle \overline{\mathcal{M}}_\varphi \rangle \equiv L_{\text{esc}}^{-1} \int_0^\infty dL e^{-L/L_{\text{esc}}} \overline{\mathcal{M}}_\varphi(L; \mathbf{B}). \end{aligned} \quad (7)$$

Note that the current conservation condition $\delta\mathcal{R}_{\text{diag}} + \delta\mathcal{R}_{\text{loop}} = -\delta\mathcal{T}_{\text{loop}}$ is fulfilled in the semiclassical limit $N, N' \gg 1$. In the absence of spin-orbit interaction we have $\overline{\mathcal{M}}_\varphi(L; \mathbf{B}) = (2s + 1) \exp(-\tilde{B}L/L_b)$, where $\tilde{B} = 2\sqrt{2}\pi B_z \mathbf{A}_0 / \Phi_0$ and \mathbf{A}_0 is the typical area enclosed by the orbit during one circulation [5, 6]. Thus the usual Lorentzian \tilde{B} -dependence is recovered by Eq. (7).

For non-vanishing spin-orbit interaction the relative quantum corrections depend on the statistical curve $\overline{\mathcal{M}}_\varphi(L; \mathbf{B})$, which characterizes the spin evolution and can be easily determined from numerical simulations. In the absence of the external field $\overline{\mathcal{M}}(L) \equiv \overline{\mathcal{M}}_\varphi(L; 0)$ changes between $\overline{\mathcal{M}}(0) = 2s + 1$ and the asymptotic value $\overline{\mathcal{M}}(\infty) = (-1)^{2s}$ [14], achieved when the particle's motion is irregular. Therefore, if the particle quickly leaves the cavity (large w, w' , small L_{esc}) or the spin-orbit interaction is too weak, then there is not enough time for the modulation factor to change from $2s + 1$, and the standard WL takes place. In the opposite limit (large L_{esc} or relatively strong spin-orbit coupling) $\overline{\mathcal{M}}(L)$ reaches its asymptotic value and $\langle \overline{\mathcal{M}}_\varphi \rangle \simeq (-1)^{2s}$. We see that for the half-integer spin the quantum correction to the conductance becomes positive due to spin-orbit interaction. This constitutes the phenomenon of *weak antilocalization*. It will be suppressed for integer spin. If $\mathbf{B} \neq 0$ then $\overline{\mathcal{M}}_\varphi(\infty; \mathbf{B}) = 0$ [14]. Hence both the perpendicular magnetic flux and the Zeeman interaction inhibit the AL. (The former destroys the interference between the orbital phases along the paths, while the latter affects the spin phases.) For a quantitative picture we need to specify the form of spin-orbit interaction.

In our numerical examples we consider the case of spin $s = 1/2$ and the Rashba spin-orbit coupling [15], which can be present in quasi-two-dimensional semiconductor heterostructures. It is described by the effective mag-

netic field $\mathbf{C} = (2\alpha_R m_e / \hbar^2) \mathbf{v} \times \hat{\mathbf{z}}$,³ where α_R is the Rashba constant, m_e is the effective mass, and \mathbf{v} is the particle velocity. In a billiard with fixed energy, \mathbf{C} is constant by magnitude. Moreover, its direction changes only at the boundary. It is convenient to characterize the relative strength of spin-orbit interaction by the mean spin-precession angle per bounce $\theta_R = 2\pi L_b / L_R$, where $L_R = 2\pi |\mathbf{v}| / C$ is the Rashba length.

In Fig. 2 (inset) we plot $\overline{\mathcal{M}}(L)$ for a chaotic desymmetrized Sinai (DS) billiard for three Rashba coupling strengths. The average was performed over 10^5 trajectories in a billiard without leads. They were started randomly at the boundary and their initial velocity had a random boundary component. We see that as the coupling strength increases, $\overline{\mathcal{M}}(L)$ reaches its asymptotic value -1 faster. In the main part of the figure we show $\overline{\mathcal{M}}(L)$ for this (curve 2) and three more systems with the same $\theta_R / 2\pi = 0.2$. Another chaotic billiard—the desymmetrized diamond (DD) [16] (curve 3)—shows a very similar behavior. This suggests a kind of *universality* for chaotic billiards. Although our Eq. (7) is valid only for chaotic cavities, the mean modulation factor $\overline{\mathcal{M}}(L)$ can be defined for other types of motion. We find that for an integrable quarter-circle (QC) billiard (curve 1) $\overline{\mathcal{M}}(L)$ oscillates around a constant value above -1 . This value is system-dependent and decreases down to -1 as θ_R increases. The oscillation frequency is independent of θ_R . For an unbounded diffusive motion (curve 4) $\overline{\mathcal{M}}(L) \simeq 3 \exp[-(\theta_R^2/3)(L/L_b)] - 1$ [14] if L_b is identified with the mean free path (Cf. Eq. (10.12) of Ref. [2]). It is worth noting that the curves 1-4 almost coincide for $L \lesssim L_b$. This happens because up to the first scattering event the particle moves along a straight line, and different types of dynamics cannot be distinguished. On a longer length scale we observe *significant qualitative differences in spin evolution in chaotic, integrable, and diffusive systems*.

In particular, the relaxation is strongly suppressed for a confined motion as compared to an unbounded (diffusive) motion with the same θ_R . This observation is supported by the following argument. In the limit $\theta_R \ll 1$ the spin movements “mimic” the particle's movements in the order θ_R^2 . If the higher-order corrections could be neglected then in the confined system the spin relaxation would saturate at $L \sim L_b$. The further decrease of $\overline{\mathcal{M}}(L)$, which is of order $(L/L_b) \theta_R^4$, is due to the Berry phase acquired by the spin wave function [3, 4]. Its effect is similar to that of the AB phase. In a chaotic system without the Zeeman interaction one finds [14]

$$\overline{\mathcal{M}}_\varphi(L; \mathbf{B}) \simeq e^{-(\tilde{B} + \tilde{\theta}_R^2)^2 L / L_b} + e^{-(\tilde{B} - \tilde{\theta}_R^2)^2 L / L_b}, \quad (8)$$

where $\tilde{\theta}_R^2 = (\mathbf{A}_0 / L_b^2) \theta_R^2 / \sqrt{2}$. The further relaxation is

³ α_R / \hbar^2 is kept constant in the formal semiclassical limit $\hbar \rightarrow 0$.

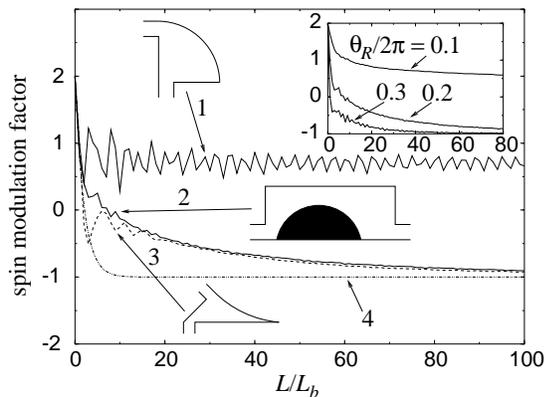


FIG. 2: Average modulation factor $\overline{\mathcal{M}}(L)$ in the quarter-circle billiard (curve 1), the desymmetrized Sinai billiard (curve 2), the desymmetrized diamond billiard [16] (curve 3), and the unbounded diffusive system with the mean-free path L_b (analytical, curve 4). The relative strength of spin-orbit interaction is $\theta_R/2\pi = 0.2$. Inset: $\overline{\mathcal{M}}(L)$ for the desymmetrized Sinai billiard at different values of θ_R .

due to the $(L/L_b)\theta_R^6$ -order terms [3, 4]. It eventually makes $\overline{\mathcal{M}}(L)$ negative and causes the AL. For a stronger interaction $\theta_R \sim 1$ the three factors (the initial relaxation, the Berry phase, and the further relaxation) work simultaneously and cannot be separated (e.g. curves 2,3 in Fig. 2).⁴

Our numerical simulations show that in integrable systems both the spin direction and the phase oscillate almost periodically as the particle moves. Therefore after a short transitional period $\overline{\mathcal{M}}(L)$ saturates. One exception that we found was the circular billiard. Here *all* the trajectories efficiently accumulate area, and the phase grows linearly in time. Hence the Berry-phase contribution is very strong, and we find $\overline{\mathcal{M}}(L) \simeq 2 \sin(x)/x$ for $\theta_R \ll 1$, where $x = \theta_R^2 L r / 2L_b^2$ and r is the radius.

The relative quantum correction to reflection (Fig. 3) in chaotic billiards $\delta\mathcal{R}/\delta\mathcal{R}^{(0)} \equiv (\delta\mathcal{R}_{\text{diag}} + \delta\mathcal{R}_{\text{loop}})/(\delta\mathcal{R}_{\text{diag}}^{(0)} + \delta\mathcal{R}_{\text{loop}}^{(0)}) = \langle \overline{\mathcal{M}}_\varphi \rangle$ is given by Eq. (7). Its dependence on θ_R for $\mathbf{B} = 0$ is similar in the DS (solid curve) and DD (dashed curve) billiards. The positive (negative) values of $\delta\mathcal{R}/\delta\mathcal{R}^{(0)}$ indicate the WL (AL). The escape length in the units of L_b is $P_c/(w+w')$, where P_c is the perimeter of the cavity (including the lead cross-sections). One also concludes that, given L_R , the AL is absent in smaller quantum dots (for fixed $P_c/(w+w')$ or $w+w'$), as supported by the experiment [17]. The Zeeman interaction (upper left inset) suppresses the AL. (It is measured by the precession angle per bounce θ_Z defined similar to θ_R .) Note the anisotropy in the field

direction. The double-peak structure in the magnetic-flux dependence (lower left inset) follows from Eqs. (8) and (7). The integrable QC billiard (dashed curve with circles) was treated in the diagonal approximation. Moreover, the length distribution, which is no longer exponential, was determined numerically [Eq. (7) is not directly applicable]. The WL-AL transition in this integrable billiard occurs at higher θ_R , compared to its chaotic counterparts.

Finally, we discuss the relationship between the semiclassical approach and the RMT [3, 4]. Equation (23) of [4] in the ballistic regime assumes that $\theta_R \ll 1$, while $\theta_R^4(P_c/w) \sim \theta_R^4 E_{\text{Th}}/N\Delta \sim 1$, where E_{Th} is the Thouless energy and Δ is the mean level spacing. Thus the RMT misses the first-bounce spin relaxation if $\theta_R \sim 1$. In addition, the RMT result contains the geometric parameters that have to be computed separately and the theory is not applicable in ballistic integrable systems. The semiclassics has a wider range of applicability including $\theta_R \sim 1$ and, thereby, smaller P_c/w . The next step could be a generalization of the semiclassical approach to disordered quantum dots where the AL will be reduced compared to the clean systems.

For the future we propose to study the power spectrum of conductance fluctuations [5]. We expect its *shape* to be independent of θ_R in an integrable system, but not in a chaotic system.

We thank M. Pletyukhov and M. Brack for many stimulating discussions and P. Brouwer for a helpful clarification. The work has been supported by the Deutsche

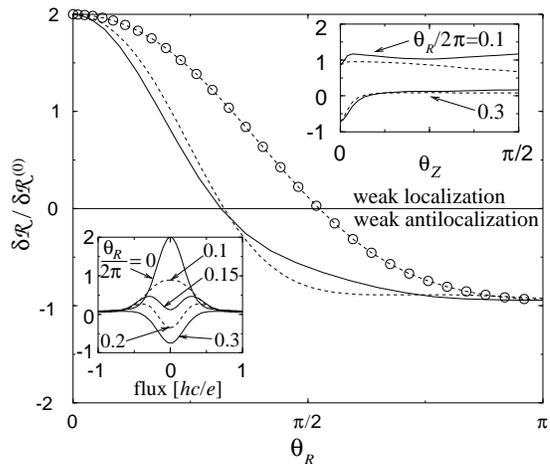


FIG. 3: Relative quantum correction to the reflection $\delta\mathcal{R}/\delta\mathcal{R}^{(0)}$ vs. spin-orbit interaction θ_R for $\mathbf{B} = 0$ in the desymmetrized Sinai (solid), diamond (dashed), and quarter-circle (dashed with circles) billiards with $P_c/(w+w') = 30$. Inset: Desymmetrized Sinai billiard. Upper right: $\delta\mathcal{R}/\delta\mathcal{R}^{(0)}$ vs. the Zeeman interaction θ_Z . The in-plane field is applied parallel (solid) and perpendicular (dashed) to the long side. Lower left: $\delta\mathcal{R}/\delta\mathcal{R}^{(0)}$ vs. perpendicular magnetic flux with $\theta_Z = 0$.

⁴ In the limit $\theta_R \ll 1$ we may have overestimated the initial relaxation, since it would vanish for closed orbits. But in this limit the θ_R^2 -order terms can be neglected anyway.

Forschungsgemeinschaft.

* E-mail: oleg.zaitsev@physik.uni-regensburg.de

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