Chiral Scars in Chaotic Dirac Fermion Systems

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Do relativistic quantum scars in classically chaotic systems possess unique features that are not shared by nonrelativistic quantum scars? We report a class of relativistic quantum scars in massless Dirac fermion systems whose phases return to the original values or acquire a 2π change only after circulating twice about some classical unstable periodic orbits. We name such scars chiral scars, the successful identification of which has been facilitated tremendously by our development of an analytic, conformal-mapping-based method to calculate an unprecedentedly large number of eigenstates with high accuracy. Our semiclassical theory indicates that the physical origin of chiral scars can be attributed to a combined effect of chirality intrinsic to massless Dirac fermions and the geometry of the underlying classical orbit.

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A remarkable phenomenon in contemporary physics is quantum scarring in classically chaotic systems. For a system that exhibits fully developed chaos in the classical limit, a typical trajectory will generate a uniform distribution in the phase space and physical space as well. Naively, one would then expect the quantum wave functions to be uniform. It was discovered by McDonald and Kaufmann [1] in 1979 in their systematic study of the quantum eigenstates of the classical stadium billiard that the physical-space distributions of the wave functions associated with many eigenenergies are highly nonuniform. In fact, due to quantum interference, the eigenstates tend to concentrate on various classically unstable periodic orbits. Such nonuniform distributions of quantum wave functions in classically chaotic systems were later named *quantum scars* by Heller [2], who also devised a random-wave or interference model to explain the phenomenon. Semiclassical theory was subsequently developed by Bogomolny [3] and Berry [4], providing a comprehensive understanding of the phenomenon. Quantum scarring in classically chaotic systems has since attracted a great deal of attention [5].

Most existing works on quantum scarring were with respect to nonrelativistic quantum systems governed by the Schrödinger equation [1–5]. In relativistic quantum systems, the basic governing equation is the Dirac equation. The question of whether scarring can occur in relativistic quantum systems exhibiting chaos in the classical limit is thus fundamental in physics. This question was partially addressed in the context of chaotic graphene [6] billiard [7], where pronounced concentrations of the wave function about distinct classical unstable periodic orbits were demonstrated in different energy regimes. However, graphene is essentially a discrete-lattice system with two nonequivalent Dirac points in the energy-momentum [$(E, \mathbf{k})$] space. Although the electronic behavior in the neighborhood of each Dirac point can be described by the Dirac equation [6], physical processes such as reflection from the system boundaries can couple the dynamics from the *two* Dirac points. In a strict sense, the underlying physics in graphene is not exactly that given by the Dirac equation. The scars uncovered in Ref. [7] are thus relativistic quantum scars only in an approximate sense. Concerning the general issue of relativistic quantum manifestations of classical chaos in the framework governed by the Dirac equation, a pioneering work was that by Berry and Mondragon [8]. They developed a boundary-integral method to solve the massless Dirac equation (for neutrinos) in closed domains such as that given by the chaotic Africa billiard but mainly addressed the issue of energy-level statistics, although an integral formula was provided to calculate the eigenstates.

In this Letter, we address the following question: Are there characteristics of relativistic quantum scars that differ fundamentally from those associated with nonrelativistic quantum scars? To make possible our search for such characteristics, we develop an analytic approach to calculating the eigenstates of massless Dirac fermions in a broad class of chaotic billiards by using the method of conformal mapping. In particular, for any shape in the class, a proper conformal mapping can transform it to a shape for which the solutions of the Dirac equation can be written down analytically. An inverse transform of the solutions thus leads to eigenstates in the original billiard. This method allows us to calculate an unprecedentedly large number of eigenvalues and eigenstates with high accuracy. Taking advantage of this powerful method, we have succeeded in identifying one such characteristic associated with the phase of the wave function. In particular, in nonrelativistic quantum systems, when a particle traverses one cycle along a scarred orbit, the associated quantum phase change is 0 or 2π. However, when we examine the various eigenstate solutions of the massless Dirac equation, we find one subclass of scarred orbits for which one complete itinerary brings about a phase change of only π. In fact, it takes two cycles for the phase of the wave function to become 2π and, for the wave function, to return completely to its original value. This relativistic quantum phenomenon is originated from the chirality of the massless Dirac fermions (as will be explained later), and consequently we name such scars *chiral scars*. We note that, despite the emergence of chiral scars, the majority of the scars are conventional in the sense that the phase change associated with one cycle is 2π. We develop a semiclassical theory to understand the physical origin of chiral scars.

Consider a massless spin-half particle in a finite domain D in the plane $\mathbf{r} = (x, y)$. Utilizing an infinite-mass term outside the domain to model the confinement of the particle motion within D, we obtain the following Hamiltonian in the position representation: $\hat{H} = -i\hbar v \hat{\boldsymbol{\sigma}} \cdot \nabla + V(\mathbf{r})\hat{\sigma}_z$, where $\hat{\boldsymbol{\sigma}} = (\hat{\sigma}_x, \hat{\sigma}_y)$ and $\hat{\sigma}_z$ are Pauli matrices. The Hamiltonian $\hat{H}$ acts on the two-component spinor wave function $\psi(\mathbf{r}) = [\psi_1, \psi_2]^T$ and it has eigenvalue E, i.e., $[-i\hbar v \hat{\boldsymbol{\sigma}} \cdot \nabla + V(\mathbf{r})\hat{\sigma}_z]\psi(\mathbf{r}) = E\psi(\mathbf{r})$. Some basic properties of the Dirac equation are the following. First, the confinement condition of imposing infinite mass outside D naturally takes into account the Klein paradox for relativistic quantum particles. Second, the reduced spatial dimension and confinement break the time-reversal symmetry of $\hat{H}$, namely, $[\hat{T}, \hat{H}] \neq 0$, where $\hat{T} = i\sigma_y \hat{K}$ and $\hat{K}$ denotes the complex conjugate. Third, for $V = 0$ in the Dirac equation, there exist plane-wave solutions whose positive-energy part has the following form:

$$\psi_{\boldsymbol{k}}(\boldsymbol{r}) = \frac{1}{\sqrt{2}} \begin{pmatrix} \exp\left(-i\frac{\theta}{2}\right) \\ \exp\left(i\frac{\theta}{2}\right) \end{pmatrix} \exp(i\boldsymbol{k}\cdot\boldsymbol{r}), \qquad (1)$$

where $\boldsymbol{k}$ is a wave vector that makes an angle θ with the x axis.

To obtain solutions of the Dirac equation, a proper treatment of the boundary condition is necessary. Letting the outward unit normal at s be $\boldsymbol{n}(s) = [\cos(\alpha), \sin(\alpha)]$ (α being the angle with the x axis, see Fig. 1), making use of the Hermiticity of $\hat{H}$, and defining $\boldsymbol{j} = v\psi^\dagger \hat{\boldsymbol{\sigma}} \psi$ as the local relativistic current, we get the vanishing current condition $\boldsymbol{j}\cdot\boldsymbol{n} = 0$ for any point s. Requiring the outward current to be zero cannot fix the boundary condition uniquely but it entails $\mathrm{Re}[\exp(i\alpha)\psi_1/\psi_2] = 0$ for all points s. Using the boundary potential as in Ref. [8], we can obtain the complete boundary condition: $\psi_2/\psi_1 = i\exp[i\alpha(s)]$.

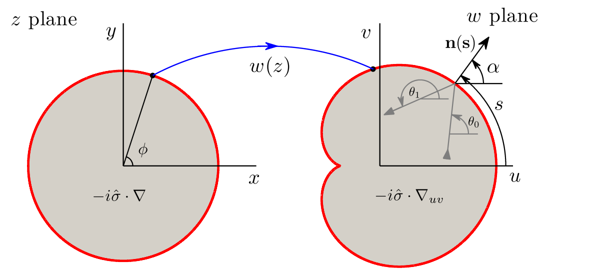

FIG. 1 (color online). Conformal transformation from the unit disk in $z = x + iy$ (z plane) to the billiard domain D in $w = u + iv$ (w plane). The boundary is generated by the mapping function Eq. (3) with parameter $\beta = 0.49$.

Consider chaotic billiards with analytic boundaries. An elementary observation [9] is that, while the Dirac equation together with the boundary condition are generally not separable in the Cartesian coordinates, for circular domains analytic solutions can be written down in terms of both eigenvalues and the eigenstate $\{\mu_{lm}, \psi_{lm}(r, \phi), l = 0, \pm 1, \pm 2, \ldots, m = 1, 2, \ldots\}$ (see the Supplemental Material [10]). Thereby, given a closed domain with analytic boundary, if a proper conformal mapping can be identified to transfer the domain into a circle, solutions can be explicitly obtained.

The billiard domain D can be defined as a conformal transformation of the unit disk in the w plane, as shown in Fig. 1; i.e., $u(x, y) + iv(x, y) = w(z) \equiv w(re^{i\phi})$ (for $r \in [0, 1]$), where $w(z)$ is an analytic function with a nonvanishing derivative in D. The boundary can be defined parametrically by $u = \mathrm{Re}[w(e^{i\phi})]$, $v = \mathrm{Im}[w(e^{i\phi})]$. The basic problem is then to solve the following stationary Dirac equation: $-i\hat{\boldsymbol{\sigma}} \cdot \boldsymbol{\nabla}_{uv}\Psi = k\Psi$, together with the boundary condition $\Psi_2/\Psi_1|_{\partial_D} = ie^{i\alpha}$, where Ψ_1 and Ψ_2 are the two components of the spinor wave function Ψ. When being acted upon by the operator $-i\hat{\boldsymbol{\sigma}} \cdot \boldsymbol{\nabla}_{uv}$, the Dirac equation becomes $-\Delta_{uv}\mathbf{1}\Psi = k^2\Psi$. Using the conformal mapping $\Delta = |dw/dz|^2\Delta_{uv}$ to transform the Dirac equation into the unit disk in the z plane, together with the definition $\Psi'(\mathbf{r}) = \Psi(u, v)$, we obtain the following form of the Dirac equation in the polar coordinates: $\Delta\Psi' + k^2T(r, \phi)\Psi' = 0$, where $T(r, \phi) = |dw/dz|^2$. To solve this equation, we expand Ψ' in terms of eigenfunctions of the unit disk: $\Psi'(r, \phi) = \sum_{l=-\infty}^{\infty}\sum_{m=1}^{\infty} c_{lm}\psi_{lm}(r, \phi)$, where c_{lm} are the expansion coefficients. Substituting this into the Dirac equation, we have $\nu_{lm}/k^2 - \sum_{l'm'} M_{lml'm'}\nu_{l'm'} = 0$, where $\nu_{lm} = \mu_{lm}c_{lm}$ and

$$M_{lml'm'} = \frac{N_{l'm'}N_{lm}}{\mu_{l'm'}\mu_{lm}} \int_0^{2\pi} d\phi \exp\{i(l' - l)\phi\} \times \int_0^1 drT(r, \phi)r\{J_l(\mu_{lm}r)J_{l'}(\mu_{l'm'}r) + J_{l+1}(\mu_{lm}r)J_{l'+1}(\mu_{l'm'}r)\}. \qquad (2)$$

Once the eigenvalues λ_n and eigenvectors $\boldsymbol{\nu}$ of the matrix $(M_{lml'm'})$ have been obtained, we get the complete solutions of the Dirac equation through the relations $k_n = 1/\sqrt{\lambda_n}$ and $c_{lm} = \nu_{lm}/\mu_{lm}$. A practical limitation is that, in actual computations, a truncated basis $\{\psi_{lm}(r, \phi)\}$, $l_{\min} \le l \le l_{\max}$, $1 \le m \le m_{\max}$, is used. Thus, extremely high energy levels and the associated eigenstates cannot be determined accurately. Nonetheless, our conformal-mapping-based method can yield an unprecedentedly large number of energy levels and the corresponding eigenstates, e.g., a basis of the size of 40 000 is used which yields about 15 000 eigenstates with high accuracy for the following analysis.

To demonstrate the working of our conformal-mapping-based method to calculate eigenenergies and eigenstates of the Dirac equation, we choose the following complex function $w(z)$ as a quadratic conformal map,

$$w(z) = \frac{1}{\sqrt{1 + 2\beta^2}}(z + \beta z^2), \qquad \beta \in \left[0, \frac{1}{2}\right), \tag{3}$$

to determine the shape of the billiard in which a massless fermion is confined. For $\beta = 0.49$, a previous work on the classical dynamics of the billiard [11] demonstrated the presence of chaos. The quadratic conformal map also has the advantage of amenability to analytic treatment where, in particular, the ϕ integration in Eq. (2) becomes straightforward and the matrix $M_{lml'm'}$ becomes nearly diagonal in l. Comparison of the energy levels calculated by our conformal-mapping method with those from the boundary-integral method [8] reveals a remarkably excellent agreement. Further validation of our method can be established by calculating and analyzing the universal behaviors of the various level-spacing statistics in chaotic billiards (see the Supplemental Material [10]).

We now present the reasoning and calculations that lead to the discovery of chiral scars. After examining a large number of relativistic quantum scars for massless Dirac fermion in chaotic billiards, we notice that a certain scarring pattern, once having appeared, tends to reappear at a different energy value. This can be understood by using semiclassical theory [12], which states that two repetitive scars associated with the same classical periodic orbit can occur when the action difference satisfies $|\Delta S| = 2\pi n\hbar$ $(n = 1, 2, \ldots)$, where $S = \oint \boldsymbol{p} d\boldsymbol{q} = \hbar kL$ and L is the length of a given periodic orbit. It can be inferred that, if one scar already appears, say, at k_0, the eigenfunctions at the wave number $k_n = k_0 \pm n\delta k$ will most likely scar, where $\delta k = 2\pi/L$. We define

$$\eta(n) = \frac{|k_n - k_0|}{\delta k} - \left[\frac{|k_n - k_0|}{\delta k}\right], \tag{4}$$

where $[x]$ denotes the largest integer less than x. According to the semiclassical theory for nonrelativistic quantum systems, the quantity η, by its definition, should exhibit only two distinct values: either close to 0 or 1. To calculate the value of η, some key characteristics of the corresponding scars are needed. Table I lists some of the key features of the calculated scars. Using the data of the most typical types of scars, i.e., scar types 2, 3, 4, and 5 in Table I, we calculate their values of $\eta(n)$ from Eq. (4). Figures 2(a)–2(l) show the results. We see that, for scar types 2 and 4, $\eta(n)$ exhibits the two values, i.e., 0 and 1, as can be anticipated from the semiclassical theory. However, for scar types 3 and 5, η can attain the additional value of $1/2$. This implies that, for this type of scar, the conventional semiclassical theory has to be modified.

TABLE I. Characteristics of the relativistic quantum scars.

Scar index[a]	L	δk	k_0	Collected number
2	4.2425	1.4810	167.3225	**104**
4-I	7.5385	0.8335	219.8747	73
4-II	5.7993	1.0843	152.2197	57
3	5.3764	1.1687	217.0473	**104**
5-I	8.4725	0.7416	189.2712	18
5-II	9.7321	0.6456	169.0422	12

[a]The relativistic quantum scars are labeled as n, the period of the corresponding classical periodic orbit, if no other configurations exist. For orbits of the same period but with different configurations, Roman numerals are used.

The origin of the type of "abnormal" scars that do not obey the conventional semiclassical quantization rules can be understood by exploring the chirality for massless Dirac fermions and the associated phase changes. In particular, for a classical periodic orbit, the chirality corresponds to the cumulative effect of reflections at the billiard wall. Consider one pair of orbits that close on themselves after N bounces but with opposite orientation, as shown schematically in Fig. 3. Based on the plane-wave description in Eq. (1), after traversing the orbit once, the associated phase change is $\Omega = \frac{1}{2}(\theta_N - \theta_0) = \Lambda\pi$, where Λ is an integer, and the total rotation $(\theta_N - \theta_0)$ can be obtained by the reflection law $\theta_n = \pi + 2\alpha - \theta_{n-1}$ for $n = 1, 2, \ldots, N$ (Fig. 1). Define $\Omega_+ - \Omega_- = (\Lambda_+ - \Lambda_-)\pi$ as the difference in the phase changes between the pair of $+$ and $-$ orbits. It was shown by Berry and Mondragon [8] that $\Omega_+ - \Omega_- = 2\Lambda_+\pi$ for even N and $\Omega_+ - \Omega_- = \pi$ for odd N. Since chirality corresponds to the situation of $(\Lambda_+ - \Lambda_-)$ being odd, where the two orbits in the pair enclose themselves with an opposite sign change, the orbit with an even number of bounces is not chiral but the orbit with an odd number of bounces is. Chirality can have a remarkable effect on scarring. To quantify this, we define an effective periodic-orbit length $L^* = \tau L$, where L is the original length of the periodic orbit and τ is a correctional factor. The nonchiral orbits with an even number of bounces correspond to $\tau = 1$. However, the chiral orbits correspond to $\tau = 2$. This means that, for chiral orbits, the quantum states as determined by the Dirac equation return to themselves after two successive circulations along the classical orbit. When the modified length is used in the semiclassical theory for type-3 scars, the values of η for all scars become concentrated on 0 and 1.

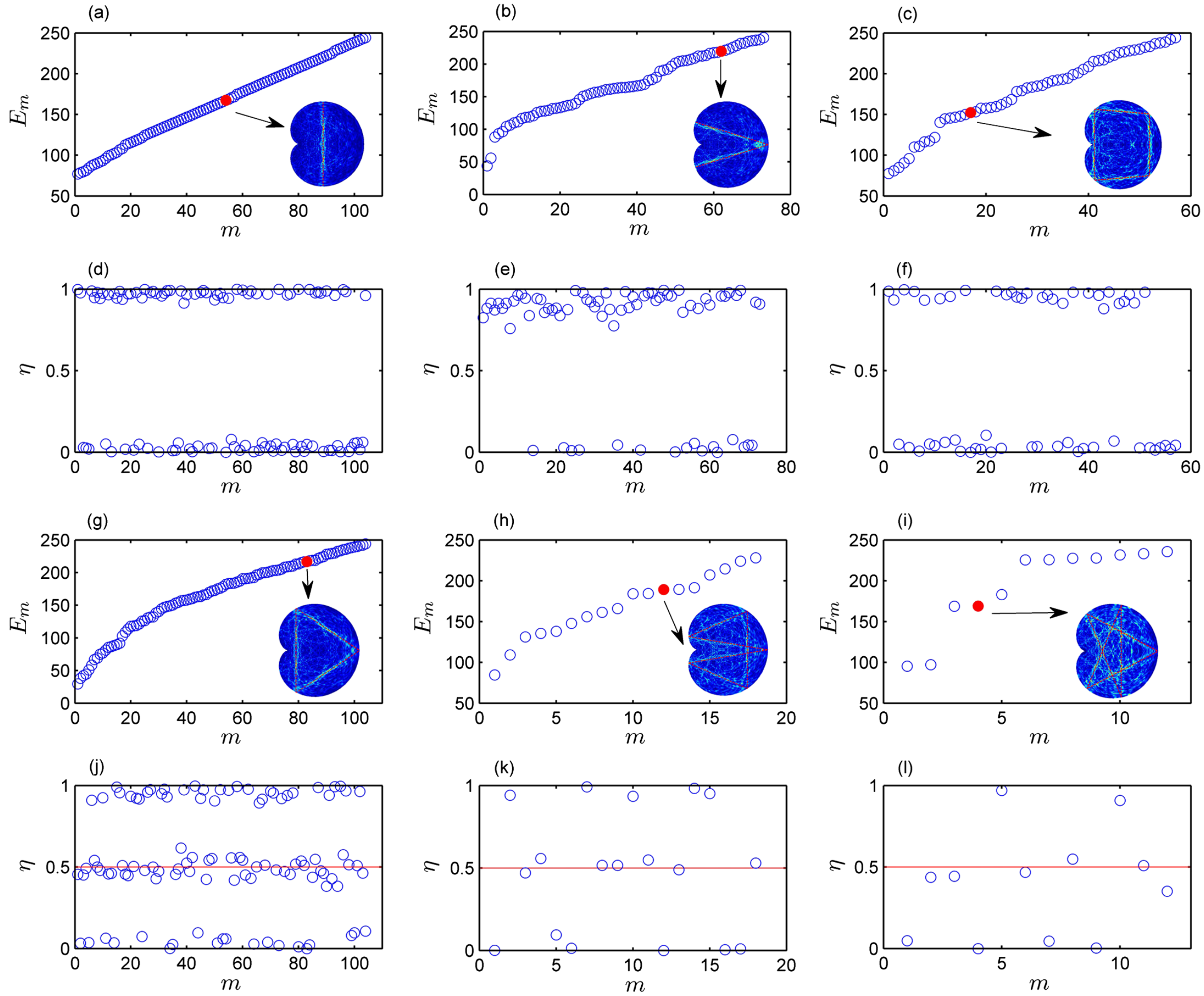

FIG. 2 (color online). (a)–(c) show the energy levels E_m versus the sequence number m for the scar types 2, 4-I, and 4-II in Table I, respectively. (d)–(f) are η versus m calculated from Eq. (4), where the relevant data are from (a)–(c), respectively. Similarly, results for the scar types 3, 5-I, and 5-II are shown in (g)–(l).

In summary, we have developed an analytic method based on conformal mapping to solve the massless Dirac equation in a broad class of closed chaotic domains. The advantage is that significantly more eigenstates can be calculated to high accuracy as compared with the previous boundary-integral or finite-difference methods. Empowered by our method, we have found a new class of relativistic quantum scars, chiral scars whose quantum phases return to their original values only after two circulations around the underlying classical unstable periodic orbits. The physical origin of chiral scars can be attributed to chirality of massless Dirac fermions coupled with the particular geometry of the underlying periodic orbit. Such scars are uniquely relativistic quantum scars and find no counterparts in nonrelativistic quantum systems.

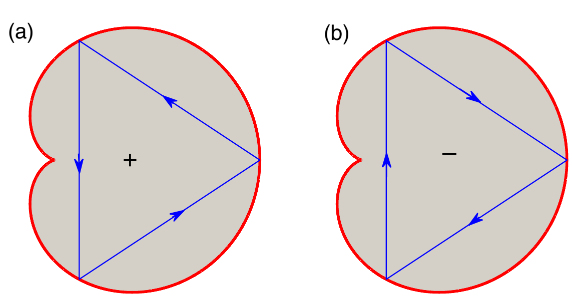

FIG. 3 (color online). Illustration of a pair of orbits with opposite orientations.

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