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Abstract – We solve the Dirac equation in two spatial dimensions in the setting of resonant tunneling, where the system consists of two symmetric cavities connected by a finite potential barrier. The shape of the cavities can be chosen to yield both regular and chaotic dynamics in the classical limit. We find that certain pointer states about classical periodic orbits can exist, which suppress quantum tunneling, and the effect becomes less severe as the underlying classical dynamics in the cavity is chaotic, leading to regularization of tunneling dynamics even in the relativistic quantum regime. Similar phenomena have been observed in graphene. A physical theory is developed to explain the phenomenon based on the spectrum of complex eigenenergies of the non-Hermitian Hamiltonian describing the effectively open cavity system.

To understand the effect of chaos in the classical limit on quantum behaviors has been a field of interest and active pursuit [1]. This field, named quantum chaos, finds applications in many fields in physics such as condensed-matter physics, atomic physics, nuclear physics, optics, and acoustics. Previous works on quantum chaos focused almost exclusively on non-relativistic quantum systems. A fundamental question is whether phenomena in non-relativistic quantum chaos can occur in *relativistic* quantum systems described by the Dirac equation. This field of relativistic quantum chaos [2] is of particular importance because of the relevance of the Dirac equation to graphene systems [3].

Recently, the remarkable phenomenon of chaos-regularized quantum tunneling has been uncovered [4], where classical chaos can suppress, significantly, the spread in the tunneling rate commonly seen in systems whose classical dynamics are regular. For example, consider the system in fig. 1, which consists of two symmetrical cavities connected by a one-dimensional potential barrier along the line of symmetry. When the classical dynamics in each cavity is integrable, for sufficiently large energy the tunneling rate can assume many
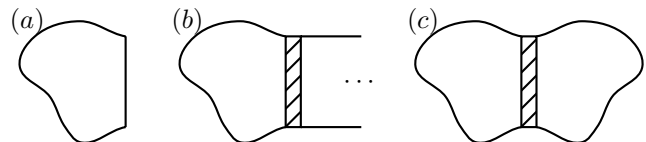

Fig. 1: (a) A closed quantum system of arbitrary shape in two dimensions, (b) the corresponding opened system, and (c) symmetric double well used in resonant tunneling computations.

values in a wide interval. Choosing the geometry of the cavity such that the classical dynamics become chaotic can greatly enhance and regularize quantum tunneling. Heuristically, this can be understood, as follows. When the potential barrier is infinite, each cavity is a closed system with an infinite set of eigenenergies and eigenstates. Many eigenstates are concentrated on classical periodic orbits, forming quantum scars [5]. For classically integrable cavity, some stable or marginally stable periodic orbits can persist when the potential barrier becomes finite so that each cavity system is effectively an open quantum system. Many surviving eigenstates correspond to classical periodic orbits whose trajectories do not encounter the potential barrier, generating extremely

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low tunneling rate even when the energy is comparable with or larger than the height of the potential barrier. The eigenstates corresponding to classical orbits that interact with the potential barrier, however, can lead to relatively strong tunneling. In a small energy interval the quantum tunneling rate can thus spared over a wide range. However, when the classical dynamics is chaotic, isolated orbits that do not interact with the potential barrier are far less likely and, consequently, the states associated with low tunneling rates disappear, effectively suppressing the spread in the tunneling rate.

In this letter, we address the question of whether chaos can regularize tunneling in relativistic quantum systems. To be concrete, we study the motion of massless Dirac fermions in the setting of resonant tunneling to facilitate comparison with the non-relativistic quantum case. To solve the Dirac equation in a confined geometry is extremely challenging, particularly due to the difficulty to incorporate zero-flux boundary conditions. We overcome this difficulty by developing a numerical scheme based on constructing a physically meaningful, Hermitian Hamiltonian. Our extensive computations reveal unequivocally the existence of surviving eigenstates that lead to extremely low tunneling rates. As for the non-relativistic quantum case, making the cavities classically chaotic can greatly regularize the quantum tunneling dynamics. To explore the practical implications, we consider resonant tunneling devices made entirely of graphene [3], and calculate the tunneling rate for different energy values. We obtain qualitatively similar results as for massless Dirac fermions. One unique feature for both the Dirac and graphene systems, which finds no counterpart in non-relativistic quantum tunneling devices, is the high tunneling rate in the regime where the particle energy is smaller than the height of the potential barrier. This is a manifestation of the Klein-tunneling phenomenon [6–8]. To explain the numerical findings, we develop a theory based on the concept of self-energies and the complex energy spectrum of the non-Hermitian Hamiltonian for the "open" cavity.

Consider the situation where a relativistic Dirac fermion is confined within a two-dimensional double-well system in which two symmetric cavities are weakly coupled by an electrical-potential barrier placed in between. The system is governed by the Dirac equation $i\hbar\partial_t\psi(t) = \hat{H}\psi(t)$, where the general form of Hamiltonian is given by $\hat{H} = c(\boldsymbol{\alpha}\cdot\boldsymbol{p}) + \beta mc^2$, and ψ is a two-component Dirac spinor. Assuming stationary solution $\psi(t) = \psi\exp(-iEt/\hbar)$, we obtain the steady-state Dirac equation $\hat{H}\psi = E\psi$. In two dimensions, $\boldsymbol{\alpha} = \boldsymbol{\sigma} = (\sigma_x, \sigma_y)$ and $\beta = \sigma_z$ are choices satisfying all anticommutation/commutation relations in Dirac/Lorentz algebra [9]. There are two major challenges in numerically solving the Dirac equation: i) a proper treatment of boundary conditions and ii) an efficient and physically meaningful discretization scheme. Firstly, for boundary conditions, we can either replace the $mc^2\sigma_z$ term by a potential

$U(\boldsymbol{r})\sigma_z$ in the Hamiltonian and let $U(\boldsymbol{r})$ go to infinity outside the domain, or use the vanishing current condition $\boldsymbol{j}\cdot\boldsymbol{n} = 0$, where $\boldsymbol{n}$ is the boundary surface normal. We obtain $\mathrm{Re}(e^{i\theta}\phi/\chi) = 0$, where ϕ and χ are the components of the Dirac spinor, $\psi = (\phi, \chi)^T$, and θ is the argument of the surface normal $\boldsymbol{n}$. It was demonstrated [10] that the condition is $\chi/\phi = i\exp(i\theta)$. When an external potential V is present, such as the barrier in our tunneling problem, E is replaced by $E - V$. Secondly, for a massless fermion, we can write the Dirac equation as

$$[v(\boldsymbol{\sigma}\cdot\boldsymbol{p}) + V]\psi = E\psi, \tag{1}$$

where we have replaced c by v for more generalized cases (*e.g.*, in graphene, the Fermi velocity is $v_F \sim 10^6\,\mathrm{ms}$). Regarding discretization, the difficulty issue is fermion doubling [11,12]. We have developed and validated an efficient discretization scheme, incorporating proper boundary conditions, for solving the Dirac equation in arbitrary geometrical confinements in $(2+1)$ dimensions. Different from the k-p models (with different flavors of the 6-band or 8-band Luttinger-Kohn model), a simple lattice grid is used to discretize the two-dimensional closed space. However, in solving massless Dirac fermion systems, a necessary ingredient designed to eliminate the fermion doubling problem is to evaluate the Dirac equations and the Dirac spinors at two different sets of square lattice points. Specifically, if one evaluates the Dirac spinors at locations (i, j), the Dirac equations have to be evaluated at $(i+1/2, j+1/2)$, otherwise one ends up with two fermions in the first Brillouin zone, which conflicts with the original single-fermion Dirac equation.

For non-relativistic quantum tunneling, due to geometric symmetry in the double-well systems, the eigenstates are either symmetric or antisymmetric about the central barrier. In this case, the tunneling rate is simply proportional to the energy splitting ΔE between the pairing symmetric and antisymmetric eigenstates [4]. However, for relativistic quantum tunneling, only in one spatial dimension can the symmetric and antisymmetric eigenstate pairs be defined. In fact, for both Dirac fermion in $(2+1)$ dimensions and graphene systems, the symmetric and antisymmetric eigenstates are not necessarily in pair. A more general, physically meaningful definition of the tunneling rate is thus needed. Our approach is the following. For an arbitrary symmetric double-well system, first we choose a random linear combination of eigenstates, denoted as $\psi = \sum_n a_n\psi_n(\boldsymbol{r})$. We then set values of ψ on the right side and barrier region to be zero and renormalize it. The new state is denoted as $\bar{\psi} = \sum_n \bar{a}_n\psi_n^L(\boldsymbol{r})$, where $\bar{a}_n$'s are the renormalized coefficients, $\psi_n^L(\boldsymbol{r}) = \psi_n(\boldsymbol{r})$, for $\boldsymbol{r}$ in the left well, and $\psi_n^L(\boldsymbol{r}) = 0$, otherwise. Next, we let this state $\bar{\psi}$ evolve with time and express it in terms of the linear combination of all eigenstates: $\bar{\psi} = \sum_m b_m\psi_m(\boldsymbol{r})$, where the index m runs through all eigenstates. The coefficient b_m can be calculated as $b_m = \int_D \psi_m^*\bar{\psi}\mathrm{d}\boldsymbol{r} = \int_L \psi_m^* \sum_n \bar{a}_n\psi_n^L\mathrm{d}\boldsymbol{r} = \sum_n \bar{a}_n \int_L \psi_m^*\psi_n\mathrm{d}\boldsymbol{r}$, where D and L denote the integration domains of the whole double well
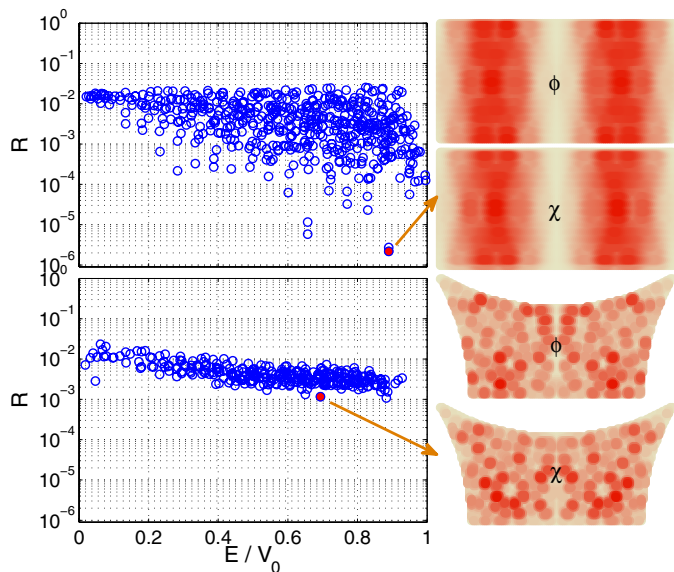
Fig. 2: (Color online) Tunneling rates and LDS patterns for massless Dirac fermion in integrable and chaotic double-well systems, where ϕ and χ are two components of the Dirac spinor. A unit system $\hbar = c = 1$ has been used in our calculations. The barrier height V_0 is about 60 under such unit system. For the rectangle double well, the width and the height are set to 2 and 1, respectively. The bow-tie chaotic shape is obtained by cutting the rectangle with three arcs such that the cut parts are all 0.3 measured on both sides of the baseline and central vertical line of the rectangle. The theoretical ratio of the left-well width to the barrier width should be 24 : 1 for the rectangle, however, this ratio may vary after discretization.

Fig. 3: (Color online) Tunneling rates and LDS patterns in integrable and chaotic graphene double-well systems, where A and B denote the two distinct types of atoms in a graphene unit cell. The tight-binding model is used in the calculation for graphene systems. The barrier height is fixed at $V_0 \sim 0.67t$ (with t denoting the nearest-neighbor hopping integral). After converting to the $\hbar = c = 1$ unit system, the geometric measures and the barrier potential are the same as the single Dirac fermion system.

and the left well, respectively. The time evolution of the state $\bar{\psi}$ is then given by $\bar{\psi}(t) = \sum_m b_m \psi_m e^{-iE_m t/\hbar}$. Because the particle state is initially confined within the left well, to characterize the tunneling process of this state, we calculate the probability that the particle may be found in the left well with respect to time, $P_L(t) = \int_L |\bar{\psi}(t)|^2 d\boldsymbol{r}$. The tunneling rate R can be determined when $P_L(t)$ reaches the minimum for the first time, *i.e.*, $R \equiv \pi \Delta P / \Delta T$, where ΔP is the probability difference between the initial value and the first minimum of $P_L(t)$, and ΔT is the time it takes to reach the minimum. This definition is general because for non-relativistic quantum tunneling where symmetric/antisymmetric eigenstate pairs do exist, it reduces to ΔE.

We now present numerical evidence for the effect of chaos on relativistic quantum tunneling. Figure 2 shows the generalized tunneling rate R *vs.* the normalized energy E/V_0 for massless Dirac fermion in the double-well barrier system for two types of geometry: one classically integrable and another chaotic. For the integrable geometry, we observe the existence of states with extremely low tunneling rates, as indicated by the arrow in fig. 2(a). These correspond to states localized nearly entirely in the left or right side of the potential barrier, which "survive" the tunneling process between the two sides, as indicated
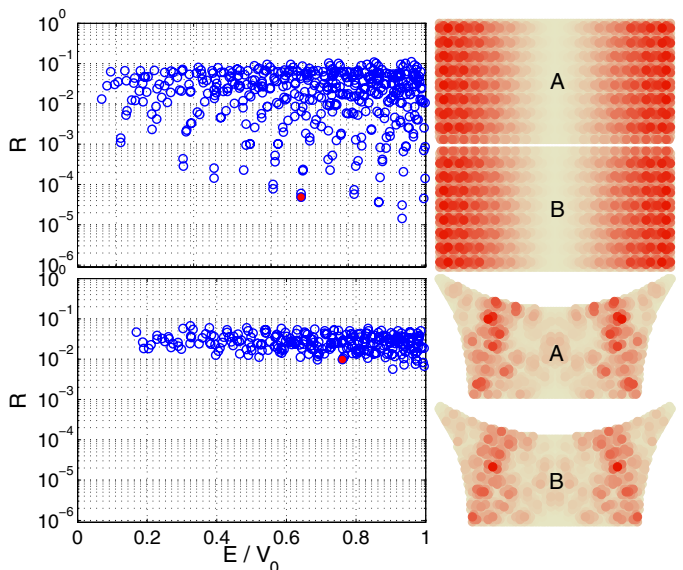
by the accompanying pattern of local density of states (LDS). We note that, in non-relativistic quantum transport, these are effectively quantum pointer states [13,14]. In relativistic quantum systems, we observe that both components of the underlying Dirac spinor exhibit a heavy concentration of the probability in orbits along which particles travel vertically back and forth on either side, parallel to the barrier. For the chaotic geometry, while signatures of pointer states can still be found, they are weak as compared with those in the integrable counterpart, as shown in fig. 2(b) and the accompanying LDS pattern. Analogous behaviors occur when the entire cavity is made of graphene, as shown in fig. 3. Thus, in both Dirac fermion and graphene systems, we observe that classical chaos can greatly suppress the spread in the quantum tunneling rate, as in non-relativistic quantum systems [4].

A common phenomenon between Dirac-fermion and graphene tunneling systems is that, for small energies, pointer states are far less likely than in non-relativistic quantum systems. Consequently, in both systems, the tunneling rate can be quite large even in the small energy regime, as shown in figs. 2 and 3. This is the direct consequence of Klein tunneling [6–8], which finds no counterpart in non-relativistic quantum mechanics where the tunneling rate tends to zero as the energy is decreased to zero [4]. Although both systems show almost identical relativistic behaviors at low energies, and both prove

chaos regularization to be a universal phenomenon across quantum systems, one should not confuse one system with the other. The difference between the two systems lies in the number of massless (quasi-)particles. It is clear that the system described by eq. (1) contains a single massless Dirac fermion. On the other hand, for a graphene system in the low-energy limit, the two electron states at different atoms (commonly called A and B) in a unit cell can be thought of as the two states of a massless quasi-particle's pseudo-spin. However, there are actually two of these massless particles close to the two distinct Dirac points. In the presence of a spatially short-range potential, the coupling between the two Dirac points becomes apparent.

To understand the effect of chaos on relativistic quantum tunneling, we develop a theory based on the self-energy concept widely employed in the study of quantum transport [15,16]. The basic observation is that pointer states generally result in low tunneling rate. Thus, when pointer states are present, the coupling between the two wells is weak. The tunneling rate can thus be approximated as the escaping rate of Dirac fermions between two nearly closed, weakly coupled wells. Let the left well be denoted by superscript (1), and the barrier together with the right well denoted by superscript (2). The Dirac equations for the whole double-well system can be written in terms of the Hamiltonians H_1 and H_2 for the separated closed wells as

$$\begin{bmatrix} H_1 & V_{12} \\ V_{21} & H_2 \end{bmatrix} \begin{bmatrix} \psi^{(1)} \\ \psi^{(2)} \end{bmatrix} = E \begin{bmatrix} \psi^{(1)} \\ \psi^{(2)} \end{bmatrix}, \tag{2}$$

where V_{ij} are the coupling matrices. Note that, if the left well were itself closed, the corresponding equation would be $H_1\psi^{(1)} = E_1\psi^{(1)}$, which becomes $(H_1 + \Sigma^R)\psi^{(1)} = E\psi^{(1)}$ when weak coupling to the right well is taken into account, where $\Sigma^R = V_{12}G^RV_{21}$ is the self-energy due to the barrier and the right well, and $G^R = (E + i\eta - H_2)^{-1}$ is the retarded Green's function. For each eigenstate in the left well, the energy shift can be obtained through first-order perturbation theory as $\langle \Sigma^R \rangle = \langle \psi^{(1)}|\Sigma^R|\psi^{(1)}\rangle$, which is typically complex. The real part of this shift changes the oscillating frequency of the corresponding eigenstate, while the imaginary part, denoted by $-\gamma$, introduces a decay factor $\exp(-c_0\gamma t/\hbar)$ in the time evolution of the probability, which describes the escaping rate of the Dirac fermions from the left to the right well. Note that, since the whole system is closed, γ only describes the transient behavior associated with particle's tunneling from left to right, with any recurring behavior neglected. If we let the right well extend to infinity so that there is no reflection, the system is equivalent to a single left well coupled with a semi-infinite lead through a potential barrier, and γ will be the tunneling rate for the single-left-well system.

To gain insights and also to validate that our proposed quantity γ is indeed proportional to the tunneling rate, we consider a one-dimensional system for which the
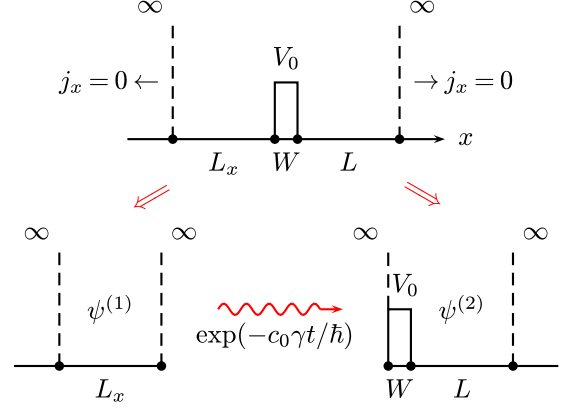

Fig. 4: (Color online) Schematic diagram for one-dimension tunneling.

Dirac equation can be solved and the self-energy and consequently γ can then be calculated analytically through the Green's function, as shown in fig. 4. Specifically, the one-dimensional Dirac equation is $(-i\hbar v\sigma_x\partial_x)\psi = (E - V)\psi$. Since the potential is zero in the left well (of width L_x), the solution is

$$\psi_n^{(1)}(x) = \frac{1}{\sqrt{L_x}}\exp\left(i\frac{\pi}{4}\right)\begin{bmatrix} \cos(k_n x - \frac{\pi}{4}) \\ i\sin(k_n x - \frac{\pi}{4}) \end{bmatrix},$$

where $k_n = (n + 1/2)\pi/L_x$. For the right part, the barrier has width W and $V = V_0$, and the right well has width L and $V = 0$. We obtain the solution

$$\psi_n^{(2)}(x) = \begin{cases} A_1 e^{i\kappa_n x}u_+ + A_2 e^{-i\kappa_n x}u_-, & \text{barrier}, \\ A_3 e^{ik_n x}u_+ + A_4 e^{-ik_n x}u_-, & \text{right well}, \end{cases}$$

where $k_n = E/(\hbar v) = [V_0W/(\hbar v) + (m + 1/2)\pi]/(L + W)$, $\kappa_n = k_n - V_0/(\hbar v)$, $u_+ = (1,1)^T$ and $u_- = (1,-1)^T$ are bases for the spinor, and the coefficients A_i are determined by the boundary conditions. Note that this is a combined solution for both $E < V_0$ and $E > V_0$. To calculate the self-energy $\langle \Sigma^R \rangle$, we discretize the space and introduce the Green's function $G^R(x_i, x_j)$. The self-energy can be expressed as [15]

$$\langle \Sigma^R \rangle = \psi_n^{(1)\dagger}(L_x - a)V_{12}G^R(L_x + a, L_x + a)V_{21}\psi_n^{(1)}(L_x - a),$$

where $x = L_x$ is the junction between the left well and the barrier, and the coupling components are $V_{12} = V_{21}^\dagger = -i\hbar v\sigma_x$. The Green's function can be calculated explicitly in the limit $L \to \infty$. After a substantial amount of algebra we obtain the following expression for the tunneling rate:

$$\gamma = -\frac{(\hbar v)^2}{2\pi L_x}\left[\cos(2ka)\,\mathrm{Im}(C) - \sin(2ka)\,\mathrm{Im}(S)\right] - \frac{\hbar v\eta}{2\pi L_x E},$$

where the quantities S and C are given by

$$S = \int_0^\infty \mathrm{d}k \frac{\sin(2\kappa a)}{E + i\eta - \hbar vk},$$

$$C = \int_0^\infty \mathrm{d}k \frac{\cos(2\kappa a)}{E + i\eta - \hbar vk}.$$
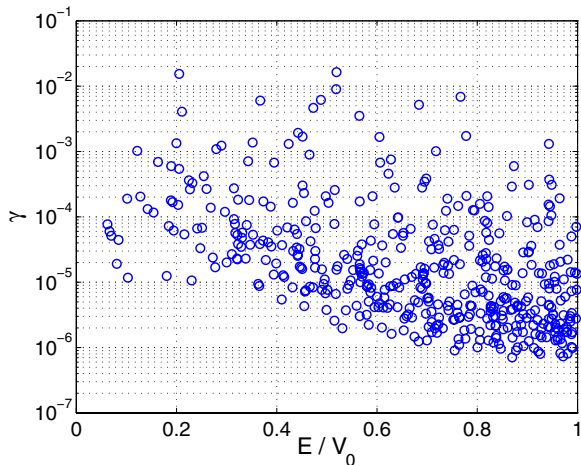
Fig. 5: (Color online) Theoretical tunneling rate γ for Dirac fermion in the two-dimensional ring system as described in the text. The eigenstates associated with the inner and outer ring regions are calculated numerically by solving the Dirac equation with proper boundary conditions. The parameters are $R_1 = 5$, $R_2 = 10$, and $V_0 = 5$. The dimensions for the outer part are $R_3 = 10.2$, and $R_4 - R_3 = 3(R_2 - R_1)$.

The integrals can be evaluated explicitly and we finally obtain $\gamma \approx \hbar v/(2L_x)$. In one spatial dimension the standard tunneling rate ΔE can also be analytically calculated through symmetry considerations. We obtain $\Delta E \approx \hbar v \pi/(2L_x)$ and consequently, $\gamma \approx \Delta E/\pi$. These analytic predictions have been verified numerically.

For tunneling systems in two spatial dimensions, even when the geometry is regular it is not possible to calculate the tunneling rate analytically, due to the entanglement of the two Cartesian coordinates in the Dirac equation. The problem is solvable only for certain special types of boundary conditions for which the variables can be separated. One particular class of such systems is tunneling between two concentric ring regions, where the first cavity is given by $R_1 < r < R_2$, the potential barrier is located in the region $R_2 < r < R_3$, and the second cavity is in the region $R_3 < r < R_4$. When all four radii are large, this ring-shaped double-well tunneling system is topologically equivalent to a rectangular double well with periodic boundary condition in one direction. We have solved the Dirac equation, calculated the Green's function and the self-energy, and finally obtained a close-form expression for the tunneling rate γ, which involves various eigenstates that can be evaluated numerically. A representative behavior of γ as a function of the energy is shown in fig. 5, which is qualitatively similar to that in the rectangular double-well system. Of particular importance to the aim of this letter are pointer states with extraordinarily low tunneling rates, which are the causes of the tunneling spread.

In summary, we have established the phenomenon of chaos-regularized tunneling in the relativistic quantum regime for both Dirac fermion and graphene tunneling systems. While tunneling in non-relativistic quantum mechanics has been well studied, there are two major challenges in investigating the phenomenon in relativistic quantum systems: solution of the Dirac equation in general two-dimensional spatial geometry and physically meaningful definition of the tunneling rate. We have overcome these difficulties and developed numerical methods and analytic theory to reveal the generic features of relativistic quantum tunneling. While we focus on resonant tunneling, the methodology developed here can be extended to other relativistic quantum transport systems, such as various electronic transport devices made of graphene.

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