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Relativistic quantum level-spacing statistics in chaotic graphene billiards

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An outstanding problem in quantum nonlinear dynamics concerns about the energy-level statistics in experimentally accessible relativistic quantum systems. We demonstrate, using chaotic graphene confinements where electronic motions are governed by the Dirac equation in the low-energy regime, that the level-spacing statistics are those given by Gaussian orthogonal ensemble (GOE) random matrices. Weak magnetic field can change the level-spacing statistics to those of Gaussian unitary ensemble for electrons in graphene. For sufficiently strong magnetic field, the GOE statistics are restored due to the appearance of Landau levels.

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A fundamental result in nonrelativistic quantum chaos is that, for systems whose classical dynamics are chaotic, their energy-level statistics correspond to those of random matrices [1,2]. In particular, if the system possesses the time-reversal symmetry, the energy-level spacings follow the distribution of those of random matrices from the Gaussian orthogonal ensemble (GOE). When the time-reversal symmetry is broken, e.g., as in the presence of a magnetic field, the level-spacing statistics are governed by the Gaussian unitary ensemble (GUE) random matrices. Both the GOE and GUE statistics have been observed experimentally for nonrelativistic quantum systems exhibiting chaotic dynamics in the classical limit [3].

In relativistic quantum mechanics, the seminal work of Berry *et al.* [4] establishes that, for massless spin-half particles such as neutrinos [5], if the classical dynamics are integrable, the level-spacing statistics are Poissonian, which are similar to those in the corresponding nonrelativistic quantum systems. However, when the classical dynamics are chaotic, the level-spacing distributions are *persistently* those of GUE, even in the absence of any magnetic field, which is due to the chiral nature of Dirac particles that breaks the time-reversal symmetry. Since its prediction over two decades ago [4], this phenomenon has not been tested experimentally, partly due to the difficulty to construct relativistic quantum systems with chaotic classical dynamics in the laboratory.

Recently, graphene, a single one-atom-thick sheet of carbon atoms arranged in a hexagonal lattice, has been realized in experiments [6]. In the low-energy regime, electronic motions in graphene are characteristic of those of relativistic massless Dirac fermions. Devices made of graphene are potentially capable of operating at much higher speed than those based on the conventional silicon electronics. Graphene confinements that have the geometric shape of chaotic billiards thus represent a potential experimental system for testing energy-level statistics in the relativistic quantum regime [7,8]. In this regard, a Poissonian type of level spacing occurs for rectangular graphene dots, which is consistent with the prediction of Berry *et al.* [4] for classically integrable systems. Increasing the strength of disorder, i.e., edge roughness or defect concentration, tends to push the distribution toward that of GOE [9]. When the disorder concentration becomes higher, a return to the Poissonian distribution occurs, due to the onset of Anderson localization [10]. It then seems quite feasible to test the prediction of Berry *et al.* for the GUE statistics of Dirac particles with classically chaotic graphene-confinement systems.

In this Rapid Communication, we address the following two fundamental questions: (1) what is the main characteristic of relativistic quantum energy-level statistics in chaotic graphene confinements, GOE or GUE? and (2) can a transition between the two types of behaviors be observed when a control parameter is changed? Our extensive computations reveal that, in the absence of magnetic field, GOE statistics arise in graphene in the relativistic quantum regime and are robust. We will argue that this can be explained by the valley symmetry in graphene systems [11]. When an external magnetic field is applied, the time-reversal symmetry is broken, causing a transition in the level-spacing statistics from those of GOE to GUE. However, as the magnetic field becomes stronger, Landau levels set in. Removing energy-level degeneracies in the Landau levels restores the GOE statistics. Our results suggest that GOE characteristics are the main feature of energy-level statistics in chaotic graphene billiards, and they are more likely to be experimentally observed.

For a graphene confinement, the tight-binding Hamiltonian is $\hat{H}=\Sigma(-t_{ij})|i\rangle\langle j|$, where the summation is over all pairs of nearest neighboring atoms [12], and $t_{ij}=t\exp[-i\frac{2\pi}{\phi_0}\int_{\mathbf{r}_j}^{\mathbf{r}_i}d\mathbf{r}\cdot\mathbf{A}]$ is the nearest-neighbor hopping energy. $\mathbf{A}=(-By,0,0)$ is the magnetic vector potential for a perpendicular uniform magnetic field under the Landau gauge, and $\phi_0=h/e=4.136\times10^{-15}$ T m^2 is the magnetic flux quanta, $t\approx2.8$ eV [13,14]. For convenience, we shall use the magnetic flux $\phi=BS$ through a hexagonal plaque as the control parameter, the area of which is $S=\sqrt{3}a^2/2=5.24$ Å^2, where $a=2.46$ Å is the lattice constant of the graphene lattice. Eigenvalues of the Hamiltonian are the energy levels in the confinement.

We shall focus on the energy spectrum around the Dirac point to capture the relativistic quantum characters of the

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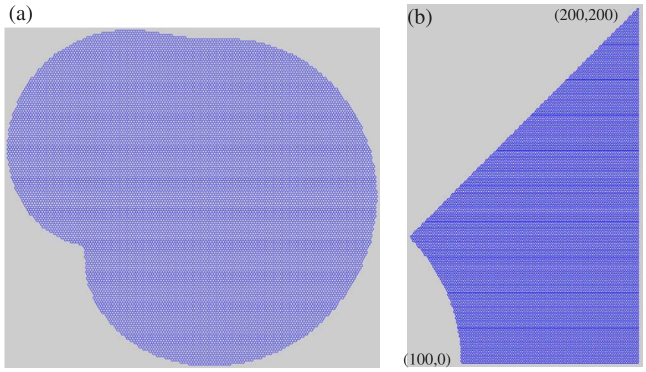

FIG. 1. (Color online) Chaotic graphene billiards. (a) Africa billiard of 42 505 atoms. The outline is determined by the equation $x+iy=70(z+0.2z^2+0.2z^3e^{i\pi/3})a$, where z is the unit circle in the complex plane. The area is $A=1117\ \text{nm}^2$. (b) 1/8 of Sinai billiard with 37 401 atoms. The coordinates are in units of lattice constant a. The area is $A=1.607\times10^4a^2=972\ \text{nm}^2$.

energy levels. This can be achieved by setting the energy in the range $0<E/t<0.4$ so that trigonal warping distortion in the $E(\mathbf{k})$ relation is minimized [15]. Our results can then be compared meaningfully with those from the relativistic neutrino billiards [4]. The presence of magnetic field modifies the energy band structure. To observe the possible transition from GOE to GUE statistics under a magnetic field while ensuring the relativistic quantum behavior, we restrict our study to the regime where the linear $E-\mathbf{k}$ relation is preserved and at the same time, the magnetic field is strong enough so that the GUE statistics may arise. We shall then consider three cases: $\phi=0$ with no magnetic field, $\phi=\phi_0/8000$ ($\sim$10 T) for weak magnetic field, and $\phi=\phi_0/800$ ($\sim$100 T) for strong magnetic field. We shall examine two classically chaotic billiard shapes that are commonly used in the study of level statistics, the Africa billiard [4] and one eighth of the Sinai billiard, as shown in Fig. 1. The boundary atoms with only one nearest neighboring atom are removed to avoid artificial scattering effects. The horizontal direction is zigzag [16].

For a nonrelativistic quantum billiard, the smoothed spectral staircase function for positive eigenvalues is given by [17] $\langle N(k)\rangle=Ak^2/4\pi+\gamma Lk/4\pi+\cdots$, where A is the area of the billiard and L is its perimeter, $\gamma=1$ (or -1) for Neumann (or Dirichlet) boundary conditions. For relativistic spin-half particle, Berry *et al.* obtained the same formula except that $\gamma=0$ [4]: $\langle N(k)\rangle=Ak^2/4\pi-1/12$. For our graphene billiard, around the Dirac point, we have $E=\hbar v_F k$, where $v_F=\sqrt{3}ta/2\hbar$. Once the eigenenergy E_n has been determined, the corresponding wave vector k_n can then be obtained. For the Africa billiard, the index of the wave vector $N(k)$ versus k is shown in Fig. 2(a) for $0<E_n/t<0.4$. A numerical fit gives $\langle N(k)\rangle=Ak^2/2\pi+37$, which differs from that for relativistic spin-half particles in a chaotic billiard in the leading "Weyl" term by a factor of two. This can be understood by noting the existence of two nonequivalent Dirac points in graphene. The difference in the fitting constant is caused by the localized edge states on the zigzag segments along the boundary. For zigzag ribbon the edge states exist when $E<E_c=\hbar v_F/L=\sqrt{3}ta/(2L)$, where L is the width of the ribbon. For our graphene billiards the diameter is about $100a$, leading to $E_c\simeq0.01t$. These states are essentially degenerate states, contributing to an artificial bias of the level-spacing distribution at small values. Therefore we set a minimum value $2E_c$ for E_n to eliminate these states.

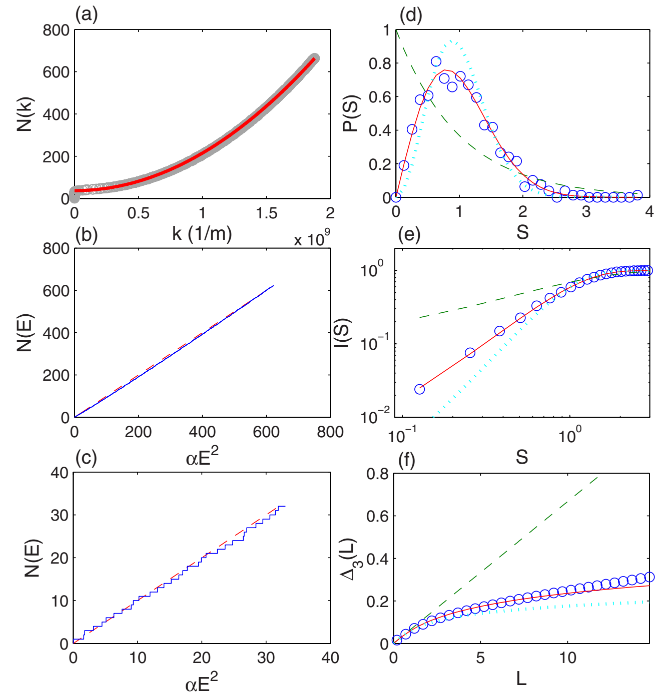

FIG. 2. (Color online) Level spacing statistics for the Africa billiard in Fig. 1(a), $\phi=0$. (a) $N(k)$ versus wave vector k for eigenenergies $0<E_n/t<0.4$ with a total of 664 energy levels (circles). The curve is semiclassical prediction. (b) Staircase function $N(E)$ versus αE^2 for calculated eigenenergies E_n (solid curve). The dashed straight line is the semiclassical prediction. (c) A zoom-in of (b) for $0.02<E_n/t<0.1$ with 33 levels. (d) Unfolded level-spacing distribution $P(S)$. (e) Cumulative unfolded level-spacing distribution $I(S)$. (f) Spectral rigidity Δ_3. (d)–(f) are for energy levels in the range of $0.02<E_n/t<0.4$ with a total of 623 levels (circles), the lines are theoretical predictions from random matrix theories: dashed line is Poisson, solid line is GOE, and dotted line is GUE. The same legend holds for subsequent figures.

Utilizing the linear energy-momentum relation for graphene, the smoothed counting staircase function with respect to the energy is $\langle N(E)\rangle=\alpha E^2+C_2$, where $\alpha=A/(2\pi\hbar^2v_F^2)$ is the unfolding normalization parameter, and C_2 is now 0. Figure 2(b) shows the staircase function of E_n and Fig. 2(c) shows a magnification of Fig. 2(b) in the range $0.02<E/t<0.1$. The dashed lines in these two panels are $\langle N(E)\rangle=\alpha E^2$. We observe a good agreement.

Now define $x_n\equiv\langle N(E_n)\rangle$ as the unfolded spectra. Let $S_n=x_{n+1}-x_n$ be the nearest-neighbor spacing and $P(S)$ be the distribution function of S_n, which satisfies $\int SP(S)dS=1$. For nonrelativistic quantum billiards, the distribution of unfolded level spacings has universal classes. In particular, if classically the system is integrable, the distribution is Poissonian [18]: $P(S)=e^{-S}$. For chaotic billiards that do not possess any geometric symmetry, the distribution follows the GOE statistics if the system has time-reversal symmetry [19,20]: $P(S)=(\pi/2)Se^{-\pi S^2/4}$, and GUE statistics if the system has no

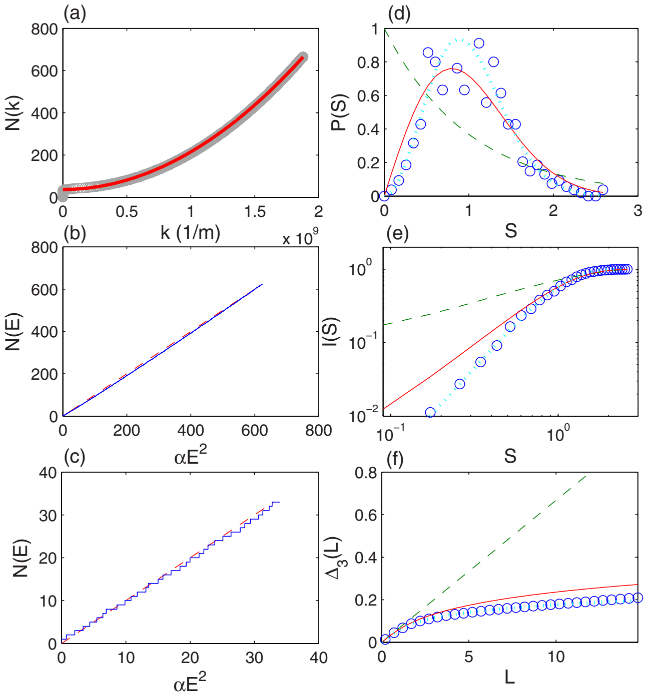

FIG. 3. (Color online) Level-spacing statistics for Africa billiard in Fig. 1(a) in the presence of weak magnetic field: $\phi=\phi_0/8000$. (a) $N(k)$ versus wave vector k for eigenenergies $0<E_n/t<0.4$ with a total of 665 energy levels. (b) Staircase function $N(E)$ versus αE^2 for calculated eigenenergies E_n (solid curve). (c) A zoom-in of (b) for $0.02<E_n/t<0.1$ with 34 levels. (d) Unfolded level-spacing distribution $P(S)$. (e) Cumulative unfolded level-spacing distribution $I(S)$. (f) Spectral rigidity Δ_3.

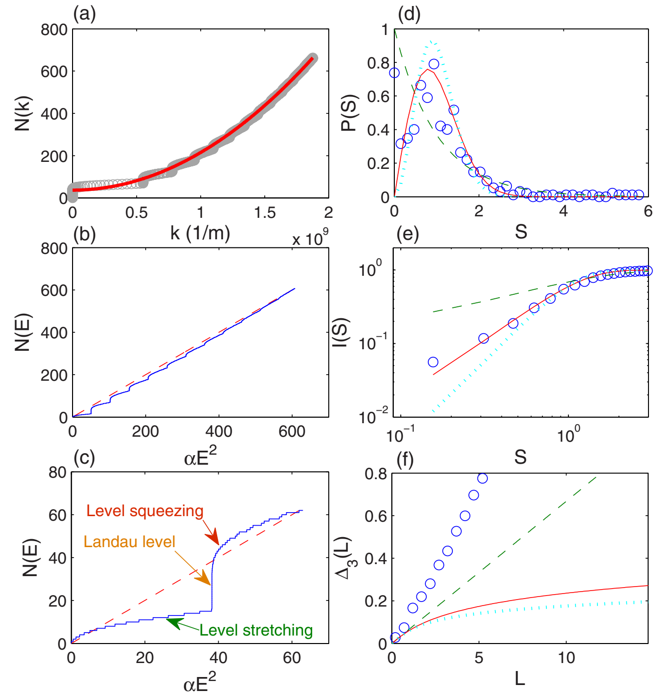

FIG. 4. (Color online) Level-spacing statistics for Africa billiard in Fig. 1(a) in the presence of a strong magnetic field: $\phi=\phi_0/800$. (a) $N(k)$ versus wave vector k for eigenenergies $0<E_n/t<0.4$ with a total of 662 energy levels. The curve is $\langle N(k)\rangle = Ak^2/(2\pi)+37$. (b) Staircase function $N(E)$ versus αE^2 for calculated eigenenergies E_n (solid curve). (c) A zoom-in of (b) for $0.02<E_n/t<0.15$ with 63 levels. (d) Unfolded level-spacing distribution $P(S)$. (e) Cumulative unfolded level-spacing distribution $I(S)$ excluding the first data point in panel (d). (f) Spectral rigidity Δ_3.

time-reversal symmetry: $P(S)=(32/\pi)S^2 e^{-(4/\pi)S^2}$. The cumulative level-spacing distribution are then obtained by $I(S)=\int_0^S P(S')dS'$. Figures 2(d) and 2(e) show, for the Africa billiard, the distribution of the unfolded level spacings and the cumulative distribution, respectively. We see that the level spacings obey the GOE statistics, not the GUE statistics as predicted for spin-1/2 Dirac particles [4]. The GOE characteristics are further supported by the behavior of the spectral rigidity $\Delta_3(L)$ defined as [21] $\Delta_3(L)=\langle \min(a,b)L^{-1}\int_{-L/2}^{L/2}dx\{N(x_0+x)-ax-b\}^2\rangle$, where the average is over x_0, which also has universal classes for nonrelativistic quantum systems. The result from the Africa graphene billiard is shown in Fig. 2(f), where we see that the GOE class represents the closest fit to the numerically obtained $\Delta_3(L)$. For 1/8 of the Sinai billiard in Fig. 1(b), we obtain essentially the same results.

The GOE characteristics in unfolded level-spacing statistics for electrons in graphene contradict the GUE statistics for neutrinos in classically chaotic billiards [4], which seems counterintuitive as both types of particles obey the same massless Dirac equation. However, since the graphene has two nonequivalent Dirac points (valleys), the time-reversal symmetry for the neutrino actually corresponds to the symplectic symmetry for graphene, which is the time-reversal symmetry in a single valley [11]. Thus the time-reversal symmetry breaking caused by the chirality of the neutrino does not imply a time-reversal symmetry breaking in graphene billiards. As a matter of fact, the time-reversal symmetry of graphene, taking into account of both valleys, is preserved in the absence of a magnetic field [11], which explains the observed GOE level-spacing statistics [22].

Adding magnetic field breaks the time-reversal symmetry of graphene, and consequently, the level-spacing distribution becomes that of GUE. Figure 3 plots the same quantities as Fig. 2 for the same Africa billiard under a weak magnetic field $\phi=\phi_0/8000$. Figures 3(a)–3(c) indicate that the energy levels agree well with the semiclassical predictions. The unfolded level-spacing statistics are shown in Figs. 3(d)–3(f), validating the GUE statistics. Essentially the same results are obtained with the Sinai billiard.

In the presence of a strong magnetic field ($\phi=\phi_0/800$), the quantization of the energy levels to Landau levels becomes important. The energy levels are clustered, leading to $\partial N/\partial E\to\infty$, as shown in the plots of staircase function [Figs. 4(a)–4(c)] as the large vertical steps. The staircase counting function remarkably deviates from the semiclassical predictions. The unfolded level-spacing distribution is shown in Figs. 4(d). The high value of first data point is originated from the spacing of energy levels within the Landau levels, which is basically 0 as compared with the normal level spacings. Figure 4(e) shows the cumulative distribution excluding the first point. The results have some deviations from GUE and are in fact closer to GOE. Intuitively, this can be understood that, while the Landau levels squeeze the energy levels around them [Fig. 4(c)], resulting in more small level spacings and a higher $P(S)$ for small S, the squeezing will at the same time stretch the energy levels in between different Landau levels since the overall slope of the staircase counting function is unchanged, yielding large level spacings and a higher $P(S)$ for large S. This forces the level-spacing distribution to go from GUE to GOE. Figure 4(f) shows the spectral rigidity, which does not fall into any of the three known categories. This is because the staircase function no longer follows the semiclassical prediction of universal classes.

In summary, we have studied the fundamental problem of energy-level statistics of chaotic graphene billiards in the relativistic quantum regime. We find that, while electrons in graphene around a Dirac point obey the same massless Dirac equation as spin-1/2 Dirac particles in the free space, the level-spacing statistics are characteristic of GOE in the absence of magnetic field, in contrast to the GUE statistics for the latter. This can be explained by the valley symmetry in graphene. Adding magnetic field breaks the true time-reversal symmetry and yields a transition in the level-spacing statistics from GOE to GUE. However, if the magnetic field is sufficiently strong, around the Dirac point where the density of states is low, the energy levels are quantized into Landau levels, which squeeze the energy levels close to the Landau levels and stretch those in between, changing the level-spacing distribution from GUE to GOE.

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