Quantum Nonlinear Dynamics in Graphene, Optomechanical, and Semiconductor Superlattice Systems

by

Lei Ying

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Graduate Supervisory Committee:

Ying-Cheng Lai, Chair
Dragica Vasileska
TingYong Chen
Yu Yao

ARIZONA STATE UNIVERSITY

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ABSTRACT

Conductance fluctuations associated with quantum transport through quantum-dot systems are currently understood to depend on the nature of the corresponding classical dynamics, i.e., integrable or chaotic. There are a couple of interesting phenomena about conductance fluctuation and quantum tunneling related to geometrical shapes of graphene systems. Firstly, in graphene quantum-dot systems, when a magnetic field is present, as the Fermi energy or the magnetic flux is varied, both regular oscillations and random fluctuations in the conductance can occur, with alternating transitions between the two. Secondly, a scheme based on geometrical rotation of rectangular devices to effectively modulate the conductance fluctuations is presented. Thirdly, when graphene is placed on a substrate of heavy metal, Rashba spin-orbit interaction of substantial strength can occur. In an open system such as a quantum dot, the interaction can induce spin polarization. Finally, a problem using graphene systems with electron-electron interactions described by the Hubbard Hamiltonian in the setting of resonant tunneling is investigated.

Another interesting problem in quantum transport is the effect of disorder or random impurities since it is inevitable in real experiments. At first, for a two-dimensional Dirac ring, as the disorder density is systematically increased, the persistent current decreases slowly initially and then plateaus at a finite nonzero value, indicating remarkable robustness of the persistent currents, which cannot be discovered in normal metal and semiconductor rings. In addition, in a Floquet system with a ribbon structure, the conductance can be remarkably enhanced by onsite disorder.

Recent years have witnessed significant interest in nanoscale physical systems, such as semiconductor superlattices and optomechanical systems, which can exhibit distinct collective dynamical behaviors. Firstly, a system of two optically coupled optomechanical cavities is considered and the phenomenon of synchronization transition
associated with quantum entanglement transition is discovered. Another useful issue
is nonlinear dynamics in semiconductor superlattices caused by its key potential ap-
plication lies in generating radiation sources, amplifiers and detectors in the spectral
range of terahertz. In such a system, transition to multistability, i.e., the emergence
of multistability with chaos as a system parameter passes through a critical point, is
found and argued to be abrupt.
I dedicate my dissertation work to my parents, my advisor, my group members and my friends. Their love is the source of my power moving me forward!
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Chapter 1

INTRODUCTION

1.1 Quantum Chaos and Transport in Two-Dimensional Dirac Systems With Various Geometries or Disorder

Recent years have witnessed a tremendous development and growth of interest in two-dimensional Dirac materials such as graphene [1, 2, 3, 4, 5, 6, 7, 8, 9], topological insulators [10], molybdenum disulfide (MoS$_2$) [11, 12], HITP [Ni$_3$(HITP)$_2$] [13], and topological Dirac semimetals [14, 15]. The quantum physics of these two-dimensional materials is governed by the Dirac equation. Especially there are tremendous recent efforts in graphene [1, 16, 3, 4, 5, 6, 9] due to its relativistic quantum physical properties and its potential for applications in nanoscale electronic devices and circuits. The study of transport in open graphene devices is thus a problem of vast interest [9]. For example, the role played by disorder in conductance fluctuations in graphene was investigated, where anomalously strong fluctuations [17] or suppression of the fluctuations [18] were reported. A recent work has revealed that, in graphene quantum dots, the characteristics of conductance fluctuations also depend on the nature of the classical dynamics similar to those for conventional two-dimensional electron-gas (2DEG) quantum-dot systems [19]. In these recent works, magnetic field is absent. The magnetic properties of graphene, however, are different from those associated with 2DEG systems. For example, in graphene the quantum Hall effect can be observed even at room temperature due to the massless Dirac fermion nature of the quasiparticles and significantly reduced scattering effects [20]. Especially, the linear energy-momentum relation [21, 22] in graphene stipulates that the Landau levels are
distributed according to $\pm \sqrt{N}$, where $N$ is the Landau index, as opposed to the proportional dependence on $N$ in 2DEG systems [23, 24, 25].

A fundamental problem in quantum transport through nanoscale devices is conductance fluctuations. Consider, for example, a quantum-dot system. As the Fermi energy of the conducting electrons is varied, the conductance can exhibit fluctuations of distinct characteristics, depending on the geometrical shape of the dot. Research in the past two decades has demonstrated that the nature of the corresponding classical dynamics can play a key role in the conductance-fluctuation pattern [26, 27, 28, 29, 30, 31, 32, 33, 19, 34, 35, 36, 37, 38, 39, 40, 41, 42]. For example, when the classical scattering dynamics is integrable or has a mixed phase-space structure, there can be sharp resonances in the conductance curve. However, when the classical dynamics is fully chaotic, the conductance variations tend to be smoother. Another tightly related area is quantum chaos, which is referred to as the study of quantum manifestations of chaotic dynamics in the corresponding classical system [43, 44], a field that has been active for more than three decades. In closed chaotic Hamiltonian systems, the basic phenomena that have been and continue to be studied include energy level-spacing statistics [45, 46, 47] and quantum scarring [48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74]. In open Hamiltonian systems, quantum chaotic scattering [40, 75, 28, 76, 41, 34, 35, 36, 77, 78, 79] has been investigated extensively. Quite recently, due to the significant development of graphene physics [1, 2, 3, 4, 7, 8, 9], relativistic quantum manifestations of classical chaos have become an interesting area of study [80, 81, 82, 83, 19, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93]. However, in these works on quantum chaos, the standard setting was that of single-particle quantum dynamics, whereas many-body effects such as electron-electron interactions were ignored. While there were also previous studies of the interplay between many-body interac-
tions and classical chaos [94, 95, 96, 97], these were exclusively for non-relativistic quantum systems described by the Schrödinger equation. To investigate the effect of chaos on relativistic quantum systems with many-body interactions has thus been an outstanding problem, yet it is not only fundamental to physics, but also important for the practical development of relativistic quantum devices. Please see more details in the introduction of Chapter 5.

An important issue in quantum transport is disorder since it is inevitable in real experiments. Disorder normally exists by environmental atoms/molecules, topographic corrugations and electron-density inhomogeneities (charge puddles) [98, 99, 100]. Disorder generally plays a negative role in quantum transport. However, some particular cases in Dirac systems indicate that disorder does not always weaken transport, such as the robust transport in topological insulators with disorder due to its topological-protected edge states [10], topological Anderson insulator [101, 102, 103, 104, 105] and disorder-assist transport in graphene ribbons caused by evanescent states [106, 107, 17, 108]. Therefore, it is more interesting to find new mechanisms in disorder-robust or disorder-enhanced transport phenomena in two-dimensional Dirac systems.

In the dissertation, Chapters 2-5 show works on quantum transport. In Chapter 2, we study conductance fluctuations in graphene quantum-dot systems in the presence of vertical magnetic field with both integrable and chaotic geometries. In Chapter 3, we propose and computationally test a practical scheme to modulate quantum conductance fluctuations in nanoscale graphene devices with rectangular geometry shape by rotating the angle between rectangular device and leads. Chapter 4 introduce the variety of spin polarization in open graphene dots with Rashba spin-orbit coupling by modifying the dot geometries. Chapter 5 uncovers the unique relativistic quantum phenomena caused by classical chaos in the presence of many-body interactions. In Chapters 6 and 7, persistent currents in two-dimensional
Dirac rings with electric disorder and novel disorder-enhanced transport in a light-irradiated graphene ribbon are investigated, respectively. Above main contents are from Refs. [85, 90, 109, 110, 111, 112]

1.2 Nonlinear Dynamics in Quantum Systems

A fundamental and important problem in physics is the understanding of the quantum manifestations of classical nonlinear and complex dynamical behaviors. In this regard, the field of quantum chaos aims to uncover and exploit the various quantum phenomena in systems exhibiting chaos in the classical limit [113, 44]. There is now a large body of literature on quantum chaos, but most works in this field focused on classical Hamiltonian systems of relatively low dimensions, addressing issues such as energy level-spacing statistics [45, 46, 47], quantum scarring [48, 49, 50, 51, 52, 53], and quantum chaotic scattering [40, 75, 28, 76, 41, 34].

The phase space dimension of complex dynamical systems can be rather high due to the number of interacting components. A higher-level description characterizing the mutual relations among the components and the emerging collective behaviors then becomes highly relevant. There are distinct types of collective dynamics in complex systems, such as synchronization [114, 115, 116, 117, 118] and antiphase synchronization [119, 120, 121, 122]. In micro- and nanoscale systems, there is growing interest in exploiting synchronization [123, 124, 125, 126, 127] for significant applications. For example, phase locking in a pair of mechanically coupled nano-beams was demonstrated [128], and the idea of using optical coupling to synchronize micro-mechanical oscillators was exploited [129, 130] for potential application in realizing massive optomechanical oscillator arrays [131, 132]. Recent years have also witnessed growing interest in the quantum manifestations of classical collective dynamics, such as quantum synchronization [133] and entanglement of qubits coupled to a driv-
en dissipative resonator [134], quantum synchronization of van der Pol oscillators with trapped ions [135], quantum-classical transition of correlations of two coupled cavities [136], quantum many-body dynamics in optomechanical arrays [137], and entanglement tongue and quantum synchronization of disordered oscillators [138].

In nonlinear dynamical systems, multistability is a common phenomenon [139, 140, 141, 142, 143, 144, 145, 146, 147, 148, 149]. Earlier works focused on low-dimensional nonlinear dynamical systems with a few [139, 140, 141, 142, 143] and many coexisting attractors [144, 145]. Recently multistability has been uncovered in nanosystems such as the electrically driven silicon nanowire [150, 147] described by nonlinear partial differential equations, as well as in a coupled system of a ferromagnet and a topological insulator [149]. The issue of controlling multistability was also addressed [151, 152, 144, 153, 148]. Multistability was uncovered in semiconductor superlattices as well [154, 155, 156].

There are a large number of nonlinear dynamical phenomena in quantum and ultra-small systems. In this dissertation, two of them, synchronization transition in two coupled optomechanical systems and multistability in semiconductor superlattices, are introduced in Chapters 8 and 9, whose primary contents were published in Refs. [157] and [157], respectively.
CONDUCTANCE FLUCTUATIONS IN GRAPHENE SYSTEMS: IS CLASSICAL DYNAMICS RELEVANT?

2.1 Introduction

There have been tremendous recent efforts in graphene [1, 16, 3, 4, 5, 6, 9] due to its relativistic quantum physical properties and its potential for applications in nanoscale electronic devices and circuits. The study of transport in open graphene devices is thus a problem of vast interest [9]. For example, the role played by disorder in conductance fluctuations in graphene was investigated, where anomalously strong fluctuations [17] or suppression of the fluctuations [18] were reported. A recent work has revealed that, in graphene quantum dots, the characteristics of conductance fluctuations also depend on the nature of the classical dynamics similar to those for conventional two-dimensional electron-gas (2DEG) quantum-dot systems [19]. In these recent works, magnetic field is absent. The magnetic properties of graphene, however, are different from those associated with 2DEG systems. For example, in graphene the quantum Hall effect can be observed even at room temperature due to the massless Dirac fermion nature of the quasiparticles and significantly reduced scattering effects [20]. Especially, the linear energy-momentum relation [21, 22] in graphene stipulates that the Landau levels are distributed according to $\pm \sqrt{N}$, where $N$ is the Landau index, as opposed to the proportional dependence on $N$ in 2DEG systems [23, 24, 25].

In this work, we study conductance fluctuations in graphene quantum-dot systems in the presence of magnetic field. Our main results are two. Firstly, in the
parameter plane spanned by the perpendicular magnetic flux and the Fermi energy, there are regions of regular and random conductance oscillations, respectively. As the Fermi energy or the magnetic flux is changed, the fluctuations can be either regular or random, implying a kind of “coexistence” of regular and irregular conductance fluctuations as a single physical parameter is varied. Secondly, an experimentally significant issue is how conductance fluctuations are affected by the size of the quantum dot in the presence of a perpendicular magnetic field. In a previous experimental study [158, 159, 160] of quantum dots of size ranging from 0.7 $\mu$m to 1.2 $\mu$m, the authors found nearly periodic conductance oscillations as the magnetic-field strength is varied. The frequency of the oscillation pattern, the so-called magnetic frequency, was found to follow a scaling relation with the edge size of the dot [158, 159, 160]. In a recent study of the magnetic scaling behavior in graphene quantum dots [161, 162], it was found that for small dots of edge size less than 0.3 $\mu$m, the magnetic frequency exhibits a scaling relation with the dot area. Here we shall focus on an important set of scarred orbits and examine the resulting conductance oscillations. We find that, for graphene quantum dots, below the first Landau level, the conductance exhibits periodic oscillations with the magnetic flux and with the Fermi energy. In fact, the magnetic frequency scales linearly with the dot size. However, the energy frequency, the inverse of the variation in the Fermi energy for the conductance to complete one cycle of oscillation, scales inversely with the dot size. Beyond the regime of periodic conductance oscillations, new sets of scarred orbits emerge and evolve as successive Landau levels are crossed, each with its own period, leading to random conductance fluctuations. The remarkable feature is that these scaling behaviors are independent of the nature of the underlying classical dynamics, i.e., regular or chaotic. Considering that a large body of existing literature points to the critical role played by the nature of the classical dynamics in conductance fluctuations
[26, 27, 28, 29, 30, 31, 32, 33, 19, 34, 35, 36, 37, 38, 39, 40, 41, 42], our finding that the presence of magnetic field can greatly suppress this sensitivity to classical dynamics is striking.

The rest of this chapter is organized as follows. Section 2.2 describes briefly the tight-binding Hamiltonian and the non-equilibrium Green’s function method to calculate the conductance for graphene quantum dots. Extensive evidence of periodic conductance oscillations and the emergence of random conductance fluctuations is presented in Sec. 2.3. In Sec. 5.4, we develop a theoretical understanding of the numerical results based on the emergence of edge states and semiclassical quantization. Conclusive remarks are presented in Sec. 6.5.

### 2.2 Graphene Quantum Dots and Conductance Calculation

We use the standard tight-binding framework [163] to compute the conductances through graphene quantum dots of various geometrical shapes, where $p_z$ orbitals and nearest-neighbor hopping are assumed. The tight-binding Hamiltonian has the form

\[ H = \sum_{i,j} -t_{ij}(c_i^{\dagger}c_j + H.c.), \]  

(2.1)

where the summation is over all nearest-neighbor pairs and $c_i^{\dagger}$ ($c_j$) is the creation (annihilation) operator, $t_{ij}$ is the hopping energy [6] from atom $j$ and to atom $i$, and the on-site energy has been set as the reference energy as it is the same for all the atoms. In the absence of magnetic field, the nearest-neighbor hopping energy is $t_{ij} = t_0 = 2.7 eV$. When a perpendicular uniform magnetic field $B$ with vector potential $A = (−By, 0, 0)$ is applied, the hopping energy is altered by a phase factor:

\[ t_{ij} = t_0 \exp(-i2\pi\phi_{i,j}), \]  

(2.2)

where $\phi_{i,j} = (1/\phi_0)\int_j^i A \cdot dl$, and $\phi_0 = h/e = 4.136 \times 10^{-15} T m^2$ is the magnetic flux quanta. For convenience, we use magnetic flux through a hexagonal plaque of
Figure 2.1: Schematic illustration of hexagonal, square and stadium shaped graphene quantum dots in a perpendicular magnetic field. Note that the magnetic field exists only in the device region.

graphene, $\phi = BS$, as a control parameter characterizing variations in the magnetic-field strength, where $S$ is the area of the hexagonal plaque composed of six carbon atoms. Thus, $S_0 = 3\sqrt{3}a_0^2/2$, where $a_0 = 1.42\text{Å}$. Here, we treat graphene devices as flat two-dimensional systems. Large ripples modify the hopping and can induce localization and additional transport fluctuations [164, 165, 166, 167, 168, 169, 170].

At low temperature, the conductance $G$ of a quantum-dot device is approximately proportional to transmission $T$ and is given by the Landauer formula [171]: $G(E) = (2e^2/h)T_G(E)$. The standard non-equilibrium Green’s function (NEGF) method [172, 173] can be used to calculate the transmission, which can be expressed by [163, 174]

$$T(E) = \text{Tr}(\Gamma_L G_D \Gamma_R G_D^\dagger),$$

(2.3)

where $G_D$ is the Green’s function of the device given by $G_D = (EI - H_D - \Sigma_L - \Sigma_R)^{-1}$, $H_D$ is the Hamiltonian of the closed device, the semi-infinite leads are accounted for by the self-energies $\Sigma_L$ and $\Sigma_R$, and $\Gamma_{L,R}$ are the coupling matrices given by

$$\Gamma_{L,R} = i(\Sigma_{L,R} - \Sigma_{L,R}^\dagger).$$

(2.4)

The local density of states (LDS) for the device is

$$\rho = -\frac{1}{\pi} \text{Im}[\text{diag}(G_D)].$$

(2.5)
To be representative, we consider graphene quantum dots of three different geometric shapes: hexagonal, square and stadium, as shown in Fig. 2.1. Hexagonal geometry is interesting due to the graphene lattice symmetry, i.e., the boundaries consist of zigzag edges only. Thus, regardless of the device size, the boundaries remain to be zigzag. The square geometry has both zigzag and armchair boundaries along the two perpendicular directions, respectively. The classical dynamics in these two structures are integrable. The stadium shaped quantum dot, however, has chaotic dynamics in the classical limit, which has been used as a paradigmatic system in the quantum-chaos literature to explore various quantum manifestations of classical chaos [43].

The geometrical parameters of the three types of devices are as follows. For the hexagonal geometry the height (the distance between the two parallel boundaries) is 10.934nm. The width of the lead is 1.136nm, which is chosen somewhat arbitrarily. For the square device the width is 10.934nm and the width of the lead is 1.136nm so that the overall size is comparable to the hexagonal dot. The size of the rectangular part of the stadium dot structure is 16.898nm×10.988nm and its lead width is 1.988nm.

2.3 Nearly Periodic Conductance Oscillations and Emergence of Random Conductance Fluctuations

Figures 2.2-2.4 are representative examples of conductance variations either with the Fermi energy for fixed magnetic flux or with the magnetic flux for fixed Fermi energy, for the hexagonal, square, and stadium dot shape, respectively. In all cases, a critical point can be identified unequivocally (denoted by either $E_1$ or $\phi_1$), where the conductance variations are nearly periodic on one side of the point and random on the other side. In particular, for all three geometrical shapes, for fixed magnetic
Figure 2.2: Conductances of the hexagonal shaped quantum dot. The height of the dot is $W_D = 10.934 \text{nm}$ and the lead width is $W_L = 1.136 \text{nm}$. The device region contains 4158 carbon atoms. (a) Conductance versus the Fermi energy $E_F$ for fixed magnetic field $\phi = 0.005\phi_0$. The energy values of the shown LDS patterns are those of the Landau levels: $E_1 = 0.2350t$, $E_2 = 0.3395t$, $E_3 = 0.4100t$ and $E_4 = 0.4730t$, respectively. (b) Conductance versus the magnetic flux $\phi$ for fixed Fermi energy $E = 0.35t$. At this energy, there are Landau levels located at $\phi_1 = 0.0115\phi_0$, $\phi_2 = 0.0057\phi_0$, $\phi_3 = 0.0037\phi_0$, and $\phi_4 = 0.0024\phi_0$ (from large to small). The corresponding LDS patterns are also shown.

For fixed Fermi energy, the conductance variations are regular for $\phi > \phi_1$ and random for $\phi < \phi_1$. Better insights into the transition from regular to random conductance variations (or vice versa) can be gained by examining the typical LDS patterns about the critical point. For example, for the hexagonal geometry, there is a circularly localized pattern at $E_1 = 0.2350t$, as shown in Fig. 2.2(a), where the conductance of the dot structure is effectively zero due to the localization of conducting electrons inside the device. Figure 2.2(a) also displays several similar, recurring LDS patterns at $E_2$, $E_3$, and $E_4$. The ratios among these energy values are $E_1 : E_2 : E_3 : E_4 =$
1 : 1.44 : 1.74 : 2.01 ≈ 1 : \sqrt{2} : \sqrt{3} : 2. We observe that the energy values are approximately proportional to $\sqrt{N}$, where $N$ is the index of $E_N$. These behaviors have also been observed for the square and stadium shaped quantum dots. For example, Fig. 2.3(a) shows, for the square geometry, occurrences of the transition between regular and random conductance fluctuations at $E_1 : E_2 : E_3 = 0.2344t : 0.3289t : 0.4021t \approx 1 : \sqrt{2} : \sqrt{3} : 2$ for fixed magnetic flux $0.005\phi_0$. The ratio is also consistent with the Landau level distribution as in Eq. (2.6) below. In Fig. 2.3(b), the Fermi energy is fixed at $E = 0.4t$, and the transition points are $\phi_1 : \phi_2 : \phi_3 = 0.01508\phi_0 : 0.00756\phi_0 : 0.00501\phi_0 = 1 : 1/1.99 : 1/3.00$, which are consistent with Eq. (2.7) (to be discussed below). For the stadium shaped device, the conductance curve shares the same features as Figs. 2.2 and 2.3. The transition points (as indicated in the figure and the caption) also fit into the same Landau level distribution as given by Eqs. (2.6) and (2.7) below. These numerical results indicate that the coexistence of regular and random conductance fluctuations and the transitions between them are determined by the Landau levels, regardless of the geometric shape of the graphene quantum dot. Note that, however, the LDS patterns do depend on the geometrical shape of the dot.

In non-relativistic quantum, 2DEG systems of infinite size, the Landau levels are distributed linearly with the level index $N$ as $E_N = (N + 1/2)(eB\hbar/m)$. However, for relativistic quantum quasiparticles in graphene, due to the linear energy-momentum relation $E = v_F k$ near the Dirac point, the Landau levels are distributed according to [175]

$$E(N) = \pm \omega_c \sqrt{N}, \tag{2.6}$$

where $\omega_c = \sqrt{2}v_F/\ell_B$ is the cyclotron frequency of Dirac fermions (electrons) and $\ell_B = \sqrt{\hbar/eB}$ is the magnetic length. When a Landau level rises, the charge carriers are localized approximately at the center of the device, leading to a near-zero conduc-
tance. The numerically obtained LDS patterns thus indicate that the critical energy values, for example, in Fig. 2.2(a), are nothing but the Landau levels.

From Eq. (2.6), we can obtain the corresponding Landau levels in terms of the magnetic flux for fixed Fermi energy:

$$B(N) = \frac{\hbar E^2}{2ev_F^2} \frac{1}{N}.$$  (2.7)

This formula can be verified by noting that, for example, as shown in Fig. 2.2(b), for fixed Fermi energy at $E = 0.35t$ in the hexagonal dot, varying the magnetic field also partitions the conductance curve into different regions with regular and random conductance fluctuations. The critical magnetic fluxes are $\phi_1 = 0.0115\phi_0$, $\phi_2 = 0.0057\phi_0$, $\phi_3 = 0.0037\phi_0$ and $\phi_4 = 0.0024\phi_0$, leading to the approximate ratios of $1 : 1/2 : 1/3 : 1/4$, which is consistent with Eq. (2.7).

2.4 Semiclassical Theory of Regular Conductance Oscillations and Universal Transition to Random Conductance Fluctuations

Our numerical computations indicate strongly that the emergence and properties of the Landau levels are key to understanding the origin of regular conductance oscillations in the presence of magnetic field. In fact, significant physical insights can be gained from the phenomenon of integer quantum Hall effect in semiconductor 2DEG systems, which is a direct manifestation of the evolution of the Landau levels. In that case, when the magnetic field strength is fixed and the Fermi energy is increased, the conductance reaches minimum when the Fermi energy is at a Landau level and takes on a much larger value when the Fermi energy is in between two neighboring Landau levels. This is contrary to the behavior of the density of the states, which is appreciable only at the Landau levels. The basic reason is that, for a quantum dot, at the Landau level the charge carriers tend to be localized in the central region.
Figure 2.3: Conductance variations in a square graphene quantum dot of side length $W_D = 10.934\text{nm}$ and lead width $W_L = 1.136\text{nm}$, which contains 4802 atoms. (a) For fixed magnetic flux, Landau levels are located at $E_1 = 0.2344t$, $E_2 = 0.3289t$ and $E_3 = 0.4021t$, and so on. In (b) where the Fermi level is fixed, the transition points are $\phi = 0.01508\phi_0$, $0.00756\phi_0$, $0.00501\phi_0$, and so on.

of the dot, and so cannot participate in the transport process. However, when the Fermi energy is in between two adjacent Landau levels, edge states arise which circulate around the boundary of the quantum dot, facilitating a strong coupling with the propagating modes in the semi-infinite leads and resulting in a large conductance. In our case, there is a new feature. Between two neighboring Landau levels, the energy difference $\Delta E_h$, where the subscript "h" stands for Hall effect, is enormous so that, besides the formation of the circular edge states associated with the quantum Hall effect, another class of circular edge states can be formed, as stipulated by the semi-classical Bohr-Sommerfield quantization condition. This introduces another energy period $\Delta E_q$, where "q" stands for quantization, in which the Bohr-Sommerfield edge states form and disappear. Since the circular edge states facilitate transport through the quantum dot and since $\Delta E_q$ is typically smaller than $\Delta E_h$, the fulfillment of
Figure 2.4: Conductance variations in the stadium geometry. The rectangular region of this chaotic dot has the dimensions $W_D = 16.898\text{nm}$ and $10.988\text{nm}$, and the lead size is $W_L = 1.136\text{nm}$. The stadium shape contains 6410 atoms. Energy Landau levels are located at $E_1 = 0.263t$, $E_2 = 0.369t$ and $E_3 = 0.4471t$, and so on for fixed magnetic flux. For fixed Fermi energy $E = 0.3t$, the magnetic Landau levels occur at $\phi = 0.0084\phi_0$, $0.0042\phi_0$, $0.0028\phi_0$, and so on.

The semiclassical quantization condition contributes to fine-scale oscillations in the conductance curve.

To exploit the Bohr-Sommerfield quantization condition for the edge states in graphene, it is convenient to modify the size of the device but keep the geometric shape unchanged. Without loss of generality, we focus on the hexagonal geometry that possesses zigzag boundaries. We choose (somewhat arbitrarily) several heights of the hexagonal devices: $W_{D1} = 19.454\text{nm}$, $W_{D2} = 10.934\text{nm}$, and $W_{D3} = 6.674\text{nm}$ with the relative ratio $W_{D1} : W_{D2} : W_{D3} = 2.9 : 1.7 : 1$. Figure 2.5 shows, for these devices, periodic conductance oscillations below the first Landau level.

Bohr-Sommerfield quantization theory stipulates that the action integral for two successive edge states satisfies the condition [176] $\Delta I = h$, where $h$ is the Planck
Figure 2.5: Conductance oscillations in hexagonal quantum dots of different sizes. The device width for (a) and (d) is $W_D = 19.454\text{nm}$ and it contains 12938 atoms, for (b) and (e) it is $W_D = 10.934\text{nm}$ and the device has 4158 atoms. In (c) and (f), the device has width $W_D = 6.674\text{nm}$ and 1616 atoms. Every sub-figure indicates the period of the regular oscillations.
constant and \( I = \oint \mathbf{p} \cdot d\mathbf{q} \). In the presence of a magnetic field with vector potential \( \mathbf{A} \), the generalized momentum is \( \mathbf{p} = \hbar \mathbf{k} + e \mathbf{A} \) and the wave vector \( \mathbf{k} \) has the same direction as \( d\mathbf{q} \). For a given periodic orbit of length \( L \), we have

\[
I = |\mathbf{p}|L = \hbar |\mathbf{k}|L + eBS, \tag{2.8}
\]

where \( S \) is the area that the periodic orbit encloses in the physical space. For a fixed magnetic-field strength, we then have \( \Delta k \cdot L = 2\pi \), where \( L \) is length of the periodic orbit. For graphene, we have \( E = \hbar v_F k \) near the Dirac point, so the relationship between the energy interval \( \Delta E_q \) due to the quantization condition and the length of the periodic orbit is

\[
\Delta E_q = \hbar v_F /L. \tag{2.9}
\]

Due to the different boundary conditions in two dimensions, we only test the ratio of the energy interval. In Figs. 2.5(a), 2.5(c) and 2.5(e), the energy intervals can be determined, giving the ratios \( \Delta E_{q1} : \Delta E_{q2} : \Delta E_{q3} = 1/L_1 : 1/L_2 : 1/L_3 = 1 : 1.76 : 2.92 \), which are quite close to the inverse ratios of the device size \( 1/W_D_1 : 1/W_D_2 : 1/W_D_3 = 1 : 1.7 : 2.9 \). Moreover, for \( L = W_D \), we can estimate the Fermi velocity \( v_F = \Delta E_q W_D /\hbar \approx 10^6 \text{m/s} \), which is close to the Fermi velocity calculated from the dispersion curve. This means that the length of the circulating orbit is comparable to the device height, indicating that the effective diameter of the orbit is smaller than that of the device. We thus see that the regular conductance oscillations are a consequence of the Bohr-Sommerfield quantization of the edge states between two Landau levels. In particular, when the quantization condition is satisfied, a strong LDS pattern emerges at the edge of the device, as shown in Fig. 2.6, which bridges with the transmitting modes in the two leads and leads to the peak value \( 2e^2/\hbar \) for the conductance. On the contrary, when the quantization condition is violated, edge states cannot form, giving rise to minimal conductance. Similarly, for fixed
Fermi energy, or equivalently, fixed wave-vector (from the dispersion relation), the quantization condition becomes $\Delta(\epsilon BS) = h$, or

$$\Delta \phi = \Delta BS = \phi_0,$$  \hspace{1cm} (2.10)

where $\phi_0 = h/e$ is the magnetic flux quanta. Since the edge states typically circulate the device boundaries, $S$ is proportional to the area of the device. From Figs. 2.5(b), 2.5(d), and 2.5(f), we obtain $\Delta \phi_1 : \Delta \phi_2 : \Delta \phi_3 = 1 : 3.2 : 9 \approx 1/W_{D1}^2 : 1/W_{D2}^2 : 1/W_{D3}^2$. Compared with the numerical results of $\Delta E_q$, the error in $\Delta \phi_q$ is larger due to our approximation of $S$. When the area surrounded by the circulating orbit is determined more precisely, we find that the magnetic quantization condition Eq. (2.10) is satisfied. Note that in the absence of magnetic field or if the field is weak, edge states occur only at zigzag boundaries. However, under a strong magnetic field (above the first Landau level), edge states can emerge for both armchair and zigzag boundaries.

From the above analysis of the Bohr-Sommerfield quantization condition, we find that the conductance oscillations are related to the Fermi energy, the magnetic-field strength, and the size of the device. To obtain a quantitative scaling relationship among those parameters, we develop the following physical analysis. Theoretically, the size of a device is related to the electron cyclotron radius at the Fermi energy, because only the electrons near the Fermi surface contribute to device transmission or conductance. The ratio of the cyclotron surrounding area and perimeter is given by \[ S/L = k_F \ell_B^2, \]  \hspace{1cm} (2.11)

where $D \equiv S/L$ can be regarded as a single parameter characterizing the device size. In a graphene system, the energy near a Dirac point is proportional to the Fermi wave-vector $k_F$: $E_F = \hbar v_F k_F$, or $k_F = E_F/(\hbar v_F)$, where the Fermi velocity is given
Figure 2.6: A hexagonal geometry device with 4158 atoms. Colors of the contour lines represent conductance $G/G_0$. The red dash lines are four Landau-levels, which divide the $G \sim E \sim \phi$ contour into several distinct regions. In each region, there are one or several conductance fluctuation patterns (patterns 1,2,3). Each conductance pattern corresponds a distinct LDS pattern.
by \( v_F = \sqrt{3}t_0a/2\hbar \) and \( a = 2.46\,\angstrom \) is the graphene lattice constant. Substituting these back into Eq. (2.11), we obtain the relationship of Fermi energy \( E \), the device size \( D \), and the magnetic flux \( \phi \) as follows:

\[
S/L = \frac{2hS_0}{\sqrt{3}e\hbar t_0} \frac{E}{\phi}, \quad (2.12)
\]

or in a different form as (for a given, fixed device size)

\[
S/L = \frac{2hS_0}{\sqrt{3}e\hbar t_0} \frac{\Delta E}{\Delta \phi}. \quad (2.13)
\]

This relation can be used to infer the characteristic size \( D \) of the device from the conductance oscillations. For example, for the hexagonal geometry, \( S = \sqrt{3}D^2/2 \) and \( L = 2\sqrt{3}D \). The scaling relation can be modified to

\[
D_{hex} = \frac{12hS_0}{\sqrt{3}e\hbar t_0} \frac{\Delta E}{\Delta \phi}, \quad (2.14)
\]

which can be readily verified numerically. In particular, since the curves shown in Fig. 2.5 are for the edge states circulating the device, we can use \( \Delta E \) and \( \Delta \phi \) from the figure to infer the corresponding values of \( D \), which yields \( D_1 = 13.926\,\text{nm} \), \( D_2 = 7.836\,\text{nm} \), and \( D_3 = 4.734\,\text{nm} \). Comparing with the actual size of the dot \( W_D \) as described in the caption of Fig. 2.5, we observe somewhat large discrepancies. However, if we compare the ratios, we have \( D_1 : D_2 : D_3 = 2.94 : 1.655 : 1 \), which are extremely close to the ratios of the actual dot sizes \( W_{D1} : W_{D2} : W_{D3} = 2.915 : 1.640 : 1 \). We also see that, for the three dot sizes, the ratio \( W_D/D \) is the same, which is about 1.4. The discrepancies in the actual size are caused by the approximation in Eq. (2.11) and by the assumption that the diameter of the circulating orbits is equal to the device size. Nevertheless, since the estimated values of \( D \) and \( W_D \) are of the same order of magnitude, it can be used to infer the dot size from the conductance oscillations versus the Fermi energy and the magnetic flux, which can be used as corroborative evidence and be compared with other direct/indirect measurements.
The scaling relation (2.14) may be feasibly observed experimentally in graphene quantum dots because, for low Fermi energy, the underlying phenomenon emerges even when the applied magnetic field is weak, i.e., \( \phi \to 0 \). For conventional semiconductor 2DEG systems with a parabolic energy-momentum relation, similar scaling can in principle be observed but only for enormous magnetic field, as we have verified numerically. In particular, for a graphene quantum dot of size \( D \sim 1\mu m \), the minimal required magnetic-field strength to observe the periodic conductance oscillations is about \( 3T \). For semiconductor 2DEG systems, we have \( E = \hbar^2 k^2 / 2m^* \) and \( D = k \ell_B^2 \). The scaling relation becomes \( D = \sqrt{2m^*E/eB} \), where \( m^* \) is the effective mass of the electron. While for a 2DEG device of the same size as \( 1\mu m \) made of GaAs/AlGaAs heterogeneous structure, the minimum magnetic field required is about \( 10T \).

To obtain a global view of the conductance oscillations/fluctuations in terms of a combination of Eqs. (2.6) and (2.7), we overlay the Landau levels on top of the contour plot of the conductance versus both energy \( E \) and magnetic flux \( \phi \) for the hexagonal dot, as shown in Fig. 2.6. We see that the Landau levels divide the whole parameter space of \( (E, \phi) \) into different regions with behaviors ranging from regular, parallel line patterns to complicated irregular patterns [177]. We have analyzed the case that the Fermi energy is below the first Landau level, where the edge states recur with the period \( \Delta E_q \), leading to regular conductance oscillations of the same energy period. For \( E_F > E_1 \), there are two sets of edge states, leading to two uncorrelated repetitive patterns, each with its own period \( \Delta E_q \). This is also manifested in Fig. 2.6 for the hexagonal dot that, in region 2 (between the first and the second Landau levels), there are two sets of conductance lines: one with the same slope as in region 1 (the overlapped gray lines) and another with a larger slope (brown lines) that originates in this region but persists in regions between higher Landau levels. In region 3 a new pattern appears, as indicated by the blue dashed lines in Fig. 2.6. The corresponding
edge states are also shown in Fig. 2.6 for these typical line segments. We see that, for a fixed magnetic flux, as the Fermi energy is increased across a Landau level, a new set of edge states appears, adding a new set of line segments in the conductance plot. Since the energy period \( \Delta E_q \) is uncorrelated for different types of edge states, as can be seen from Fig. 2.6, the conductance will fluctuate randomly when there are many sets of edge states. This explains the transition from regular conductance oscillations to random conductance fluctuations, as shown in panel (a) of Figs. 2.2-2.4. A similar analysis can be carried out when the magnetic flux is varied [panel (b) of Figs. 2.2-2.4]. Since the transition is caused by the crossing of Landau levels and the variation of the edge states, it holds regardless of the detailed geometric shape of the quantum dot and the nature of the underlying classical dynamics, i.e. integrable or chaotic. The transition can thus be characterized as universal.

While our discussion has been focused on the hexagonal dot, here we briefly show that the same mechanism leading to regular conductance oscillations and the transition to random fluctuations holds for other geometries as well. To demonstrate this in a comprehensive manner, we show in Fig. 2.7 the conductance in the \((\phi, E)\) plane for all the three cases. We see that the conductance is symmetric with respect to reversal of the magnetic flux \( T(\phi) = T(-\phi) \) due to the two-terminal characteristic of our device [163]. The patterns of the conductance oscillations and fluctuations for the three cases are apparently similar, due to the fact that the patterns are all partitioned by the Landau levels [e.g., Eq. (2.6)] that do not depend on the geometric details of the device. However, the fine structures can be different. Firstly, below the first Landau level, the slopes of the line patterns indicate the size of the device because the edge states are exactly circulating the “edge” of the device (Fig. 2.6), which are slightly different for the three cases. Secondly, above the first Landau level, the details of the conductance patterns are more distinct. This is because, in contrast
Figure 2.7: (a-c) Conductance $G(E, \phi)$ for the hexagonal, square and stadium shaped graphene quantum dots, respectively, where the colors indicate the values of the conductance.
to the edge states below the first Landau level, these states are now more dispersive and also depend on the shape of the device (comparing the LDS patterns in Figs. 2.2-2.4). Thirdly, conductance fluctuations in the chaotic stadium billiard tend to be more smooth as compared with those in the two integrable cases [81, 178]. This feature is especially pronounced in the small-ϕ regime. When the classical dynamics is chaotic, the characteristic energy scale in the conductance-fluctuation pattern of the underlying quantum dot tends to be much larger [19], leading to a smoother variation. For quantum dots with integrable or mixed dynamics, there are sharp resonances in the conductance-fluctuation curves. This can be seen, e.g., from the sudden change of the color scale from blue to red, or vice versa, in Fig. 2.7(b) for ϕ ~ 0. [In the chaotic case, the change in the color scale is much more smooth, as shown in Fig. 2.7(c)]. In addition, in the chaotic graphene quantum dot, there is level repelling, which can also be seen from Fig. 2.7(c) in the ϕ ~ 0 regime where the conductance lines tend to avoid each other, a feature that is absent in both Figs. 2.7(a) and 2.7(b).

2.5 Conclusion

Previous works on conductance fluctuations associated with transport through nanoscale, quantum-dot systems emphasized the difference between situations where the underlying classical dynamics are chaotic or integrable [26, 27, 28, 29, 30, 31, 32, 33, 19, 34, 35, 36, 37, 38, 39, 40, 41, 42]. A general understanding is that Fano-type [179] of sharp resonances typically occur in dot systems with integrable classical dynamics, and chaos can effectively smooth out these resonances quantum-mechanically. This picture holds for both 2DEG and graphene systems in which the quantum dynamics are non-relativistic and can be relativistic, respectively, and it has been suggested recently [84] that altering classical chaos can effectively modulate quantum transport in terms of conductance-fluctuation patterns.
We find that the presence of magnetic field can alter the existing understanding of the quantum manifestations of classical chaos in that the difference in the quantum transport as caused by different types of classical dynamics can diminish. As a result, universal behaviors emerge. The remarkable phenomenon has been observed in graphene quantum dots of integrable and chaotic geometries. In particular, the conductance curves contain both regular oscillations and random fluctuations, and the transition is caused by the emergence of new edge states when crossing the Landau levels. In the region of regular oscillation, the periods in the Fermi energy and in magnetic flux are related to the size of the device in a universal manner, regardless of the nature of the corresponding classical dynamics. The key to this universal scaling is the quantization of classically circulating edge orbits, which does not depend on the specific details of the geometrical shape of the dot. The details do appear in the fine-scale variations, where the random conductance fluctuations are typically smoother when the classical dynamics is chaotic.
Chapter 3

EFFECT OF GEOMETRICAL ROTATION ON CONDUCTANCE FLUCTUATION IN GRAPHENE QUANTUM DOTS

3.1 Introduction

Quantum transport is fundamental to the development of nanoscale devices. Given a nanostructure, a large number of factors can affect the quantum-transport dynamics, such as the Fermi energy, the geometrical shape of the dot, external electrical and/or magnetic field, etc. [180, 181]. Devising effective, experimentally feasible methods to modulate or control quantum transport is a problem of tremendous interest at the present.

A key quantity underlying many quantum-transport processes is conductances. Consider a two-dimensional nano-scale device such as a graphene [1, 16, 3, 4, 5, 6, 9] quantum dot or a more traditional semiconductor 2DEG (two-dimensional electron gas) structure [180]. When the device is connected through electron waveguides (or leads) to electron reservoirs (i.e., contacts) to form a circuitry, various conductances can be defined with respect to voltage biases among the contacts together with the corresponding currents. Hall conductance in the presence of a perpendicular magnetic field is one such example. At low temperatures the conductances can be related to the corresponding quantum transmission [163] that depends on the electronic and device parameters. As a result, the conductances will also depend on these parameters. In the common situation in nanoscience where the size of the device is less than the phase-relaxation length, quantum interference is important, which can lead to significant fluctuations in the conductances with respect to the parameter variations.
A critical issue is how the conductance fluctuation pattern may be modulated or controlled. In this regard, a recent work has suggested the idea of exploiting classical transient chaos for quantum conductance modulation [85].

In this chapter, we propose and computationally test a practical scheme to modulate quantum conductance fluctuations in nanoscale transport devices. We focus on graphene quantum dots. A dot structure typically consists of a device area of certain geometrical shape, such as a rectangle, and a number of leads connected to the device. Consider the common setup where a pair of semi-infinite, co-linear leads connected to the device on the left- and right-hand side, respectively, as shown schematically in Fig. 3.1. Our basic idea is to exploit the relative orientation between the device and the leads for modulating conductance fluctuations. For example, Fig. 3.2(a) shows a situation where the device has been rotated with respect to the leads by an angle $\theta$. For different angles, the conductance-fluctuation patterns can be quite different.

In particular, when a physical parameter such as the Fermi energy $E$ is varied, conductance $G$ changes accordingly. For different values of $\theta$, the fluctuation patterns of $G$ with $E$ will in general be different. It is convenient to write $G(E;\theta)$. For a fixed value of $\theta$, the degree of the fluctuating behavior of the conductance with $E$ can be characterized by the standard autocorrelation function

$$C(\Delta E, \theta) = \frac{\langle (G(E;\theta) - \overline{G})(G(E + \Delta E;\theta) - \overline{G}) \rangle}{\langle (G(E;\theta) - \overline{G})^2 \rangle},$$  

(3.1)

where $\Delta E$ is a small energy interval, $\overline{G}$ is the mean of conductance, and the average $\langle \cdot \rangle$ is taken over a large energy interval. The half-width of $C(\Delta E, \theta) = 0.5$, denoted by $\varepsilon$, will depend on the device angle $\theta$, so we write $\varepsilon(\theta)$. Our hypothesis is that $\varepsilon$ will depend markedly on $\theta$, meaning that the degree of the conductance fluctuations can be effectively modulated by varying $\theta$. 

[26, 27, 28, 29, 30, 31, 32, 33, 19, 34, 35, 36, 37, 38, 39, 40, 41, 42].
Figure 3.1: (a) Schematic illustration of a graphene quantum dot. (b) For a square quantum dot tilted with respect to the orientation of the left and right semi-infinite leads, construction of layer-based tight-binding Hamiltonians for recursive Green’s function calculation. The device consists of layer 1 to layer $N$, while the left lead is from $-\infty$ to layer 0 and the right lead is from layer $N+1$ to $\infty$.

In order to test the hypothesis, we study a rectangular graphene quantum dot as a prototypical system, and use the standard tight-binding Hamiltonian and non-equilibrium Green’s function approach [163] to calculate the conductance. To facilitate computations to gain high efficiency, especially for dots of relatively large sizes under systematically varying orientations, we develop a layer-based non-equilibrium Green’s function approach, which decomposes the whole dot region into successive layers perpendicular to the direction of the semi-infinite leads and then calculates the Green’s function of individual layers, one after another. This allows the conductance of arbitrarily large dots to be computed in an extremely efficient manner, insofar as the number of atoms in each layer is not prohibitively large, which is usually the case for typical graphene quantum dots of experimental interest. Our systematic computations reveal that the degree of conductance fluctuations can be modulated by geometrical rotations.

In Sec. 5.2, we describe our layer-based recursive Green’s function method for
efficient computation of conductance fluctuations at arbitrary rotation angles. In Sec. 9.3, we demonstrate that device rotation can be used to modulate the conductance-fluctuation pattern. Conclusion is presented in Sec. 6.5.

3.2 Experimental Scheme and Numerical Method

A graphene device can be formed by cutting into a large graphene sheet, as shown in Fig. 3.2. While graphene sheet can be obtained by repeatedly peeling from multilayer graphite [1], the chemical vapor-deposition (CVD) method [16, 182, 183, 184, 185] can be used to grow a graphene device into any desirable shape, greatly facilitating the interaction between theoretical and experimental research. A possible scheme of experimentally realizing our system is as follows. A number of Ni layers are first cut into the desired geometries with rotation angle $\theta$ systematically varying from $-\pi/4$ to $\pi/4$, as shown in Fig. 3.2(a). Next, the Ni layers are placed on SiO$_2$/Si layers and processed chemically, as shown in Fig. 3.2(b). Graphene devices with pre-determined rotational angles are then synthesized, which are ready for conductance measurement.

At low temperatures, the conductance $G$ of a quantum dot is proportional to the quantum transmission $T$, as given by the Landauer formula [171, 163]:

$$G(E) = (2e^2/h)T(E).$$  \hspace{1cm} (3.2)

Transmission is usually calculated by the non-equilibrium Green’s function (NEGF) method [172, 173]. For a graphene quantum dot system consisting of a device region and two semi-infinite leads (left lead and right lead) as shown in Fig. 3.1(a), the transmission can be conveniently calculated through the self-energies [163]. In particular, let $H_D$ be the finite Hamiltonian matrix describing the device in the tight-binding framework. The Green’s function of the device is given by

$$G_D = (EI - H_D - \Sigma_L - \Sigma_R)^{-1},$$  \hspace{1cm} (3.3)
Figure 3.2: (a) Schematic diagram: a square graphene device with two leads is generated by cutting into a large graphene sheet. The angle $\theta$ is adjustable. (b) Typical process of experimental graphene growth. Left are three nano-layers made of Si, SiO$_2$, Ni, respectively. The nickel layer is shaped as device and lead geometry. The layers are heated to 1000$^\circ$C with flowing reaction gas (CH$_4$/H$_2$/Ar) mixtures. After cooling down to room temperature, a mono-layer graphene is pasted on upper layer. Etching the Ni and SiO$_2$ layers makes the graphene device fall down on Si layer. (c) Local atomic configurations near a device-lead interface for $\theta = 0^\circ$, 22.5$^\circ$, 30$^\circ$ and 40$^\circ$. 
where \( \Sigma_L \) and \( \Sigma_R \) are the self-energies associated with the left and right leads, respectively. Let \( V_{L,R} \) be the coupling matrix between the left (right) lead with the device, the self-energies can be calculated by the following Dyson’s equations [174, 186, 187]:

\[
\Sigma_{L,R} = V_{L,R}^\dagger (E - H_D - \Sigma_{L,R})^{-1} V_{L,R}.
\]

(3.4)

The transmission is then given by

\[
T(E) = \text{Tr}(\Gamma_L G_D \Gamma_R G_D^\dagger),
\]

(3.5)

where \( \Gamma_{L,R} \equiv i(\Sigma_{L,R} - \Sigma_{L,R}^\dagger) \). The local density of states (LDS) for the device is

\[
\rho_D = -\frac{1}{\pi \text{Im}[\text{diag}(G_D)]},
\]

(3.6)

Although the above procedure is standard, for large graphene quantum dots (e.g., length scale of 100 nm), the size of the Hamiltonian matrix \( H_D \) will be large, making the computation extremely demanding, especially in terms of the memory requirement. We are thus led to develop a layer-by-layer type of recursive Green’s function (RGF) method to calculate the transmission and the local density of states. The basic idea is to divide a given (large) device into smaller units or layers. The specific way to choose the division can be highly flexible, depending on the geometrical shape of the device region. A well-designed, physically meaningful division scheme can help accelerate the computation tremendously. An example is shown in Fig. 3.1(b), where a square device tilted with respect to the orientation of the left and right leads (horizontal direction) is divided into \( N \) layers. The left and right leads can be conveniently labeled as layer 0 and layer \( N + 1 \), respectively. In this RGF method, each layer \( j \) \((j = 1, \ldots, N)\) is considered as a separated device and its nearest neighboring layers \( j-1 \) and \( j+1 \) are regarded as the local left and right “leads” connecting to the device, respectively. The Green’s function \( G_j \) for layer \( j \) is determined by the Fermi energy

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Figure 3.3: For a square device of side length $L = 60.5a_0$, where $a_0$ is the lattice constant of graphene, dimensionless conductance $G(E)$ as a function of the Fermi energy, where the conductance is normalized by $G_0 = 2e^2/h$, and the corresponding autocorrelation curves: (a,b) $\theta = 0$, (c,d) $\theta = 22.5^\circ$, (e,f) $\theta = 30^\circ$ and (g,h) $\theta = 45^\circ$. (i) LDS patterns corresponding to the black circles in (g).

and the self-energies from its “leads.” Carrying out the calculation of the Green’s function layer-by-layer, we can assemble the Green’s function for the original (large) device. A detailed formulation of RGF method can be found in Appx. A.
3.3 Results

To be concrete, we consider a square-shaped graphene device of side length $L = 60.5a_0$, where $a_0 = \sqrt{3}a \approx 0.246$ nm is the lattice constant and $a$ denotes the C–C bond length in graphene. Two leads of width $W = 11a$ are connected to the central regions of the left and right sides of the device, where the angle $\theta$ is a control parameter that can be varied in the range $[-\pi/4, \pi/4]$. The leads are graphene nano-ribbons that can have either zigzag or armchair boundaries. For a fixed value of $\theta$, we calculate the conductance $G(E)$, normalized by $G_0 = 2e^2/h$, as a function of the Fermi energy $E$. Figure 3.3 shows the conductance-fluctuation patterns and the corresponding auto-correlation functions for $\theta = 0^\circ$, $22.5^\circ$, $30^\circ$ and $40^\circ$. We observe that rotation can affect the fluctuation pattern markedly. For example, for $\theta = 0^\circ$, the conductance curve appears more smooth. For $\theta = 40^\circ$, the fluctuations are sharper. The fluctuation patterns can be characterized by the autocorrelation functions in terms of the the half-width $\varepsilon$. We have $\varepsilon = 0.005t$ for $\theta = 0^\circ$, but it reduces to $\varepsilon = 0.001t$ for $\theta = 40^\circ$, where $t$ is the nearest-neighbor hopping energy of the graphene lattice.

We note that the conductance fluctuations in Fig. 3.3(g) is unusually strong as compared with other cases, in the sense that the conductance is nearly zero for most energy values and reaches maximum values for relatively fewer energy values, and the transitions between near-zero and maximum values appear quite abrupt with respect to change in the energy. The main reason is that, for relatively large rotational angles (e.g., $\theta = 40^\circ$), the boundary mismatch between the graphene leads and device induces strong backscattering except for those energy values where edge states can form. The LDS pattern of an edge state is shown in Fig. 3.3(i) on the left-hand side, while a strong backscattering state is shown on the right-hand side where we observe essentially zero electron density in the device region.
Figure 3.4: For zigzag leads and device with zigzag boundary at $\theta = 0$, contour plot of the normalized conductance in the two-dimensional parameter plane $(\theta, E)$: (a) full-range plot where the color represents the conductance value. The red dashed lines divide the conductance-fluctuation pattern into three regions, (b) magnification of part of (a).
To obtain a comprehensive picture, we show in Fig. 3.4(a) a contour plot of the conductance in the two-dimensional parameter space \((\theta, E)\), where the leads of the rotated device have zigzag boundaries. We observe that, for \(\theta\) in different regions, the conductance-fluctuation patterns with the Fermi energy can be characteristically different, indicating the role of device rotation in modulating the conductance fluctuations. From a different standpoint, for a fixed Fermi energy, the conductance can be viewed to fluctuate with \(\theta\). In particular, in the low-energy regime, the conductance varies relatively slowly with \(\theta\), but significant fluctuations of the conductance with \(\theta\) occur in the large energy regime. Approximately, we can divide the contour plot in Fig. 3.4(a) into three distinct regions: \(\theta < -\pi/6\), \(-\pi/6 \leq \theta \leq \pi/6\), and \(\theta > \pi/6\), which are marked by the red dashed lines. The critical angles \(\pm \pi/6\) arise because of the hexagonal lattice structure of the leads (graphene ribbons) with zigzag boundaries. In the range \(-\pi/6 \leq \theta \leq \pi/6\), there are two symmetrical regions in the contour plot with nearly uniformly low conductance values and only a few small regular islands of high conductance values in the low Fermi-energy region \((E \leq 0.08\ell)\).

In the two mostly low-conductance areas, the rare points of high conductance values form approximately parabolic curves, as can be seen from the contour plot in Fig. 3.4(b). As the square device is rotated, its boundary changes from totally zigzag or totally armchair type at \(\theta = 0\) to a mixture of both. For a given value of \(\theta\), only for a few energy values are the conductance values appreciable. The pattern of relatively high values of the conductance is also symmetric with respect to \(\theta = \pi/12\). The reason is that, when the rotation angle reaches \(\theta = \pi/6\), the orientation of the leads coincides with the armchair boundary of the device, and the angle \(\pi/12\) corresponds to the “most” mixed boundaries. In fact, the parabolic curves in Fig. 3.4(b) are a consequence of the formation of the edge states in the graphene device, as shown in Fig. 3.5. Along each parabolic curve, although the connecting angle between the
Figure 3.5: Transmission contours about angle $\theta$ and energy $E$. The blue dashed lines link the transmission peaks. The black circles represent the LDS patterns of the entire parabolic blue lines. The energies for the LDS patterns 1, 2, 3, 4, 5, and 6 are $E_1 = 0.008t$, $E_2 = 0.0242t$, $E_3 = 0.0435t$, $E_4 = 0.052t$, $E_5 = 0.016t$ and $E_6 = 0.0319t$, respectively, and the corresponding angles are $\theta_1 = 25.65^\circ$, $\theta_2 = 26.10^\circ$, $\theta_3 = 24.30^\circ$, $\theta_4 = 3.60^\circ$, $\theta_5 = 4.95^\circ$ and $\theta_6 = 6.75^\circ$.

device and the leads is systematically chanced, the LDS patterns indicate localization of electronic states about the corners of devices, which are similar to each other. For example, in Fig. 3.5, patterns 1 and 4, patterns 2 and 5, and patterns 3 and 6 exhibit similar edge states. In the black area in Fig. 3.4, there are no edge states.

When the ribbons have armchair boundaries and the device’s boundaries are also armchair initially (at $\theta = 0$), we observe qualitatively similar patterns to those in Fig. 3.4(a), but the trend of conductance changes is opposite, as shown in Fig. 3.6. The reason can be attributed to the distinct electronic behaviors for different types
Figure 3.6: For armchair leads and device with armchair boundary at $\theta = 0$, contour plot of the normalized conductance in the two-dimensional parameter plane ($\theta$, $E$): (a) full-range plot where the color represents the conductance value. The red dashed lines divide the conductance-fluctuation pattern into three regions, (b) magnification of part of (a).
of boundaries. In particular, at low energy, electrons are localized near the zigzag edges [? ], so a change from zigzag to armchair boundary can reduce the conductance gradually, as can be seen from the three LDS patterns in Fig. 3.7. Conceptually, the zigzag boundaries act as channels, while the armchair boundaries behave as barriers to these channels. For \( \theta = 30^\circ \) and the initial zigzag device connected to zigzag leads, the electrons travel through the channel smoothly to pass the device, giving rise to large conductances, as the middle LDS pattern in Fig. 3.7(b) indicates, where the light blue dash lines mark the potential channels. Hence, as shown in Fig. 3.4(a), the average conductance at \( \theta = 30^\circ \) is larger than those at other angles. In a graphene system, the Fermi energy follows \( E \sim k \sim 1/\lambda \), where \( \lambda \) is the electron wavelength.

When the device is rotated away from the initial setting, say to \( \theta = 22.5^\circ \), a large number of barriers (armchair boundaries) arise, as indicated in Fig. 3.2(b), which the electrons cannot cross. Indication of this behavior can also be seen from the left LDS pattern in Fig. 3.7, where few electrons extend into the device due to the barriers. When the angle is changed, cases such as that illustrated by the third LDS pattern in Fig. 3.7 can arise.

To quantify the effect of rotation on the conductance-fluctuation pattern, we calculate the energy autocorrelation function \( C(\Delta E, \theta) \) for each fixed value of rotation angle \( \theta \) and plot the half-width \( \varepsilon \) as a function of \( \theta \). The energy range for performing the average in Eq. (3.1) is chosen to be \([0.05t, 0.1t]\). The result is shown in Fig. 3.7. For comparison, result from a 2DEG system of the same geometry and size (corresponding effectively to square-lattice system in the tight-binding framework) is also included. We see that, for the graphene system, the half-width depends sensitively on the rotation angle, especially for large angles, although the dependence is relatively weak in the angle range \( \theta \in [-\pi/6, \pi/6] \). The sensitivity originates from the fact that, in graphene, electron mobility is extremely direction-dependent. As a result,
Figure 3.7: For system with zigzag boundaries, half width of the energy autocorrelation function versus the angle of rotation $\theta$. Result from a conventional semiconductor 2DEG system of the same geometry and size is included for comparison (dashed curve). Three representative LDS patterns for Fermi energy $E = 0.07t$ and $\theta = 0^\circ$, $22.5^\circ$ and $40^\circ$ are shown to illustrate the conducting channels.

A slight change in the graphene lattice orientation will result in a drastic change in the conductance. In fact, it is a general property of graphene that small structural perturbations at the atomic level, such as adding or removing one atom, would affect the conductance significantly [174, 188]. In contrast, for the corresponding 2DEG system, the dependence of the half-width on the rotation angle is much more smooth, due to the isotropic nature of the electrons’ traveling direction.

An issue is the effect of impurity or disorder [189, 83]. When a small amount of impurity is present, conductance may be enhanced on average because the random scattering induced by impurity can break the localized, resonance-type of LDS pat-
terns \cite{83} that typically lead to extremely sharp conductance fluctuations. However, for large amounts of impurity, strong localization can set in, reducing significantly the conductance. Thus an optimal amount of impurity can maximize the conductance \cite{83}. For a fixed amount of impurity in the device, the average value of the conductance may change but the variations of the conductance with respect to device rotation are expected to remain qualitatively the same.

Another interesting issue concerns the interplay between the conductance-fluctuation pattern and the size of the quantum dot. This is especially relevant when a perpendicular magnetic field is present. In particular, for a quantum dot of given geometrical shape, the conductance can vary periodically with the strength of the magnetic field, the frequency of which, the so-called magnetic frequency, depends on the dot size \cite{158, 159, 160}, and in fact follows a linear scaling relation \cite{161, 162}. The origin of the scaling can be attributed to the interplay between the Landau levels and some pronounced quantum pointer states \cite{85}. In our case, rotation of the quantum-dot device can lead to the emergence of different groups of quantum pointer states. Thus, in the presence of a magnetic field, the magnetic frequency is expected to depend on the dot size linearly but the associated slope will depend on the angle of rotation.

Varying the device aspect ratio $W/L$, insofar it is small, does not affect the effect of device rotation on conductance-fluctuation patterns. When the shape of the device is changed, the fluctuation pattern may change characteristically. For example, if the shape is such that the corresponding classical dynamics is chaotic, the conductance fluctuations will be more smooth as compared with the case where the classical dynamics is regular \cite{85}. However, rotation can still have a significant effect on the conductance-fluctuation pattern, regardless of the geometric shape of the quantum dot.
3.4 Conclusion

The conductance of a nano-scale quantum dot depends on many parameters such as the Fermi energy, the strength of external magnetic field (if there is one), and the details of the geometry of the structure, etc. Conductance fluctuations are thus an issue of both fundamental interest and practical significance. Especially, in the development of nanoscale quantum-transport device for circuit and sensor implementations, it is desirable to be able to modulate the conductance-fluctuation patterns depending on the specific application requirements. Recently it has been suggested that classical chaos can be exploited to control the statistical characteristics of conductance fluctuations in both semiconductor 2DEG and graphene quantum dots [85].

We have suggested an experimentally realizable scheme to modulate conductance fluctuations in quantum-dot devices. Our idea is to exploit geometrical rotation of the device relative to the leads, which is tested computationally using two-terminal graphene and conventional semiconductor 2DEG systems. To overcome the challenge of computing systematically the conductance in multiple parameter space (e.g., the Fermi energy and the device rotation angle) for relatively large devices, we have developed a layer-based recursive Green’s function method. Our study indicates that geometrical rotation can have a drastic effect on the autocorrelation width of the conductance-fluctuation pattern, and the dependence is more sensitive for graphene device. Qualitatively, the mechanism of modulation can be understood by the emergence of the edge states in graphene systems. Control of quantum transport dynamics, especially in graphene systems, is a problem of great importance in the development of all sorts of nano-scale devices, and our geometry-based method represents a simple but effective scheme in this pursuit.
Chapter 4

ENHANCEMENT OF SPIN POLARIZATION BY CHAOS IN GRAPHENE QUANTUM DOT SYSTEMS

4.1 Introduction

In a two-dimensional (2D) solid state system, when the potential in the direction perpendicular to the 2D plane is asymmetric, the atomic spin-orbit coupling can lead to a momentum-dependent splitting of the spin bands, a phenomenon known as the Rashba effect [190] or the Rashba-Dresselhaus effect [191]. This effect can be exploited for manipulating spin in various settings such as electrical spin injection [192], 2D superconducting devices [193], spin modulation through an electrical field [194], spin filtering [195], and spin field effect transistor [196]. In two-dimensional Dirac materials of current interest such as graphene [1, 3, 4, 6, 8, 197], topological insulators [198], and molybdenum disulfide (MoS$_2$) [11, 12], intrinsic or extrinsic spin-orbit interactions of various degrees can arise. The interaction typically leads to energy splitting and can result in fascinating phenomena such as the spin Hall effect [199, 200], weak anti-localization [201, 202], spin-flipping scattering and spin polarization [203, 204, 205].

There are two types of spin-orbit coupling: intrinsic and external. In graphene, the intrinsic spin-orbit coupling is usually quite weak, but significant interaction (e.g., characterized by energy splitting on the order of 200meV) can be realized [206, 207, 208] through the Rashba effect by depositing graphene on the surface of Ni(111) or Ir(111). Rashba spin-orbit interaction preserves the time-reversal symmetry but breaks the inversion symmetry in the direction perpendicular to the two-dimensional material plane, and has wide applications in spin transport devices [209, 210, 211, 212,
213, 214, 215]. For example, for a two-terminal (source-drain) system with a Rashba field in the middle region, electrons of pure spin (say, spin up) are injected from the source and enter the central region. The Rashba coupling causes the electron spin to precess. When these electrons move into the drain terminal, some of them will have their spin flipped down. The flipping process leads to imperfect spin polarization. The degree of the spin polarization can then be modulated by the Rashba interaction strength.

In addition to the Rashba interaction strength, the geometric shape of the central interaction region can affect the electron scattering dynamics and, consequently, can have an effect on spin polarization. For convenience, we call the central region where the Rashba coupling exists, the \textit{scattering region}. Domains of different geometry can lead to characteristically distinct types of classical dynamics. For example, if the scattering region is rectangular, the underlying classical dynamics is integrable (or regular). However, a simple addition of two semicircular segments on two opposite sides of the rectangle leads to the stadium geometry, for which the classical dynamics is chaotic without any stable periodic orbits. If, a small circular region at the center of a square is converted into a classically forbidden region (e.g., through the application of a localized electrical potential), the domain becomes that of a Sinai billiard [216, 217], for which the classical dynamics is fully chaotic with all periodic orbits being unstable. \textit{The main result of this chapter is that chaos can enhance spin polarization, a beneficial property that can be exploited for spintronics applications.}

We focus on a class of two-terminal graphene devices with Rashba interactions occurring in the central scattering region whose geometrical shape can be chosen to yield distinct types of dynamics in the classical limit. The shape of the scattering region is that of the cosine billiard [218, 36, 219, 19] with an upper and a lower hard boundaries at $y(x) = W + (M/2)[1 - \cos (2\pi x/L - \pi)]$ and $y = 0$, respectively, for
\(-L/2 \leq x \leq L/2\). To make the scattering region symmetrical, we choose the lower boundary to be \(y(x) = \pm W + (M/2)[1 - \cos(2\pi x/L - \pi)]\) for \(-L/2 \leq x \leq L/2\), and the lead width is accordingly \(2W\). The type of the classical dynamics in the billiard can be controlled by the parameter ratios \(W/L\) and \(M/L\). For example, for \(W/L = 0.18\) and \(M/L = 0.11\), there are both stable and unstable periodic orbits, and the classical phase space is mixed (nonhyperbolic) with both chaotic regions and KAM islands. However, for \(W/L = 0.36\) and \(M/L = 0.22\), all periodic orbits are unstable and the classical dynamics is fully chaotic (hyperbolic). Given a billiard shape, we construct the Hamiltonian incorporating Rashba interaction and use the Green’s function method to calculate the conductance and spin polarization for systematically varied strength of the Rashba interaction. We find that, classical chaos can not only smooth the fluctuations of the spin polarization with the Fermi energy, but more importantly, can enhance the average spin polarization. We provide a heuristic argument based on semiclassical theory to understand the chaos-induced enhancement effect.

4.2 Hamiltonian and Calculation of Spin Polarization

In the tight-binding framework, the Hamiltonian of the graphene system with Rashba spin-orbit interaction (RSOI) is given \([199]\) by \(H = H_0 + H_R\), where the first and second terms describe the electron hopping and RSOI, respectively. The explicit forms of \(H_0\) and \(H_R\) are

\[
H_0 = -t \sum_{(i,j):\sigma} c_{i,\sigma}^\dagger c_{j,\sigma},
\]

\[
H_R = i\Delta_R \sum_{(i,j):\sigma,\overline{\sigma}} (s_{\sigma,\overline{\sigma}} \times d_{ij})_z c_{i,\sigma}^\dagger c_{j,\overline{\sigma}},
\]

where, \(c_{i,\sigma}^\dagger (c_{j,\sigma})\) is creation (annihilation) operator, \(\sigma(\overline{\sigma}) = \uparrow (\downarrow)\) or \(\downarrow (\uparrow)\), \(d_{ij}\) is the vector from site \(i\) to site \(j\), and \((\cdots)_z\) represents the \(z\) component of the vector.
quantity in the parenthesis. The hopping energy is \( t = 2.8\text{eV} \) and \( \Delta_R \) is the strength of RSOI. We define the region with \( \Delta_R > 0 \) as the RSOI region. For convenience, we call the region for which \( \Delta_R = 0 \) the NR region.

The spin conductance of an open NR-RSOI-NR system can be calculated from the Green’s function technique and the classic Landauer-Büttiker formula

\[
G(E) = \frac{e^2}{h} \text{Tr}[\Gamma_L G^r \Gamma_R G^a],
\]

(4.2)

where \( \Gamma_{L(R)} = i[\Sigma_{L(R)}^r - \Sigma_{L(R)}^a] \), and \( G^r(a) \) is the retarded (advanced) Green’s function of the central scattering region, which are given by

\[
G^r = (G^a)^\dagger = [E - H_C - \Sigma^r_L - \Sigma^r_R]^{-1}.
\]

(4.3)

We use the recursive Green’s function method with high computational efficiency [85, 90]. The conductance can be obtained as [212, 220]

\[
\begin{pmatrix}
G_{11} & G_{12} \\
G_{21} & G_{22}
\end{pmatrix},
\]

(4.4)

where \( G_{11(22)} = G_{\uparrow(\downarrow)} = G_{\uparrow\uparrow(\downarrow\downarrow)} + G_{\uparrow\downarrow(\downarrow\uparrow)} \) and the total conductance is given by \( G_{\text{tot}} = G_\uparrow + G_\downarrow \). The non-diagonal element \( G_{12(21)} \) contains the projection of the spin polarization into the \((x,y)\)-plane. The spin polarization \( \mathbf{P} = [P_x, P_y, P_z] \) can be calculated through [221, 213, 220]

\[
\begin{align*}
P_z &= \frac{G_{11} - G_{22}}{G_{11} + G_{22}}, \\
P_x - iP_y &= \frac{2G_{21}}{G_{11} + G_{22}}.
\end{align*}
\]

(4.5)

4.3 Numerical Results

We vary two parameters: the Fermi energy \( E \) and the Rashba interaction strength \( \Delta_R \). The range of \( E \) is between zero and a fraction of \( t \), the nearest-neighbor hopping energy of graphene, and the maximum value of \( \Delta_R \) is set to be \( 0.07t \approx 200\text{meV} \), which is the currently experimentally achievable value [206, 207, 208].
Figure 4.1: The total conductance and spin polarization versus the Fermi energy for a nonhyperbolic (a,c) and a hyperbolic (b,d) graphene quantum dot. In both cases, the Rashba interaction strength is $\Delta_R = 0.07t \approx 200\text{meV}$ and the unit conductance is $G_0 = 2e^2/h$. The geometric parameters for the nonhyperbolic and hyperbolic dots are $(W/L = 0.18, M/L = 0.11)$ and $(W/L = 0.36, M/L = 0.22)$, respectively, with $W = 40a$ and $a = 0.142\text{nm}$, and their dot shapes are illustrated in the insets in (a) and (b). The dashed boundaries are symmetrical with respect to solid boundaries about $y = 0$, and the scattering region is defined as the region in between the two vertical line segments. The blue, red and green curves correspond to the $x$, $y$ and $z$ components of the spin polarization. The gray dotted lines highlight the identical locations of the resonant peaks in the conductance and spin-polarization curves.

Effect of chaos and Rashba interaction on conductance and spin-polarization fluctuations. Figures 4.1(a) and 4.1(b) show the conductance fluctuation patterns with the Fermi energy for the nonhyperbolic and hyperbolic dot systems, respectively, where the Rashba interaction strength is $\Delta_R = 0.07t \approx 200\text{meV}$ for both cases. For graphene quantum dots, a previous work [19] that did not treat Rashba interactions showed that, fully developed chaos can eliminate sharp (Fano) resonances in the conductance curve and lead to smooth fluctuations. Comparing the conductance curves in Figs. 4.1(a) and 4.1(b), we see that the same holds: chaos can make the conductance fluctuations dramatically more smooth even in the presence of Rashba interaction. A similar behavior occurs for all three components, $[P_x, P_y, P_z]$, of the spin polarization, as shown in Figs. 4.1(c) and 4.1(d). In particular, Fig. 4.1(c) exhibits Fano-like resonances in the spin polarization for the nonhyperbolic dot system, while the resonances entirely disappear when the classical dynamics becomes
Figure 4.2: Width of resonance $\gamma_\alpha$ for nonhyperbolic [squares, panels (a) and (c)] and hyperbolic [circles, panels (b) and (d)] quantum dot systems. The Rashba interaction strength is $\Delta_R = 0$ for (a,b) and $\Delta_R = 0.07t$ for (c,d). Blue and red colors correspond to the cases where the Rashba interaction is absent and present, respectively. The gray dashed lines divide the complex plane of $E_\alpha^c$ into three regions for the purpose of qualitative analysis.
hyperbolic, as shown in Fig. 4.1(d). Note that, in the window of the Fermi energy from 0.16t to 0.19t, the \( y \)-component of the spin polarization for the hyperbolic case maintains at a stable and relatively high level: \( P_y \approx 0.4 \), but this behavior does not occur for the nonhyperbolic system. As we will demonstrate, this stable region leads to a markedly higher value of the average spin polarization for the hyperbolic case as compared with the nonhyperbolic case. Note that, the results shown in Fig. 4.1 are for zigzag boundaries in the horizontal direction. Since the average spin polarization is obtained over the energy range with two transverse modes (which is not close to the Dirac point), the edge type has little effect on the average spin polarization. In fact, our computations indicate that using armchair boundaries yields essentially the same result.

To understand the effect of chaos on fluctuations in the conductance and spin polarization, we calculate the width of the resonances \[19, 92\] from the non-Hermitian Hamiltonian of the corresponding open system. In particular, the Hamiltonian \( H_C \) of the central scattering region is Hermitian with a set of real eigenvalues denoted as \( \{E_{0\alpha}|\alpha = 1, \cdots, N\} \), where \( N \) is the size of the Hamiltonian matrix (the number of carbon atoms in the graphene lattice in the scattering region). For the open system, the Hamiltonian matrix is \( H_{tot}^c(E_0) = H_C + \Sigma_L^c(E_0) + \Sigma_R^c(E_0) \), where \( \Sigma_L^c(E_0) \) and \( \Sigma_R^c(E_0) \) are the complex self-energy matrices associated with the left and right leads, respectively, which characterize the coupling between the states in the scattering region and those in the leads. Solving the eigenvalues of \( H_{tot}^c(E_0) \), we obtain a set of complex numbers \( \{E_{c\alpha}|\alpha = 1, \cdots, N\} \), where \( E_{c\alpha} = E_{0\alpha} - \Delta_\alpha - i\gamma_\alpha \). The imaginary part of \( E_{c\alpha} \) characterizes the coupling strength between the states in the scattering region and in the leads, which effectively measures \[19, 222\] the resonance width \( \gamma_\alpha \). If \( \gamma_\alpha \) is small, e.q., less than \( 10^{-4}t \), a sharp, Fano-type of resonance emerges in both the conductance and spin-polarization curves. If \( \gamma_\alpha \) is relatively large, e.g., larger
than $10^{-3}$, the conductance and spin-polarization variations would be smooth.

Figures 4.2(a-d) show, for the nonhyperbolic and hyperbolic systems, the locations of various eigenvalues $E^c_\alpha$ in its own complex plane, for two cases where the Rashba interaction is absent and present with strength $0.07t$, respectively, where we choose $E_0 = 0.2t$ from the energy range in Fig. 4.1. Based on values of $\gamma_\alpha$, qualitatively we can divide the complex plane into three regions: regions I-III, corresponding to $\gamma_\alpha < 10^{-4}t$, $10^{-4}t \leq \gamma_\alpha \leq 10^{-3}t$, and $\gamma_\alpha > 10^{-3}t$, respectively, which are specified with the dashed lines. Roughly, the values of $\gamma_\alpha$ in regions I and II correspond to the Fano-like resonances in the conductance and spin-polarization curves [Fig. 4.1(c)], while those in region III correspond to the smooth variations [Fig. 4.1(d)]. For the nonhyperbolic dot, as shown in Figs. 4.1(a,c), without Rashba interaction, some values of $\gamma_\alpha$ are located in region I [Fig. 4.1(a)]. Generally, Rashba interaction can increase the width of the resonance [223]. In the presence of the interaction [Fig. 4.1(c)], the values of $\gamma_\alpha$ tend to increase slightly, but there are still a number of values in region II. For the hyperbolic dot, as shown in Figs. 4.1(b,d), without or with Rashba interaction, no eigenvalue is located in region I and almost no eigenvalues are in region II. In fact, almost all values of $\gamma_\alpha$ are located in region III, giving rise to smooth conductance and spin-polarization variations.

Signatures of the band splitting and the weak anti-localization effects can be seen in Fig. 4.2, which are caused by the RSOI. In particular, the Fano-type resonance is caused by the interplay between the quasi discrete energy levels from the quantum dot and the continuous background of the semi-infinite leads [224]. As the Rashba coupling strength is tuned up, a single discrete level splits into two. As a result, for both nonhyperbolic and hyperbolic quantum dots, the number of the Fano-type of resonances doubles [c.f., dot doubling in Figs. 4.2(c,d)]. However, we note that a sharp resonance corresponds to a pointer state in which the electrons is localized in
Figure 4.3: Average spin polarization versus Rashba interaction strength (a) for integrable (black dashed curve), nonhyperbolic (blue dashed-dotted curve), and hyperbolic (red solid curve) quantum dots, (b) for rectangular (blue dashed-dotted curve) and Sinai billiard (red solid curve) dot systems. The maximum spin polarization of integrable dots, $P^m_y$, is equal to 0.347 in (a) and 0.09 in (b). The side length of the rectangular billiard dot is $D = 118a$ and the lead width is $W = 6.5a$. The radius of the circular hard disk in the Sinai billiard system is $R = 0.258L$.

the dot region, but the ROSI can smooth out the resonance. This is because of the weak anti-localization effect [201, 202], which reduces the degree of localization and consequently broadens the width of the sharp resonances. In fact, as can be seen from Fig. 4.2, comparing with the case where there is no RSOI, the values of the imaginary eigen energies $\gamma_\alpha$ with the RSOI in regions I and II are generally higher. In general, as the electron energy is increased, the total conductance will increase, reaching higher conductance plateaus [225].

Enhancement of spin polarization by chaos. In our coordinate setting, the $y$ component of the spin polarization, $P_y$, is much larger than the $x$ and $z$ components.
To be concrete, we focus on $P_y$. For both nonhyperbolic and hyperbolic dot systems, $P_y$ fluctuates with the Fermi energy. A surprising finding is that, for a relatively large energy interval, e.g., $0.15 \leq E/t \leq 0.25$, the average spin polarization tends to be larger for the hyperbolic system. For example, for $\Delta_R = 0.07t$, we have $\langle P_y \rangle \approx 0.275$ for the nonhyperbolic dot and $\langle P_y \rangle \approx 0.302$ for the hyperbolic dot. This is indication that chaos can enhance the average spin polarization. The average spin polarization is obtained over the energy range covering two subbands. The reason to choose a relatively small lead width for the rectangular and the Sinai billiard systems in Fig. 4.3(b) was to reduce the effect of the lead on the scattering properties of the specific geometric domains to maximize the contrast between classical integrable and chaotic dynamics.

To obtain a better understanding of the role of chaos in enhancing spin polarization, we make the quantum dot system symmetric in $y$ so that the $x$- and $z$-components of the spin polarization vanish, while keeping the length of the scattering region unchanged [221]. Figure 4.3(a) shows $\langle P_y \rangle$ versus $\Delta_R$ for the symmetrical hyperbolic, nonhyperbolic and integrable dot systems, where $P_y$ is averaged over the energy range $0.083 \leq E/t \leq 0.141$ in which there are two modes in the leads. As $\Delta_R$ is tuned up from zero, $\langle P_y \rangle$ increases initially and then plateaus at a maximum value. For the integrable and nonhyperbolic dots, the curves of $\langle P_y \rangle$ versus $\Delta_R$ are nearly identical. The remarkable phenomenon is that the average spin polarization for the hyperbolic dot is consistently larger than that for the nonhyperbolic or integrable dots.

To demonstrate the generality of the phenomenon of enhancement of spin polarization by chaos, we study a characteristically different class of quantum dot systems subject to Rashba spin-orbit interaction. In particular, a rectangular quantum dot, as shown in the inset of Fig. 4.3(b), has classically integrable dynamics. However,
Figure 4.4: (a) Schematic diagram of transmission behavior at the RSOI-NR interface. (b) The $y$-component of the spin polarization, $P_y(\theta)$, versus the outgoing angle for $\Delta R/E = 0.005$ (blue), 0.025 (red) and 0.05 (green). Dashed lines represent the maximum outgoing angles for different values of $\Delta R/E$.

when a circular hard disk is introduced at the center of the rectangle, the classical dynamics becomes that of the Sinai billiard, which is fully chaotic [216, 217]. The lead width is chosen to be small to minimize the effect of the leads on the scattering properties, so as to maximize the effect of the classical dynamics on spin transport. Calculations show that, depending on the strength of the Rashba interaction, $P_y$ can be either positive or negative. We thus focus on $\langle |P_y| \rangle$, where the average is again taken over the energy range in which the semi-infinite leads permit two modes: $0.696 \leq E/t \leq 0.965$. As shown in Fig. 4.3(b), the normalized $\langle |P_y| \rangle$ values (by its maximum for the integrable case) for the chaotic case is markedly larger than that for the integrable case, for all possible values of $\Delta R$. For $\Delta R \approx 0.04t$, chaos induced enhancement in the average spin polarization reaches maximum.
4.4 Semiclassical Argument for Enhancement of Spin Polarization by Chaos

In our system, a spin-up/down electron enters the RSOI region from the left lead, where the Rashba interaction leads to spin precession. For simplicity, we assume that each scattering event changes only the propagation direction of the electron (as for the situation of classical reflection) and does not affect the spin precession. Due to the surface reflections experienced by the electron at the hard boundaries, the electron will scatter into the right lead with certain outgoing angle, on which the transmission coefficients \( t_{\sigma_R,\sigma_L} \) depends, where \( \sigma_{L,R} \) denote the spin states at the left and right leads, respectively. The angle-dependent transmission coefficients give rise to angle-dependent spin polarization. Spin polarization generation can then be treated as a refraction process at the RSIO-NR interface, as shown as schematically in Fig. 4.4(a).

The Hamiltonian of a Dirac fermion with RSOI is given by
\[
H = H_0 + H_R = \hbar v_F (\sigma_x k_x + \sigma_y k_y) + \Delta_R (\sigma_x s_y - s_x \sigma_y),
\]
where \( v_F \) is the Fermi velocity. The energy dispersion is given by \( E = k \) for the NR region if we set \( \hbar = v_F = 1 \). In the RSOI region, due to the Rashba effect, the energy band splits into two subbands: \( k_\pm = \sqrt{E^2 + \Delta_R^2} \) and the eigen wavefunction is a linear superposition of the \( \pm \) states:
\[
\Psi_R = c_+ \psi_+ + c_- \psi_-,
\]
where \( c_\pm \) and \( \psi_\pm \) are the expansion coefficients and the eigenfunctions associated with the \( \pm \) states, respectively. Following a previous work [226], we set \( c_+ = c_- = 1/\sqrt{2} \). The transmission coefficient \( t_{\sigma_R,\sigma_L} \) can then be obtained by imposing appropriate boundary conditions. The three components of the spin polarization are given by [212, 221, 227]
\[
P_x = \frac{2e^2}{\hbar G} \sum_{\sigma_L} t_{\sigma_L}^* t_{\sigma_L}^\prime,
\]
\[
P_y = \frac{(G_{\uparrow\uparrow} + G_{\uparrow\downarrow}) - (G_{\downarrow\uparrow} + G_{\downarrow\downarrow})}{G},
\]
\[
P_z = \frac{G_{\uparrow\uparrow} + G_{\downarrow\downarrow} - G_{\uparrow\downarrow} - G_{\downarrow\uparrow}}{G},
\]
where the total conductance is given by \( G_{tot} = G_{\uparrow\uparrow} + G_{\downarrow\downarrow} + G_{\uparrow\downarrow} + G_{\downarrow\uparrow} \) and \( G_{\sigma_R\sigma_L} = \ldots \)
\( e^2/h|t_{\sigma R\sigma L}|^2 \). Figure 4.4(b) shows the \( y \)-component of the spin polarization, \( P_y \), versus the outgoing angle \( \theta \), where we observe a valley at the central region. As the RSOI strength is increased, the width of the valley in the \( P_y \) curve narrows down and the maximum value of \( P_y \) gradually increases. Note that \( P_z(\theta) \) vanishes. For a system with an angular symmetry, we have \( P_x(\theta) = P_x(-\theta) \) and, hence, \( P_z(\theta) \) does not contribute to the spin polarization [221, 227].

If the electronic wavelength is much smaller than the device size, i.e., \( \lambda_e \ll L \), the electron motion can be described as that of a classical particle, rendering applicable a semiclassical approximation. For a chaotic domain, its boundary plays the role of random scattering sources for the electron. As a result, the electron trajectories extend all over the domain. Since the system is open, the electron has a finite average dwelling time \( \tau_{dwell} \) in the RSOI region. However, for a nonhyperbolic/integrable domain, quantum pointer states [68, 186, 228, 229] can arise. As a result, the classical quantity \( \tau_{dwell} \) diverges. For the electrons that do escape, the angle distribution can be characteristically different from that of the chaotic case, as shown schematically in Figs. 4.5(a) and 4.5(b). To verify this, we numerically calculate the distribution of outgoing angles, \( f(\theta) \), for both nonchaotic and chaotic systems, as shown in Fig. 4.5(c), where the classical particles are initialized from the left lead with their incident angles and \( y \) locations chosen randomly and uniformly. We see that \( f_\theta \) is flatter for the chaotic domain and cosine-like for the nonchaotic domain. A fourth-order polynomial fit of the angle distribution gives \( f_\theta = -0.057\theta^4 - 0.033\theta^2 + 0.416 \) and \( f_\theta = 0.024\theta^4 - 0.260\theta^2 + 0.504 \) for the chaotic and nonchaotic domains, respectively.

The average spin polarization can be calculated from

\[
\langle P_y \rangle = \frac{1}{2\theta_m} \int_{-\theta_m}^{\theta_m} f(\theta)P_y(\theta)d\theta, \tag{4.7}
\]

where \( \theta_m \) is the maximum outgoing angle, as indicated in Fig. 4.4(b). Figure 4.5(d)
Figure 4.5: (a,b) Schematic illustration of classical outgoing trajectories for the nonchaotic and chaotic quantum dot systems. (c) Numerically obtained angle distribution of the outgoing classical particles (blue - nonchaotic; red - chaotic), where the green solid and brown dashed curves are fourth-order polynomial fitting curves for the respective cases. (d) The average $y$ spin polarization versus the RSOI strength (blue dashed curve - nonchaotic, red solid curve - chaotic). The maximum average spin polarization for the nonchaotic case is $P_y^m \approx 0.075$. 
shows the average spin polarization versus $\Delta R$, where we see that for the chaotic device it has higher values than those for the nonchaotic systems, in agreement with the numerical results in Fig. 4.3(a).

Figure 4.6(a) shows the outgoing angle distributions for the rectangular and Sinai billiard systems. For the former, the outgoing angle distribution is identical to that of the incident angles. For the Sinai system, the escaping probability is larger (smaller) for large (small) outgoing angles. The fitting functions are $f(\theta) = -0.120\theta^6 + 0.363\theta^4 - 0.284\theta^2 + 0.368$ and $f(\theta) = -0.775\theta^8 + 4.142\theta^6 - 7.059\theta^4 + 3.843\theta^2 + 0.056$ for rectangular and the Sinai systems, respectively. Figure 4.6(b) shows the average spin polarization versus the RSOI strength for the two cases. In general, chaos has a more pronounced effect on spin polarization for large outgoing angles. When the angle distribution is taken into account, this leads to enhanced average spin polarization.

Would it be possible to obtain an explicit analytic expression for the average spin polarization? To address this question, we note that, in general, the spin polarization depends on the angle in a sophisticated way, and it seems not feasible to carry out the integration in Eq. (4.7) analytically so as to obtain an explicit formula for the average spin polarization. However, the behavior of the average spin polarization can be assessed by numerically integrating Eq. (4.7). Our results indicate unequivocally that the average spin polarization can be enhanced by chaos. Note that Eq. (4.7) is obtained based on semiclassical considerations, which is approximate with respect to the results from the tight-binding Hamiltonian. Practically, it may not be necessary to write down an explicit formula for the average spin polarization.

4.5 Conclusion and Discussion

Quantum chaos is referred to as the study of quantum manifestations of chaotic behaviors in the corresponding classical system [43, 44], a field that has been extreme-
Figure 4.6: (a) Angle distribution of the outgoing classical particles for the rectangular (blue squares) and Sinai (red circles) dot systems, with the respective polynomial fitting curves. (b) The $y$ component of the average spin polarization versus the RSOI strength (blue dashed curve - rectangular dot; red solid curves - Sinai dot). The maximum average spin polarization for the rectangular system is $P^m_y = 0.0024$.

This work investigates the role of chaos in quantum transport in graphene systems subject to Rashba spin-orbit interaction (RSOI), an important quantum effect in solid state systems [190, 191]. Using the setting of a two-terminal graphene quantum dot where RSOI occurs in the central dot region, we focus on the average spin polar-
ization, a key quantity in the study of spintronic devices. By varying the geometric shape of the dot region, we generate a spectrum of characteristically distinct classical behaviors such as integrable (regular), mixed, and fully developed chaotic dynamics. The quantum dot setting thus represents a generic platform to study the interplay among classical chaos, RSOI, and relativistic quantum mechanics. We find that, in the presence of RSOI, chaos can significantly reduce the sharp fluctuations in the spin polarization (e.g., as the Fermi energy is varied) that occur when the corresponding classical system is regular. A remarkable phenomenon is that, in the experimentally feasible range of the variation of the Rashba interaction strength, the average spin polarization for the chaotic dot can be markedly larger than that for the regular or mixed dot. We develop a semiclassical understanding of the phenomenon of chaos enhanced spin polarization. In particular, a key quantity that determines the average spin polarization is the angle distribution of the outgoing electrons at the interface between regions where RSOI is present and absent, respectively. We find that the angle distribution generated by classical chaos favors the spin alignments.

Our finding has practical values for developing graphene or other 2D Dirac material-based spintronic devices, such as nanoscale magnetic sensors using the mechanism of the Datta-Das transistor \([231, 232]\). In particular, due to its high mobility and weak intrinsic spin-orbit coupling, graphene can preserve the spin orientation of spin-polarized electrons over long distances (e.g., \(\sim 4\mu m\) at room temperature and even up to \(\sim 200\mu m\) at low temperature) \([233, 234, 235, 236, 237, 238]\). However, for a RSOI-based graphene device, the high spin-polarized currents can lead to variable magnetoresistances when the device is connected to a ferromagnetic material. The relatively large range of variation in the magnetoresistances can be used to develop magnetic sensors for reading magnetic information at a higher speed.
To study quantum chaos in the presence of many-body interactions, in this paper we use the standard Hubbard model with on-site repulsive Coulomb interactions. This paradigmatic model to treat interacting particles in a lattice was originally proposed [239] to describe the transition between conducting and insulating systems. For electrons in a solid, comparing with the conventional tight-binding model representing a single electron Hamiltonian, the Hubbard model contains a potential term to include the many-body effect through the mechanism of on-site Coulomb interaction [240, 241]. There has been a great deal of interest in the Hubbard model due to its relevance to frontier problems in condensed matter physics such as high-temperature superconductivity and the trapping of untracold atoms in optical lattices [240]. As we demonstrate in this chapter, while the Hubbard model is much more challenging and sophisticated than the tight-binding model, it can serve as a paradigm to gain significant physical insights into many-body relativistic quantum manifestations of distinct type of classical dynamics.

To be concrete, we focus on graphene systems and study the particular phenomenon of quantum resonant tunneling. The typical setting of a quantum tunneling system consists of two symmetric potential wells separated by a potential barrier in between, as shown schematically in Fig. 5.1. The whole system, which includes the left and right wells as well as the barrier, is closed, and its geometrical shape can
be chosen to yield characteristically distinct types of dynamics in the classical limit. For example, if the whole system has a rectangular domain, the classical dynamics is integrable, but fully developed chaos can arise if the system has a stadium or a bowtie shape. It was discovered that, in both nonrelativistic [242] and relativistic [86] quantum, single-electron tunneling systems, classical chaos can regularize quantum tunneling dynamics. Here by “regularizing” we mean that the spread in the tunneling rate in any small energy interval, typically seen in the integrable geometry, can be greatly suppressed when the underlying geometry becomes chaotic. A unique feature in the relativistic case, as demonstrated in Ref. [86], 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.

In spite of the recent results on regularization of quantum tunneling by chaos [242, 86] in the single particle framework, whether the same can be achieved when many-body interactions are present was unknown prior to this work. More generally, the interplay among chaos, many-body interactions, and relativistic quantum mechanics is a fundamental yet outstanding issue that we aim to address here. There are two main findings: (1) emergence of a class of localized, spin-polarized, relativistic quantum states in classically integrable domains, which find no counterpart in the single-particle framework, and (2) effective removal of these states by classical chaos. A more detailed explanation of these findings is as follows.

In order to uncover the unique relativistic quantum phenomena caused by classical chaos in the presence of many-body interactions, we first study the class of integrable systems of rectangular shape [Fig. 5.1(a)]. Since the whole system is closed, we calculate the eigenenergies and investigate various eigenstates from the mean-field Hubbard Hamiltonian. A striking finding of this work is emergence of a class of eigenstates with near zero tunneling rate. In particular, for such an eigenstate, the spin-up and
spin-down wavefunctions are typically separated, i.e., the spin-up electrons reside in only one potential well while the spin-down electrons reside in the other. As a result, if the initial state is spin-up in one potential well, it is localized and will stay in the same well practically for an infinite amount of time with little quantum tunneling. When the potential term characterizing the on-site Coulomb interactions is removed so that the Hamiltonian becomes that of the tight-binding type, such localized states no longer exist, indicating strongly that they are the result of electron-electron interactions and consequently a distinct many-body phenomenon. We derive an approximate theory, based on the simplified picture of one-dimensional tunneling of massless Dirac fermions, to explain the physical origin of the localized states. We further find that, when the geometrical shape is that of stadium [Fig. 5.1(b)] or bowtie [Fig. 5.1(c)] so that the classical dynamics is chaotic, the localized states are effectively removed and the tunneling rates become significant. This means that, classical chaos is capable of destabilizing the localized states. In addition to the classically integrable and fully chaotic domains, we have also considered a class of domains, the mushroom billiard [Fig. 5.1(d)], in which the classical dynamics is mixed (or nonhyperbolic) with coexisting regular and chaotic components in the phase space [243, 93]. We show that, due to the chaotic component, quantum tunneling can be regularized and enhanced. From the standpoint of device development such as graphene-based resonant-tunneling diodes, the localized states present an obstacle to effective tunneling and such states are therefore undesirable. From this perspective, classical chaos may be regarded as advantageous.

In Sec. 5.2, we describe the mean-field Hubbard model and our method to compute the tunneling rate and tunneling probability for graphene systems. In Sec. 9.3, we present evidence for polarized states with near-zero tunneling rate as induced by many-body interactions in classically integrable domains and demonstrate that chaos
Figure 5.1: Schematic illustration of four classes of geometrical domains for graphene billiards studied (a) rectangle, (b) stadium, (c) bowtie and (d) mushroom. The respective classical dynamics are integrable (a), chaotic with neutral periodic orbits (b), hyperbolic with all periodic orbits being unstable (c), and nonhyperbolic with mixed phase space (d). The thin gray region along a symmetric line represents the potential barrier.

can regularize the quantum many-body tunneling dynamics. In Sec. 5.4, we present a physical theory based on solutions of the Dirac equation to understand the emergence of polarized states. Conclusions and discussion are presented in Sec. 6.5.

5.2 Methods: Mean-Field Hubbard Model and Quantum Tunneling

5.2.1 Mean-Field Hubbard Hamiltonian

We consider $p_z$ orbitals contributing to $\pi$-electron hopping in the graphene honeycomb lattice. Each orbital can have two electrons at most, one spin up and another spin down. To capture the essential physics of electron-electron interactions in graphene while keeping the model tractable, we take into account nearest-neighbor hopping terms and electron Coulomb repulsion at the local site. The tight-binding
Hubbard Hamiltonian has the following standard form [244]:

\[
H = -t \sum_{\langle i,j \rangle, \sigma} c_{i,\sigma}^\dagger c_{j,\sigma} + V(x, y) \sum_{i, \sigma} c_{i,\sigma}^\dagger c_{i,\sigma} + U \sum_{i, \sigma} n_{i,\sigma} n_{i,\bar{\sigma}},
\]

where the summation of \(\langle i,j \rangle\) is with respect to all nearest-neighbor pairs, the index \(\{\sigma, \bar{\sigma}\}\) denotes spin up and down electrons, \(c_{i,\sigma}^\dagger (c_{j,\sigma})\) is the creation (annihilation) operator, \(n_{i\sigma} = c_{i,\sigma}^\dagger c_{i,\sigma}\) is the number operator, the nearest-neighbor hopping energy is \(t = 2.8\text{eV}\), \(V(x, y)\) is the location dependent external electric potential, and \(U\) is the Coulomb energy describing the interaction between a spin-up and a spin-down electrons at the same site. While the Hubbard Hamiltonian provides a somewhat simplified picture of electron-electron interactions in the corresponding system, the analysis and computations become extremely difficult even for moderate system size with only tens of atoms. For relatively large system size, approximation must be employed to gain physical understanding of the system behaviors. A standard approach is to use the mean-field approximation, where the Hamiltonian (5.1) is modified to [245, 246, 247, 248, 249, 250]

\[
H_{MF} = -t \sum_{\langle i,j \rangle, \sigma} c_{i,\sigma}^\dagger c_{j,\sigma} + V(x, y) \sum_{i, \sigma} c_{i,\sigma}^\dagger c_{i,\sigma} + U \sum_{i, \sigma} \langle n_{i,\bar{\sigma}} \rangle n_{i,\sigma}.
\]

Physically, the mean-field Hamiltonian describes the situation where a spin-up electron at site \(i\) interacts with the average spin-down electron population \(\langle n_{i\downarrow} \rangle\) at the same site, and vice versa. The mean field Hubbard model is effectively a variation of the unrestricted Hartree-Fock approximation [251]. There have been recent efforts in comparing the various aspects of the mean-field Hubbard model with those from first-principle or quantum Monte-Carlo calculations, with the conclusion that the mean-field approximation is generally valid for graphene systems [250, 249], especially in the weakly coupling regime [246, 252]. It is thus justified to choose the
parameter $U$ below the critical Coulomb repulsion $U_c = 2.2t$. In this work, we use $U = 1.2t$ [250].

System (5.2) can be solved iteratively, as follows. At half-filling and zero temperature, the average density of electrons with spin $\sigma$ at atom $i$ is defined as $\langle n_{i,\sigma} \rangle = \sum_{n=1}^{N/2} \rho_{i,\sigma}(E_n)$, where $N$ is the total number of eigenstates with a given spin, and $\rho_{i,\sigma}(E_n) = |\psi_{i,\sigma}^n|^2$ is the local density of states (LDS) at site $i$ for the $n$th eigenstate $\psi_{i,\sigma}^n$. Starting from an initial condition of $\langle n_{i,\sigma} \rangle$ for spin $\sigma$, the Hamiltonian in (5.2) is complete for spin $\sigma$ and yields a new set of eigenstates $\{E_n, \psi_{\sigma, n}^i, n = 1, \cdots, N\}$, which can then be used to calculate $\rho_{\sigma}(E_n)$, leading to a new set of $\langle n_{i,\sigma} \rangle$. Using $\langle n_{i,\sigma} \rangle$ as the initial condition, the Hamiltonian in (5.2) can be used to solve the set of eigenstates for spin $\sigma$, yielding a new set of average density $\langle n_{i,\sigma} \rangle$ of electrons for spin $\sigma$. We then iterate the process until $\langle n_{i,\sigma} \rangle$ and $\langle n_{i,\bar{\sigma}} \rangle$ reach a steady state. To be concrete, we choose the initial configuration of the system to be that of an anti-ferromagnetic state, where the initial values of $\langle n_{i,\downarrow} \rangle$ are chosen to be $+1/−1$ at sublattice $A/B$, respectively. The local spin density at site $i$ is $m_i = (\langle n_{i,\uparrow} \rangle - \langle n_{i,\downarrow} \rangle)/2$. In our model, the number of electrons is fixed, so the total spin density of the whole system is given by $M = \sum_{i=1}^{N} m_i = M^L + M^R = 0$, where $M^L$ and $M^R$ represent the total spin density at the left and the right sides of the potential barrier, respectively.

### 5.2.2 Integrable, Chaotic, and Nonhyperbolic Domains

We consider four types of geometrical domains with distinct classes of classical dynamics, as illustrated in Fig. 5.1. For meaningful comparison of results, we set the sizes of the billiards to be approximately the same. The first type is rectangular graphene billiard with integrable classical dynamics. The parameters of the system are $L = 161a = 22.86\text{nm}$ (armchair boundaries) and $D = 85a = 12.05\text{nm}$ (zigzag boundaries), where $a = 1.42\text{Å}$ is the distance between two neighboring carbon atoms.
and the lattice constant is $a_0 = \sqrt{3}a$. The total number of atoms is $N = 10692$. The second type is stadium billiard with parameters $L = 22.862\text{nm}$, $D = 12.052\text{nm}$, and $N = 9452$. The underlying classical dynamics is chaotic but with an infinite number of neutrally stable periodic orbits, corresponding to particles bouncing back and forth vertically at the rectangular portion of the billiard. The third type is bowtie billiard, which is cut from a rectangle graphene sheet of 14.5nm by 7.2nm by circles of radius $r = 32.7\text{nm}$, and the domain contains 10946 carbon atoms. For the bowtie billiard, the classical dynamics is fully chaotic (hyperbolic) with all periodic orbits being unstable. The fourth type is the mushroom billiard with a mixed classical phase space (nonhyperbolic classical dynamics [243, 93]), i.e., there are coexisting chaotic sets and KAM tori. The radius of the semicircle is $R = 11.86\text{nm}$, and the stem of the mushroom has the sizes 11.86nm by 5.93nm. The total number of carbon atoms contained in the mushroom billiard is 10620.

In the quantum regime, classical chaos is fundamentally suppressed due to the quantum uncertainty or finite Planck constant that effectively leads to “discretization” of the classical phase space. This should be contrasted with the discretization of the physical or configuration space through a crystal lattice. In general, any such discretization scheme is incompatible with chaos because classically, the Planck constant is effectively zero and motion can occur on arbitrarily fine scales, but this difficulty is somewhat alleviated due to the finite Planck constant in the quantum regime. Only in the limit of large geometric dimensions as compared to the lattice constant will the effect of chaos be manifested in the quantum behaviors. For the geometrical domains shown in Fig. 5.1, we test different sizes and find that the pertinent quantum phenomena are quantitatively the same insofar as the system is sufficiently large, e.g., with more than 7000 atoms.

For all four types of billiards, a thin potential barrier is placed along a symmetric
line of the system. Let $x$ specifies the direction perpendicular to the symmetric line, the potential function can be written as $V(x) = V_0[\Theta(x - L/2 + w/2) - \Theta(x - L/2 - w/2)]/2$, where $\Theta$ is the Heaviside step function. Effectively, the whole billiard system thus has a double quantum-well (QW) structure. We set (somewhat arbitrarily) $V_0 = 0.766t$ and $w = 2.5a$ in all calculations.

### 5.2.3 Characterization of Tunneling

For nonrelativistic single particle quantum systems, the tunneling phenomenon and the effect of classically chaotic dynamics can be conveniently studied by considering symmetric quantum billiards with a potential barrier placed along the line of symmetry. In such a situation, the eigenstates are either symmetric or antisymmetric, and they appear in pairs. A particle will tunnel through completely from one side to another, and then back and forth, generating an oscillating pattern. The tunneling dynamics can then be fully characterized by the tunneling rate, which can be expressed in terms of the corresponding energy splittings of the symmetric-antisymmetric tunneling pairs [242]. In relativistic quantum systems, the symmetric and antisymmetric eigenstates do not necessarily come in pairs. In this case, the tunneling rate can be calculated, for each eigenstate, by setting a special type of corresponding initial state localized on one side of the barrier. The tunneling rate can be determined through the time evolution of such an initial state. This method is general, as for nonrelativistic quantum tunneling systems, the results agree completely with those calculated by the symmetric-antisymmetric energy splitting method [86]. When many-body interactions are included, the method needs to be modified further. Especially, the interactions can effectively be represented by a mean-field potential $U\langle n_i, \pi \rangle$ for a $\sigma$ electron. With respect to tunneling, there is then an extra potential that is different for spin up and spin down electrons. This extra potential breaks
the mirror symmetry and induces localized states with diminishing tunneling. As a result, an additional quantity, the tunneling probability, together with the tunneling rate, is needed to fully describe the tunneling phenomena in relativistic many-body quantum systems.

To be specific, the method developed for single-electron tunneling in Dirac fermion and graphene systems [86, 93] can be readily adopted to systems described by the Hubbard Hamiltonian. Firstly, we solve the eigenenergy values and eigenstates from $H_\sigma |n\rangle_\sigma = E_{n\sigma} |n\rangle_\sigma$, where $H_\sigma$ is the mean-field Hamiltonian in Eq. (5.2) and $\langle n_i, \sigma \rangle$ are the steady-state values. An arbitrary state $|\psi\rangle_\sigma$ can then be written as a linear combination of the eigenstates: $|\psi\rangle_\sigma = \sum_n a_n |n\rangle_\sigma$, where $a_n$ denotes a set of normalized coefficients. Second, for each eigenenergy value $E_{n\sigma}$ and its associated eigenstate, we define a new wavefunction: $\psi_{n, \sigma}(r)$, such that the corresponding probability is concentrated entirely on one side of the barrier, say, the left side:

$$\psi_{n, \sigma}(x, y) = \begin{cases} C |n\rangle_\sigma, & x \leq (L - w)/2 \\ 0, & \text{otherwise}, \end{cases}$$

(5.3)

where $C$ is a normalization constant. This new, asymmetrical wavefunction can be expanded in the original base of eigenstates: $|\psi\rangle_{n, \sigma} = \sum_k b_k |k\rangle_\sigma$, where $b_k$ is a set of expansion coefficients given by $b_k = \langle k | \psi \rangle_\sigma$. The time evolution of the wavefunction $|\psi\rangle_{n, \sigma}$ is then given by

$$|\psi(t)\rangle_{n, \sigma} = \sum_k b_k e^{-iE_k t/\hbar} |k\rangle_\sigma.$$  

(5.4)

In general, $b_n$ is significantly larger than other coefficients. Depending on the original state, there can be two, three, or a few coefficients that are well separated from the rest of the coefficients that are negligible. As a result, the summation of Eq. (5.4) can effectively be evaluated using a small number (usually tens) of states with appreciable coefficients.
Starting from Eq. (5.4), the left-well probability $P_L^\sigma(t)$ can be written as

$$
P_L^\sigma(t) = \langle \bar{\psi}(t) | \psi(t) \rangle_{n,\sigma}^L = \sum_{k,k'=1}^{N} b_k b_{k'} \langle k | k' \rangle_{\sigma}^L e^{-i(E_{k'} - E_k)t},
$$

(5.5)

where the upper index $L$ indicates integration over the left well only and $b_k$ is real. Since $|\psi(t)\rangle_{n,\sigma}$ can be approximated by a few terms, the sum in Eq. (5.5) can be approximated by a few terms as well. From direct numeric calculation, we find that most of the states can be approximated by either two or three eigenstates, with few exceptions.

Say, initially, we choose an initial state entirely in the left well: $P_L^\sigma(t = 0) = \langle \bar{\psi}(0) | \psi(0) \rangle_{\sigma}^L = 1$, where the upper index $L$ denotes the integration over the region on the left side of the barrier, i.e., $x \leq (L + w)/2$. For $t > 0$, the tunneling process begins so that the probability $P_L^\sigma(t)$ decreases with time and reaches its first minimum value $P_{\text{min}}^L$ at time $t = \Delta T$. The tunneling rate is conveniently determined by $R = 1/\Delta T$, where the Planck’s constant has been normalized to unity: $\hbar = 1$. Defining $\Delta P = 1 - P_{\text{min}}^L$, we see that $\Delta P$ is the portion that tunnels to the right side of the barrier. The rate $R$ and tunneling probability $\Delta P$ characterize the tunneling process completely.

Similarly, one can choose an initial state that is localized in the right-hand side of the barrier: $P_R^\sigma(t = 0) = \langle \bar{\psi}(0) | \psi(0) \rangle_{\sigma}^R = 1$, examine the time evaluation $P_R^\sigma(t)$, and determine the tunneling rate accordingly. Due to symmetry, we have $P_L^\sigma = P_R^\bar{\sigma}$, so it is necessary to focus only on the tunneling from the left side for spin-up and spin-down states to obtain a complete picture of the quantum tunneling dynamics.
5.3 Results

5.3.1 Polarization of Spin Wavefunctions Associated with Confined States

To gain intuition, we first study confined states in the absence of any potential barrier for the rectangular geometry. Representative results are shown in Fig. 5.2(a), where the profiles of the probability density in the horizontal direction for electrons with different spins are presented. From Fig. 5.2(a), we observe that the confined states are not polarized, i.e., the spin-up and spin-down wavefunctions are nearly identical in their spatial distributions in the entire domain. The small difference between the spin-specific wavefunctions diminishes for $E \to t$, where $t$ is the nearest-neighbor hopping energy in the graphene lattice.

We next investigate the case where there is a narrow potential barrier at the center of the rectangular graphene flake. A surprising phenomenon is that, due to a combined effect of electron-electron interactions and the potential barrier, there are eigenstates in which the spin-up and spin-down electrons become strongly polarized. For example, for the case shown in Fig. 5.2(b), the spin-down (up) electrons tend to focus on the left (right) side of the barrier only. While the case shown in Fig. 5.2(b) corresponds to wavevector $k_x \approx 2\pi/L$, other polarized states can be found for $k_x \approx \pi n/L$ ($n = 4, 6, \cdots$). This polarization phenomenon occurs only for the original eigenstates of even parity ($n = 2, 4, 6, \cdots$) in the absence of potential barrier. For eigenstates of odd parity ($n = 1, 3, 5, \cdots$) originally, introduction of a potential barrier does not generate spin polarization.

The polarized states appear in pairs. For example, if there is a polarized state in which the spin-up electrons concentrate on the left quantum well (spin-down electrons on the right well), there will be a corresponding polarized state that somewhat mimics a reflected version of the original state, e.g., represented by a wavefunction for which
Figure 5.2: Spin-up-down are denoted by red/solid and blue/dashed curves, respectively. (a) probability density profile of the 5849th eigenstate at $y = D/2$ without a potential barrier, where it extends in both potential wells, (b) probability density profile of the 5860th eigenstate at $y = D/2$ with a potential barrier of height $V_0 = 0.766t$ and width $w = 2.5a$ at $x = 0$ (represented by the gray rectangle). In (b), there is spin polarization, i.e., spin-up electrons reside in the right well and spin-down electrons reside in the left well. The corresponding eigenenergies are $E_{5849} \approx 0.6819t$ for (a) and $E_{5860} \approx 0.6924t$ for (b). The insets in both panels show the corresponding LDS patterns in the entire domain. Note that the wavefunctions have a zigzag appearance because they are plotted for both graphene sublattices, denoted by $A$ and $B$. (A plot of the wavefunction on one sublattice would appear more smooth.)

the spin-up electrons concentrate on the right well. The energy difference between the paired states are typically small. Figure 5.3(a) shows the energy levels of the polarized-state pairs. The red and blue bars with arrow (indicating spins) located at the left or the right side denote that the electrons are mainly polarized at the left or the right quantum well, respectively. For the specific initial condition used, the average local spin density is positive at the right boundary, and negative at the left boundary. Because of the repulsive Coulomb interaction between the electrons, the polarized state with spin-up electrons residing at the right well has a lower energy,
Figure 5.3: (a) Eigenenergy levels versus the eigenstate index. The red and blue bars with up and down arrows, respectively, represent a pair of polarized states \((n = 5760 \text{ and } m = 5765)\), where the corresponding eigenenergies are \(E_n = 0.6203t\), \(E_{n+1} = 0.6204t\), \(E_m = 0.6235t\) and \(E_{m+1} = 0.6237t\). The black bar without any arrow corresponds to a non-polarized state. (b,c) Probability densities for the polarized state pairs \((n, n+1)\) and \((m, m+1)\), respectively. Note that the energy difference for each pair is quite small.

while its counterpart has a higher energy. Typical polarized states are shown in Fig. 5.3(b-c). The accumulation of edge states contributes to the polarized average spin density (magnetic moments) of the graphene sheet. When polarization of the confined states emerges, the polarized magnetic moments remain approximately the same. The reason is that, for each pair, the magnetic moments of the polarized states nearly cancel each other.

The basic physical mechanism for the emergence of the localized spin-polarized states can be understood by employing the Dirac equation \([1, 2, 3, 4, 7, 8, 9]\):

\[
-iv_F[\sigma \cdot \mathbf{p} + V]\psi = E\psi, \tag{5.6}
\]
where $v_F$ is the Fermi velocity of electrons in graphene, $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ are the Pauli matrices, the components of the spinor wavefunction $\psi = [\psi_A, \psi_B]$ correspond to the pseudospins that characterize whether the electron resides on sublattice $A$ or $B$, respectively, and the term $V$ represents the mean-field potential due to a combined effect of the barrier potential and the edge potential caused by the intrinsic magnetic moments of spin electrons. It can be demonstrated that the Coulomb repulsive interaction leads to anti-ferromagnetic steady states (mostly edge states) at the graphene sublattices, with net spin-up electrons residing on the zigzag boundary on one side, while spin-down electrons residing on the other zigzag boundary. These steady states can in turn be regarded as an effective potential that breaks the left-right reflection symmetry. However, this symmetry breaking can be subdued as a shift of the system. When a potential barrier is applied, it introduces into the system a natural reference point that makes this shift unlikely, yielding spin polarized confined states. These states often appear in pairs so that their magnetic moments cancel each other. Details of the solutions of the Dirac equation and their physical analysis are presented in Sec. 5.4.

5.3.2 Tunneling Rate and Probability of Spin-Polarized States

When a potential barrier is placed in a closed domain, electrons can tunnel through from one side of the barrier to another. For graphene systems, a systematic method for numerically calculating the tunneling rate has been developed recently [86] in the single-electron, tight-binding framework.

Our numerical computation reveals a striking phenomenon: when electron-electron interactions are present, the tunneling probability $\Delta P$, the portion of the state that can tunnel into the other side of the barrier, can be extremely small, e.g., $\Delta P \sim 10^{-4}$, as shown in Fig. 5.4(a). This should be contrasted to the case of single-electron tun-
Figure 5.4: $1/\Delta T$ versus $\Delta P$ for two cases where (a) there are electron-electron interactions as described by the Hubbard model and (b) there is only a single electron in the system.

Corresponding to the extremely small values of $\Delta P$, the tunneling rate $1/\Delta T$ that characterizes the “speed” of tunneling assumes also extremely small values. The reason that $\Delta P$ can be so small for electrons with Coulomb interactions lies in the emergence of the spin-polarized states. In particular, in a single-electron tunneling system, because of the left-right reflection symmetry, the eigenfunction also has even or odd symmetry, and the probabilities for the electron to reside in the left and right wells are equal. When renormalizing the left part of the wavefunction for the situation where the electron initially is located in the left well, the symmetry stipulates that the electron will eventually tunnel to the right side as there is no mechanism to contain it only within the left well. However, for the many-body case where electron-electron interactions are present, the graphene zigzag edge at the opposite boundaries bear different magnetic moments, positive on one side and negative on the other side. Spin-up and spin-down electrons will then “feel” different potentials at the bound-
aries, leading to the left-right reflection symmetry breaking and, consequently, to the emergence of spin-polarized states. For example, consider an eigenstate associated with spin-up electrons residing mostly in the left well. Because it is an eigenstate, the time evolution of the probability in the left well, $P_L$, will be a constant and approximately equal to 1. That is, it is a spin polarized and localized state. We can then deduce that, for spin-up electrons in the left well initially, the associated state will have a significant component in the spin-polarized states, with a high probability $P_L$ in the left well at all times, resulting in extremely small values of $\Delta P$. For comparison, we have also computed the tunneling rate for the single-electron case, as shown in Fig. 5.4(b). In this case, while the tunneling rate can be small, the tunneling probability $\Delta P$ is generally large. We note that, in addition to the strongly localized states, there are also states that are less localized, resulting in relatively larger values of $\Delta P$. These states can be either spin polarized or non-polarized.

A careful examination of Fig. 5.4(a) reveals that the data points can be categorized into three classes, depending on the patterns of their distribution in the $(1/\Delta T, \Delta P)$ plane. These different tunneling behaviors correspond to distinct time evolutions of the probability $P_L(t)$ for electrons in the left well. In particular, for classes I and II in Fig. 5.4(a), $P_L(t)$ is a cosine function, while for class III, $P_L(t)$ is a zigzag curve. In Sec. 5.4, we develop a theory to understand the distinct behaviors in the time evolution of $P_L$.

### 5.3.3 Regularization of Tunneling by Chaos

Our understanding of the spin-polarized confined states in the rectangular graphene indicates that many-body interactions are key to the emergence of such states. These states have a significant effect on the quantum tunneling dynamics. Especially, for the rectangular graphene billiard, not only can the tunneling rate be negligibly small
Figure 5.5: Tunneling rates $1/\Delta T$ versus $\Delta P$ for (a) stadium and (b) bowtie graphene billiards. The green dashed horizontal line indicates the separation of the two classes of spin polarized (lower) and unpolarized (upper) states. The black solid up- and down-triangles correspond to the typical LDS patterns in each class for spin-up and -down states, respectively.
(corresponding to large values of $\Delta T$), but also the tunneling magnitude $\Delta P$. While our analysis suggests that other physical factors, such as the potential barrier and the pseudospin degree of freedom of graphene, also play a role in the formation of the localized spin-polarized states, many-body interactions are the single most important factor. This is because, without such interactions, the tunneling rate and magnitude can typically be appreciable in graphene systems of the same geometry [86]. Does this mean that, in any realistic graphene system where many-body interactions are inevitably present, tunneling is far less likely? If this were the case, it would be difficult to develop graphene-based tunneling device. Here, we shall show that *this difficulty can be overcome by taking advantage of classical chaos*. In particular, we demonstrate that, when the geometry of the domain is such that the corresponding classical dynamics is chaotic, both the tunneling rate and magnitude can be significantly enhanced, suggesting that chaotic geometries are favorable if fast and sizable tunneling is needed when developing graphene tunneling devices. Since the effective geometrical shape of the domain can be modulated by external means, such as atomic probe [253] or gate voltage, control of quantum tunneling dynamics in the presence of many-body interactions can be achieved by using chaos.

Figure 5.5 shows the tunneling rates for a stadium-shaped and a bowtie-shaped graphene billiards, where the latter is fully chaotic in that all classical periodic orbits are unstable. As compared with the rectangular billiard, for both types of chaotic billiards, the points in the plot of the tunneling rates $1/\Delta T$ versus $\Delta P$ in Fig. 5.5 are more concentrated in both dimensions. The concentration is more compact for the bowtie billiard (the “more chaotic” domain). More specifically, some pronounced features of Fig. 5.5 are the following.

Firstly, as compared with the rectangular domain, the tunneling rates associated with the chaotic domains are greatly enhanced, e.g., from about $10^{-6}$ in Fig. 5.4 to
Figure 5.6: Tunneling rates $1/\Delta T$ versus $\Delta P$ for the nonhyperbolic mushroom billiard. The green dashed horizontal lines indicate the separation of the data points into three different classes. The middle and lower classes correspond to the chaotic components. The upper class is originated from the stem of the mushroom billiard. The black solid up- and down-triangles correspond to the LDS patterns for spin-up and spin-down states in the right-side panels, respectively.

about $10^{-4}$ in Fig. 5.5. Comparing Figs. 5.5(a) with 5.5(b), we see that overall, the tunneling rates for the “more chaotic” bowtie billiard are even larger.

Secondly, the range of $\Delta P$ is reduced in the chaotic cases in the sense that, as compared with the rectangular domain, the minimum value of $\Delta P$ is larger and its maximum value becomes smaller. For the stadium and bowtie domains, the ranges are from 0.1 to 0.9 and from 0.2 to 0.8, respectively. A common feature is that the localized states with extremely small values of tunneling rate no longer exist. In fact, the maximal local spin densities are comparable for all three types of domains: 0.1565, 0.1507, 0.1691 for rectangular, stadium, and bowtie billiards, respectively. Thus, the nearly perfect spin polarized states in the integrable domain have been effectively eliminated by chaos!

Thirdly, for the integrable case, as shown in Fig. 5.4, the points in the plot of
$1/\Delta T$ versus $\Delta P$ are grouped into three classes. For both types of chaotic domain, as shown in Fig. 5.5, the points only belong to two classes. The first class is for $1/\Delta T \sim 10^{-2}$, which is similar to case III for the rectangular domain in that the eigenstates are not polarized but distributed equally between the left and the right wells. It might be tempting to regard the lower points in Fig. 5.5 (especially in the side panels) as corresponding to some sort of spin-polarized states. However, in contrast to the rectangular case in which the states are either antiphase (class I) or having identical phases for $A$ and $B$ atoms (class II), the eigenstates for the chaotic cases do not have such a clear cut for the relative phases, but assume randomized values between 0 and $\pi$.

We conclude that, when electron-electron interactions are taken into account in a graphene system, chaos can not only regularize the tunneling rate as in situations where such interactions are neglected [242, 86, 93], but also regularize the polarization and mix the relative phase between the states associated with the two distinct sublattices.

In realistic quantum devices, nonhyperbolic dynamics with mixed phase space [40, 75, 28, 76, 41, 34, 35, 36, 77, 78, 79] can be expected to arise typically. Here we investigate the tunneling dynamics in classically nonhyperbolic systems in the presence of electron-electron interactions. We choose the mushroom billiard, a mathematically proved nonhyperbolic system [243], as shown in Fig. 5.1(d). A potential barrier is placed along the vertical symmetric line. Figure 5.6 shows the tunneling rate $1/\Delta T$ versus $\Delta P$. The points are scattered in three regions, which are separated by the horizontal dashed lines. The middle and the lower parts are similar to the two regions for the chaotic cases in Fig. 5.5. Specifically, the middle part corresponds to nonpolarized states, while the lower part corresponds to the polarized states. The upper region, which is absent for both integrable and chaotic cases, corresponds to
the integrable part of the mushroom billiard in the stem region. From Fig. 5.6, the minimum value for $\Delta P$ is about 0.3, which is larger than those for both chaotic cases. For the mushroom billiard, the classical periodic orbits generally cross both the left and the right parts, thus strong polarized states are less likely to form, leading to relatively larger values of $\Delta P$. These results are quantitatively similar to those in absence of electron-electron interactions [93].

5.4 Theory

5.4.1 Emergence of Polarized States - Mean-Field Theory

The unit cell of the honeycomb lattice of graphene has two nonequivalent carbon atoms, $A$ and $B$, resulting in two Dirac points in the wave vector space: $K(K') = (2\pi/\sqrt{3}a_0, \pm 2\pi/3a_0)$. In the vicinity of a Dirac point, the dispersion relation is linear: $E = \pm \hbar v_F |k|$, where $v_F$ is the Fermi velocity of electrons in graphene, and $k$ denotes the deviation in the momentum from the Dirac point. Neglecting the coupling between the two Dirac points, the quantum dynamics of the quasiparticles in graphene are described by the Dirac equation [1, 2, 3, 4, 7, 8, 9], Eq. 5.6. The electron-electron interaction can be treated by the mean-field Hubbard Hamiltonian. In particular, the states of electrons of spin $\sigma$ are affected by the mean-field electron density of the opposite spin $\langle n_{i,\overline{\sigma}} \rangle$. This density has appreciable values only at the zigzag edges and it is in fact exponentially small inside the domain [Fig. 8.1(a)]. As a result, effectively the electron-electron interaction can be described by the following square potential function $\varepsilon_\sigma M(x)$ [Fig. 8.1(b)]:

$$M(x) = \begin{cases} 
+M_0, & x < \Delta l \\
-M_0, & x > L - \Delta l \\
0, & \text{otherwise}
\end{cases}$$ (5.7)
where \( \varepsilon = \varepsilon_{\uparrow(\downarrow)} = +1(-1) \) for spin up (down), \( M_0 \) is the effective value of \( \langle U \langle n_{\sigma}(\pi) \rangle \rangle \) close to the zigzag boundary, \( U \) is a parameter characterizing the Coulomb interaction in the mean-field Hubbard Hamiltonian, and \( \Delta l \sim a \) is the width of the effective potential. Note that the effective potential felt by the spin-up and spin-down electrons are opposite to each other. The overall potential for spin \( \sigma \) electrons can thus be expressed as \( \tilde{V}_\sigma = V(x) + \varepsilon_\sigma M(x) \), and the mean-field Dirac Hamiltonian near the Dirac point \( K(K') \) is given by

\[
H_{K(K'),\sigma} = v_F \begin{pmatrix}
\tilde{V}_\sigma & -i \partial_x \mp \partial_y \\
-i \partial_x \pm \partial_y & \tilde{V}_\sigma
\end{pmatrix}.
\]  
(5.8)

For notational clarity, we shall use small letters \( \epsilon, \tilde{v} \) and \( m \) to denote the energy \( E \), potential \( \tilde{V} \), and \( M \) divided by \( \hbar v_F \). Note that, the Hamiltonian with the effective potential \( \varepsilon_\sigma M(x) \) no longer has the left-right reflection symmetry. However, it has the combined symmetry of simultaneous reflection and spin interchange. It is thus only necessary to consider spin-up electrons, because the states of spin-down electrons can be obtained straightforwardly by the symmetry operation: \( \psi_\downarrow(x) = \psi_\uparrow(-x) \).

For the \( K(K') \) valley, the bulk eigenstate of the Dirac Hamiltonian Eq. (5.8) is given by [254]

\[
[\psi_A^{(l)}, \psi_B^{(l)}]^T = e^{ik \cdot r}[1, \mp e^{\pm i\phi}]^T
\]

associated with energy \( E = \pm \hbar v_F |k| \), or \( \epsilon = \pm |k| \), where \( \phi = \tan^{-1} k_y/k_x \). Under the influence of the total potential \( \tilde{V} \), the wavevector in the \( x \)-direction becomes

\[
k_x = \sqrt{(\epsilon - \tilde{v})^2 - k_y^2}.
\]

The solutions of the Dirac equations for the armchair or zigzag graphene nanoribbons can be found in Refs. [7, 255]. For the armchair boundaries, the wavevector \( k_y \) is related with the length \( D \) in the \( y \) direction by \( k_y \rightarrow k_n = n_y \pi / D - 4\pi / 3a_0 \), where
\( n_y = 0, \pm 1, \pm 2, \ldots \). For an armchair nanoribbon, \( k_n \) is thus independent of the potential \( \tilde{V} \) and \( k_x \), and the wavefunction in the \( y \)-direction can be separated as

\[
[\psi_A, \psi_B]^T = e^{ik_n y}[\phi_A, \phi_B]^T,
\]

where

\[
\begin{pmatrix}
\phi_A \\
\phi_B
\end{pmatrix} = \begin{pmatrix}
\frac{1}{\epsilon_\gamma}[a_\gamma(k_n - z)e^{zx} + b_\gamma(k_n + z)e^{-zx}] \\
a_\gamma e^{zx} + b_\gamma e^{-zx}
\end{pmatrix}.
\]

The coefficients \( a_\gamma \) and \( b_\gamma \) in Eq. (5.9) represent the amplitudes of the wavefunction in the region \( \gamma \) and \( \epsilon_\gamma = \epsilon - \tilde{\nu} \) is the relative energy, where \( \gamma = L, R, C \) stand for the left, the right and the central barrier regions, respectively. For confined and edge states, we have \( z = k_x \) and \( z = ik_x \), respectively.

For zigzag graphene ribbons, the wave vector \( k_x \) parallel to the armchair edges couples with \( k_n \) if the potential \( \tilde{\nu} \) is equal to zero or a constant. In this case, the relationship between the two wavevectors in orthogonal directions is given by [255]

\[
(k_n - z)/(k_n + z) = \exp(\mp 2Lz),
\]

for the \( K(K') \) point, respectively. A simplified condition of \( k_x \) for confined states can be rewritten as [255, 7] \( k_x = \pm \tan^{-1}(k_x/k_n) \) for the \( K(K') \) valley.

We first focus on the solution in the \( K \) valley and the case without central barrier. In this case, \( k_n \) is determined by the width \( D \) of the domain but, due to the effective potential \( M(x) \) close to the zigzag boundaries, it is infeasible to obtain an exact expression for \( k_x \). Note that the width of this potential, \( \Delta l \), is typically much smaller than the length \( L \) of the device and is also smaller than the wavelength in the \( x \) direction. The following approximations can then be justified. In particular, we assume that the ratio between the wave amplitude is a constant: \( a_\gamma/b_\gamma = -1 \), and the potential \( \tilde{\nu} \) is also a constant for the whole system, which are valid for the case without the central potential barrier. Within distance \( \Delta l \) to the boundaries \( x = -L/2 \)
Figure 5.7: (a) Illustration of a rectangular graphene domain of length $L$ and width $D$ with a potential barrier in the middle. The zigzag and armchair edges are along the $x-$ and $y-$axis, respectively. The filled red (blue) circles at the right (left) zigzag boundaries denote the positive (negative) magnetic moments, the radii of which represent the strength of the spin density. (b) The effective potential profile $\tilde{V}_1(x)$ at the position $y = D/2$ for spin-up electrons, where the positive and negative potentials near the boundaries represent the strength of the respective spin density, which approach the value of $M_0 (-M_0)$ at the left (right) zigzag edges in (a). The effective potential for spin-down electrons is reversed at the boundaries as compared with that for spin-up electrons.
and \( L/2 \), the wavefunction can then be written as

\[
\begin{pmatrix}
\phi_A \\
\phi_B
\end{pmatrix} \approx a_{\gamma} \begin{pmatrix}
\frac{1}{\epsilon_{\gamma}} [-2z + 2k_nzx] \\
zx
\end{pmatrix}
\]

by first-order linear approximation. In these regions, the only difference from the case where the effective potential is absent lies in the wavevector or the wavelength, i.e., \( k_{x}^{\pm} = \sqrt{(\epsilon \pm m) - k_n^2} \). Since, what matters here is only the phase change in the wavefunction, we can assume that the wavevector is unchanged but the length of this potential region is changed, say, from \( \Delta l \) to \( \Delta \tilde{l}^{\pm} \) for the right and left boundaries, respectively. We have

\[
\Delta \tilde{l}^{\pm} = (k_x/k_{x}^{\pm})\Delta l.
\]

As a result, the wavevectors \( k_{\gamma} \) takes on the same value as for the case without the potential \( m \) and the only difference is the change in the effective width, \( \Delta l \). In particular, at the left boundary, \( \Delta l \) shrinks to \( \Delta \tilde{l}^- \) and, at the right boundary, \( \Delta l \) expands to \( \Delta \tilde{l}^+ \). This is illustrated in Fig. 5.8(a) in the zoom-in insets, which show the comparison between the real wavefunction (black solid curve) and the effective wavefunction (red dashed curve) in the potential regions. Based on these observations, we can effectively transform the system into a new system without potential \( m \), but with the boundaries shifted by a displacement \( \delta_{1(2)} \), as shown schematically in Fig. 5.8(a). The effective boundary displacement can be determined as

\[
\delta_1 = \Delta l - \Delta \tilde{l}^- \quad \text{and} \quad \delta_2 = \Delta \tilde{l}^+ - \Delta l.
\]

The physical meaning is that the wavefunctions of spin-up electrons are shifted toward the right (positive axis) by the amount \( \delta = (\delta_1 + \delta_2)/2 \). We shall see that, because of this relative shift, when a potential barrier is placed in the middle of the domain, the equivalent system with shift breaks the left-right reflection symmetry, which is
the key to the emergence of spin polarized states. Note that, if the energy \( \epsilon \) is close to the potential value \( m \), the wavevector \( k_x^- \) will be purely imaginary and the wavefunction near the left boundary has an exponential form, which differs from a normally propagating wavefunction. But this does not affect our analysis.

Next, we consider the case where a potential barrier is placed along the symmetric line of the domain and provide an explanation for the emergence of the spin-polarized states. To be concrete, we choose a narrow potential barrier of width \( w = 2.5a = 0.016L \) and place it at \( x = 0 \). From the above analysis, \( x = 0 \) is no longer the center of the equivalent system, as the boundaries have been shifted to the right by the displacement \( \delta \) so that the widths of the left- and right-side quantum wells become \( W_1 \approx (L - w)/2 - \delta \) and \( W_2 \approx (L - w)/2 + \delta \), respectively. Equivalently, the electron-electron interaction system with a symmetric double well structure can be transformed into a single-electron system with asymmetric double wells.

For an asymmetric double-well system, the standard wavefunctions for graphene [Eq. (5.9)] satisfy the boundary conditions:

\[
\phi_{A(B)}^L(-L_1/2) = \phi_{A(B)}^R(L_2/2) = 0,
\]

where \( L_{1,2} = 2W_{1,2} + w \). We obtain

\[
b^L = -a^L e^{-ik_x L_1} \quad \text{and} \quad b^R = -a^R \frac{k_n^r}{k_n^l} e^{ik_x L_2},
\]

where \( k_n^\pm = k_n \pm ik_x \), \( k_n = n_y \pi/D + 4\pi/3a_0 \), and \( k_x \) is to be determined. The continuity conditions at the barrier interfaces are

\[
\phi_{A(B)}^L(-w/2) = \phi_{A(B)}^C(-w/2),
\]

\[
\phi_{A(B)}^R(w/2) = \phi_{A(B)}^C(w/2).
\]

When Eq. (5.11) is applied, the equations of \( a = [a^L, a^R, a^C, b^C]^T \) can be reorganized
as $\mathbf{A} \cdot \mathbf{a} = 0$, with $\mathbf{A}$ given by

$$
\mathbf{A} = \begin{pmatrix}
\frac{\epsilon'}{\epsilon} [k_n^- e^{-ik_x \frac{w}{2}} - k_n^+ e^{-ik_x L_1^-}] & 0 & -k_n^- e^{-i\beta \frac{w}{2}} & -k_n^+ e^{i\beta \frac{w}{2}} \\
e^{-ik_x \frac{w}{2}} - e^{-ik_x L_1^-} & 0 & -e^{-i\beta \frac{w}{2}} & -e^{i\beta \frac{w}{2}} \\
0 & \frac{\epsilon'}{\epsilon} [k_n^- e^{ik_x \frac{w}{2}} - k_n^- e^{ik_x L_2^-}] & -k_n^- e^{i\beta \frac{w}{2}} & -k_n^+ e^{-i\beta \frac{w}{2}} \\
0 & e^{ik_x \frac{w}{2}} - k_n^+ e^{ik_x L_2^-} & -e^{i\beta \frac{w}{2}} & -e^{-i\beta \frac{w}{2}} \\
\end{pmatrix},
$$

(5.13)

where $L_{1,2} = L_{1,2} - w/2$, $\beta = \sqrt{k_n^2 - \epsilon'^2}$, $\epsilon' = v_0 - \epsilon$, and $v_0 = V_0/\hbar v_F$ is the barrier height. In order to have non-trivial solutions of $\mathbf{a}$, the matrix $\mathbf{A}$ should satisfy the condition $\det |\mathbf{A}| = 0$, which in turn solves the only unknown parameter $k_x$. In general, a pair of solutions can be found near $2n\pi/L$, where $n$ is an integer corresponding to the mode number in each quantum well. The final step in our analysis is to obtain the coefficients $\mathbf{a}$. Solving for $a^L/a^R$, we obtain their relative values as

$$
a^L = \frac{\epsilon'}{\epsilon} k_n^- [1 - e^{-ik_x(w-L_2)}] - (k_n + \beta)[1 - \frac{k_n^-}{k_n^+} e^{-ik_x(w-L_2)}],
$$

$$
a^R = e^{(ik_x+\beta)w} \left\{ \frac{\epsilon'}{\epsilon} k_n^- [1 - \frac{k_n^+}{k_n^-} e^{ik_x(w-L_2)}] - (k_n + \beta)[1 - e^{ik_x(w-L_1)}] \right\}. \quad (5.14)
$$

The relative values of $b^{L-R}$ can be obtained from Eq. (5.11). With these coefficients, the wavefunction in the $x$-direction can be obtained from Eq. (5.9).

These theoretical predictions can be compared with numerical results from the mean-field Hubbard Hamiltonian for spin-up wavefunctions, as shown in Fig. 5.8(b-c). We obtain a good agreement.

There are several issues associated with experimental realizations. One is the size of the potential barrier. In our simulation, we set the width of barrier to be 0.4nm, which may be too small for a gate potential to be applied, as the current experimental techniques would allow the minimum width of top gate to be about 10nm [256]. Nonetheless, based on the theoretical prediction in Eq. (5.14), the spin-polarized
Figure 5.8: (a) Illustration of the shift in the wavefunction caused by the effective potential $M(x)$. The black solid vertical lines are the actual domain boundaries. The gray dashed lines represent the effective boundaries. The black solid curves show the actual probability of an evenly confined spin-up state without the potential barrier, and the red dashed curves represent the effective wavefunction after the “shift.” (b, c) Anti-phase and in-phase wavefunctions for sublattice $A$ and $B$, respectively, where red circles represent the simulation results from the mean-field Hubbard Hamiltonian and the gray solid and dashed curves are predictions from theory [Eqs. (5.9,5.11,5.14)]. The parameters are $v_0 = 2.045/a$, $\Delta l = 2a$, $m_0 = 0.2/a$, and the resulting boundary shift is $\delta = 0.032a$. The wavefunction mode in the $y$-direction is chosen to be $n_y = 16$ for (b) and $n_y = 112$ for (c). The numerical results are from the (arbitrarily chosen) states $n = 5547$ and 5548 for (b) and $n = 5568$ and 5569 for (c).
state is not affected by the width of the central potential barrier: it only depends on the ratio of barrier width $w$ and device length $L$. This allows an experimental study of the localization phenomenon if we enlarge $w$ and $L$ proportionally so that $w$ is sufficiently large, say, 15nm. Another consideration is that the barrier in an experimental realization may not be a square potential but with small deformations. This, however, does not present any serious challenge because the spin-polarized states are stable due to the edge magnetic moments. As a result, the polarized states can still exist and similar regularization effects of chaos should persist.

5.4.2 Tunneling Rate of Spin-Polarized States

From Eq. (5.4), we have the time evolution of the wavefunction $|\psi\rangle_{n,\sigma}$. Then, the left-well probability $P^L_\sigma(t)$ is given by Eq. (5.5). Since $|\psi(t)\rangle_{n,\sigma}$ can be approximated by a few terms, the sum in Eq. (5.5) can be approximated by a few terms as well. From direct numerical calculation, we find that most of the states can be approximated by either two or three eigenstates, with few exceptions. Particularly, for classes I and II (e.g., Fig. 5.4), we can approximate $|\psi\rangle_{k,\sigma}$ by two eigenstates only:

$$|\psi\rangle_{k,\sigma} \approx b_k |k\rangle_\sigma + b_{k'} |k'\rangle_\sigma,$$

and the expansion coefficients satisfy the relation

$$b_k^2 + b_{k'}^2 \approx 1. \quad (5.15)$$

In this case, $|k\rangle_\sigma$ and $|k'\rangle_\sigma$ are symmetric pairs: $|k(-x)\rangle_\sigma \approx |k'(x)\rangle_\sigma$, as demonstrated in Fig. 5.9(a-b). We then have

$$\langle \psi | \psi \rangle_{k,\sigma} = \langle \psi | \psi \rangle^L_{k,\sigma} = 1 \approx b_k \langle \psi | k \rangle^L_\sigma + b_{k'} \langle \psi | k' \rangle^L_\sigma.$$

Comparing this equation with Eq. (5.15), we get $\langle \psi | k \rangle^L_\sigma \approx b_k$, and $\langle \psi | k' \rangle^L_\sigma \approx b_{k'}$. Note that $\langle \psi | k \rangle^L_\sigma \approx b_k$ is equivalent to $|k\rangle^L_\sigma = b_k |\psi\rangle^L_\sigma$, as the former can be obtained by
Figure 5.9: $P_L(t)$ for spin-up states corresponding to $n = 5858$ (a), 5826 (b) and 5692 (c), and their projected states with the corresponding weighting coefficients. The green dashed-dotted curves are fitted from Eq. (5.16) (a,b) and Eq. (5.17) (c).
multiplying $\langle \psi | L \rho | \psi \rangle$ to the latter. Similarly, we have $|k'\rangle_L = b_{k'} |\psi\rangle_L$. Substituting these relations back into Eq. (5.5), we obtain the time evolution of left-side probability as

$$P^L_\sigma(t) \approx b_k^4 + b_{k'}^4 + 2b_k^2 b_{k'}^2 \cos(\Delta E \cdot t),$$

(5.16)

where $\Delta E = E_{k'} - E_k$. Note that $\langle k'| k\rangle_L$ is not zero because the integration is with respect to the left well only. Thus, the $P^L_\sigma(t)$ curve is a standard cosine-type function.

At $t = 0$, we have $P^L_\sigma = b_k^4 + b_{k'}^4 + 2b_k^2 b_{k'}^2 = (b_k^2 + b_{k'}^2)^2 \approx 1$. We see that $P^L_\sigma(t)$ reaches its first minimum at $\Delta T = \pi/\Delta E$, which is

$$P^L_\sigma = b_k^4 + b_{k'}^4 - 2b_k^2 b_{k'}^2 = (b_k^2 - b_{k'}^2)^2.$$

As a result, the tunneling probability into the right well is given by $\Delta P = 4b_k^2 b_{k'}^2$.

To validate our approximation, we select two typical states ($k = 5858$ and $5826$) that can be well approximated by two eigenstates, $|k\rangle_\sigma$ and $|k'\rangle_\sigma$, calculate $b_k$ and $b_{k'}$, and compare the approximate result Eq. (5.16) with the accurate result Eq. (5.5) of the time evolution of $P^L_\sigma(t)$, as shown in Figs. 5.9(a,b). We observe a good agreement.

Both type-I and type-II classes have the cosine time evolution of $P^L_\sigma$, but they are well separated in the $1/\Delta T, \Delta P$ plane. The main reason lies in the phase difference between the wavefunctions on the sublattices $A$ and $B$. Particularly, the phases can have $\pi$ difference, or they can be the same, as illustrated by the eigen wavefunctions in Figs. 5.9(a,b). Due to the phase differences, the energy difference $\Delta E$ (thus the tunneling rate $R$) differs as well. For the eigen wavefunctions with anti-phase with respect to $A$ and $B$, the energy difference is considerably smaller than that for the case of identical phases, resulting in the separation exemplified in Fig. 5.4(a).

For class III pattern, the quantity $|\psi(t)\rangle_{k,\sigma}$ can be approximated by three eigenstates,

$$|\psi\rangle_{k,\sigma} \approx b_k |k\rangle_\sigma + b_{k'} |k'\rangle_\sigma + b_{k''} |k''\rangle_\sigma,$$
where \( b_{k''} \) is comparable to \( b_{k'} \), and they are smaller than \( b_k \). Normalization condition requires

\[
b_k^2 + b_{k'}^2 + b_{k''}^2 \approx 1.
\]

For this class, the states are generally not polarized and they distribute approximately evenly in the left and the right well. We thus have

\[
\langle \ell | \ell \rangle_L^L \approx \langle \ell' | \ell' \rangle_L^L \approx \langle \ell'' | \ell'' \rangle_L^L \approx 1/2.
\]

Substituting this relation into Eq. (5.5), we obtain the time evolution of the left-well probability as

\[
P^L_\sigma(t) \approx b_k^2 \langle \ell | \ell \rangle_{\sigma}^L + b_{k'}^2 \langle \ell' | \ell' \rangle_{\sigma}^L + b_{k''}^2 \langle \ell'' | \ell'' \rangle_{\sigma}^L + 2b_k b_{k'} \langle \ell | \ell' \rangle_{\sigma}^L \cos (\Delta E' \cdot t)
\]

\[
+ 2b_k b_{k''} \langle \ell | \ell'' \rangle_{\sigma}^L \cos (\Delta E'' \cdot t)
\]

\[
\approx 1/2 + 2b_k b_{k'} \langle \ell | \ell' \rangle_{\sigma}^L \cos (\Delta E' \cdot t) + 2b_k b_{k''} \langle \ell | \ell'' \rangle_{\sigma}^L \cos (\Delta E'' \cdot t),
\]

where \( \Delta E' = E_{k'} - E_k \), \( \Delta E'' = E_{k''} - E_k \), \( b_k \)'s, \( \langle \ell | \ell' \rangle_{\sigma}^L \), and \( \langle \ell | \ell'' \rangle_{\sigma}^L \) can be determined numerically. A representative case is shown in Fig. 5.9(c) with both accurate result in Eq. (5.5) and the approximation in Eq. (5.17). It can be seen that the approximated results agree with those from the exact calculation reasonably well. For more complicated cases that have four and more large coefficients of \( b_k \), the above approximation method is still valid, which has been verified by direct numeric calculations.

5.5 Conclusion and Discussion

A fundamental problem in nonlinear dynamics and quantum physics is the manifestation of classical chaos in quantum systems in the presence of many-body interactions. This issue has been studied but only for non-relativistic quantum systems [94, 95, 96, 97]. We address this problem in relativistic quantum mechanics.
using graphene systems in the setting of resonant tunneling, where the electron-electron Coulomb interactions are described by the mean-field Hubbard Hamiltonian. A resonant tunneling system consists of two symmetric potential wells separated by a potential barrier, and the geometric shape of the whole domain can be chosen to generate integrable or chaotic dynamics in the classical limit. By calculating a large number of eigenenergies and eigenstates, we uncover a class of localized spin-polarized states with near-zero tunneling in the classically integrable systems (e.g., those of rectangular domains). The physical origin of the spin-polarized states can be attributed to the a combined effect of electron-electron interaction, the pseudo-spin freedom of graphene sublattices, and the potential barrier. Note that the localization phenomenon is somewhat similar to the general localization effect in one-dimensional fermion systems, i.e., the addition of an arbitrary weak barrier at a given point effectively freezes the tunneling through the barrier [257]. However, the underling mechanism in our case is different.

We show that the traditional quantity to characterize quantum tunneling dynamics, namely the tunneling rate, is inadequate for describing the tunneling behavior associated with the localized spin-polarized states. In fact, the tunneling strength is also necessary. For the spin-polarized states, not only can the tunneling rate be negligibly small, but also the tunneling strength. For these states, the spin-up and spin-down electrons are separated in space by the potential barrier. As a result, if an electron occupies a spin-up state, it will remain so for all times. This should be compared with the case of absence of many-body interactions, where the tunneling strength can typically be much larger.

When the geometry is changed so that the classical dynamics becomes chaotic, the spreads in both the tunneling rate and strength are greatly suppressed. The states with extremely small tunneling rate and strength are effectively removed. Study of
three representative systems with a chaotic component in the classical limit indicates that a more chaotic system has a stronger ability to regularize the tunneling dynamics. The main message is then that chaos can significantly enhance the tunneling process in realistic situations where electron-electron interactions are present. This implies that classical chaos is capable of facilitating greatly relativistic quantum tunneling, which is desirable in the development of nano-scale devices such as graphene-based resonant-tunneling diodes.

Finally, we wish to discuss and justify the mean-field approach to solving the Hubbard model for graphene systems. Firstly, in Ref. [250], it was indicated that the self-consistent mean-field approach is accurate when the Hubbard interaction strength $U$ is not too large. In our study, we used $U = 1.2t$, which is well within the regime of validity of the mean-field Hubbard model, i.e., $U \lesssim 2t$.

Secondly, Ref. [252] investigated the dynamical properties of edge-state magnetism in graphene systems. It also compared the results of static spin polarization from the mean-field theory with those from the quantum Monte-Carlo (QMC) approach. A main conclusion of Ref. [252] is that the results from the two approaches agree well in static properties and even in terms of the dynamic properties, but for narrowest ribbons.

In general, the Hubbard model is paradigmatic in that it really does capture the electron-electron interactions in graphene systems and the self-consistent mean-field approach is effective to analyze the effects of the interactions. In fact, a recent paper investigated edge spin-polarization for large systems, e.g., $10^4$ carbon atoms and it concluded that if the environment time scale $\tau_{env}$ is much shorter than $\tau_{qd}$, the system is pushed into the same classical Néel-like state again and again. As a result, the state cannot decay, which is known as the quantum Zeno effect [258]. Furthermore, our results do not require perfect spin polarization at opposite zigzag edges. In presence
of quantum fluctuations, if there are noticeable remanent edge magnetic states, which introduce left-right asymmetry to the spin electrons, with the central potential barrier the eigenstates will be spin-polarized for the left and the right domains.
ROBUSTNESS OF PERSISTENT CURRENTS IN TWO-DIMENSIONAL DIRAC SYSTEMS WITH DISORDERS

6.1 Introduction

Persistent or permanent currents, i.e., currents requiring no external voltage with zero resistance, were traditionally thought to occur only in superconductors. However, about three decades ago, it was theoretically predicted [259] that such dissipationless currents can emerge in normal metallic or semiconductor ring systems subject to a central Aharonov-Bohm (AB) magnetic flux [260]. In particular, if the ring size is smaller than the quantum phase coherent length, the electron motion in the entire domain become ballistic, effectively eliminating scattering and leading to a persistent current. While the environmental temperature needs to be sufficiently low to reduce inelastic scattering from phonon-electron and/or electron-electron interactions for the currents to be observed [259, 261, 262, 263], the metallic material itself remains “normal” (i.e., not superconducting). The remarkable phenomenon of persistent currents was subsequently observed experimentally in a large variety of settings [264, 265, 266, 267, 268, 269, 270, 271], all being nonrelativistic quantum systems.

Persistent currents in nonrelativistic quantum systems, however, are vulnerable to material impurities, fundamentally limiting the phenomenon to systems at or below the mesoscopic scale. Indeed, in real materials disorders are inevitable, which can dramatically reduce the phase coherent length due to enhanced random scattering. In general, random disorders can induce the phenomenon of level repulsion, opening
energy gaps and destroying the conducting state. As a result, disorders in metallic or semiconductor systems, 1D or 2D, tend to diminish the persistent currents [272, 273, 274, 275, 276, 277, 278]. For example, as the strength of the disorder is increased, the current decays exponentially to zero [272, 278].

Recent years have witnessed a tremendous development and growth of interest in 2D Dirac materials such as graphene [1, 2, 3, 4, 7, 8, 9], topological insulators [10], molybdenum disulfide (MoS$_2$) [11, 12], HITP [Ni$_3$(HITP)$_2$] [13], and topological Dirac semimetals [14, 15]. The quantum physics of these 2D materials is governed by the Dirac equation, and there were studies of persistent currents, e.g., in graphene [279, 280, 281, 282, 283, 284, 285, 286, 287, 288] and other Dirac materials [289, 290]. The effects of boundary deformation on the persistent currents were recently investigated [230], where it was found that, even when the deformation is so severe that the corresponding classical dynamics in the 2D domain becomes fully chaotic, persistent currents can sustain. The physical origin of the so-called superpersistent current [230] can be attributed to the emergence and robustness of a type of quantum states near the boundaries of the domain, which carry a large angular momentum and are essentially the whispering gallery modes (WGMs) that arise commonly in optical systems [291, 292, 293, 294] and can occur nonrelativistic quantum electronic systems [295] as well. The Dirac WGMs apparently are insensitive to boundary deformations, which may be intuitively understandable by considering the zero flux boundary condition required for nontrivial, physically meaningful solutions of the Dirac equation. In spite of these efforts, an open issue concerns the effects of bulk disorders on persistent currents in 2D Dirac systems. In particular, since there are random scattering sources inside the domain with a finite probability of occurrence even near the boundary, it is not apparent whether the Dirac WGMs and hence the persistent current can still exist.
In this chapter, we investigate the effects of random disorders on persistent currents in 2D relativistic quantum systems. Specifically, we consider a Dirac ring domain with a vertical magnetic flux through the center, as shown in Fig. 6.2(a). To completely constrain a Dirac fermion within the domain, we impose the infinite mass boundary condition originally introduced by Berry [296] into the study of chaotic neutrino billiard, which is experimentally realizable through proper ferromagnetic insulation [297]. We assume uncorrelated disorders throughout the domain, which can be simulated using localized, random electric potential impurities uniformly distributed in the domain, as illustrated in Fig. 6.2(b). In an experiment, for a given material neither the strength nor the density of the disorders can be readily adjusted. However, the sample size can be controlled. Classically, under a vertical magnetic field, the electron moves along circular trajectories in the domain. For a larger ring sample, the electron encounters more disorders in one complete rotation. In terms of rotational motion, increasing the density of the disorders is equivalent to enlarging the outer radius of the ring domain. Following this heuristic consideration, we fix the disorder strength as well as the domain size but systematically vary the density of the disorders. For convenience, in our computations we set the total number of disorders in the whole domain as a control parameter, and solve the Dirac equation to obtain the magnitude of the persistent current as a function of the number of disorders. For comparison with the nonrelativistic quantum counterpart, we solve the Schrödinger equation under the same setting. Our main results are the following. For the Dirac ring system, as the number of the disorders is systematically increased, the average current decreases slowly initially and then plateaus at a finite nonzero value, indicating that the persistent current is robust. We demonstrate that WGMs are the physical mechanism responsible for the robust current. In contrast, in the nonrelativistic quantum ring system, the WGMs are sensitive and fragile to the dis-
orders, leading to a rapid and exponential decay of the current to zero. We develop a physical theory based on the quasi-one-dimensional approximation to understand the striking contrast in the behaviors of the current in Dirac and Schrödinger rings. Our findings have important implications: (1) Dirac WGMs are robust and topologically protected states in relativistic quantum systems, and (2) persistent current in Dirac rings can potentially occur in realistic systems of large sizes.

In Sec. 9.2, we describe the Hamiltonian for a 2D Dirac ring and the numerical method to calculate the persistent current. In Sec. 7.3, we demonstrate the robustness of the current against random disorders and the emergence of WGMs. In Sec. 6.4, we justify a quasi-1D approximation and derive a physical theory to understand the drastically contrasting decaying behaviors in Dirac and Schrödinger ring systems. In Sec. 6.5, we present conclusions and a discussion about the possibility of observing persistent currents in Dirac systems of large size (e.g., beyond the mesoscopic scale).

6.2 Model Hamiltonian and Simulation Setting

We consider a 2D Dirac ring domain where an AB magnetic flux passes through the central region, as shown schematically in Fig. 8.1(a). The Dirac Hamiltonian subject to a magnetic field is

$$\mathcal{H} = \mathcal{H}_0 + U(r) = \hbar v(\hat{p} + eA) \cdot \hat{\sigma} + V(r)\sigma_z + U(r), \quad (6.1)$$

where $\hat{p} = -i\hbar \partial/\partial r$ is the momentum operator, $\hat{\sigma} = [\sigma_x, \sigma_y, \sigma_z]^T$ is the “vector” of Pauli matrices, and $A = \Phi \partial (-\ln |r|) / \partial r$ is the magnetic vector potential and $\Phi$ is the AB magnetic flux. The disorders are modeled as a random electrical potential function $U(r)$, and the mass potential that confines the Dirac particle in the domain is $V(r)$, where $V = \infty$ for $r < R_1$ or $r > R_2$. In the polar coordinates, the stationary
Dirac equation in the ring domain can be written as (in the units $\hbar = v = 1$)

\[
\begin{pmatrix}
  i[U(r, \theta) - \varepsilon] & e^{-i\beta}(\partial_r - \frac{i}{r}\partial_\theta + \frac{\Phi/\Phi_0}{r}) \\
  e^{i\beta}(\partial_r + \frac{i}{r}\partial_\theta - \frac{\Phi/\Phi_0}{r}) & i[U(r, \theta) - \varepsilon]
\end{pmatrix} \cdot \Psi(r, \theta) = 0,
\]

where $\varepsilon$ denotes the eigenenergy, and the relevant lengths are normalized by the outer radius $R_2$ (e.g., the inner radius becomes $\xi = R_1/R_2$). In the absence of random disorders, the Dirac equation in the ring domain can be solved analytically: its solutions are

\[
\Psi(r, \theta) = [\psi^-(r, \theta), \psi^+(r, \theta)]^T
\]

where $\bar{m} = m + \Phi/\Phi_0$ is the effective quantum number of the angular momentum $m = \pm 1/2, \pm 3/2, \pm 5/2 \ldots$, is the eigenvalue of the momentum operator $\hat{J}_z = -i\partial_\theta + \sigma_z$.

The infinite mass boundary condition leads to following relation between the two components of the spinor wavefunction [296]:

\[
\psi^+/\psi^- = i\text{sgn}(V) \exp(i\theta).
\]

The radical part of the whole wavefunction can be expressed as a set of Haknel functions [see Eq. (C.3) in Appendix].

Treating the random disorders as perturbation, we have

\[
\sum_{i,j} \langle j | \mathcal{H} | i \rangle = \sum_i E_i^{(0)} + \sum_{i,j} \langle j | U(r, \theta) | i \rangle,
\]

where $E_i^{(0)}$ and $| i \rangle$ are the eigenvalue and eigen wavefunction of the unperturbed Hamiltonian $H_0 = H_{U=0}$, respectively. The energy levels of the perturbed system can be solved numerically using the Hamiltonian in Eq. (6.5). The concrete parameter setting in our simulation is the following. We model the random disorders
using a set of uncorrelated Gaussian potential functions: 

\[ U(r, \theta) = \sum_{s=1}^{N} U_s(r_s, \theta_s) = \sum_{s=1}^{N} u_s e^{-\delta r^2/2\sigma^2}, \]

where \( s \) and \( N \) are the index and the total quantity of random impurities. \( \sigma \) and \( u_s \) are the size and the height of a single electric impurity, respectively. We set the cutoff radius of any disorder to be \( \delta r \leq 3\sigma \) and the mean radius of each disorder to be \( (R_2 - R_1)/20 \). The strength of the disorders is randomly chosen from the interval \([-u_m/2, u_m/2]\), where \( u_m \) depends on the average spacing of the first ten energy levels, \( \Delta E_{10} \).

For convenience, we use the superscripts “\( D \)” and “\( S \)” to denote results for the Dirac and Schrödinger equations, respectively. Our computation gives \( \Delta E_{10}^{(S)} \approx 10\Delta E_{10}^{(D)} \) for \( \xi = 1/2 \). The maximum number of disorders is chosen to be 500 to avoid complete coverage of the ring domain by them. The rms value of the persistent current associated with the \( n \)th energy level is given by [261]

\[ I_n = \sqrt{\langle I_n^2(\Phi) \rangle}, \quad (6.6) \]

where \( I_n(\Phi) = -\partial E_n(\Phi)/\partial \Phi \) is the flux-dependent persistent current associated with the \( n \)th energy level.

### 6.3 Results and Qualitative Understanding

Figures 6.2(a) and 6.2(b) show, for the Dirac and Schrödinger systems, respectively, the average amplitude of the persistent current versus the number \( N \) of random disorders, which are calculated using 100 statistical realizations. The error in the calculated value of the current amplitude is about \( 10^{-2} \). In both cases, the current amplitude decays exponentially for \( 0 < N \leq 350 \): \( I_n \sim I_n^0 \exp[-\gamma^{(D,S)}N] \), with the distinct feature that the decay rate for the Dirac system is about half of that for the Schrödinger system: \( \gamma^{(D)}/\gamma^{(S)} \approx 1/2 \). A more remarkable feature is that, for the Dirac system, after an initial exponential decay, the current amplitude approaches...
Figure 6.1: (a) Schematic of a ring domain with an AB magnetic flux through the center. The light blue color denotes the regions of infinite mass. Red and blue loops illustrate the eigenstates near the outer and inner boundaries, respectively. (b) Schematic illustration of random disorders that are uniformly distributed in the ring region, with their strength denoted with different colors.

Figure 6.2: The average rms amplitude of the persistent current versus the number of the disorders for (a) Dirac (denoted as “D”) and (b) Schrödinger (denoted as “S”) rings, respectively, for fixed disorder strength $u_{\text{in}}^{(D,S)} = 300 \Delta E_{\text{10}}^{(D,S)}$. Experimentally the Dirac ring can be fabricated by placing a ferromagnetic insulator of proper shape on the surface of a topological insulator [230].
a constant value of about $10^{-1}$ (which is about one order of magnitude larger than the numerical error) for $N \geq 350$, but for the corresponding Schrödinger system the current amplitude effectively decays to zero. We see that, as there are more random disorders in the domain (or equivalently, as the domain size is increased), the decaying behavior of the persistent current is characteristically different for the Dirac and Schrödinger systems: for the former the current is robust and continues to exist (in spite of deterioration in the amplitude) but for the latter the current quickly diminishes. That is, persistent current in the Dirac system is topologically protected against random disorders.

In relativistic quantum systems, the phenomenon of Klein tunneling can be expected, which has a strong manifestation in the behavior of the persistent current in 1D systems with random impurities [298]. This is because, in one dimension, the incident “angle” of a wave on an impurity is zero so that the condition for Klein tunneling is always satisfied. However, in two dimensions, there can be a wide distribution of the incident angle [299] on a random potential, and the angle range for Klein tunneling is quite limited. In our setting, the potential field of an electric disorder is Gaussian, rendering highly unlikely Klein tunneling. To provide further evidence that Klein tunneling plays little role in sustaining persistent current in the Dirac ring system with disorders, we set the impurity potential to be attractive in the range $[-u_m, 0]$ and obtain essentially the same result as in Fig. 6.2(a).

The physical mechanism for persistent current to sustain in the Dirac ring system with random disorders can be attributed to a set of WGM states near the domain boundaries, which can be verified by examining the local density of states (LDS) and the local current density (LCD) that can be calculated [296] as $j(r, \theta) = \Psi^\dagger(r, \theta) \hat{\sigma} \Psi(r, \theta)$. The LDS and LCD distributions are shown in Fig. 6.3, where the WGM characteristics of the boundary states are apparent. In general, a Dirac fermion
tends to stay near one of the infinite mass boundaries with a high probability, due to the zero-flux boundary condition. For a Dirac ring domain without any random disorder, the intrinsic circular symmetry stipulates identical radial wavefunction for different angular modes. In this ideal case, the WGMs tend to “attach” to the boundaries. Random disorders break the circular symmetry and, as a result, the WGMs tend to be detached from but they are still near the boundaries. In general, the LDS and LCD patterns depend on the wavevector and the detailed distribution of the random disorders. For comparison, we also plot the LDS and LCD patterns for the Schrödinger ring and its LCD is calculated by $j(r, \theta) = \Psi^\dagger(r, \theta)(\hat{\nabla} + A)\Psi(r, \theta)$. As shown as the LDS and LCD patterns in Figs. 6.3 (e,f), the LCD is localized by disorder.

To further understand the robustness of the WGMs in the Dirac ring domain against random disorders, we examine the wavefunctions at higher energy levels. Without any disorder, while the LDS pattern “attaches” to the boundary, its radial wavefunction of high levels ($n \geq 9$) is typically maximized in the interior of the domain, as shown by the dashed black curves in Figs. 6.4(a,b). Random disorders attenuate significantly the LDS in the interior region but it is significant near the boundaries, as shown by the green curves in Figs. 6.4(a,b).

A fundamental feature of the Dirac system, which is absent in the Schrödinger counterpart, is the spin texture. We find that the spin texture associated with the WGMs is hardly affected by the random disorders. For a 2D Dirac system (e.g., the surface of a 3D topological insulator), the spin orientation is given by $s(r, \theta) = \Psi^\dagger(r, \theta)\hat{S}\Psi(r, \theta)$, with $\hat{S} = (1/2)(\sigma_y, -\sigma_x, \sigma_z)$. As shown by the blue arrows in Figs. 6.5(b,c), the spin orientations of the WGMs near the inner and outer boundaries are parallel to their respective normal vectors. (For non-boundary states, the spin orientations are random.) The robustness of the spin orientation against
random disorders can again be attributed to the zero-flux boundary condition that allows the states with definite spin orientation to close on itself after completing a circular path to ensure constructive interference. That is, the infinite mass boundaries in the Dirac system tend to “protect” the spin orientation for WGM type of boundary states.

6.4 Physical Understanding of Robust Persistent Current

For a circular Dirac domain, in the absence of random disorders the energy level $\varepsilon$ depends on the angular momentum quantum number $m$, $\varepsilon = \varepsilon(m)$. If the thickness of the quantum ring is not large, as an approximation [301] one can assume that the disorders have little effect on the radial component $\chi(r)$ of the eigenfunctions but they can affect significantly the azimuthal component $\phi(\theta)$. A general wavefunction
**Figure 6.4:** Panels (a) and (b) shows the radial wavefunctions of the “clean” system (gray dashed) of the 22nd and the 25rd levels, respectively. The red curves in (a,b) show the corresponding average radial wavefunctions for the case where there are 100 random disorders in the domain.

**Figure 6.5:** The spin orientations corresponding to the LDS patterns in Fig. 6.3. The locations of the states in (b) and (c) are indicated by the blue crosses in (a). (d) Schematic of spin orientations at radical cross section with homogeneous LDS.
from the Dirac equation can be written as a linear combination of the eigenfunctions:
\[ \Psi(r, \theta) = \sum_n \phi_n(\theta) \chi_n(r), \]
where \( \chi_n(r) \) is the eigenfunctions of the Bessel’s equation (see Appx. C for details), and \( \phi_n(\theta) \) is the azimuthal wavefunction associated with the original quantum number \( m \) of the angular momentum in the absence of disorders.

The orthogonality condition for \( \chi_{n,m}^\pm(r) \) is (Appendices A and B)
\[ \int_\xi^1 \frac{1}{r} \chi_{n',m}^\pm(r) \chi_{n,m}^\pm(r) dr = \delta_{n',n}. \]

Utilizing this condition and eliminating the radial partial terms in Eq. (6.2), we obtain the governing equation for the quasi 1D azimuthal wavefunction as
\[ \partial_\theta \phi_{n,m}(\theta) = \hat{G} \phi_{n',m}(\theta), \quad \text{(6.7)} \]
where \( s \) is the index of the random disorders, \( n \) and \( n' \) are the energy level indices, \( \Gamma_{n',m}^{(s)} \) is the scattering integral associated with the radial component:
\[ \Gamma_{n',m}^{(s)}(r_s) = -\int_\xi^1 \chi_{n,m}^- * (r) U_s(r, \theta) \chi_{n',m}^+(r) dr \]
\[ = \int_\xi^1 \chi_{n,m}^+ * (r) U_s(r, \theta) \chi_{n',m}^-(r) dr. \quad \text{(6.9)} \]

This approximative procedure is schematically illustrated in Fig. 6.6 (a). For simplicity, we set the potential for the random disorders as
\[ U(r, \theta) = \sum_s U_s(r_s, \theta_s) = \sum_s \left( u_s/r \right) \delta(r - r_s) \delta(\theta - \theta_s), \]
which yields
\[ \Gamma_{n',m}^{(s)} = -u_s \chi_{n,m}^- * (r_s) \chi_{n',m}^+(r_s) \delta(\theta - \theta_0). \]

For comparison with the nonrelativistic quantum counterpart, we note that for a Schrödinger domain, the azimuthal equation is [301]
\[ (\partial_\theta^2 + m^2) \phi_n(\theta) = \sum_s \sum_{n'} \Gamma_{n',m}^{(s)} \phi_{n'}(\theta), \]
\[ 105 \]
where
\[ \Gamma^{(s)}_{n'n,m} = u_s \chi^*_{n',m}(r_s) \chi_{n,m}(r_s) \delta(\theta - \theta_s). \]

Having obtained a quasi 1D equation that approximately describes the effects of the random impurities, Eq. (6.7), we are in a position to set up a quantum transport model, which is analogous to the transfer matrix method of Schrödinger systems. In particular, the transfer operator associated with the random impurities for one complete rotation in the ring domain is defined as [302, 106]
\[ \phi(\theta = 2\pi) = \mathcal{T} \phi(\theta = 0), \]
where
\[ \mathcal{T} = \mathcal{T}^{(N+1)}_p \prod_{s=N}^{1} \mathcal{T}^{(s)}_p \mathcal{T}^{(s)}_m, \]
the operators \( \mathcal{T}^{(s)}_p \) and \( \mathcal{T}^{(s)}_m \) represent propagating and scattering procedures and they can be obtained from the first-order Neumann solution [303, 304, 305] of the azimuthal Dirac equation (6.7) as
\[ \phi(\theta_s') = \hat{Q} \exp \left[ \int_{\theta_s}^{\theta_s'} \hat{G}(\theta) \right] \phi(\theta_s) \]
with \( \hat{Q} \) denoting the Dyson ordering operator and \( \hat{G} \) being an angle-dependent operator. In general it is extremely difficult to obtain the solutions of Eq. (6.11). To gain insights, we set \( \hat{Q} = 1 \) so as to obtain the following expressions:
\[ \mathcal{T}^{(s)}_p = \begin{pmatrix} e^{i(\theta_s - \theta_s - 1)(m-1/2)} & 0 \\ 0 & e^{i(\theta_s - \theta_s - 1)(m+1/2)} \end{pmatrix}, \]
\[ \mathcal{T}^{(s)}_m = \begin{pmatrix} \cos \Gamma^{(s)}_{nn',m} & -ie^{i\theta} \sin \Gamma^{(s)}_{nn',m} \\ -ie^{-i\theta} \sin \Gamma^{(s)}_{nn',m} & \cos \Gamma^{(s)}_{nn',m} \end{pmatrix}. \]
Note that these expressions are different than those from the Schrödinger counterpart.
To carry out the analysis further, we have that the transfer matrix associated with the magnetic flux periodicity for \( \theta = 0 \) is given by
\[ \mathcal{T}_\Phi = e^{i2\pi \Phi/\Phi_0} \mathcal{I}. \]
Thus the relationship $m = m(\varepsilon)$ in the presence of random disorders can be solved from

$$\det[T - T_\Phi] = 0. \quad (6.14)$$

In our heuristic analysis, we make the diagonal approximation: $n = n'$, to avoid generating any additional energy crossings [301].

Figure 6.7(a) shows the relation between the determinant of the difference of the transfer matrices, $\det[T_D - T_\Phi]$, with the angular momentum quantum number $m$. In the absence of random disorders, Eq. (6.14) only has a single solution, which corresponds to the energy crossing point. With random disorders, energy repulsion occurs, leading to a split in the original angular momentum quantum number: $\Delta m$,
Figure 6.7: (a) The angular momentum quantum number $m$ versus the value of the determinant of the transfer matrix, $\text{Det}[T_D - T_\Phi]$, for two cases where there is no disorder (dashed gray curves) and where there are 300 disorders (solid red curves). (b) Decaying behavior of $1 - \Delta m$ with the number $N$ of random disorders for Dirac ($u_m^{(D)} = 0.03$) and Schrödinger ($u_m^{(S)} = 0.075$) systems on a semilogarithmic scale.

on which the amplitude of the persistent current depends. Note that the range of $\Delta m$ is $[0, 1]$. For a small value of $\Delta m$, the energy repulsion is weak so that a large current can be maintained. On the contrary, for a large value of $\Delta m$ the current amplitude becomes small. Roughly, the current amplitude is proportional to $1 - \Delta m$.

Figure 6.7(b) shows the decreasing behavior of $1 - \Delta m$, on a semi-logarithmic scale, with the number of disorders. We see that the exponential decay rate is much smaller for the Dirac system than for the Schrödinger counterpart. For a relatively large value of $N$ (e.g., $N \approx 400$), for the Dirac system the quantity $1 - \Delta m$ stops to decay but plateaus at a small (but nonzero) value, indicating a strong sustainability of the persistent current against random disorders. In a striking contrast, for the Schrödinger system, the value of $1 - \Delta m$ decays rapidly to zero, indicating that the persistent current in the nonrelativistic quantum ring is vulnerable to random
disorders. These results are consistent with those from direct numerical calculations
(Fig. 6.2).

Our analysis based on the quasi-1D equation provides a heuristic method to estimate the decay rate of the persistent current as the number $N$ (or density) of random disorders is increased. For an initial range of $N$, for both the Dirac and Schrödinger systems, the decaying behavior of the current can be written as $I_n/I_0^n = A \exp(-\gamma N)$, where the decay rate is $\gamma \sim \langle \Gamma_n \rangle$. Thus the ratio of decay rates between the Dirac and Schrödinger systems is approximately given by

$$\frac{\gamma_n^{(D)}}{\gamma_n^{(S)}} \approx \frac{\langle \Gamma_n^{(D)} \rangle}{\langle \Gamma_n^{(S)} \rangle},$$

(6.15)

where

$$\langle \Gamma_n^{(D)} \rangle = \int_\xi^1 dr\chi_n^{-}\chi_n^{+},$$

$$\langle \Gamma_n^{(S)} \rangle = \int_\xi^1 drr\chi_n^{(S)*}\chi_n^{(S)}.$$   

In a Dirac ring, the upper and lower components of the radical wavefunction have a large phase difference for low energy levels, as shown in Figs. 6.6 (b,c). As a result, we have

$$\langle \Gamma_n^{(D)} \rangle < \langle \Gamma_n^{(S)} \rangle.$$  

For example, for the 2nd and 3rd energy levels, we have

$$\gamma_{2,3}^{(D)} / \gamma_{2,3}^{(S)} \approx \langle \Gamma_{2,3}^{(D)} \rangle / \langle \Gamma_{2,3}^{(S)} \rangle \approx 1/2,$$

which agrees approximately with the numerical results in Figs. 6.2(c,d).

6.5 Conclusion and Discussion

For a ring domain with a magnetic flux through the center, persistent current can arise due to the AB effect. This work investigates the effect of random disorders
on persistent current in relativistic quantum (Dirac) ring systems. There are two reasons to investigate the impact of random disorders. First, in any realistic materials random disorders are inevitable. In nonrelativistic quantum systems the disorders have a devastating effect on the persistent currents, so they can only be observed in systems of sufficiently small size (e.g., smaller than the phase coherence length of the material). For relativistic quantum systems, there is a recent work on the effects of random disorders on persistent currents in one dimension [298]. It is of interest to understand the effect in experimentally more feasible 2D systems. Second, in order to assess the feasibility of observing persistent currents in large systems, one can study the impact of random disorders of systematically increasing density, as to solve the Dirac equation under a magnetic field in a large system can be extremely computationally demanding. These points can be elaborated through the following discussion of the main results of this work and their implications.

Previous theoretical and experimental results on persistent currents in nonrelativistic quantum (Schrödinger) systems revealed that the currents are sensitive and thus vulnerable to disorders. A natural question is then whether persistent currents can be more “sustainable” in relativistic quantum systems. Through direct numerical calculation of the persistent current for both Dirac and Schrödinger ring systems with systematically varying number (or density) of random disorders, we find that persistent currents in the Dirac system are significantly more robust than those in the Schrödinger counterpart. While for both systems, as the number of random disorders is increased from zero, the current amplitude decays exponentially, there are two key characteristic differences between relativistic and nonrelativistic quantum cases. First, the rate of decay is much smaller in the Dirac than in the Schrödinger system. Second, for the Dirac ring the exponential decay is terminated when the number of random disorders becomes large and is subsequently replaced by a plateaued behavior
with a finite current amplitude, but in the Schrödinger ring the exponential decay continues until the current effectively becomes zero. The underlying quantum states providing a “sustained” persistent current in the Dirac system are found to be a WGM type of boundary states. We developed a physical theory, based on a quasi 1D approximation, to explain the distinct current decaying behaviors in Dirac and Schrödinger systems. Specifically, under this approximation the effect of random disorders can be assessed and the persistent current can be calculated through a scattering integral over the radial dimension that involves the product of the two components of the relativistic quantum spinor. These findings suggest the extraordinary robustness of persistent current in the Dirac system, implying that the underpinnings of the current, i.e., the WGM states, are topologically protected against random disorders.

Our calculations uncovered that, for both Dirac and Schrödinger rings, the interior states are vulnerable to random disorders. It is the zero-flux boundary condition that renders the WGM boundary states robust in the Dirac system. (In the Schrödinger system boundary states cannot form due to the Dirichlet boundary condition.) It is possible to observe the sustaining boundary states experimentally by exploiting, e.g., the surface states of 3D topological insulators. Especially, a ring domain can be formed through deposition of ferromagnetic insulating materials on the surface of the topological insulator. Another finding is that the spin orientations of the WGM states are hardly affected by random disorders, which may have implications for relativistic quantum spintronic devices.

An important implication of our finding lies in the possibility to observe persistent current in Dirac systems of large sizes. In Schrödinger materials (normal metals or semiconductors), the current can arise but only when the device size is smaller than the phase coherence length to ensure that the electron trajectories are ballistic. When the device is larger than this scale, the inevitable random scattering due to impurities
will make the current dissipated away and diminish to zero. However, the robustness of the persistent current in the Dirac system implies that the relativistic quantum phenomenon can occur in larger devices, possibly on the macroscopic scale. This can be argued by noting that, as the ring size is increased, the number of scattering events that a particle experiences in one circulating motion will increase. From the standpoint of scattering, increasing the density of random disorders for fixed device size is equivalent to enlarging the device. For strong random disorders, Anderson localization sets in [306], prohibiting currents inside the domain. However, because of the strong boundary currents in Dirac fermion systems, it is possible that the persistent current will not vanish.

In real experiments, such a 2D Dirac ring can be realized by surface states of Bi$_2$Te$_3$/Bi$_2$Se$_3$, whose Fermi velocity is $v_F \approx 7 \times 10^5 m/s$ [307, 308, 309]. In our simulation, the Gaussian-like disorder is analogy of charge puddles with single puddle size 30nm and strength 10meV [309] in the surface states of Mn/Ca-doped Bi$_2$Te$_3$/Bi$_2$Se$_3$ materials. In the pure Bi$_2$Te$_3$/Bi$_2$Se$_3$ materials, the strength of charge puddles should be smaller than the puddle strength in the doped materials and thus we set as $u_m/2 = 5meV$. In our numerical simulation, if high disorder density, say 400 – 500 single impurities, is considered, the disorder pattern is really similar to the charge puddles in the experimental observation [309]. The maximum strength of charge puddles is given by $u_m = 300\Delta E_{10}$, with $\Delta E_{10} = \hbar v_F \Delta k_{10}/R_2$, where $k_{10}R_2 = 0.45$ and $R_2$ is the outer radius of the ring. Now, the outer radius $R_2$ can be estimated as $R_2 = 300 \times 0.45\hbar v_F u_m \approx 6\mu m$. As a result, the estimated size of the Dirac ring is $D = 2R_2 = 12\mu m$, which is much larger than the size of normal metallic or semiconductor rings with persistent currents observed in previous experiments [264, 265, 266, 267, 268, 269, 270, 271].

In addition, in a clean Dirac ring with size $D = 12\mu m$, the persistent currents of
one energy level can be estimated as $I_n^0 \sim 2\Delta E_{10}/\Phi_0 = 0.45 \times h v_F/(R_2 \Phi_0) \approx 3nA$, where $\Phi_0 = h/e \sim 4 \times 10^{-15} Tm^2$ is the magnetic flux quantum. If 500 impurities are taken into account, the persistent currents still remain at a finite value, $I_n \approx 0.1I_n^0 \approx 0.3nA$. Then, the total persistent currents in experimental measurements are given by $I = \sum_{n=1}^{N} I_n$, where $N$ depends on the Fermi energy of the Dirac ring. For example, if the Fermi energy is taken as $E = 1meV$, there are several energy levels included. The total persistent currents are $I \sim 1nA$, which could be observable in experiments by using SQUID techniques [264, 265, 266, 267, 269, 270].
Chapter 7

DISORDER-ENHANCED TRANSPORT IN A LIGHT-IRRADIATED
GRAPHENE RIBBON

7.1 Introduction

As an external light irradiates on graphene-like or other spin-orbit systems, a dynamical topological insulator state may be arisen and it firstly reported in 2009 [310]. Such a non-trivial state with time-periodic nature can be represented by Floquet theory and it is also so-called Floquet topological insulator (FTI). More recently, various properties about FTIs, such as transport [311, 312, 313, 314], edge states [315, 316, 317, 318], topological transitions [319, 320], dynamical polarizability [321], modulated and disorder-induced FTIs [322, 323, 105], valleytronics [324], and local pseudospin textures [325], were theoretically investigated. In addition, a recent experiment observed Floquet-Block states on the surface of a topological insulator [326].

The transport of Floquet systems is nonequilibrium [327, 311] and it is quite different from the case of static systems. For example, a short light-irradiated Dirac ribbon can show a superdiffusive behavior caused by evanescent modes. In addition, a phenomenon of disorder-enhanced transport in light-irradiated bulk graphene [319], by breaking the spatial-temporal symmetry, distinguishes from the case of non-irradiated systems, where disorder-enhanced transport may be observed in a short structure with assist of evanescent states [328, 106, 17], or in a system with pointer states caused by some specific conditions, such as specific scattering sources [68, 329] or an external magnetic field [83, 85]. However, such a phenomenon is not explained in detail and
the conductance enhanced by disorder is extreme tiny ($\Delta G \ll 2e^2/h$). What’s more, the bulk transport cannot completely represent more practical ribbon structure.

In this work, with above motivations, a light-irradiated graphene ribbon structure with onsite disorder connected with two doped leads, is taken into account. In general, the FTI is on the verge of weak topological insulator [330, 331] and, here, we only focus on weak-disorder regime. In Sec. 7.2, the Floquet theory, model and nonequilibrium transport are introduced. The disorder-enhance transport in a ribbon structure is exhibited and explained in Sec. 7.3, where left-right asymmetrical transport is studied with partial disorder as well.

7.2 Floquet Theory, Model, and Nonequilibrium Transport

The time-dependent Hamiltonian with an uniform light irradiation is given by $H(t) = v_F \sigma \cdot [p + (e/c)A(t)]$, where $v_F$ is Fermi velocity and $A(t) = eA_0/h(\cos \Omega t, \sin \Omega t)$ is a time-dependent vector potential to represent the rotating electric field with $E(t) = \partial A(t)/\partial t$. $\Omega$ is the frequency of light and $A_0$ is the light intensity. The time-dependent Schrödinger equation is written as $H_F(t)|\Psi(r, t)\rangle = [H(t) - i\partial_t]|\Psi(r, t)\rangle = 0$, where $H_F(t)$ is the Floquet Hamiltonian. Since $H(t)$ is periodic, the wavefunction can be expressed as the Floquet states $|\Psi_\alpha(r, t)\rangle = e^{i\varepsilon_\alpha t}|\Phi_\alpha(r, t)\rangle$ and $\varepsilon_\alpha$ is the quasienergy. Then, the Schrödinger equation reduced to $H(t)|\Phi_\alpha(r, t)\rangle = \varepsilon_\alpha|\Phi_\alpha(r, t)\rangle$, where $|\Phi_\alpha(r, t+T)\rangle = |\Phi_\alpha(r, t)\rangle$ and $T = 2\pi/\Omega$ is the period. Thus, the wavefunction can be expressed in the discrete Fourier form as ($\hbar = c = 1$)

$$|\Phi_\alpha(r, t)\rangle = \sum_m e^{im\Omega t}|\varphi^m_\alpha(r)\rangle,$$  \hspace{1cm} (7.1)

where $|\varphi^m_\alpha(r)\rangle$ is static and the normalization of Floquet states is taken as $\sum_m \langle \varphi^m_\alpha | \varphi^m_\beta \rangle = \delta_{\alpha\beta}$. Then the Schrödinger equation of the Floquet states in the discrete Fourier form
Figure 7.1: The schematic diagram of a two-terminal undoped graphene nanoribbon with length $L$ and width $W$, irradiated by a circularly polarized light with strength $A_0$ and frequency $\Omega$. The black random dots denote the onsite potential disorders. Left and right leads are non-irradiated regions as light illumination is by electrodes on top of leads. $V_{L,R}$ represent doping at left and right leads, respectively.

$$\sum_m H_{nm}^F |\varphi_m^\alpha\rangle = \varepsilon_\alpha |\varphi_n^\alpha\rangle,$$  \hspace{1cm} (7.2)

where $H_{nm}^F = n\Omega \delta_{nm} + 1/T \int_0^T dt e^{i(n-m)\Omega t} H(t)$ and the integral means all terms in that equation are time-average. By transformed into a discrete Fourier series, as a result, the Floquet states are quantized in time dimension and the traditional Hilbert space is extended into the Sambe space [332].

In the tight-binding framework, the time-dependent Hamiltonian is given by

$$H(t) = - \sum_{ij,s} \gamma_{ij}(t)c_{ij,s}^\dagger c_{ij,s} + \sum_{i,s} u_i c_{i,s}^\dagger c_{i,s},$$  \hspace{1cm} (7.3)

where $c_{i,s}^\dagger (c_{i,s})$ is the creation(annihilation) operator and $s = \uparrow, \downarrow$. The hopping energy is driven by the vector potential and it is given by $\gamma_{ij} = \gamma_0 \exp[iA_{ij}(t)]$, where $A_{ij}(t) = e/h(r_j - r_i)$. $u_i$ is the onsite disorder potential at site $i$, which is taken from an uniform distribution in the region $[-U_0/2, U_0/2]$ with $\langle u_i \rangle = 0$ and $\langle u_i u_j \rangle = (U_0^2/12)\delta_{ij}$.

For a two-terminal structure, the “scattering” region is irradiated by a circular-
Figure 7.2: (a) Average conductance $\langle G \rangle$ versus disorder strength $U_0$. Blue rightward and red leftward triangles denotes the $L \rightarrow R$ and $R \rightarrow L$ conductances, respectively. Black curve corresponds to the mean conductance $G$. $G_{\text{def}}$, represented by the blue curve, corresponds to the case with a $r = W/2$ semicircle defect as shown in Fig. 8.1. The green dashed curve is a fitting curve based on Born approximation. The arrows at $\varepsilon = 0$ and $\Omega/2$ in the inserted quasienergy bandstructure correspond to FTI states. The parameters are $L = 70a_0$, $W = 50a$, $A_0 = 0.15$ and $\Omega = 0.8\gamma_0$, where $a_0 = \sqrt{3}a = 2.46\text{Å}$ is lattice constant of graphene. (b) Average conductance versus $A_0$ and $U_0$. The red dashed curve fits conductance peaks.

Polarly polarized light. The leads, covered by electrodes in real experiments, are non-irradiated. This is a non-equilibrium system, in which photon absorption and emission are involved. The transport procedure is that electrons are injected from left lead with Fermi energy $E$ and, with influences by light, some of electrons may excite from both left and right leads with energy $E + k\hbar\Omega$, where $k$ is the number of photon absorption or emission. Then the zero-temperature conductance is evaluated by $G = (G_{RL} + G_{LR})/2$, where $G_{\nu\mu}(E) \equiv G_{\nu\mu}(E) = G_0 \sum_k T_{\nu\mu}^{(k)}(E)$ and $T_{\nu\mu}^{(k)}(E) = Tr[\Gamma_{\nu}^{(k)}(E) G_{1N}^{(0)}(E) G_{1N}^{(k)}(E)]$. The detailed numerical method is introduced in Appx. A.
Before introducing our results, a couple of detailed settings for this model should be presented. Firstly, to effectively measure the conductivity of irradiated region, the leads are doped so that more transverse modes are injected from left/right leads as far as possible. In our numerical simulation, the doping for left and right leads are $V_L = V_R = \gamma_0$. Secondly, the length of irradiated region $L$ should be long enough that transport of evanescent states can be neglected for avoiding the influence from evanescent states. The length-width ratio $L/W \gtrsim 2.5$ is used in our simulation and it is numerically confirmed. Thirdly, be aware that the conductance $G$ is time-average since an integral over time coordinate was applied and $\langle \cdots \rangle$ represents disorder average.

Disorder-enhanced transport—Fig. 7.2(a) shows the average conductance versus the strength of disorder, where a typical and abnormal consequence is the disorder-enhance transport. At beginning, at low disorder range, the average conductance is enhanced until reaching a peak value near $U_0/\Omega = 0.7$ with increase of disorder strength $U_0$. After the maximum point, caused by strong localization, the conductance monotonically decays at large disorder range. With uniform disorder, this systems is statistically spatial-symmetrical and thus relation $\langle G_{RL} \rangle = \langle G_{LR} \rangle$ is valid. We also consider a nanoribbon with a semicircular defect, as shown as the black dashed curve in Fig. 8.1, and the conductance $G_{def}$ is always smaller than $G$. It indicates that strong defects cannot eliminate the disorder-enhanced transport and the enhanced conductance is determined by the effective width of the ribbon structure.

To systematically investigate the effect of irradiated light, a surf diagram of conductance versus $A_0$ and $U_0$ is shown in Fig. 7.2 (b). If $A_0 = 0$, there is no conductance enhancement effect with increase of disorder strength and the conductance always re-
mains at a tiny value. When the irradiated light is applied, even with low intensity, a non-trivial FTI state is induced and the disorder-free conductance rapidly raises up to a finite value near $G_0$. When disorder is taken into account, the average conductance thereupon increases. At low intensity regime, this FTI state is not robust enough that the effect of disorder-enhanced conductance is weak and a dominated factor is the localized effect. Thus, the conductance monotonically decays as well. When light intensity is impressive, say $A_0 > 0.04$, the disorder-enhance conductance is considerable as well. The conductance peak obey a fitting relationship as $G_{\text{max}} \approx 3A_0^{1/3}$ and its projection on $(A_0, U_0)$ plane is approximately a straight line $U_0/\Omega - 5A_0 = 0$.

Our results distinguish from the bulk transport of graphene reported previously, where disorder-enhanced transport is caused by breaking the entwined spatial-temporal symmetry only at the $\Gamma$ point [319]. In our work, the giant disorder-enhanced conductance in a zigzag ribbon occurs not only at the $\Gamma$ point but at any light with low-intensity, say $A_0 < 0.5$. Even at strong intensity regime, $A_0 \geq 1$, disorder-enhanced transport can be observed under some sets of parameters as well. Please see additional results in Appx. A.

This phenomenon corresponds to the case of an undoped zigzag graphene ribbon, but it is not always valid on other energy levels. Depended on our numerical confirmation, the phenomenon of disorder-enhance transport usually occurs near the quasienergy $\varepsilon/\Omega = N/2$, where $N$ is an arbitrary integer. If the quasienergy of the irradiated region is raised up or depressed down to the levels with many bulk states, transport will be monotonically weaken with increase of disorder strength. This is because the bulk states are sensitive to weak disorder. Another condition to keep this phenomenon is that the light frequency $\Omega$ should less than bandwidth of tight-binding model. Otherwise, the conductance will stabilize at a finite value for weak disorder range. In addition, we also numerically confirm the results in armchair ribbons and
there is no qualitative change by the modification of boundary conditions.

*Understanding in Born approximation*—The reason of this disorder-enhanced conductance is different from previous static cases. We can understand it based on the first-order Born approximation (BA), where single resonance Hamiltonian is considered and the effective Hamiltonian is reorganized by disorder. The average self-energy of disorder is given by

\[
\Sigma_{\text{dis}}(z, \mathbf{k}) = \int_{FBZ} d\mathbf{k}' \langle U_{\text{dis}}(\mathbf{k}, \mathbf{k}') G_0^F(z, \mathbf{k}') U_{\text{dis}}(\mathbf{k}', \mathbf{k}) \rangle.
\] (7.4)

The non-diagonal elements represent the coupling between different Floquet channels. Under approximation of weak irradiation \( A_0 \ll 1 \), an effective coupling strength is obtained as

\[
\tilde{A}_\pm = A_0 (1 + \alpha_\pm U_0^2),
\] (7.5)

where \( \alpha_\pm(\Omega, A_0) \) is an integral over the first Brillouin Zone with relation \( \alpha_+ = \alpha_-^\dagger \). Please see details in Appx. B. The self-energy of disorder thus incidents that disorder positively contributes the coupling of Floquet states and it results in the enhancement of transitions between different Floquet states. In general, if the conductance is simply enhanced by the change of the coupling elements, the enhanced conductance would approximately be proportional to \( U_0^2 \). By setting a fair parameter, a green dashed curve, \( \langle G \rangle \approx (1 + |\alpha_\pm| U_0^2) G_{U_0=0} \), is fitted in Fig. 7.2(a).

Now, based on the result from Born approximation, it is not difficult to understand the phenomenon of disorder-enhanced transport. Fig. 7.3(a) shows a schematic diagram of transport procedure, where the levels at \( m \) coordinate represent Floquet channels and waved curves denote the photon absorption/emission procedures. For instance, electrons are injected from on Floquet channel \( m = 0 \) at left lead and the probability of photon absorption/emission is enhanced by the disorder in the light-irradiated region. As a result, the transmission from \( m = 0 \) to Floquet channel \( k \) is
Figure 7.3: (a) Band diagram for schematically illustrating the nonequilibrium transport for a two-terminal irradiated system. Electrons are injected at left lead with Floquet channel $m = 0$ and, after irradiated by light at scattering region, leak at right lead with Floquet channels $m = 0, \pm 1, \pm 2, \cdots$ The red waved curves denote the photon absorption and emission between different Floquet channels and the gray arrows represent transport in Floquet channels. (b) The surface Green’s function $g_{1N}^k$ for describing the contact between slice 1 and $N$ with absorbing $k$ photons in a closed nanoflake, which are illustrated by inserted diagram.

enhanced, where $|k| > 1$. The total conductance is a summation of transmission $T^{(k)}$ and, therefore, the conductance is enhanced as well by the disorder.

However, at present, another factor which might enhance transport is unbeknown. It is possible that the transport also can be enhanced by disorder breaking mismatching of wavefunctions between irradiated and non-irradiated regions. To confirm the correction of theory, we numerically calculate, for a closed nanoflake, the surface Green’s function $G_{1N}^k$, where $k$ corresponds to the transition from Floquet states $m = 0$ to $k$, as shown as the illustrated diagram in Fig. 7.3(b). The surface Green’s function $G_{1N}$, is a block matrix of $G^F(z) = [z + i\eta - H^F]^{-1}$. Its normalized expression as $g_{1N}^k = G_{1N}^k / \sum_m G_{1N}^m$. We calculate $10^3$ sets of disorder realizations for each $U_0$ and then average them. As expected, the normalized surface Green’s function $g_{1N}^{(k)}(E)$ with $|k| > 1$ is gradually raised with increase of disorder strength and therefore, the
**Figure 7.4:** (a) Band diagram for schematically illustrating the nonequilibrium transport for a two-terminal irradiated system with partial disorder. The upper and lower diagrams respectively describe $L \rightarrow R$ and $R \rightarrow L$ transport. $L_{dis}$ is the length of partial disorder and $d_{dis}$ is the distance between disorder region and left lead. The LDS pattern on various Floquet channels are averaged by 10 sets of disorder with $U_0/\Omega = 1.6$, $L = 80a_0$, $L_{dis} = 30a_0$ and $d_{dis} = 2a_0$. (b) Average conductance versus the disorder strength with $\Omega = 0.8\gamma_0$, $A_0 = 0.15$ and $L_{dis} = 20a_0$ for a graphene zigzag ribbon with $L = 70a_0$ and $W = 50a$. (c) Average conductance versus the location of partial disorder with $L_{dis} = 30a_0$ for a graphene zigzag ribbon. Other parameters are same to (b). The average conductance is calculated from 200 disorder realizations.

Matching problem is not the main factor in this system.

*Asymmetrical transport with partial disorder*—Instead of the case with disorder spread over all irradiated region, a partial disorder, with length $L_{dis}$ and distance from left lead $d_{dis}$, is applied, as shown as the schematic diagrams in Fig. 7.4(a). In that schematic, the upper and the lower diagrams represent $L \leftarrow R$ and $R \rightarrow L$ transports, respectively. Here, we schematically give an example with partial disorder closed to the left lead. Let us focus on the distribution of local density of states (LDS) on different Floquet channels at first. For $m = 0$ Floquet channel, on account of wavefunction mismatching at disorder interfaces, the LDS is extremely high near interfaces and is low at the rest of area. There is almost no effect caused by disorder on Floquet channel $m = 0$. Nevertheless, LDS at disordered domain is remarkably
enhanced on channels $m = \pm 1$ and collectively elevated on channels $|m| > 1$. This consequence agrees with understanding from BA approximation.

For a driven system, the $L \rightarrow R$ and $R \rightarrow L$ transports are generally unequal [327]. Now we will explain why $G_{RL}$ and $G_{LR}$ are asymmetric in the system with partial disorder. Note that on channel $m = 0$, the conductance $G_{\beta \alpha}^{(0)}$ is low due to its low LDS at non-terminal region. Thus, for a $L \leftarrow R$ transport, electrons are injected at the left lead and accumulate near left lead. Due to a larger LDS overlap area at left side between Floquet channels $m = 0$ and $m = \pm 1$, electrons can transmit more from Floquet channel $m = 0$ to channel $m = \pm 1$. This keeps more probability that electrons transmit from $m = \pm 1$ to higher-level Floquet channels. As a result, $G_{RL}^{(|k|>0)}$ are remarkably enhanced by this left-hand partial disorder, as show as the curved arrows in Fig. 7.4 (a). On the contrary, for the $R \rightarrow L$ transport, lower overlapped area of LDS between channels $m = 0$ and $m = \pm 1$, and less electrons can jump to high-level channels. Therefore, this asymmetrical disorder can lead to the difference between $G_{RL}$ and $G_{LR}$. Based on above understanding, $G_{RL}$ can be cut down via increasing $d_{\text{dis}}$ and while $G_{LR}$ does not show any remarkable changes.

To justify above predictions, our numerical results in Fig. 7.4(b), show that the values of $G_{RL}$ and $G_{LR}$ gradually drift apart as $U_0$ increases and their ratio can reach to $G_{RL}/G_{LR} \approx 2$. Meanwhile, the average conductance $\langle G \rangle$ is slightly enhanced by disorder. In addition, as varying $d_{\text{dis}}$, the difference between $G_{RL}$ and $G_{LR}$ can be modulated. Fig. 7.4 (c) shows the conductance with varied $d_{\text{dis}}$, where $G_{RL}$ and $G_{LR}$ are monotonously decreasing and increasing, respectively, and cross at left-right symmetrical point $d_{\text{dis}} = 20a_0$. 

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7.4 Conclusion

In summary, graphene, driven by a light, may show properties of FTIs, which is called Floquet topological insulator due to its time-periodic nature represented by Floquet theory. Here, a light-irradiated graphene ribbon connected with two doped leads is considered. We set the length of irradiated region is long enough that transport is not contributed by evanescent states, even with onsite disorder in tight-binding framework. Based on our numerical simulation, the conductance can be enhanced with the increase of disorder strength until reaching a maximum value. This unusual phenomenon can be understood in Born approximation, where the disorder reorganizes Floquet Hamiltonian and effectively change the coupling elements between different Floquet states. That means disorder promotes the photon absorption or emission and, thus, the nonequilibrium transport is accordingly enhanced. This phenomenon distinguishes from the case of bulk graphene, where disorder-enhanced transport is caused by breaking the entwined spatial-temporal symmetry only at the $\Gamma$ point [319]. In irradiated graphene ribbons, it is general to observe the phenomenon of disorder-enhanced transport with $A_0 < 0.5$. Finally, a phenomenon of left-right asymmetrical transport in a same system with partial disorder is investigated and an understanding is proposed by analyzing LDS patterns in different Floquet channels. This understanding perfectly agrees with our numerical results.
8.1 Introduction

In physics, various transition phenomena induced by changes in system parameters are basic and relevant. Examples are phase transitions in statistical physics and bifurcations to distinct dynamical states including chaos. Suppose the complex system of interest exhibits a transition from one type of collective dynamical behavior to another, and further assume that quantum effects cannot be neglected (e.g., for a nanoscale system). What are the quantum manifestations of the transition? To address this general question in a concrete setting, we consider a class of physical systems of considerable recent interest: optomechanical systems \[333, 334, 335, 336, 337, 338, 339, 340, 341, 342, 343, 344, 345, 346, 347\].

A single optomechanical system consists of an optical cavity and a nanoscale mechanical oscillator, typically a cantilever. When a laser beam is introduced into the cavity, a resonant optical field emerges, exerting a radiation force on the mechanical cantilever, causing it to oscillate. The mechanical oscillations in turn change the length of the optical cavity, hence its resonant frequency. There is thus a coupling between the the optical and mechanical degrees of freedom. This coupling, or interaction, can in fact lead to the cooling of the mechanical oscillator, a subject of intense recent research \[348, 349\]. Here, we consider the setting of two optomechanical subsystems mutually coupled through a optical fiber \[350\] as shown in Fig. 8.1, and both subsystems are driven by a common driving laser beam. This photon-photon
coupling could be sundry experimentally, such as two coupled fibre-taper waveguides [351, 352]. Further, it is interesting to research on optomechanical crystals by arraying a series of optomechanical subsystems due to its many potential applications [353, 354]. Utilizing the Heisenberg equations of motion, we describe each optomechanical subsystem by a set of nonlinear equations of four dynamical variables in the phase space: the real and complex components of the optical field, and the position and velocity of the mechanical cantilever. The classical phase space dimension of the coupled optomechanical system is thus eight. In our analysis, synchronization occurs when the normalized power $\lambda$ of the common driving laser is relatively low. But as $\lambda$ is increased through a critical point $\lambda_c$, a transition to antiphase synchronization occurs, this being a novel phenomenon in optomechanics that can be tested experimentally with potential applications in integrated optomechanical systems [346]. To uncover the quantum manifestations of the transition, we study and pay particular attention to quantum entanglement between the two coupled optomechanical subsystems. Calculation of the entanglement measures [347] associated with various optical and mechanical degrees of freedom reveals a distinct type of quantum manifestation of the synchronization transition: as the transition point is crossed, the maximum entanglement measure is continuous but its derivative with respect to the parameter $\lambda$ is discontinuous. This is characteristic of a second-order phase transition. In spite of the recent works on quantum synchronization, the second-order nature of the quantum change associated with transition in the classical collective dynamics has not been identified before. Since it is not necessary to drive the individual optomechanical subsystems into highly nonlinear regimes for the synchronization transition to occur, it is feasible to test our findings experimentally.
8.2 Models

We consider two identical optomechanical subsystems coupled through an optical fiber [350], as shown in Fig. 8.1. Each individual system is a Fabry-Perot cavity with one fixed and one movable mirrors. We assume that there is only one photon mode with frequency $\omega = 2\pi c/L$, where $L$ is the length of each cavity. The Hamiltonian of the whole coupled system can be divided into three parts: $H = H_a + H_b + H_c$. The sub-Hamiltonians $H_{a(b)}$ describe the individual subsystems. We have $H_a + H_b = \Delta_0(a^\dagger a + b^\dagger b) + (\omega_m/2)((p_1^2 + q_1^2) + (p_2^2 + q_2^2)) + G_0(a^\dagger a q_1 + b^\dagger b q_2)$, where $a^\dagger$ ($b^\dagger$) and $a$ ($b$) are the creation and annihilation operators, respectively. The first and second terms of $H_a + H_b$ describe the cavity and mechanical modes, respectively, and the last term represents the nonlinear coupling between the optical and mechanical modes in each subsystem caused by the radiated pressure. The coupling
between the two subsystems is linear, which can be described by the Hamiltonian
\[ H_c = \lambda (a\dagger b + b\dagger a). \]
The dynamics of the coupled system are governed by the quantum Langevin equations [346]:
\[ \partial \hat{O}/\partial t = i[\hat{H}, \hat{O}] + \hat{N} - \hat{H}_{diss}, \]
where \( \hat{N} \) is the quantum fluctuation operator, \( \hat{H}_{diss} \) characterizes the dissipation, and \( \hat{O} = p_1, q_1, a \) denotes the operators for the left cavity and \( p_2, q_2, b \) for right cavity, where \( p_{1,2} = \dot{q}_{1,2}/\omega_m \). The set of quantum Langevin equations is then given by
\[
\begin{align*}
\dot{p}_1 &= -\omega_m q_1 + G_0 a\dagger a - \gamma_m p_1 + \xi_1, \\
\dot{a} &= -\left(\kappa + i\Delta_0\right) a + i G_0 a q_1 + E - i \lambda b + \sqrt{2\kappa a^m}, \\
\dot{p}_2 &= -\omega_m q_2 + G_0 b\dagger b - \gamma_m p_2 + \xi_2, \\
\dot{b} &= -\left(\kappa + i\Delta_0\right) b + i G_0 b q_2 + E - i \lambda a + \sqrt{2\kappa b^m},
\end{align*}
\]
where \( \kappa \) is the decay rate of each cavity, \( \gamma_m \) is the mechanical damping rate, and the laser detuning is given by \( \Delta_0 = \omega_c - \omega_0 \). Here \( \omega_c \) and \( \omega_0 \) are respectively the frequencies of the cavity mode and of the driving laser, and \( E = E_0 + E_1 \cos (\Omega t) \) is the driven external field. The driven frequency is \( \Omega = 2\omega_m \). The vacuum radiation input noise \( a^m \) and \( (b^m) \) are stochastic processes [355] described by \( \langle a^m(t)a^{m\dagger}(t') \rangle = \langle b^m(t)b^{m\dagger}(t') \rangle = \delta(t - t') \), and the Hermitian Brownian noise operator is characterized by its autocorrelation function, in the Markovian approximation [356], as \( \langle \xi_{1,2}(t)\xi_{1,2}(t') + \xi_{1,2}(t')\xi_{1,2}(t) \rangle / 2 = \gamma_m (2\bar{n} + 1) \delta(t - t') \), where \( \bar{n} = 1/[\exp (h\omega_m/k_BT) - 1] \). The mechanical and optical noise operators have zero mean values.

### 8.3 Phase Transition in Classical Dynamics

To uncover the transitions in the classical dynamics, we solve the deterministic version of the quantum Langevin equations, i.e., without the noise terms in Eq. (8.1), for the following experimental parameter setting [336, 357]: \( L = 25 \text{mm}, F = 1.4 \times 10^4 \), \( \omega_m = 2\pi \times 10^6 \text{Hz}, Q = 10^6 \) and \( m = 150 \text{ng} \). We use a red detuned laser \( \Delta_0 \simeq \omega_m \) and
Figure 8.2: (a,b) Time evolution of the mechanical operators $\hat{q}_{1(2)}$, and (c,d) the real and (e,f) imaginary parts of the optical operators $\hat{a}(\hat{b})$. There is a transition from synchronization to antiphase synchronization as the coupling parameter $\lambda$ passes through the critical point $\lambda_c \approx 0.39082$. The left and right columns correspond to $\lambda = 0.388$ (before the transition) and 0.398 (after the transition), respectively. Note that there is a phase difference $\pi$ in all panels in the right column. Especially, for (d,f), the optical fields exhibit a period-2 behavior. A $\pi$ phase shift will make the solid and dashed traces overlap with each other completely.
its wavelength $\lambda = 1064\text{nm}$. Then, the modulation coefficients $E_n (n = 0, \pm 1)$ in Eq. (8.1) are given by $E_n = \sqrt{2\kappa P_n / (\hbar \omega_0)}$ with the power of the associated sidebands $P_0 = 10 \times 10^{-3}\text{W}$ and $P_{\pm 1} = 0.5 \times 10^{-3}\text{W}$, where decay rate $\kappa = \pi c / (2FL)$ and light velocity $c = 3.0 \times 10^8\text{m/s}$. In numerical, we normalize above parameters by $\omega_m$ and thus, $\gamma_m/\omega_m = 1 \times 10^{-6}$, $G_0/\omega_m = 3.7726 \times 10^{-6}$, $\Delta_0/\omega_m = 1$, $\kappa/\omega_m = 0.107$, $E_0/\omega_m = 6.042 \times 10^4$, $E_1/\omega_m = 1.351 \times 10^4$, and $\Omega/\omega_m = 2$. In later calculation for quantum entanglement, we set $\bar{n} = 0.05$. We find that, as the coupling parameter $\lambda$ is increased through a critical value $\lambda_c \approx 0.39082$, there is a transition from in-phase to antiphase synchronization. Figures 8.2(a-f) show the time evolution of various dynamical variables for two different values of $\lambda$: one before the transition ($\lambda = 0.388$, left column) and another after the transition ($\lambda = 0.398$, right column). We observe that, in the synchronized (in phase, left column) state, the system exhibits limit-cycle oscillations. In the antiphase synchronization state (right column), the system exhibits period-2 oscillations.

To understand the transition from synchronization to antiphase synchronization, we plot the bifurcation diagrams of various dynamical variables versus the coupling parameter $\lambda$, as shown in Fig. 8.3(a), where the red and green curves correspond to peak and valley values of the real and imaginary parts of the photon operator $a$ and $b$, respectively. We observe a Hopf bifurcation at the transition point. The bifurcation behavior of the mechanical operator $q_{1(2)}$ appears slightly more complicated than that associated with the optical operator. On both sides of the critical point $\lambda_c$, each mechanical variable has two branches, but the oscillation amplitude becomes larger as $\lambda$ is increased through $\lambda_c$. The black dashed curves indicate the behaviors of the unstable oscillations about $\lambda_c$, whose amplitudes remain unchanged through the transition. Note that, in the real quantum system, due to existence of noise, the unstable state, as well as continuation of steady state before critical point,
Figure 8.3: (a) Bifurcation diagrams for the mechanical variables \( q_{1,2} \), the real \( a_r \) and \( b_r \), red curves) and imaginary parts of the cavity operators \( a_i \) and \( b_i \), green curves). The black dashed lines indicate the unstable state after the transition. The basin structures before and after the synchronization transition are also shown, where the pink and light blue areas correspond to the in-phase and antiphase synchronization states, respectively. (b,c) Extraction of Hopf bifurcation at the transition point, where \( q_1 \) and \( q_1^0 \) represent the stable and unstable time evolution of left mechanical mode, respectively, after the critical point \( \lambda_c \), in arbitrary unites. (d) Transverse Lyapunov exponents (TLEs) versus the coupling parameter \( \lambda \), where the blue solid curves correspond to the two largest TLEs and the black dashed line indicates the largest TLE of the unstable state after the transition. The pink and light blue backgrounds correspond to synchronized and anti-phase synchronized states, respectively.
would disappear. Also shown in Fig. 8.3(a) are the basin structures. In particular, for $\lambda < \lambda_c$, the in-phase synchronized state is the only stable state in the system but it becomes unstable for $\lambda > \lambda_c$, where antiphase synchronization state becomes stable. Figure 8.3(b) shows a magnification of the bifurcation diagram of the mechanical variables. As shown schematically in Fig. 8.3(c), the bifurcation at $\lambda_c$ can be understood as a continuation of the modulation due to the driven optical field and the occurrence of a standard Hopf bifurcation at $\lambda_c$ superimposed on the original oscillations. Since the frequencies of the driven optical field and the limit-cycle oscillations generated by the Hopf bifurcation are incommensurate, the combination of the two leads to period-2 oscillations in both cavities but with the phase difference of $\pi$. The bifurcation at $\lambda_c$ is thus not a period doubling bifurcation.

The stabilities of the collective motions about the transition point can be characterized by the transverse Lyapunov exponents (TLEs) [358]. As shown in Fig. 8.3(d), the largest nontrivial TLE associated with the synchronized state is negative before the transition but it becomes positive after the transition. The synchronized state is thus stable for $\lambda < \lambda_c$ but it is unstable for $\lambda > \lambda_c$. At the transition, where the antiphase synchronization state is born, its largest nontrivial TLE is zero but decreases linearly past the transition point. The antiphase synchronization state is thus stable for $\lambda > \lambda_c$.

8.4 Quantum Manifestation of the Synchronization Transition

To characterize the quantum manifestation of the collective transition at $\lambda_c$, we measure the degree of quantum entanglement, which is defined as the logarithmic negativity (LN) [359]. It can be calculated through the covariance matrix $V(t)$ whose time evolution is governed by [357]

$$
\frac{dV(t)}{dt} = A(t)V(t) + V(t)A^T(t) + D,
$$

(8.2)
Figure 8.4: (a,b) Time evolution of the measure of quantum entanglement between the optical and mechanical modes for $\lambda = 0.388$ and 0.398, respectively. (c) Maximum quantum entanglement measure (maximum logarithmic negativity) versus $\lambda$. (d) Illustration of quantum entanglement between different modes in the two cavities, where, respectively, “M” and “C” stand for mechanical and optical cavity modes, indices “1” and “2” denote the mechanical modes from the left and the right subsystems, and “a” and “b” represent the optical modes in the left and the right cavities. The solid arrows mean there are quantum entanglement between the two modes with colors corresponding to those in (a,b). The dashed lines indicate lack of quantum entanglement.
where $D = \text{diag}[0, \gamma_m(2\bar{n} + 1), \kappa, \kappa, 0, \gamma_m(2\bar{n} + 1), \kappa, \kappa]$, and the matrix $A$ is

$$A = \begin{bmatrix} A_1 & A_c \\ A_c & A_2 \end{bmatrix},$$  

(8.3)

with

$$A_{1,2} = \begin{bmatrix} 0 & \omega_m & 0 & 0 \\ -\omega_m & \gamma_m & \text{Re}(G_{a,b}) & \text{Im}(G_{a,b}) \\ -\text{Im}(G_{a,b}) & 0 & -\kappa & \Delta_{a,b} \\ \text{Re}(G_{a,b}) & 0 & -\Delta_{a,b} & -\kappa \end{bmatrix},$$  

(8.4)

and

$$A_c = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \lambda \\ 0 & 0 & -\lambda & 0 \end{bmatrix}.$$  

(8.5)

The matrix elements are written as $G_{a,b} = \sqrt{2}G_0 \langle a, b(t) \rangle$ and $\Delta_{a,b} = \Delta_0 - G_0 \langle q_{1,2}(t) \rangle$. The elements of the covariance matrix $V(t)$ at one time step are given by $V_{ij} = \langle u_i u_j + u_j u_i \rangle/2$, where $u_i = \delta O_i = O_i - O_i^s$ with $O_i = q_1, p_1, a_r, a_i, q_2, p_2, b_r$ or $b_i$ and the upper index “$s$” stands for “stable state.” For our coupled optomechanical system, the covariance matrix contains information about quantum entanglement among two mechanical and two optical modes; thus its size is $8 \times 8$. The covariance matrix can be expressed as

$$V = [V_{ij}]_{8 \times 8} = \begin{bmatrix} I_1 & C_{1a} & C_{12} & C_{1b} \\ C_{a1} & I_a & C_{a2} & C_{ab} \\ C_{21} & C_{2a} & I_2 & C_{2b} \\ C_{b1} & C_{ba} & C_{b2} & I_b \end{bmatrix},$$  

(8.6)

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where $I_i$ and $C_{ij}$ are $2\times2$ matrices and $C_{ij} = C_{ji}^T$. Thus, the covariance matrix for two entangled modes is given by

$$v_{ij} = \begin{bmatrix} I_i & C_{ij} \\ C_{ij}^T & I_j \end{bmatrix},$$

where $I_{i,j}$, and $c_{ij}$ are $2 \times 2$ matrices. For convenience, we use the indices $(i,j) = (1,2)$ and $(i,j) = (a,b)$ to specify the mechanical and optical modes, respectively, for the left and right side subsystems. For example, “1b” denotes the entanglement between the mechanical mode on the left side and the optical mode on the right side, and “a2” denotes the entanglement between the optical mode on the left side and the mechanical model on the right side, and so on. The LN value between any two modes is given by

$$EN_{ij} = \max[0, -\ln (2\eta_{ij})],$$

where $\eta_{ij} = \sqrt{\Sigma_{ij} - [\Sigma_{ij}^2 - 4|v_{ij}|]^{1/2}}/\sqrt{2}$ and $\Sigma_{ij} = |I_i| + |I_j| - 2|C_{ij}|$. Physically meaningful LN values fall in the unit interval $[0,1]$, where zero means absence of any degree of entanglement and the unity value indicates perfect entanglement. Negative LN values may appear in the calculations, which are physically meaningless. In this case, the actual values are zero.

Note that, during calculation of logarithmic negativity, the quantum steady state for the fluctuations should be a zero-mean bipartite Gaussian state [360]. For verifying the validation of this method under parameters in our simulation, we repeatedly solve Eq. (8.1) with noise terms by the second-order Heun method [361] and find that all of fluctuations around steady oscillations $\delta O_i$ obey Gaussian distribution.

Figures 8.4(a) and 8.4(b) show the time evolution of the various LN measures for $\lambda = 0.388$ and 0.398, respectively. We see that there is strong entanglement between the mechanical and optical modes in the same cavity, and cross-cavity entanglement
occurs only between modes of the same nature. In other words, there is no entanglement between the mechanical (optical) mode in the left cavity and the optical (mechanical) mode in the right cavity in details. Based on our results, in general, entanglement is much stronger between modes in the same cavity than those across the cavities. For clarification of this results, Figure 8.4(c) shows the maximum LN values associated with four different pairs of modes: 1a, 2b, 12, and ab, as functions of the inter-cavity coupling parameter $\lambda$ about the transition point, where the 1a and 2b values are identical due to symmetry.

The remarkable phenomenon is the occurrence of a “cusp” type of behavior in all four functions at the transition point where the derivatives of the functions are not continuous. This is characteristic of second-order phase transition. Especially, the situation considered is optical coupling between the two cavities. Due to the intra-cavity coupling between the optical and mechanical modes, there is considerable amount of quantum entanglement between the mechanical modes in the two cavities. As the intercavity coupling is strengthened towards the transition point in which the classical dynamics is in-phase synchronization, the degree of entanglement between the mechanical modes increases. But after the transition, classical antiphase synchronization sets in, and this leads to a decrease in the degree of entanglement between the mechanical modes in the two subsystems. Such a cusp catastrophe of quantum entanglements between two identical subsystems is remarkably similar to quantum phase transition (QPT) of Dicke model [362, 363, 364]. In Dicke Hamiltonian, it is a nonlinear coupling between bosonic mode and ensemble of two-level atoms. While in our optomechanical model two identical subsystems are linearly coupled. Nevertheless, understandings of QPT in Dicke model are helpful to explain QPT in our system. In Dicke model, quantum entanglement divergence behavior is similar to transition in the quantum cusp catastrophe theory around its bifurcating fixed point.
and the Dicke Hamiltonian also has a classical cusp singularity in the catastrophe theory [363, 347]. Here, in this coupled system there is no such singular behavior. In classical limit, this phase transition can be simplified as a hopf-like bifurcation. In quantum limit, it corresponds to a transition of phonon number and Wigner density due to appearance of self-induced oscillation [365]. Under whole coupling parameter, there is a common state, as well as background state, driven by the modulated laser, which bridge quantum entanglements between two optomechanical subsystems. As increase of coupling strength until critical point, emergency of a new state excited by strong coupling ($\lambda \geq \lambda_c$) begins to strengthen or weaken the entanglements built by this background state. As a result, continuity of quantum entanglement is broken and a cusp catastrophe appears.

The transition point can be modulated by changing the amplitude $E_1$ of the driving laser for the optomechanical subsystems, as shown in Fig. 8.5(a). As $E_1$ is increased, the maximum values of LN also increase, signifying stronger entanglement between the two cavities. For the special case of $E_1 = 0$, before the transition the classical dynamics reaches a steady state with little quantum entanglement, but antiphase synchronization state sets in at some critical point of the inter-cavity coupling parameter. In this case, the degree of inter-cavity entanglement between the optical modes tends to increase after the onset of antiphase synchronization, as shown in Fig. 8.5(b).

8.5 Conclusion

To summarize, we uncover a transition from in-phase to antiphase synchronization in a system of two optically coupled optomechanical cavities. The emergence of the antiphase synchronization state is shown to be a result of a Hopf bifurcation from an oscillatory state. Calculations of the quantum-entanglement measures for various
Figure 8.5: Effect of driving laser power on the transition point: (a) Maximum LN values between the mechanical modes for laser amplitude $E_1 = E_1^0, 1.1E_1^0, 1.2E_1^0, 1.3E_1^0$ (from lower to upper curves), where $E_1^0/\omega_m = 1.351 \times 10^4$. The gray dashed line indicates a linear relation between the critical points $\lambda_c$ and $E_1$.
(b) Maximum LN values between the optical modes in the two cavities versus $\lambda$ for $E_1 = 0$.

Combinations of the mechanical and optical modes reveal a second-order phase transition type of change at the critical point. In a more general context, our work addresses the fundamental issue of quantum manifestations of transitions among distinct types of collective behaviors in classically complex dynamical systems, an emerging area that deserves further efforts.
Chapter 9

MULTISTABILITY, CHAOS, AND RANDOM SIGNAL GENERATION IN SEMICONDUCTOR SUPERLATTICES

9.1 Introduction

A semiconductor superlattice consists of a periodic sequence of thin layers of different types of semiconductor materials, which was conceived by Esaki and Tsu [366] with the purpose of being able to engineer the electronic properties of the structure. Specifically, a superlattice is a periodic structure of coupled quantum wells, where at least two types of semiconductor materials with different band gaps are stacked on top of each other along the so-called growth direction in an alternating fashion [367, 368]. For a structure consisting of two materials, e.g., GaAs and AlAs, the regions of GaAs serve as quantum wells while those of AlAs are effectively potential barriers. As a result, the conduction band of the whole system exhibits spatially periodic modulation with the period given by the combined width of the quantum well and the barrier, which is typically much larger than the atomic lattice constant. If the widths of the barriers are sufficiently small, the quantum wells are strongly coupled through the mechanism of quantum tunneling, effectively forming a one-dimensional energy band in the growth direction. Because of the relatively large spatial period of the superlattice as compared with the atomic lattice spacing, the resulting Brillouin zones and the bandwidths are much smaller than the inverse of the atomic lattice constant, leading to a peculiar type of band structure: the miniband. For larger barrier width, the quantum wells are weakly coupled so that resonant tunneling of electrons between adjacent wells occurs and becomes dominantly sequential. When an external voltage
(bias) is applied, electronic transport can occur, making superlattice appealing to investigating and exploiting various transport phenomena [369]. More generally, the unique perspective or freedom to design electronic properties makes semiconductor superlattices a paradigm to study many phenomena in condensed matter physics and device engineering [370].

While electronic transport in semiconductor superlattices should be treated quantum mechanically in principle, the presence of an external field and the many-body effect through the electron-electron Coulomb interaction make a full quantum treatment practically impossible. An effective approach to modeling transport dynamics in the superlattice system is through the force-balance equation [371, 372, 373, 374, 375, 376, 377, 378, 379, 380], which can be derived either from the classical Boltzmann transport equation [374, 375] or from the Heisenberg equation of motion [381, 382]. In spite of a quantum system’s being fundamentally linear, the self-consistent field caused by the combined effects of the external bias and the intrinsic many-body mean field becomes effectively nonlinear [383, 384]. In the high field transport regime, various nonlinear phenomena including chaos can arise [369]. In the past two decades, there were a host of theoretical and computational studies of chaotic dynamics in semiconductor superlattices [369, 384, 385, 386, 383, 387, 388, 389, 390, 391, 392, 393, 394, 395, 396, 397]. The effects of magnetic field on the nonlinear dynamics in superlattices were also investigated [398, 399, 400]. Experimentally, a number of nonlinear dynamical behaviors were observed and characterized [401, 368, 402, 403, 404].

A key application of semiconductor superlattices is to fill the so-called “THz” gap, i.e., to develop radiation sources, amplifiers and detectors [405, 406, 407, 408, 409] from 0.1 to 10 THz, the frequency range in which convenient radiation sources are not readily available [410, 411, 412, 413]. In particular, below 0.1 THz electron transport based devices are typical, and above 10 THz devices based on optical transitions...
(e.g., solid state lasers) are commonly available. Since in general, chaotic systems can be used as random number generators [414, 415, 416, 417, 418, 419, 420, 150, 421], ubiquity of chaos in semiconductor superlattices implies that such systems may be exploited for random signal generation in the frequency range corresponding to the THz gap. Motivated by this, in this work we are led to investigate the dynamics of energetic or “hot” electrons in semiconductor superlattices. Specifically, we study the setting where the system is subject to strong $dc$ and $ac$ fields so that dynamical resonant tunneling occurs effectively in a quasi-one-dimensional superlattice. Due to the strong driving field, a space charge field is induced, which contains two nonlinear terms in the equation of motion. The main issue that we address is that of reliability and robustness, i.e., for a given parameter setting, what is the probability to generate chaos from a random initial condition? We find that, for the common case of a single $ac$ driving field, onset of chaos is typically accompanied by the emergence of multistability in the sense that there are coexisting attractors in the phase space which are not chaotic. Using the ensemble method to calculate the maximum Lyapunov exponent, we distinguish the regular from the chaotic attractors. The probability for a random initial condition to lead to chaos is finite but in general is not close to unity. Due to the simultaneous creation of the basin of attraction of the chaotic attractor, the transition to multistability with chaos, as a system parameter passes through a critical point, is necessarily abrupt. Likewise, the disappearance of multistability is abrupt, as the typical scenario for a chaotic attractor to be destroyed is through a boundary crisis [422], which is sudden with respect to parameter variations. From the point of view of random signal generation, multistability is thus undesired. We find, however, that an additional driving field, e.g., of an incommensurate frequency, can effectively eliminate multistability to guarantee the existence of open parameter regions in which the probability of generating chaos from random initial conditions
is unity. We also find that, due to multistability, weak noise can suppress chaos but strong noise can lead to chaos with probability one.

We note that, in nonlinear dynamical systems, multistability is a common phenomenon [139, 140, 141, 142, 143, 144, 145, 146, 147, 148, 149]. Earlier works focused on low-dimensional nonlinear dynamical systems with a few [139, 140, 141, 142, 143] and many coexisting attractors [144, 145]. Recently multistability has been uncovered in nanosystems such as the electrically driven silicon nanowire [150, 147] described by nonlinear partial differential equations, as well as in a coupled system of a ferromagnet and a topological insulator [149]. The issue of controlling multistability was also addressed [151, 152, 144, 153, 148]. Multistability was uncovered in semiconductor superlattices as well [154, 155, 156]. The multistability phenomenon studied in the present work, however, is associated with the dynamics of hot electrons.

9.2 Model

In weakly-coupled superlattices in which sequential resonant tunneling is the main transport mechanism, chaos can arise and its potential use for random number generator has been proposed [368, 387, 370]. In our work, we focus on the strongly-coupled regime, in which miniband conduction is the primary contribution to transport.

Using the force-balance equation [423] for an $n$-doped semiconductor quantum-dot superlattice, we write the dynamical equation for the electron center-of-mass velocity $V_c(t)$ as

$$
\frac{dV_c(t)}{dt} = -\left[\gamma_1 + \Gamma_c \sin (\Omega_c t)\right] V_c(t)
$$

$$
+ \frac{e}{M(E_e)} \left[ E_0 + E_1 \cos (\Omega_1 t) + E'_1 \cos (\Omega'_1 t) + E_{sc}(t) \right],
$$

(9.1)

where $\gamma_1$ is the momentum-relaxation rate constant, $\Gamma_c$ comes from the channel-conductance modulation with $\Omega_c$ being the modulation frequency, $M(E_e)$ is the energy-
dependent averaged effective mass of an electron in the superlattice, \( \mathcal{E}_e(t) \) is the average energy per electron, \( E_0 \) is the applied dc electric field, \( E_1 \) and \( E'_1 \) are the amplitudes of the two external ac fields with frequencies \( \Omega_1 \) and \( \Omega'_1 \), respectively, and \( E_{sc}(t) \) is the induced space-charge field due to the excitation of plasma oscillation. Here, the statistical resistive force [423] has been approximated by the momentum relaxation rate. Based on the energy-balance equation, one can show [424] that \( \mathcal{E}_e(t) \) satisfies the following dynamical equation

\[
\frac{d\mathcal{E}_e(t)}{dt} = -\gamma_2 \left[ \mathcal{E}_e(t) - \mathcal{E}_0 \right] + eV_c(t) \left[ E_0 + E_1 \cos(\Omega_1 t) + E'_1 \cos(\Omega'_1 t) + E_{sc}(t) \right],
\]  

(9.2)

where \( \gamma_2 \) is the energy-relaxation rate constant and \( \mathcal{E}_0 \) is the average electron energy at the thermal equilibrium, and the thermal energy exchange of the electrons with the crystal lattice [424] is approximately described by the \( \gamma_2 \) term. Applying the Kirchoff’s theorem to a resistively shunted quantum-dot superlattice [383], we obtain [425] the dynamical equation for the induced space-charge field \( E_{sc}(t) \) as

\[
\frac{dE_{sc}(t)}{dt} = -\gamma_3 E_{sc}(t) - \left( \frac{en_0}{\epsilon_0 \epsilon_b} \right) V_c(t),
\]  

(9.3)

where \( \gamma_3 \), which is inversely proportional to the product of the system resistance and the quantum capacitance, is the dielectric relaxation rate constant [425], \( n_0 \) is the electron concentration at the thermal equilibrium, and \( \epsilon_b \) is the relative dielectric constant of the host semiconductor material. The exact microscopic calculations of \( \gamma_1 \) and \( \gamma_2 \) in the absence of space-charge field were carried out previously [426] based on the semiclassical Boltzmann transport equation and the coupled force-energy balance equations [390], respectively. Equivalent quantum calculations of \( \gamma_1 \) and \( \gamma_2 \) can also be done through the coupled force balance and the Boltzmann scattering equations [423].

Within the tight-binding model, the single-electron kinetic energy \( \varepsilon_k \) in a semi-
conductor quantum-dot superlattice can be written as

\[ \varepsilon_k = \frac{\Delta}{2} \left[ 1 - \cos(kd) \right], \quad (9.4) \]

where \( k \ (|k| \leq \pi/d) \) is the electron wave number along the superlattice growth direction, \( \Delta \) is the miniband width, and \( d \) is the spatial period of the superlattice. This energy dispersion relation gives \[423\]

\[ \frac{1}{M(E_e)} = \left\langle \frac{1}{\hbar^2} \frac{d^2\varepsilon_k}{dk^2} \right\rangle = \frac{1}{m^*} \left[ 1 - \left( \frac{2}{\Delta} \right) E_{e}(t) \right], \quad (9.5) \]

where \( m^* = 2\hbar^2/\Delta d^2 \) and \( |1/M(E_e)| \leq 1/m^* \).

For numerical calculations, it is convenient to use dimensionless quantities. Specifically, we introduce \( v(\tau) = (m^* d/\hbar) V_c, \ w(\tau) = [(2/\Delta) E_{e} - 1], \ f(\tau) = (ed/\hbar \omega_0) E_{sc}, \) and \( \tau = \omega_0 t \) with \( \omega_0 = 1 \text{ THz} \) being the frequency scale. In terms of the dimensionless quantities, the dynamical equations of the resonantly tunneling electrons in the superlattice become

\[
\frac{dv(\tau)}{d\tau} = -b_1 v(\tau) \left[ 1 + a_2 \sin(\bar{\Omega} \tau) \right] \\
- \left[ a_0 + a_1 \cos(\Omega \tau) + a'_1 \cos(\Omega' \tau) + f(\tau) \right] w(\tau), \\
\frac{dw(\tau)}{d\tau} = -b_2 [w(\tau) - w_0] \\
+ \left[ a_0 + a_1 \cos(\Omega \tau) + a'_1 \cos(\Omega' \tau) + f(\tau) \right] v(\tau), \\
\frac{df(\tau)}{d\tau} = -b_3 f(\tau) - a_3 v(\tau),
\]

where \( w_0 = [(2/\Delta) E_{e} - 1] = -1, \ b_1 = \gamma_1/\omega_0, \ b_2 = \gamma_2/\omega_0, \ b_3 = \gamma_3/\omega_0, \ a_0 = \omega_B/\omega_0, \)
\( a_1 = \omega_s/\omega_0, \ a'_1 = \omega'_s/\omega_0, \ a_2 = \Gamma_c/\gamma_1 \) and \( a_3 = (\Omega_c/\omega_0)^2 \) are all positive real constants. The field related parameters are \( \omega_B = eE_0d/\hbar, \ \omega_s = eE_1d/\hbar, \ \omega'_s = eE'_1d/\hbar, \ \Omega = \Omega_1/\omega_0, \ \Omega' = \Omega'_1/\omega_0, \ \bar{\Omega} = \Omega_c/\omega_0, \) and \( \Omega_c = \sqrt{e^2 n_0/m^* \epsilon_0 \epsilon_b}, \) where the last quantity is the bulk plasma frequency. The fields are assumed to be turned on at \( t = 0 \). The initial conditions for Eq. (9.6) are \( v(0) = v_0, \ f(0) = f_0 \) and \( w(0) = w_0 \).
Figure 9.1: Evidence of multistability: multiple coexisting attractors and their basins of attraction. (a) Schematic diagram of multistability resulting from different choices of the initial conditions \( v_0, w_0 \) and \( f_0 \). Two distinct sets of initial conditions, \((v_0, w_0, f_0)\) and \((v'_0, w'_0, f'_0)\) chosen from a cube in the \((v, w, f)\) space, can result in a stable steady state and chaos, respectively. The dashed blue and yellow traces signify that the asymptotic state is a regular steady state (blue) and a chaotic attractor (yellow), respectively, as indicated by the distribution of the maximum Lyapunov exponent calculated from a large number of initial conditions. (b,c) Basins of attraction of the steady state and the chaotic attractor in the \((v_0, w_0)\) plane for a systematically varying set of values of \( f_0 \) (for \( f_0 \in [-1, 1] \) in increment of 0.2) for \( a_1 = 1.9 \) and \( a_1 = 2.3 \), respectively. The ranges of \( v_0 \) and \( w_0 \) are \(|v_0| \leq 1\) and \(|w_0| \leq 1\). Other parameters for both (b) and (c) are \( a_0 = 2.23, a'_1 = a_2 = 0, a_3 = 7.48, b_1 = 0.28, b_2 = b_3 = 2.85 \times 10^{-2} \), and \( \Omega = 1.34 \).

9.3 Results

9.3.1 Evidence of Multistability

In the absence of the space-charge field \( E_{sc}(t) \) from the plasmon excitation, Eqs. (9.1) and (9.2) become linearly-coupled equations. In such a case, the electron dynamics can be solved exactly [426] by using the semiclassical Boltzmann transport equation subject to a strong \( dc + ac \) field, where there is an interplay between the phenomena of Bloch oscillations and dynamical localization, which play an important role in the transport dynamics. When the space charge field \( E_{sc}(t) \) was included, the
motions of hot electrons in the quantum-dot superlattice can exhibit chaotic behaviors [383]. The relaxation rates in Eqs. (9.1) and (9.2), $\gamma_1$ and $\gamma_2$, can be evaluated using the coupled force-energy balance equations [390], where the two-dimensional phase diagram of the driving amplitude and frequency in the absence of the $dc$ field, as well as their dependence on the lattice temperature, were computed and analyzed.

The dimensionless Eq. (9.6) represents a nonlinear dynamical system with $f(\tau)w(\tau)$ and $f(\tau)v(\tau)$ as the specific nonlinear terms. While, in principle, all system parameters can be adjusted, experimentally certain parameters are not readily susceptible to changes, especially those characterizing the material properties such as $\gamma_{1,2,3}$. Adjustable are the parameters associated with the driving $dc/ac$ electric field such as $a_0$, $a_1$, $a'_1$, and the frequencies $\Omega$ and $\Omega'$.

To search for multistability, we use the method of ensemble simulations by which we choose a large number of random initial conditions and determine the asymptotic state for each initial condition. As shown schematically in Fig. 9.3.1(a), under the same parameter setting, two initial conditions can lead to two completely different attractors, one regular and another chaotic. For better visualization of the basins of the distinct attractors, we select a number of parallel planes in the dynamical variables $(v, w)$ for a set of systematically varying values of the third variable $f$. Figure 9.3.1(b) shows, for $a_1 = 1.9$ ($E_1 < E_0$), the basin structures of 11 such planes, where we find two final states: one steady state (blue) and another chaotic (yellow) attractors. A general feature is that the basin structures appear quite irregular, and there are approximately equal numbers of initial conditions that lead to each of the two distinct attractors. As the amplitude of the modulated field is increased to $a_1 = 2.3$ ($E_1 > E_0$), the number of initial conditions that lead to the chaotic attractor is apparently more than that to the steady state attractor, as shown in Fig. 9.3.1(c). For both Figs. 9.3.1(b) and 9.3.1(c), for $f_0 > 0$ there is an open area near $(v_0, w_0) = (0, 0)$
Figure 9.2: Examples of chaotic dynamics associated with multistability: (a-d) Four representative trajectories evolving toward a chaotic attractor in the three-dimensional phase space. The initial conditions are \((v_0, w_0, f_0) = (-0.2, -0.2, -0.6)\) for panels (a,c) and \((0, 0.2, 0.4)\) for panels (b,d). The value of the bifurcation parameter is \(a_1 = 1.9\) for (a,b) and \(a_1 = 2.3\) for (c,d). Other parameters are \(a_0 = 2.23, a_1' = a_2 = 0, a_3 = 7.48, b_1 = 0.28, b_2 = b_3 = 2.85 \times 10^{-2},\) and \(\Omega = 1.34.\)

which belongs to the basin of the chaotic attractor, indicating a high probability for the system trajectory to land in this attractor and henceforth ubiquity of chaos associated with hot electron motions in the superlattice. Representative examples of the evolution towards a chaotic attractor are shown in Figs. 9.2(a-d).

9.3.2 Abrupt Transition to Multistability with Chaos

To determine the nature of the distinct asymptotic attractors of the system, we use the standard maximum (nontrivial) Lyapunov exponent \(\lambda_m\), where a positive and a negative value indicates a chaotic and a regular attractor, respectively. The time-dependent Jacobian matrix of Eq. (9.6) is
\[ \mathcal{A}(\tau) = \]

\[
\begin{pmatrix}
-b_1 [1 + a_2 \sin(\Omega \tau)] & -a_0 + a_1 \cos(\Omega \tau) + a'_1 \cos(\Omega' \tau) + f(\tau) & -w(\tau) \\
 a_0 + a_1 \cos(\Omega \tau) + a'_1 \cos(\Omega' \tau) + f(\tau) & -b_2 & v(\tau) \\
 -a_3 & 0 & -b_3
\end{pmatrix}
\]

(9.7)

The maximum Lyapunov exponent can be calculated through

\[
\frac{d\mathbf{x}(\tau)}{d\tau} = \mathcal{A}(\tau) \cdot \mathbf{x}(\tau),
\]

(9.8)

where \( \mathbf{x} \) is a unit tangent vector.

Statistically what is the route to chaos for hot electron motion in the superlattice as a system (bifurcation) parameter is changed, and how likely is multistability? From the standpoint of relative basin volumes, the transition must be abrupt because, when a chaotic attractor emerges (e.g., through the standard period doubling route \([427]\)), its basin is created simultaneously. Thus, if we calculate the probability for a random trajectory to land in the chaotic attractor versus the bifurcation parameter, we expect to see an abrupt increase in the probability from zero to a finite value as the parameter passes through a critical point. This has indeed been found in the superlattice system, as shown in Figs. 9.3(a) and 9.3(c) for fixed \( a_0 = 2.23 \) and \( a_1 \) increasing systematically from 1.0 to 3.0. Specifically, shown in Fig. 9.3(a) are the values of the maximum Lyapunov exponent \( \lambda_m \) versus \( a_1 \) from a large number of random initial conditions chosen from a unit cube \( |v_0, w_0, f_0| < 1 \) in the phase space. Figure 9.3(b) shows the probability of having \( \lambda_m > 0 \) versus \( a_1 \). For \( a_1 \approx 1.65 \), we observe an abrupt increase in the probability of having chaos. Similarly, disappearance of chaos (e.g., through the typical mechanism of boundary crisis \([422]\)) must also be abrupt because, as a chaotic attractor is destroyed, its basin disappears simultaneously as it is absorbed into the
Figure 9.3: Transition to chaos and multistability. (a) For fixed $a_0 = 2.23$, the values of the maximum Lyapunov exponent $\lambda_m$ calculated from an ensemble of initial conditions versus $a_1$ for $1.0 \leq a_1 \leq 3.0$. (b) A similar plot but for fixed $a_1 = 2.13$ and $a_0$ varying in the range $[1.0, 2.4]$. (c) For $a_0 = 2.23$, the probability versus $a_1$ for a random trajectory to land in a chaotic attractor. (d) A plot similar to that in (c) but for fixed $a_1 = 2.13$ and varying $a_0$. Other parameters are $a'_1 = a_2 = 0$, $a_3 = 7.48$, $b_1 = 0.28$, $b_2 = b_3 = 2.85 \times 10^{-2}$, and $\Omega = 1.34$. From (a) and (c), abrupt emergence of chaos at $a_1 \approx 1.65$ and abrupt disappearance of chaos at $a_1 \approx 2.45$ can be seen (see text for the reason of the “abruptness”). The dips in the probability curve of chaos for $a_1 \approx 2.0$ and $a_1 \approx 2.15$ are due to periodic windows. Abrupt emergence and disappearance of multistability associated with chaos also occur for fixed $a_1 = 2.13$ and varying $a_0$, as shown in (b) and (d).
basin of the coexisting regular attractor. This behavior occurs for $a_1 \approx 2.45$, as shown in Fig. 9.3(c). Since the probability of having chaos is never unity, we see that multistability arises for $1.65 \leq a_1 \leq 2.45$ (except for the values of $a_1$ corresponding to the occurrence of periodic windows), in which a chaotic and a regular attractors coexist.

Abrupt emergence and disappearance of multistability associated with chaos also occur for fixed $a_1 = 2.13$ and varying $a_0$, as shown in Figs. 9.3(b) and 9.3(d). We see that the maximum probability of landing in a chaotic attractor is relatively small as compared with that for Figs. 9.3(c). Even if the system has settled into chaotic motion, due to multistability external disturbances can “push” it our of chaos, which is undesired for random signal generation.

9.3.3 Reliable and Robust Chaos with Quasiperiodically Driving Fields and the Effect of Noise

The simultaneous emergence of chaos and multistability presents a difficulty in exploiting semiconductor superlattices for applications in random signal generation, a task that requires reliable, robust, and persistent chaotic behaviors. However, due to the coexisting non-chaotic attractor, there is a finite probability that a randomly chosen initial condition would not lead to a chaotic trajectory. Even when the system has settled into a chaotic attractor, random disturbances can drive it out of chaos. Through extensive simulations, we find that, if the system is under a single ac driving, it is unlikely that the probability of having chaos can reach unity in any open interval. However, we find a relatively simple, experimentally feasible way to eliminate multistability in such a way that the only attractor in the system is chaotic. In particular, when the system is subject to a second ac driving field of incommensurate frequency, transition to chaos can be achieved but without the occurrence of multistability.
Figure 9.4: Occurrence of reliable and robust chaos with probability one under quasiperiodic driving. When a second ac driving field of amplitude $a'_1$ and frequency $\Omega' = \sqrt{2}$ is applied to the superlattice system, open parameter intervals emerge in which the probability of generating chaos from a random initial condition is unity. (a) Statistical counts of the maximum Lyapunov exponent and (b) probability of generating chaos versus $a'_1$. Other parameters are $a_0 = 2.23$, $a_1 = 2.3$, $a_2 = 0$, $a_3 = 7.48$, $b_1 = 0.28$, $b_2 = b_3 = 2.85 \times 10^{-2}$, and $\Omega = 1.34$.

Figures 9.4(a,b) demonstrate the occurrence of chaos with probability one when the superlattice system is under quasiperiodic driving, i.e., when a second ac driving field, $a'_1 \cos(\Omega'\tau)$, is present for $\Omega' = \sqrt{2}$. In particular, Fig. 9.4(a) shows, for systematically varying amplitude $a'_1$, the possible values of the maximum Lyapunov exponent where, for each fixed value of $a'_1$, the distinct values of the exponent from a large number of initial conditions are displayed. Figure 9.4(b) shows the probability of generating chaos versus the driving amplitude $a'_1$, where we see that there are open parameter intervals in which the probability is one. Thus, in spite of the periodic windows, in these open intervals the only attractor of the system is chaotic, effectively eliminating multistability. Due to the openness of the parameter inter-
Figure 9.5: Statistical properties of chaos for random signal generation. Under quasiperiodic driving ($\Omega = 1.34$ and $\Omega' = \sqrt{2}$), (a) distribution of the values of a chaotic time series $f(\tau)$. The green dashed curve is a fitted Gaussian with mean $\mu = -0.9$ and variance $\sigma^2 = 0.1$. (b) Autocorrelation of the chaotic time series, where $\Delta \tau$ is the time difference $\tau - \tau'$ and $d\tau$ is the time step used in the numerical integration of the equations of motion. Other parameters are identical to those in Fig. 9.4.

vals for chaos, generic perturbation will not drive the system out of chaos, making it suitable for random signal generation. Figure 9.5(a) presents an example of the statistical distribution of the values associated with a typical chaotic signal, which is approximately Gaussian. Figure 9.5(b) shows the autocorrelation of the signal, which exhibits a desired decaying behavior.

In weakly-coupled systems [428, 429], noise can induce chaos. We find, however, that in strongly coupled systems noise, depending on its amplitude, can either suppress or enhance chaos. In particular, due to multistability, weak noise tends to "kick" a chaotic trajectory out of its basin of attraction and drives the system to the coexisting regular attractor. If noise is sufficiently strong, the system can be driven
Figure 9.6: Effect of noise on multistability and chaos. When noise of zero mean is applied to the voltage driving, for weak noise chaos is suppressed but it is enhanced for strong noise. In the latter case there are open parameter intervals in which the probability of generating chaos from a random initial condition is unity. (a) Statistical counts of the maximum Lyapunov exponent and (b) probability of generating chaos versus $a_1'$. Other parameters are the same as for Fig. 9.4 except $a_1' = 0$. A simple mechanical system illustrating the interplay among noise, multistability, and chaos is included in (b) - see text for details.

out of the basin of the regular attractor towards the chaotic attractor. In either case, multistability is destroyed, as under noise there is only a single attractor that can be either regular or chaotic depending on the noise amplitude. To demonstrate this phenomenon, we apply uncorrelated noise $a_0 \rightarrow a_0 + a^{in}(t)$ with a Gaussian distribution to the voltage driving, where $\langle a^{in}(t)a^{in}(t') \rangle = \sigma^2 \delta(t-t')$. We find, for $0.06 \leq \sigma \leq 0.56$ (the weak noise regime for the particular parameter setting), the stable steady state is the only attractor in the system as noise can drive a chaotic trajectory into the stable steady state attractor. In contrast, in the strong noise regime ($\sigma \geq 0.56$), the chaotic attractor is the only attractor in the system. The phenomena can be
intuitively illustrated using a simple mechanical system in which a particle moves in an asymmetrical double potential well system. As indicated in Fig. 9.6(b), the stable steady state and the chaotic attractor are represented by the deep and shallow well, respectively. Weak noise can drive the particle from the shallow well and kick it into the deep well with a lower energy, but the opposite cannot occur due to the weakness of noise and the well depth. However, for strong noise, the random energy can be sufficient to excite particle out of the deep well. We remark that noise induced chaos is a well documented phenomenon in nonlinear dynamics (see, for example, Refs. [430, 431, 432, 433, 434, 435]).

9.3.4 Physical Mechanism of Chaos and Multistability

The physical mechanism for the evolution of the basin structure toward a more chaos dominated one [Fig. 9.3.1(c)] as the ac driving amplitude is increased can be understood, as follows. From Eq. (9.1), we find that the quantity \(1/M(\mathcal{E}_e)\) controls the switching between the in-phase (acceleration with \(dV_c/dt > 0\)) and the out-of-phase (deceleration with \(dV_c/dt < 0\)) electron motions with respect to the driving \(dc + ac\) field. Equation (9.2) also indicates that the in-phase and out-of phase motions are associated with the increase (field-power absorption) and decrease (field-power amplification) in the average electron energy \(\mathcal{E}_e (\geq 0)\). A change in \(\mathcal{E}_e\) directly leads to \(M(\mathcal{E}_e) > 0\) for \(0 \leq \mathcal{E}_e < \Delta/2\) or \(M(\mathcal{E}_e) < 0\) for \(\Delta/2 < \mathcal{E}_e \leq \Delta\). This gives rise to an upper limit for the velocity amplitude \(|V_c|\).

In the absence of the \(ac\) field, by neglecting decays and the space-charge field, we get from Eqs. (9.1) and (9.2)

\[
\frac{d^2 V_c(t)}{dt^2} + \omega_B^2 V_c(t) = 0 ,
\]

(9.9)

where \(\omega_B = eE_0d/\hbar\) is the Bloch frequency. The \(dc\) field can thus drive the electrons
into periodic Bloch oscillations with the frequency $\omega = \omega_B$ due to the periodic superlattice band structure. In the presence of an external ac field, the combination of the $E_1 \cos(\Omega_1 t) E_e(t)$ term in Eq. (9.1) and the $E_1 \cos(\Omega_1 t) V_c(t)$ term in Eq. (9.2) will generate many harmonic ac fields in the system. Specifically, including the primary ac field but still neglecting decays and the space-charge field in Eqs. (9.1) and (9.2), we obtain its $n$th harmonics in the oscillating $V_c(t)$ with the frequency $\omega = n\Omega_1$ and the amplitude $|V_c| \sim (eE_1 d/\hbar \Omega_1)^{2n-1}/(2n - 1)!!$, where $n = 2, 3, \cdots$. These harmonic ac fields interact with the electron Bloch oscillations by forming multiple resonances at $\omega = \omega_B \pm n\Omega_1$. Note that, without any harmonics, the system dynamics is similar to that of a forced pendulum, which can typically have chaotic motion for large driving amplitude and low frequency. For small values of $E_1$, i.e., $(eE_1 d/\hbar \Omega_1) < 1$, we anticipate only a few periodic oscillating modes associated with the isolated multi-resonances, which manifest themselves as islands (or gaps) in the $E_1-\Omega_1$ plane. As the driving force is increased ($E_1 > E_0$) and the driving frequency is decreased ($\Omega_1 < \Omega_B$), a large number of enhanced harmonic ac modes emerge in the system for $(eE_1 d/\hbar \Omega_1) > 1$. In such a case, the multiple resonance-induced islands in the $E_1-\Omega_1$ phase space are widened and become overlapped. As a result, the electron motion switches from a periodic-dominant pattern to a chaotic-dominant one.

Equation (9.3) contains a self-consistent oscillating space-charge field $E_{sc}(t)$, whose amplitude $|E_{sc}|$ tends to grow with the amplitude $|V_c|$ of the electron velocity. From the combination of the $E_{sc}(t) E_e(t)$ term in Eq. (9.1) and the $E_{sc}(t) V_c(t)$ term in Eq. (9.2), we expect much higher harmonics of the primary ac field to develop rapidly in the system insofar as $(eE_1 d/\hbar \Omega_1) \geq 1$. In fact, a straightforward calculation indicates $|E_{sc}| \sim (eE_1 d/\hbar \Omega_1)^{\alpha_n}$, where the sequence $\alpha_n = 2\alpha_{n-1} + \alpha_{n-2}$ with $\alpha_1 = 1$ and $\alpha_2 = 3$ diverges fast with $n$ [i.e., $\lim_{n \to \infty} (\alpha_n/\alpha_{n-1}) = 1 + \sqrt{2}$]. In short, by including the self-consistent oscillating space-charge field, the superlattice system will be driven
quickly into a chaotic regime insofar as $\Omega_c/\Omega_1$ is large and the condition $eE_1d/h\Omega_1 > 1$ is met.

We remark that, in the miniband approach, the balance equation Eq. (9.1) is valid only if the electric field in the superlattice is homogeneous. With such an electric field, the system dynamics is generally unstable when the $dc$ differential conductivity is negative - the so-called NDC instability [378, 395]. The normalized $dc$ current density $j_{dc}^\Omega/j_p$ in the superlattice can be estimated using the Esaki-Tsu characteristic and the Tucker relations [436, 370, 437, 438, 439, 440]. For the static case with only $dc$ driving field $a_0$, the parameters in our simulation are located in the NDC instability regime. However, with an $ac$ driving, transport can be enhanced by a quantized energy (“photon”) caused by the $ac$ field. As a result, the differential conductivity is not always negative for large values of $a_0$ [441, 442]. The differential conductivity becomes
positive for \( a_0 = n\Omega \), where \( n = 1, 2, \cdots \). Using the same parameter setting as in Figs. 9.3(b,d), we find that, near \( a_0 = 1\Omega \approx 1.34 \), the regime of chaos (gray regime in Fig. 9.7) covers completely the positive differential conductivity regime, indicating the existence of parameter regimes of chaos but without the NDC instability and, as such, the NDC instability may not be a contributing factor to chaos. Indeed, since our model is based on a single miniband, it precludes any NDC effect. In addition, the field domain effect is expected to be small if the period of the superlattice is short and the number of periods is not too large. A complete analysis of the NDC instability and its possible interplay with chaotic dynamics is beyond the scope of the present work.

9.4 Conclusion and Discussion

Semiconductor superlattices, due to their potential applications as radiation sources, amplifiers, and detectors in the THz spectral range, have been extensively studied. There has also been a great deal of effort in investigating nonlinear dynamics in superlattice systems. Especially, chaos has been demonstrated as a generic behavior, suggesting the possibility of random signal generation in the THz range. For such applications it is desired that chaos be reliable and robust in the sense that disturbances to the system shall not drive it out of chaos. In spite of the previous works in this field, the issues have not been addressed of whether chaos in semiconductor superlattice is reliable and robust and if not, what can be done to overcome the difficulty.

The main result of our work is demonstration that, for resonant tunneling dynamics of energetic electrons in semiconductor superlattices subject to an external periodic driving field, chaos and multistability go side by side in the sense that they emerge and disappear simultaneously as a system parameter is changed. Due to the creation of the basin of attraction associated with the birth of a chaotic attractor, the
transition to multistability is necessarily abrupt. As a result of multistability, for any given parameter the probability of generating chaos from a random initial condition will in general not be close to unity. We develop a heuristic physical understanding for the emergence of chaos and multistability. To eliminate multistability and ensure that chaos is the only outcome for any random initial condition, we find that the approach of applying quasiperiodic $ac$ driving can be effective. Experimentally it may be feasible to apply a second $ac$ electric field to drive the superlattice system. Our work demonstrates that robust chaos can emerge, making semiconductor superlattice with quasiperiodic driving a potential candidate for random signal generation in the THz range.
REFERENCES


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APPENDIX A

LAYER-BASED RECURSIVE GREEN’S FUNCTION METHOD
Starting from the left side of the device, the self-consistent Dyson equation \( \Sigma_{l,r} = V_0^\dagger (E - H_0 - \Sigma_{l,r})^{-1} V_0 \) solves the self-energy of layer 1, denoted by \( \Sigma_{l,1} \), due to the left lead, where \( V_0 \) is the coupling matrix between the left lead and the first layer of the device. The Green’s function of layer 1, taking into account the self-energy \( \Sigma_{l,1} \), is then given by

\[
G_{l,1}(E) = (E I - H_{11} - \Sigma_{l,1})^{-1}, \quad (A.1)
\]

where \( H_{11} \) is the Hamiltonian of layer 1. Similarly, the self-energy of layer 2 due to its local left lead, which is in fact layer 1, is given by

\[
\Sigma_{l,2} = H_{21} G_{l,1}(E) H_{12} = H_{12}^\dagger G_{l,1}(E) H_{12}, \quad (A.2)
\]

where \( H_{12} \) is the coupling matrix from layer 2 to layer 1. We can thus obtain the Green’s function of layer 2 taking into account the self-energy from the “new” left lead, which now includes layer 1 (non-uniform leads). Repeating this recursive procedure, we can obtain the self-energies of layers 3, 4, and so on. In general, for layer \( j = 1, ..., N-1 \), we can use the following equation repeatedly:

\[
G_{l,j}(E) = (E I - H_{jj} - \Sigma_{l,j})^{-1}, \quad (A.3)
\]

\[
\Sigma_{l,j+1} = H_{j+1,j} G_{l,j}(E) H_{j,j+1}, \quad (A.4)
\]
to get the self-energy \( \Sigma_{l,N} \) for the left lead of layer \( N \). From the Dyson equation, we can also obtain the self-energy of layer \( N \) due to the right lead, \( \Sigma_{r,N} \). Regarding the layer \( N \) itself as a device, we can calculate its Green’s function

\[
G_N(E) = (E I - H_{NN} - \Sigma_{l,N} - \Sigma_{r,N})^{-1}, \quad (A.5)
\]

and its coupling matrices \( \Gamma_l = i(\Sigma_{l,N} - \Sigma_{l,N}^\dagger) \) and \( \Gamma_r = i(\Sigma_{r,N} - \Sigma_{r,N}^\dagger) \). The transmission \( T \) of this layer, which is the same as the transmission for the original whole device, is given by

\[
T(E) = \text{Tr}(\Gamma_l G_N \Gamma_r G_N^\dagger). \quad (A.6)
\]

The local density of states (LDS) can also be calculated using the RGF method in a layer-by-layer formulation. In particular, for layer \( j \), one can compute the self-energy \( \Sigma_{l,j} \) by using Eqs. (A.3) and (A.4) recursively. Similarly, starting from the right hand side, by repeatedly applying

\[
G_{r,j}(E) = (E I - H_{jj} - \Sigma_{r,j})^{-1}, \quad (A.7)
\]

\[
\Sigma_{r,j-1} = H_{j-1,j} G_{r,j}(E) H_{j-1,j-1}, \quad (A.8)
\]

we get the self-energies \( \Sigma_{r,j} \) from the right lead for layer \( j \). The Green’s function \( G_j(E) \) for this layer taking into account both left and right leads is \( G_j(E) = (E I - H_{jj} - \Sigma_{l,j} - \Sigma_{r,j})^{-1} \). The LDS for this layer is then

\[
\rho_j = -\frac{1}{\pi} \text{Im}[\text{diag}(G_j)], \quad (A.9)
\]

and the LDS for the whole device is given by

\[
\rho = [\rho_1, \rho_2, ..., \rho_N]. \quad (A.10)
\]
Note that the Green’s functions obtained in Eqs. (A.3) and (A.7) are incomplete in a sense that they incorporate the self-energies from either the left or the right lead and thus cannot be used to derive the LDS.

The merits of this layer-based recursive RGF method lie in its time and memory efficiency for large device simulations, its high accuracy, and the flexibility to treat device of arbitrarily geometrical shape. The method is not limited to the calculation of transport properties for open systems. In fact, by imposing the zero-contact condition at the boundaries of the leads, this RGF method can be adopted to closed system calculations of eigenvalues and eigenstates. Extensive tests indicate that the recursive NEGF method outperforms the conventional NEGF method in the computational efficiency by up to three orders of magnitude. For example, the ratio of the CPU times required for calculating the LDS patterns in Fig. 3.5 by using the conventional method and the recursive method is about 800, which is typical for conductance and LDS calculations reported in Chapter 3.
APPENDIX B

CALCULATION OF SPIN POLARIZATION AT THE INTERFACES BETWEEN THE FREE AND RASHBA INTERACTION REGIONS
The continuous Hamiltonian of Dirac fermion with RSOI is given by \( H = \hbar v_F (\sigma_x k_x + \sigma_y k_y + \Delta_R (\sigma_x s_y - s_x \sigma_y)) \). There are two eigenvalues: \( k_\pm = \sqrt{E^2 \mp E \Delta_R} \), with their normalized eigen wavefunctions given by

\[
\psi_\pm = N_\pm \left[ \left( \frac{1}{E} e^{i \theta} \right) | \uparrow \rangle \pm i \left( \frac{E}{k_\pm} e^{2i \theta} \right) | \downarrow \rangle \right] e^{i k \cdot r}, \tag{B.1}
\]

where \( N_\pm = \frac{1}{\sqrt{2[1 + (E/k_\pm)^2]}} \) is a normalization constant and \( \theta = \arctan(k_y/k_x) \). Due to the RSOI, the nondiagonal elements are finite and thus the ratio of spin-up and -down state is equal to unity. The eigen wavefunction can be written as

\[
\psi_{\uparrow, \downarrow} = \left[ \begin{array}{c} 1 \\ e^{i \phi} \end{array} \right] | \uparrow, \downarrow \rangle e^{i \mathbf{q} \cdot \mathbf{r}}. \tag{B.2}
\]

The ratio can thus be arbitrary.

We consider a pure spin state incident from the left lead into the RSOI region and finally reaching the right-hand NR region, as shown in Fig. 4.4(a). The wavefunction in the RSOI and the right-hand NR regions can respectively be written as

\[
\Psi_R = c_+ \psi_+(\phi_+) + c_- \psi_-(\phi_-) + r_+ \psi_+(-\phi_+) + r_- \psi_-(-\phi_-), \quad \Psi_{\sigma L}^\sigma = t_{\uparrow, \sigma L} \psi_+(\theta) + t_{\downarrow, \sigma L} \psi_-(\theta). \tag{B.3}
\]

At the RSOI-NR interface \( (x = 0) \), the boundary condition is

\[
\Psi_R(x) = \Psi_{\sigma L}^\sigma(x), \tag{B.4}
\]

leading to solutions: \([r_+, r_-, t_{\uparrow, \sigma L}, t_{\downarrow, \sigma L}]^T\), where we set \( c_+ = c_- = 1/\sqrt{2} \) for the cases of \( \sigma_L = \uparrow \) and \( \downarrow \). As a result, we have \( t_{\sigma R, \uparrow} = t_{\sigma R, \downarrow} \). Note that the coefficients satisfy the relation \( r_+^2 + r_-^2 + t_{\uparrow, \sigma L}^2 + t_{\downarrow, \sigma L}^2 \approx c_+^2 + c_-^2 \).
APPENDIX C

ORTHONORMALITY OF RADIAL WAVEFUNCTIONS
The radial component of a Dirac spinor in 2D is governed by
\[
\left( -\frac{d}{dr} + \frac{\hat{m}-1/2}{r} \frac{d}{dr} + \frac{\hat{m}+1/2}{r} \right) \chi = i\varepsilon \chi. \tag{C.1}
\]

The two decoupled equations for the upper and lower components of the radial wavefunction can be written as \( H^i \chi = 0 \), where
\[
\begin{align*}
\left[ \frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} + \left( \varepsilon^2 - \frac{(\hat{m} - 1/2)^2}{r^2} \right) \right] \chi^-_{n,m} &= 0 \\
\left[ \frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} + \left( \varepsilon^2 - \frac{(\hat{m} + 1/2)^2}{r^2} \right) \right] \chi^+_{n,m} &= 0. \tag{C.2}
\end{align*}
\]

The solutions of these equations can be expressed in terms of a set of Hankel functions:
\[
\begin{pmatrix} \chi^-_m \\ \chi^+_m \end{pmatrix} = \frac{1}{\sqrt{N}} \begin{pmatrix} H^{(1)}_{m-1/2}(\varepsilon r) + \alpha H^{(2)}_{m-1/2}(\varepsilon r) \\ iH^{(1)}_{m+1/2}(\varepsilon r) + i\alpha H^{(2)}_{m+1/2}(\varepsilon r) \end{pmatrix}, \tag{C.3}
\]
where the coefficient \( \alpha \) and the normalized coefficient \( N \) are given by
\[
\alpha = -\frac{H^1_{m+1/2}(\varepsilon \xi) + H^1_{m-1/2}(\varepsilon \xi)}{H^2_{m+1/2}(\varepsilon \xi) + H^2_{m-1/2}(\varepsilon \xi)} = -\frac{H^1_{m+1/2}(\varepsilon) - H^1_{m-1/2}(\varepsilon)}{H^2_{m+1/2}(\varepsilon) - H^2_{m-1/2}(\varepsilon)}, \tag{C.4}
\]
\[
N_m = 2\pi \int_\xi^1 r dr (|\chi^-_m|^2 + |\chi^+_m|^2),
\]
respectively, with \( \chi^1_{1,2} \) denoting the unnormalized radial wavefunctions. Consider two different pairs of quantum numbers: \( m_i, \varepsilon_i \) and \( m_j, \varepsilon_j \), where \( i \neq j \). Substituting them into Eq. \( (C.2) \), we can obtain the corresponding pairs of states as \[301\]
\[
(m_j^2 - m_i^2) \int_\xi^1 \frac{dr}{r} \chi^\pm_{m_j}(r) \chi^\mp_{m_i}(r, \varepsilon_i) = (\varepsilon_j^2 - \varepsilon_i^2) \int_\xi^1 r dr \chi^\mp_{m_i}(r, \varepsilon_i) \chi^\pm_{m_j}(r, \varepsilon). \tag{C.5}
\]

Setting \( \varepsilon_i = \varepsilon_j = \varepsilon \), we have \( m_{i,j} = m_{i,j}(\varepsilon) \) and
\[
[m_j^2(\varepsilon) - m_i^2(\varepsilon)] \int_\xi^1 \frac{dr}{r} \chi^\pm_{m_j}(\varepsilon) \chi^\mp_{m_i}(\varepsilon) = 0. \tag{C.6}
\]

For nondegenerate energy levels, if \( m_i(\varepsilon) \neq m_j(\varepsilon) \), the integral with the weight \( 1/r \) is zero. For \( m_i(\varepsilon) = m_j(\varepsilon) \), the integral can assume an arbitrary value and, for convenience, we can set it to be unity. As a result, the orthonormal condition becomes
\[
\int_\xi^1 \frac{dr}{r} \chi^\pm_{m_j}(\varepsilon) \chi^\mp_{m_i}(\varepsilon) = \delta_{i,j}. \tag{C.7}
\]

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leading to the normalized condition

\[ N_m^{\pm'} = 2\pi \int_\xi^1 \frac{dr}{r} |\chi_m^{\pm'}|^2, \quad (C.8) \]
APPENDIX D

AZIMUTHAL EQUATION WITH RANDOM DISORDERS IN THE DIRAC RING SYSTEM
Substituting the entire wavefunction into the Dirac equation in the polar coordinates with random disorders [Eq. (6.2)], we have the equations for the upper and lower components of the spinor as

\[
\begin{align*}
\phi_{n,m}^+ \left( \partial_r + \frac{\Phi}{\Phi_0} \right) \chi_{n,m}^+ - \chi_{n,m}^+ \frac{i}{r} \partial_\theta \phi_{n,m}^+ &= 0, \\
+ie^{i\theta} \phi_{n,m}^- (U_s - \varepsilon) \chi_{n,m}^- = 0, \\
\phi_{n,m}^- \left( \partial_r - \frac{\Phi}{\Phi_0} \right) \chi_{n,m}^- + \chi_{n,m}^- \frac{i}{r} \partial_\theta \phi_{n,m}^- &= 0,
\end{align*}
\]

(D.1)

Since Eq. (C.1) can be expressed as

\[
\begin{align*}
\left( \partial_r + \frac{\Phi}{\Phi_0} \right) \chi_{n,m}^+ &= -\frac{m+1/2}{r} \chi_{n,m}^+ + i\varepsilon \chi_{n,m}^-, \\
\left( \partial_r - \frac{\Phi}{\Phi_0} \right) \chi_{n,m}^- &= -\frac{m-1/2}{r} \chi_{n,m}^- + i\varepsilon \chi_{n,m}^+,
\end{align*}
\]

(D.2)

we can eliminate the term in the radial dimension: \( \partial_r \chi^\pm \). In particular, making the approximation \( e^{i\theta} \phi_{n}^- \approx \phi_{n}^+ \), we can express the azimuthal equation in matrix form

\[
\sum_n \frac{1}{r} \begin{pmatrix} \partial_\theta - i(m-1/2) & 0 \\ 0 & \partial_\theta - i(m+1/2) \end{pmatrix} \begin{pmatrix} \phi_{n}^- \chi_{n,m}^- \\ \phi_{n}^+ \chi_{n,m}^+ \end{pmatrix} = \sum_n \begin{pmatrix} 0 & e^{-i\theta} U_s(r, \theta) \\ e^{i\theta} U_s(r, \theta) & 0 \end{pmatrix} \begin{pmatrix} \phi_{n}^- \chi_{n,m}^- \\ \phi_{n}^+ \chi_{n,m}^+ \end{pmatrix}.
\]

(D.3)

Multiplying \( \int_\xi^1 dr \chi_{n,m}^- * \) and \( \int_\xi^1 dr \chi_{n,m}^+ * \) on both sides of the upper and lower components, respectively, and using the orthonormal condition in Eq. (C.7), we can simplify the azimuthal equation for the Dirac system as

\[
\begin{pmatrix} \partial_\theta - i(m-1/2) & 0 \\ 0 & \partial_\theta + i(m+1/2) \end{pmatrix} \phi(\theta) = \sum_s \sum_{n'} \int_\xi^1 dr \chi_{n',m}^- * U_s(r, \theta) \chi_{n,m}^+ \phi.
\]

(D.4)
APPENDIX E

SCATTERING MATRIX METHOD FOR THE SCHRÖDINGER SYSTEM
Based on the same approximation as for the Dirac system, we have the azimuthal equation for the Schrödinger case as [301]

\[(\partial^2_{\theta} + m^2)\phi_n(\theta) = \sum_s \sum_{n'} \Gamma^{(s)}_{n'n,m} \phi_{n'}(\theta), \quad (E.1)\]

where \(\Gamma^{(s)}_{n'n,m} = u_s\chi^{*}_{n',m}(r_s)\chi_{n,m}(r_s)\delta(\theta - \theta_s)\). The orthonormal condition is [301]

\[\int_0^1 dr (1/r) \chi_{m_j(\varepsilon)}^*(r,\varepsilon)\chi_{m_i(\varepsilon)}(r,\varepsilon) = \delta_{i,j}. \]

The azimuthal wavefunction of the Schrödinger system with an impulsive impurity satisfies the boundary conditions

\[\phi_n(\theta^+_s) = \phi_n(\theta^-_s), \quad (E.2)\]

Similar to the Dirac system, we make the diagonal approximation: \(n = n'\). To avoid numerical divergence, we use the scattering matrix method. In particular, for propagation along a free path and scattering with an impurity, the respective scattering matrices can be obtained from Eq. (E.2):

\[S_P^{(s)} = \begin{pmatrix} 0 & e^{i(\theta_s - \theta_{s-1})m} \\ e^{-i(\theta_s - \theta_{s-1})m} & 0 \end{pmatrix}, \quad (E.3)\]

\[S_M^{(s)} = \begin{pmatrix} \Gamma^{(s)}_{n'n,m}e^{2im} & 2m \\ 2m - \Gamma^{(s)}_{n'n,m}e^{-2im} & \Gamma^{(s)}_{n'n,m} \end{pmatrix}, \quad (E.4)\]

The total scattering matrix is given by

\[S = S_P^{(N+1)} \otimes S_M^{(N)} \otimes S_P^{(N)} \otimes \cdots \otimes S_M^{(1)} \otimes S_P^{(1)}. \quad (E.5)\]

If we consider two scattering matrices defined by

\[S_i = \begin{pmatrix} r_i & t_i' \\ t_i & r_i' \end{pmatrix}, \quad S_j = \begin{pmatrix} r_j & t_j' \\ t_j & r_j' \end{pmatrix}. \quad (E.6)\]

The compounded scattering matrix \(S_{ij} = S_i \otimes S_j\) can be calculated as [443, 444, 445]

\[S_{ij} = \begin{pmatrix} r_i + t_i'r_j(1 - r_j'r_i)^{-1}t_i & t_i'(1 - r_j'r_i)^{-1}t_i \\ t_j(1 - r_j'r_i)^{-1}t_i & r_j' + t_jr_i'(1 - r_j'r_i)^{-1}t_j' \end{pmatrix}. \quad (E.7)\]

Combining the total scattering matrix for a set of random disorders with the scattering matrix associated with the magnetic flux

\[S_\Phi = \begin{pmatrix} 0 & e^{-i2\pi\Phi/\Phi_0} \\ e^{i2\pi\Phi/\Phi_0} & 0 \end{pmatrix}, \quad (E.8)\]
we have [444, 445]

\[ \text{Det}[S - S_\phi] = 0, \quad (E.9) \]

from which the angular momentum quantum number \( m \) and its split value \( \Delta m \) can be solved.
APPENDIX F

FLOQUET GREEN’S FUNCTION
The time-dependent Schrödinger equation for an irradiated system connected with leads is given by

\[
\begin{align*}
H(t) - i \frac{\partial}{\partial t} - i \Gamma/2 | \Phi_\alpha(t) \rangle &= (\varepsilon_\alpha - i \eta_\alpha) | \Phi_\alpha(t) \rangle \\
H(t) - i \frac{\partial}{\partial t} + i \Gamma/2 | \tilde{\Phi}_\alpha(t) \rangle &= (\varepsilon_\alpha + i \eta_\alpha) | \tilde{\Phi}_\alpha(t) \rangle
\end{align*}
\] (F.1)

where the self-energy \( \Gamma \) represents the influence of leads and it can be obtained by highly convergent schemes [446]. Due to its time-periodic nature, the wavefunction can be written as

\[
| \Phi_\alpha(t) \rangle = \sum_{m=-\infty}^{+\infty} e^{i m \Omega t} | \phi^m_\alpha \rangle,
\] (F.2)

where \( | \phi^m_\alpha \rangle \) is static. The time-partial and time-dependent terms in Eq. (F.3) can be eliminated by utilizing Eq. (F.2) and making an integral over a time period. Thus, a time-dependent system is transferred into a static-like system and it can be expressed as

\[
\begin{align*}
(\varepsilon_\alpha - i \eta_\alpha + n \Omega - i \Gamma/2) | \phi^m_\alpha \rangle &= \sum_m (H_{n-m}) | \phi^m_\alpha \rangle \\
(\varepsilon_\alpha + i \eta_\alpha + n \Omega + i \Gamma/2) | \tilde{\phi}^m_\alpha \rangle &= \sum_m (H_{n-m}) | \tilde{\phi}^m_\alpha \rangle
\end{align*}
\] (F.3)

where \( H_n = (1/T) \int_0^T H(t) \exp[in \Omega t] dt \). The Floquet Green’s function is given by

\[
\mathcal{G}_n = \sum_{\alpha} \sum_{m} \frac{| \phi^{n-m}_\alpha \rangle \langle \tilde{\phi}^m_\alpha |}{E - \varepsilon_\alpha + i \eta_\alpha - m \Omega}.
\] (F.4)

In numerical calculation, a matrix framework is more efficient. The retard Green’s function of whole system is given by

\[
G^r = \frac{I}{E + i \eta + \Omega - H - i \Gamma/2},
\] (F.5)

where

\[
\begin{align*}
\mathbf{H} &= \begin{pmatrix}
\ddots & \ddots & \ddots & \ddots \\
\ddots & H_0 & H_1 & \ddots \\
\ddots & H_{-1} & H_0 & \ddots \\
& \ddots & \ddots & \ddots \\
& & +1 \Omega & 0 & -1 \Omega \\
\end{pmatrix}, \\
\mathbf{\Gamma} &= \begin{pmatrix}
\ddots & \ddots & \ddots & \ddots & \ddots \\
\Gamma(E + \Omega) & \ddots & \ddots & \ddots & \ddots \\
\ddots & \Gamma(E) & \ddots & \ddots & \ddots \\
\ddots & \ddots & \Gamma(E - \Omega) & \ddots & \ddots \\
\ddots & \ddots & \ddots & \ddots & \ddots \\
\end{pmatrix}, \\
\mathbf{G} &= \begin{pmatrix}
\ddots & \ddots & \ddots & \ddots & \ddots \\
\mathcal{G}_{11} & \mathcal{G}_{01} & \mathcal{G}_{-11} & \ddots & \ddots \\
\ddots & \mathcal{G}_{10} & \mathcal{G}_{00} & \mathcal{G}_{-10} & \ddots \\
\ddots & \ddots & \mathcal{G}_{1-1} & \mathcal{G}_{0-1} & \mathcal{G}_{-1-1} \\
& \ddots & \ddots & \ddots & \ddots \\
\end{pmatrix}
\end{align*}
\] (F.6)
$G_{0k}$ can be written as $G^{(k)}$. We use recursive Green’s function scheme for numerical efficiency [447, 90]. Finally, the transmission is given by

$$T^{k}_{\mu\nu}(E) = Tr \left[ \Gamma^{(k)}_{\nu} G^{(k)}_{1N}(E) \Gamma^{(0)}_{\mu} G^{(k)}_{1N} \right],$$  \hspace{1cm} \text{(F.7)}

where $\mu(\nu) = L, R$. Fig. F.1 shows the result of conductance with a high light intensity $A_0 = 1$. 
Figure F.1: (a) Average conductance $\langle G \rangle$ versus disorder strength $U_0$. Blue rightward and red leftward triangles denotes $G_{RL}$ and $G_{LR}$, respectively. Black curve corresponds to the average conductance $G = (G_{RL} + G_{LR})/2$. $G_{\text{defect}}$, represented by the blue curve, corresponds to the case with a $r = W/2$ semicircle defect as shown in Fig. 8.1. The parameters are $L = 122a$, $W = 50a$, $A_0 = 1$ and $\Omega = 1.533\gamma_0$. (b) Floquet spectrum with the same parameters in (a). Red and blue curves correspond to FTI states. (c,d) show Floquet conductance $G_{RL}^{(k)}$ and $G_{LR}^{(k)}$, respectively.
The single resonant Floquet Hamiltonian is given by

\[ H^F = \begin{pmatrix} H_{\text{eff}} + \Omega & V_+ \\ V_- & H_{\text{eff}} \end{pmatrix}, \]  

(G.1)

with

\[ H_{\text{eff}} = \begin{pmatrix} \Delta_0 & k_- \\ k_+ & -\Delta_0 \end{pmatrix}, \]  

(G.2)

where \( k_\pm = k_x \pm ik_y \) and \( \Delta_0 = v_F^2 A_0^2 / \Omega \) is a topological mass. The Floquet Green’s function without disorder is given by

\[ G^F_0(z, k) = [z - H^F(k)]^{-1}. \]  

(G.3)

Then, the disorder potential in real space is written as

\[ U_{\text{dis}}(r) = \sum_i \begin{pmatrix} u_i^A \delta(r - r_i^A) \\ 0 \\ u_i^B \delta(r - r_i^B) \end{pmatrix}, \]  

(G.4)

where \( u_i^{A,B} \) are uniformly taken in the range \([-U_0/2, U_0/2]\) and thus they satisfy the relationship,

\[ \langle u_i^{A,B} \rangle = 0, \]  

(G.5)

\[ \langle u_i^s u_j^{s'} \rangle = U_0^2 \frac{1}{12} \delta_{ij} \delta_{ss'}, \]  

(G.6)

where \( s, s' = A, B \). Then substitute the Floquet Green’s function and disorder potentials into

\[ \Sigma_{\text{dis}}(z, k) = \int_{FBZ} d\mathbf{k}' U_{\text{dis}}(k, k') G^F_0(z, k') U_{\text{dis}}(k', k), \]  

(G.7)

with assumptions \( z \to 0 \) and \( A_0 \ll 1 \). The non-diagonal block of effective Hamiltonian \( \tilde{H}^F = H^F + \Sigma_{\text{dis}} \) is written as

\[ \tilde{V}_+ = \begin{pmatrix} 0 & \tilde{A}_+ & 0 \\ A_0 + \tilde{A}_+ & 0 \\ 0 & 0 \end{pmatrix}, \quad \tilde{V}_- = \begin{pmatrix} 0 & 0 \\ A_0 + \tilde{A}_- & 0 \\ 0 & 0 \end{pmatrix}, \]  

(G.8)

where

\[ \tilde{A}_\pm = A_0 \left( 1 + \alpha_\pm U_0^2 \right), \]  

(G.9)

and

\[ \alpha_\pm = -\frac{\Omega}{12} \int_{FBZ} \frac{k_\pm dk}{(k_+ k_- + \Delta_0^2)(k_+ k_- + \Delta_0^2 - \Omega^2)}. \]  

(G.10)
Lei Ying is a PhD candidate in Electrical Engineering at Arizona State University. He obtained his Bachelor degree in Physics and studied as Master student in theoretical physics at Lanzhou University in 2010 and 2011, respectively. His research interests are quantum transport, theoretical condensed matter physics, photonics, quantum chaos and nonlinear dynamics. His research work has been published on physical journals, including Physical Review series and Journal of Physics: Condensed Matter. He also served as referee of various journals, such as Phys. Rev. A, EPL, AIP advances, etc.