Quantum Nonlinear Dynamics and Chaos in Photonic and Nano Systems

by

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ABSTRACT

This dissertation aims to study and understand the effect of nonlinear dynamics and quantum chaos in graphene, optomechanics, photonics and spintronics systems.

First, in graphene quantum dot systems, conductance fluctuations are investigated from the respects of Fano resonances and quantum chaos. The conventional semi-classical theory of quantum chaotic scattering used in this field depends on an invariant classical phase-space structure. I show that for systems without an invariant classical phase-space structure, the quantum pointer states can still be used to explain the conductance fluctuations. Another finding is that the chaotic geometry is demonstrated to have similar effects as the disorders in transportations.

Second, in optomechanics systems, I find rich nonlinear dynamics. Using the semi-classical Langevin equations, I demonstrate a quasi-periodic motion is favorable for the quantum entanglement between the optical mode and mechanical mode. Then I use the quantum trajectory theory to provide a new resolution for the breakdown of the classical-quantum correspondences in the chaotic regions.

Third, I investigate the analogs of the electrical band structures and effects in the non-electrical systems. In the photonic systems, I use an array of waveguides to simulate the transport of the massive relativistic particle in a non-Hermitian scenario. A new form of Zitterbewegung is discovered as well as its analytical explanation. In mechanical systems, I use springs and mass points systems to achieve a three band degenerate band structure with a new pair of spatial separated edge states in the Dice lattice. A new semi-metal phase with the intrinsic valley-Hall effect is found.

At last, I investigate the nonlinear dynamics in the spintronics systems, in which the topological insulator couples with a magnetization. Rich nonlinear dynamics are discovered in this systems, especially the multi-stability states.
To my parents
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1. QUANTUM CHAOTIC SCATTERING IN GRAPHENE SYSTEMS IN THE ABSENCE OF INVARIANT CLASSICAL DYNAMICS

1.1. Introduction

Quantum chaos is a field that explores the quantum manifestations of various chaotic behaviors of Hamiltonian systems in the classical limit [1–3]. In open Hamiltonian systems, a fundamental type of chaotic behaviors is transient chaos [4], which leads to chaotic scattering. Quantum chaotic scattering, referred to as the study of quantum behaviors caused by chaotic scattering in the corresponding classical system [5–16], is highly relevant to a number of fields in physics, such as atomic physics, condensed matter physics, and acoustics.

The major characteristic that distinguishes a quantum system from its classical counterpart is that in quantum mechanics, the system is characterized by a nonzero value of the Planck constant. Let $\hbar$ denote the Planck constant nondimensionalized by normalizing to characteristic length and momentum values, so that $\hbar \to 0$ corresponds to the classical limit, $\hbar \ll 1$ to the semiclassical regime, and $\hbar \sim 1$ to the fully quantum mechanical regime. To study the quantum manifestation of classical Hamiltonian chaos, the semiclassical regime is of particular importance because this is the regime where both quantum and classical effects are relevant. Historically, of particular interest are signatures of chaotic scattering when the same system is treated quantum mechanically in the semiclassical regime [5,6,8,10].

The fundamental quantity characterizing a quantum scattering system is the scattering matrix, or the S-matrix, whose elements are the transition probabilities between quantum states of the system before and after the scattering. The formulation of the S-matrix in terms of classical quantities had been of great interest in chemical physics even before chaos started attracting wide attention. The seminal contribution by Miller [17], who obtained a formula for S-matrix elements in terms of
purely classical quantities in the semiclassical regime for reactive scattering systems, became the fundamental tool in the study of quantum chaotic scattering. Given a system that exhibits chaotic scattering in the classical limit, the S-matrix elements in the semiclassical regime exhibit random fluctuations as some physical parameters of the system, such as the energy of the scattering particle or the strength of some externally applied magnetic field, change in a classically small but quantum-mechanically large range. Depending on whether classical scattering is hyperbolic or nonhyperbolic [4], the statistical properties of the fluctuations in the S-matrix elements can be quite distinct [5, 6, 8, 10, 16]. In particular, the fluctuation patterns can be characterized by the energy-correlation function, where a faster decay of the function from unity as the energy difference is increased points to more severe fluctuation patterns. In their seminal work, Blümel and Smilansky [5] showed that the energy-correlation function is related to the decay law of trajectories in the classical phase space as Fourier-transform pairs. Thus, if classical trajectories decay faster from the scattering region, the energy-correlation function decreases more slowly from unity, and vice versa.

A tacit assumption employed in previous works on quantum chaotic scattering is that, as a physical parameter such as the particle energy changes, the classical dynamics is invariant so that the decay law remains unchanged, rendering meaningful its Fourier transform. Such situations arise in physical systems, for example, transport of electrons through a quantum dot in the absence of magnetic field where the corresponding classical dynamics is essentially that of a open billiard and so does not depend on the electron energy. However, when a magnetic field is present, the characteristics of classical dynamics can change drastically with the particle energy. In particular, in an early work, Breymann, Kovács and Tél studied the chaotic scattering of charged particles in an open three-disk billiard subject to a perpendicular magnetic field [18], which is effectively a three-terminal quantum-dot system in the presence of a magnetic field. Classically, since the Lorentz force
depends on both the particle energy and the magnetic field, even for a fixed magnetic field strength the dynamics will depend on the energy. We thus face a challenge that, as the particle energy is systematically changed, there is no unique classical correspondence. Quantum mechanically, the scattering matrix elements will exhibit fluctuations with the particle energy, but Fourier-transform formula relating the energy autocorrelation function and classical particle decay law is no longer applicable. How can then the fluctuation patterns be characterized and understood?

To investigate quantum chaotic scattering in lack of invariant classical dynamics, in this paper we use quantum-transport systems in two-dimensions in the presence of a perpendicular magnetic field as a paradigm. To be concrete, we shall study multiple terminal (lead) graphene [19–23] quantum dots and focus on the conductance that is a function of scattering-matrix elements, as given by the Landauer formula [24, 25]. For convenience, we call the quantum dot region excluding the semi-infinite leads the device region. In the terminology of scattering physics, such a region is called scattering region, and we shall use both terms quite arbitrarily in this paper. For a fixed magnetic-field strength, as the Fermi energy of the conducting electrons increases, the underlying chaotic scattering dynamics in the classical limit can change its characteristics, and the quantum conductance can exhibit significant fluctuations. Our main result is that the fluctuation patterns can be characterized and understood by the behaviors of the complex eigenvalues of the non-Hermitian Hamiltonian of the whole open system. In particular, when leads are not present so that the quantum-dot system is closed, the device Hamiltonian describing this closed system is Hermitian so that all eigenenergies are real. The effect of a semi-infinite lead, however, can be treated by constructing the corresponding self-energy through the non-equilibrium Green’s function formalism [25]. When all the self-energy terms corresponding to multiple leads are combined and inserted in the device Hamiltonian, the resulting Hamiltonian is no longer Hermitian and typically possesses complex
eigenenergies. We shall demonstrate that, even for our situation where there is no unique classical dynamics, the magnitude of the imaginary parts of the eigenenergies provides a reasonable characterization of the conductance-fluctuation patterns. A particular feature is that, when eigenvalues with extremely small imaginary parts emerge, sharp conductance fluctuations occur in a nearly abrupt fashion over small energy scales.

In Sec. 1.2, we describe our model of multi-terminal graphene quantum dots, study its classical phase-space structure, and briefly review the non-equilibrium Green’s function (NEGF) method for quantum transmission or conductance calculation. In Sec. 1.3, we argue that the standard semi-classical treatment breaks down due to lack of invariant classical dynamics and then present an alternative theory based on the spectral properties of the non-Hermitian Hamiltonian of the open quantum-dot system. Numerical support is provided in Sec. 1.4. Concluding remarks are offered in Sec. 1.5.

1.2. Model

1.2.1. Classical Dynamics

Without loss of generality, we use the symmetric, three-terminal quantum-dot system as a prototypical model to address the issue of conductance fluctuations in lack of invariant classical dynamics. Classically, the system consists of a scattering region and three semi-infinite leads separated angularly by $2\pi/3$, as shown schematically in Fig. 1. The scattering region is specified by the black heavy lines, the boundaries of which consist of three circular arcs, where the centers of the respective circles are located at the three corners of an equilateral triangle, the coordinates of which are $(-d/\sqrt{3}, d), (-d/\sqrt{3}, -d), (2d/\sqrt{3}, 0)$, respectively. The radius of each circle is $r$. We assume that the quantum-dot system is made entirely of graphene, so we choose the geometric parameters $d$ and $r$ in terms of the lattice constant of graphene: $d = 199a_0$ and $r = 110\sqrt{3}a_0$, where $a_0 = 1.42\text{Å}$.
is the distance between two nearest neighbor carbon atoms in graphene [19]. The boundary walls are infinitely hard, rendering elastic scattering off the walls. The semi-infinite leads are also assumed to be made of graphene. A perpendicular magnetic field is uniformly applied in the circular region enclosed by the blue-dashed lines in Fig. 1, the radius of which is \( d/\sqrt{3} \). Due to the dependence of the Lorentz force on particle velocity and hence on particle energy, the classical dynamics depends on the energy as well. This means that, for the quantum-dot system, as the Fermi energy is varied, the corresponding classical phase-space structure will change [18]. In classical simulations, the electron moves effectively in free space, so its energy is given by \( E = \frac{1}{2}mv^2 \) and the cyclotron radius is \( r = \frac{mv}{eB} \), where \( m \) is the vacuum mass of the electron and \( v \) is the Fermi velocity.

For a fixed magnetic field and a given energy, the chaotic invariant set in the classical phase space can be numerically calculated, as follows. Without collision with the wall, the electron trajectory is a circle defined by the cyclotron radius. Let \((p, q)\) be the coordinates of the center of the circle, say, before a collision. After the collision, it is only necessary to calculate the new center coordinates in terms of those before the collision and system parameters. Let \((x_i, y_i)\) be the center of the boundary circle on which the collision occurs. The angle between \((p, q)\) and the collision point on the wall with respect to \((x_i, y_i)\) can be written as \( \theta = \theta(p, q, x_i, y_i) \). The center coordinates of the electron cyclotron orbit after the collision, \((p', q')\), can be determined by rotating the point \((p, q)\) with respect to \((x_i, y_i)\) by \(2\theta\) clockwise (or counterclockwise, depending on the direction of the magnetic field). In particular, we have

\[
\begin{align*}
p' &= x_i + (p - x_i) \cos(2\theta) - (q - y_i) \sin(2\theta) \\
q' &= y_i + (p - x_i) \sin(2\theta) + (q - y_i) \cos(2\theta),
\end{align*}
\]

(1.1)

where \( \beta = \theta \) if the magnetic field is upward and \( \beta = -\theta \) for downward magnetic field. Since the system is open, chaos is transient and the underlying chaotic invariant set is non-attracting, which can be calculated, for example, by using the sprinkler method [4]. Figure 2 shows, for a fixed
Fig. 1. Geometry of a three-terminal quantum dot system. The boundary of the device is denoted by the black heavy lines. A perpendicular magnetic field is applied in the circular region defined by the blue dashed lines. The system is made entirely of graphene. The corresponding classical dynamics is effectively that of an open billiard system with three outgoing channels.
magnetic field specified by the magnetic flux $\phi$, some representative chaotic sets for different values of the Fermi energy, where $\phi/\phi_0 = 0.0019$ and $\phi_0 = h/e = 4.136 \times 10^{-15} T m^2$ is the magnetic flux quanta. Here, for convenience of quantum calculations, we use the magnetic flux quanta to normalize the magnetic flux. For graphene, the magnetic flux is $\phi = BS$, where $S = 3\sqrt{3}a_0^2/2$ is the area of one honeycomb unit cell composed of six carbon atoms. For convenience, the electron Fermi energy is also normalized by the hopping energy in the tight-binding model of the graphene lattice, which is $t = 2.7eV$ [19].

1.2.2. Calculation of Quantum Transmission and Conductance

We use the NEGF formalism [25] to calculate the conductance of the multi-terminal quantum-dot system. The Green’s function is defined as

$$(EI - H)G(E) = I,$$  \hspace{1cm} (1.2)$$

where $H$ is the Hamiltonian of the whole system of device and semi-infinite leads, $E$ is the eigenvalue, and $I$ is the identity matrix. In order to calculate the various conductances between different pairs of leads, we need to calculate the Green’s function of device itself under the influence of the semi-infinite leads. The standard methodology is to introduce the non-Hermitian self-energy terms associated with the leads into Eq. (1.2). Let $H_D$ be the device Hamiltonian. For three terminals, the NEGF of the device, $G_D(E)$, can then be expressed by

$$G_D(E) = [EI - H_D - \Sigma_{L_1} - \Sigma_{L_2} - \Sigma_{L_3}]^{-1},$$  \hspace{1cm} (1.3)$$

where $\Sigma_{L_i}, (i = 1, 2, 3)$ are the self-energy terms associated with the three leads, respectively.

For the graphene device, the tight-binding Hamiltonian is

$$H_D = \sum_{\langle i,j \rangle} -t_{ij}(c_i^\dagger c_j + H.c.),$$  \hspace{1cm} (1.4)$$
Fig. 2. For fixed magnetic field specified by $\phi/\phi_0 = 0.0019$, representative chaotic sets for four different values of the Fermi energy: (a) $E/t = 0.05$, (b) $E/t = 0.15$, (c) $E/t = 0.25$, and (d) $E/t = 0.35$, where $p$ and $q$ are the coordinates of center points of the electron trajectory. We observe that the chaotic sets are characteristically distinct.
where $t_{ij} = t$ is the hopping energy between nearest neighbor site of electron, $\langle i,j \rangle$ indicates that only the nearest neighbor pairs contribute to the whole energy, and $c_i^\dagger$ and $c_i$ are the creation and annihilation operators on site $i$, respectively. When a perpendicular uniform magnetic field is applied, the hopping energy is changed to

$$t_{ij} = te^{-i2\pi\phi_{ij}},$$

(1.5)

where

$$\phi_{i,j} = \frac{1}{\phi_0} \int_j^i A \cdot dl,$$

and $A$ is the corresponding vector potential. At the hard-wall boundaries of the device, as both the potential and its first derivative are infinite, the coupling elements in the Hamiltonian are zero. At the boundaries between the device and the leads, since the leads are also made of graphene, the coupling elements in the Hamiltonian matrix are finite and can be written down explicitly.

The self-energy terms $\Sigma_{L_i}$, which describes the effects of leads on the transport property through the device, can be solved self-consistently using a standard iteration procedure [26,27]. In particular, we first calculate the surface retarded Green’s functions of the three leads ($g_{L_i}$) using

$$g_{L_i} = [E^+ I - H_0 - H_c \Lambda]^{-1} \quad i = 1$$

$$g_{L_i} = [E^+ I - H_0 - H_c \Lambda]^{-1} \quad i = 2, 3,$$

(1.6)

where $E^+ = E + i\eta(\eta \to 0^+)$, $H_0$ is the Hamiltonian of one unit cell of the lead, $H_c$ is the coupling matrix between two neighboring unit cells, and $\Lambda$ and $\bar{\Lambda}$ are the so-called appropriate transfer matrices which can be calculated iteratively [25]. The self-energy functions $\Sigma_{L_i}(E)$ are given by

$$\Sigma_{L_i} = H_{L_i,D}^\dagger g_{L_i} H_{L_i,D},$$

(1.7)

where $H_{L_i,D}$ is the coupling matrix between the $i$th lead and the device. The size of $H_{L_i,D}$ is $n_{L_i} \times N_D$, where $n_{L_i}$ is the number of atoms per unit cell of the $i$th lead and $N_D$ is the total number
of atoms in the device. Note that only the elements associated with the boundaries between the
device and the leads are non-zero. The NEGF of the device can then be obtained by Eq. (1.3).

The quantum transmission of the three-terminal quantum-dot system is given by [25, 26]

\[ T_{ij}(E) = \text{Tr}[\Gamma_{L_i} G_D \Gamma_{L_j} G_D^\dagger], \]  

(1.8)

where

\[ \Gamma_{L_i} = i[\Sigma_{L_i} - \Sigma_{L_i}^\dagger], \]  

(1.9)

and the subscript in \( T_{ij}(E) \) indicates the transmission is from the \( j \)th lead to the \( i \)th lead. Corresponding to the transmission \( T_{ij} \), the conductance can be calculated by using the classic Landauer formula [24]:

\[ G_{ij}(E) = \frac{2e^2}{h} T_{ij}(E). \]  

(1.10)

Due to rotational symmetry of the three-terminal quantum-dot system, we discuss the transport properties between an arbitrary pair of leads, e.g., from lead 2 to lead 1, i.e., \( T_{12}(E) \) and \( G_{12}(E) \).

The local density of states (LDOS) at site \( i \) can be obtained through

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

(1.11)

where \( G_D(i, i) \) is the diagonal matrix element of the Green’s function at the \( i \)th site.

When the device is large, e.g., with ten thousands atoms, the device Hamiltonian matrix is also large and the required computation for the Green’s function can become quite demanding. We use the recursive Green’s function (RGF) method to calculate the transmission in a layer-by-layer manner. In particular, we divide the device into a large number of graphene layers and calculate the Green’s function of each layer. In so doing the effect of all other layers and the leads are treated as some kind of self energies. The advantage is basically to replace computations of large matrix
by those associated with a large number of small matrices, leading to marked improvement in the computational efficiency.

1.3. Theory

1.3.1. Breakdown of Semiclassical Theory of Quantum Chaotic Scattering in Lack of Invariant Classical Phase-Space Structure

The fundamental quantity in the semiclassical theory of quantum chaotic scattering is the energy-correlation function of the S-matrix. Let \( s(E) \) be an arbitrary element of the S-matrix \( S(E) \), which depends on the Fermi energy \( E \). The energy-correlation function is

\[
C(\Delta E) = \frac{\langle s^*(E)s(E + \Delta E) \rangle_E}{\langle |s(E)|^2 \rangle},
\]

(1.12)

where \( s^*(E) \) is the complex conjugate of \( s(E) \), \( \langle \cdot \rangle_E \) denotes average over a classically small but quantum-mechanically large energy interval, say \( \Delta E \), and \( \Delta E \ll \Delta E \) is a small energy increment.

The seminal result of Blümel and Smilansky in their semiclassical treatment [5] is that \( C(\Delta E) \) can be calculated by the Fourier transform of the classical particle-decay law \( P(t) \):

\[
C(\Delta E) \sim \int P(t)e^{-i\Delta Et/\hbar}dt.
\]

(1.13)

For fully chaotic (hyperbolic) scattering, particle decay from the scattering region is exponential: \( P(t) \sim e^{-\kappa t} \), where \( \kappa \) is the escape rate associated with the underlying transient chaos [4]. Substituting the exponential-delay law into Eq. (1.13) gives a Lorentzian type of energy-correlation function \( C(\Delta E) \), which is flat for \( \Delta E \to 0 \) [5]. For nonhyperbolic chaotic scattering where chaotic set and Kolmogorov-Arnold-Moser (KAM) islands coexist so that the decay law is algebraic [28–32], \( C(\Delta E) \) decreases fast from unity as \( \Delta E \) is increased from zero [8].

We thus see that, while the semiclassical theory is powerful for revealing the quantum manifestations of classical chaotic scattering, Eq. (1.13), relies on the system’s possessing a well-defined,
unique particle decay law associated with the classical scattering dynamics as the particle energy is changed. For quantum-dot systems this is indeed the case in the absence of any magnetic field. However, as demonstrated in Sec. 1.2.1, when a magnetic field is present, the classical phase-space structure changes with the energy, so does the particle decay law. The formulation of the semiclassical theory of quantum chaotic scattering, Eq. (1.13), no longer holds.

1.3.2. Spectral Theory of Quantum Chaotic Scattering in the Presence of Magnetic Field

A key quantity in determining the transmission or conductance through a quantum-dot system is the self-energy terms, which effectively reduce an infinite open system to a finite one. However, as can be seen from Eq. (1.7), the self-energy matrices $\Sigma_{L_i} (i = 1, 2, 3)$ are not Hermitian, which is a consequence of the coupling between quantum states in the device and the continuum environment (leads) [33]. Nonetheless, the device Hamiltonian $H_D$ describes a closed system specified by the finite scattering region, as shown in Fig. 1, so it is Hermitian and defines the following eigenvalue problem:

$$H_D \psi_{0\alpha} = E_{0\alpha} \psi_{0\alpha},$$

(1.14)

where the subscript $\alpha$ denotes the eigenvalue index, and the eigenvalues $E_{0\alpha}$ and the eigenfunctions $\psi_{0\alpha}$ are all real. The time evolution of an eigenfunction is governed by

$$i\hbar \frac{\partial}{\partial t} \psi_{0\alpha}(t) = E_{0\alpha} \psi_{0\alpha}(t),$$

(1.15)

for which the solution is

$$\psi_{0\alpha}(t) = \psi_{0\alpha}(0)e^{-i\frac{E_{0\alpha}}{\hbar} t}.$$  

(1.16)

For the entire open quantum-dot system where electrons go through the device from one lead to another, the Hamiltonian is not Hermitian. The eigenvalue problem can be written as

$$[H_D + \Sigma_{L1} + \Sigma_{L2} + \Sigma_{L3}] \psi_{\alpha} = E_{\alpha} \psi_{\alpha},$$

(1.17)
where the eigenvalue $E_\alpha$ is complex and the eigenfunctions $\psi_\alpha$ no longer form an orthonormal set. We can express the energy as

$$E_\alpha = E_{0\alpha} - \Delta_\alpha - i\gamma_\alpha,$$

(1.18)

where $\Delta_\alpha$ represents the shift in the energy from the corresponding value in the closed device system as caused by the leads and $\gamma_\alpha$ is the imaginary part of the eigenvalue $E_\alpha$. In order to have a more quantitative expression for $\Delta_\alpha$ and $\gamma_\alpha$, we can treat the self-energy terms as a small perturbation and keep only the first-order terms [16]. After some standard calculation we can obtain

$$\Delta_\alpha + i\gamma_\alpha \approx -\langle \psi_{0\alpha} | \Sigma_L | \psi_{0\alpha} \rangle,$$

(1.19)

where $\Sigma_L = \Sigma_{L1} + \Sigma_{L2} + \Sigma_{L3}$. We thus have

$$\gamma_\alpha \approx -\text{Im}(\langle \psi_{0\alpha} | \Sigma_L | \psi_{0\alpha} \rangle) = -\langle \psi_{0\alpha} | \text{Im}(\Sigma_L) | \psi_{0\alpha} \rangle$$

(1.20)

which shows explicitly that the imaginary part of $E_\alpha$ is induced by the leads. Since the self-energy term $\Sigma_L$ represents the coupling between the device and leads, only the boundary parts of $\psi_{0\alpha}$ contribute to the value of $\gamma_\alpha$. This means that the wavefunctions which describe delocalized states always have a stronger coupling with the leads than those describing strong localized states; that is, strongly localized states have much smaller $\gamma_\alpha$ values than delocalized states. In previous works, the quantity $\gamma_\alpha$ has been used in the study of conductance fluctuations [33–35].

Our idea is that, even when the classical phase-space structure varies with the Fermi energy (or any parameter, with respect to which conductance fluctuations are examined) so that a semiclassical understanding is not available, the quantity $\gamma_\alpha$ can be used to characterize and understand the fluctuation patterns. To gain insights, it is useful to examine the origin of sharp resonances in the conductance-fluctuation curve, for regular and chaotic dynamics in the classical limit. It has been known that sharp conductance fluctuations in open, nanoscale transport devices are typically caused
by quantum pointer states, resonant states of finite but long lifetime formed inside the nanostructure [36–41]. These resonant states are in fact a kind of Fano resonance [42]. For example, for a quantum-dot system whose classical dynamics is regular or contains a significantly regular component, there are stable periodic orbits. If the dot geometry is closed, highly localized states can form around the periodic orbits, forming quantum scars [43–47]. When leads are attached to the quantum dot so that the system becomes open, some periodic orbits can still survive, leading to resonant states, or quantum pointer states. Since the corresponding classical orbits are stable, the resonant states can have long lifetime, leading to weak coupling with the leads. As a result, narrow resonances can form about the energy values that are effectively the eigenenergies in the corresponding closed system. When a modification to the dot geometry is introduced so that the underlying classical dynamics becomes fully chaotic, no stable periodic orbits can exist. While scars can still be formed around classically unstable periodic orbits in the closed system [43–47] (even in graphene and Dirac fermion systems [48,49]), the corresponding resonant states in the open system generally will have much shorter lifetimes, effectively eliminating the narrow resonances in the conductance fluctuation pattern.

The interplay between conductance fluctuations and quantum pointer states, as discussed above, does not require an invariant classical phase-space structure. Consequently, the emergence of pointer states, mathematically characterized by the quantity $\gamma_\alpha$, provides a reasonable way to understand the conductance-fluctuation patterns for quantum-dot systems in the presence of a magnetic field.

1.4. Results

Figure 2 shows that, in the presence of a magnetic field of flux strength $\phi/\phi_0 = 0.0019$, as the Fermi energy of the electron is increased, the underlying chaotic set in the classical limit changes
Fig. 3. (a-d) Normalized conductance (by \( G_0 = 2e^2/h \)) versus the Fermi energy for our three-terminal graphene quantum-dot system for small energy intervals around \( E/t = 0.05, 0.15, 0.25, \) and 0.35, respectively. The conductance-fluctuation patterns are quite different for different energy values, due to the characteristic difference in the corresponding phase-space structure (Fig. 2).

The characteristics of the conductance-fluctuation patterns then depend on the energy value. An example is shown in Fig. 3, where we observe quite distinct behaviors of conductance fluctuation. For instance, for energy values in a small interval about \( E/t = 0.05 \) [Fig. 3(a)], the normalized conductance is near unity and there is hardly any fluctuation. However, for energy values about, say \( E/t = 0.25 \), there are sharp, resonance-type of variations in the conductance, as shown in Fig. 3(c). We notice that the corresponding chaotic invariant set for \( E/t = 0.25 \) is much extensive in the phase space than that associated with \( E/t = 0.05 \). In fact, for high energy values, there are large-size KAM islands in the phase space [18].
The magnetic flux is $\phi/\phi_0 = 0.0019$. The four vertical bands correspond to the four cases of conductance fluctuations in Figs. 3(a-d), respectively. For the first band around $E/t = 0.05$, the values of $\gamma_\alpha$ are all large (about $10^{-2}$), giving rise to the smooth conductance variation in Fig. 3(a).

Much smaller values of $\gamma_\alpha$ appear in the remaining three vertical bands, leading to significant conductance fluctuations as in Figs. 3(b-d). The three colors in each band specify different ranges of the values of $\gamma_\alpha/t$.

We now demonstrate that the local conductance-fluctuation patterns exemplified in Figs. 3(a-d) can be understood through the imaginary part of the complex energy eigenvalue, $\gamma_\alpha$, as discussed in Sec. 1.3. For clarity, we plot $\gamma_\alpha$ versus $Re(E_\alpha)$ in units of $t$, where $\gamma_\alpha/t$ is on a logarithmic scale, as shown in Fig. 4. We notice the following three features: (1) the range of variation in $\gamma_\alpha/t$ is over six orders of magnitude, (2) a substantial fraction of large values of $\gamma_\alpha/t$ appear to follow a curve that plateaus approximately for $\gamma_\alpha/t \leq 10^{-2}$, and (3) the eigenvalues with smaller imaginary parts begin to appear for $E/t \approx 0.15$. 

Fig. 4. 
Imaginary part $\gamma_\alpha$ of complex eigenvalues of the non-Hermitian Hamiltonian for the three-terminal graphene quantum-dot system versus the real part, where $\gamma_\alpha$ is represented on a logarithmic scale.
Mathematically, the imaginary part of the complex eigenenergy contributes an exponential decay factor to the wavefunction. Physically this means that the electrons entering the device from one lead will eventually scatter out of the device into leads, and the imaginary part of eigenvalue effectively the inverse of the lifetime of electrons in a particular state in the device [25]. Another physical significance of $\gamma_\alpha$ is that it characterizes the width of Fano resonance that occurs commonly in quantum-dot systems [33]. From Fig. 3, we can see that there are two kinds of fluctuations: smooth variations and sharp fluctuations. The smooth variations are caused by fully chaotic scattering and the values of the corresponding transmission into all leads are of the order of unity, due to coherent superposition of overlapping resonances. In terms of the complex eigenenergy, the transmission in this case corresponds to some poles with large imaginary parts. The sharp fluctuations are caused by the strongly localized states in the devices, for example, Fano resonances. The coupling between such a strongly localized state and the leads is in general quite weak so that the imaginary part of $E_\alpha / t$ becomes extremely small, typically on the order $10^{-3} \sim 10^{-8}$. To verify these features, we have calculated many LDS patterns for a large number of energy values. For smooth transmission variations, the LDS patterns are typically not localized in the scattering region, as exemplified in Fig. 5(a). In fact, in this case, boundary states prevail, a typical feature of graphene [19]. However, for sharp fluctuations in the transmission, highly localized LDS patterns are common, examples of which are shown in Figs. 5(b-d).

The coupling between discrete states in the device with continuum in the open leads, however, is not the only condition under which Fano resonances may be observed. The Fermi energy of electrons has to reach a threshold to activate the first level of the discrete system (closed device), which can be seen in the presence of a magnetic field because such levels are in fact the Landau levels of the system [50]. From Fig. 4, for example, extremely small values of $\gamma_\alpha$ start to appear.
Fig. 5. Local density of states in the three-terminal graphene quantum-dot system for different Fermi energies: (a) $E/t = 0.05$, (b) $E/t = 0.1474$, (c) $E/t = 0.245$, and (d) $E/t = 0.355$. 
around $Re(E_\alpha)/t = 0.15$, which is caused by the emergence of the first Landau level about that energy. The pattern in Fig. 5(b) is in fact that associated with the first Landau level at energy $E/t = 0.1474$. As the energy is increased through the second and third Landau levels, the physics remains the same even though the scattering process becomes more complicated due to chaos, phases change of paths, and their superpositions etc. These results indicate that the values of the imaginary part of the complex eigenenergies of the non-Hermitian Hamiltonian explains well the conductance-fluctuation patterns in the presence of a magnetic field, even when the underlying classical dynamics varies with the Fermi energy.

To demonstrate the generality of using the complex eigenenergies of the non-Hermitian Hamiltonian to characterize conductance fluctuations in the absence of classically invariant phase-space structure, we present results with a four-terminal graphene quantum-dot system, as shown in Fig. 6. In particular, the geometry of the system is shown in Fig. 6(a), where the scattering (device) region is denoted by thick black curves and the region in which the perpendicular magnetic field is applied is represented by the blue dashed circle. Figure 6(b) shows the values of the eigenenergies in the complex plane, where we see that for $E > 0$, eigenvalues with extremely small imaginary part begin to appear after the first Landau level arises for $E/t \geq 0.13$. A representative strongly localized state, corresponding to the filled red circle in Fig. 6(b), is shown in Fig. 6(c), whose coupling with the leads is weak. The corresponding local conductance-fluctuation pattern is shown in Fig. 6(d), where the vertical red dashed line corresponds to the real energy value of the filled red circle in Fig. 6(b). Overall, we observe similar behaviors to those in the three-terminal system.

1.5. Conclusion

We have argued that a foundational result in the conventional semiclassical theory of quantum chaotic scattering, namely the formula of the energy autocorrelation function of S-matrix element,
Fig. 6.
Conductance fluctuations and characterization in a four-terminal graphene quantum-dot system under a perpendicular magnetic field of flux $\phi / \phi_0 = 0.0019$. (a) Geometry of the system (same legend as in Fig. 1), (b) complex eigenvalue spectrum, (c) localized density of states for $E/t = 0.1444$, (d) Local conductance fluctuations from the left to the upper leads about the first Landau level, i.e., $E/t = 0.1444$. The filled red circle in (b) and the violet dash line in (d) correspond to $E/t = 0.1444$. 
breaks down when a magnetic field is present, for example, in a multi-terminal quantum-dot system. The basic reason is that the semiclassical formula relies on the assumption that the corresponding classical chaotic set, or more broadly the classical phase-space structure, remains unchanged in the range where the energy is varied. However, under a magnetic field the classical phase-space structure depends on the energy [18]. The main contribution of this paper is an alternative framework to understand quantum chaotic scattering in situations where the classical phase-space structure varies with energy (or any other physical parameter, with respect to which the fluctuations of the $S$-matrix elements are of interest).

Utilizing multi-terminal graphene quantum dots as a prototypical class of systems, we articulate that quantum chaotic scattering can be physically characterized by the complex eigenvalues of the non-Hermitian Hamiltonian of the underlying system. A quantum-dot system can in general be decomposed into two parts: a closed device or scattering region and the set of semi-infinite electronic waveguides (or leads). The device Hamiltonian is Hermitian and permits a discrete set of eigenvalues, but the leads possess a continuum of energy spectrum mathematically described by complex self-energy terms. Adding the self-energies to the device Hamiltonian leads to a non-Hermitian Hamiltonian describing the entire open quantum system, whose eigenvalues are in general complex. The key physics to quantum chaotic scattering is that the inverse of the imaginary part of a complex eigenvalue is nothing but the lifetime of the corresponding eigenstate in the scattering region. Thus, when an energy eigenvalue possesses an extremely small imaginary part, the corresponding eigenstate has a long lifetime, which is effectively a strongly localized state. The coupling between such a localized state and the leads, or the quantum “environment” of the device, must necessarily be weak. This leads to an abrupt change in the transmission or conductance over an extremely small energy scale, the so-called Fano resonance [39–42]. Overall, in order to explain a
numerically calculated or experimentally observed conductance-fluctuation pattern in quantum-dot systems under a magnetic field, one can calculate the complex eigenenergies of the corresponding non-Hermitian Hamiltonian. Energy regions in which the eigenenergies exhibit small imaginary parts are the regions where severe conductance fluctuations can be anticipated.
2. CONDUCTANCE STABILITY IN CHAOTIC AND INTEGRABLE QUANTUM DOTS
WITH RANDOM IMPURITIES

2.1. Introduction

In the development of nano-scale quantum devices, an important issue is stability against random perturbations such as various types of impurities. While the impurities can be reduced to certain extent through the improvement and refinement of the underlying fabrication process, it is of interest to uncover alternative mechanisms to enhance the device stability. The purpose of this paper is to show that classical chaos can be exploited to generate devices that are relatively more stable in the quantum regime than those exhibiting integrable dynamics in the classical limit.

To be concrete, we study quantum dot systems, an essential type of structures in nano-electronic devices. Such a system consists of a central scattering region, or a dot region, and a number of electronic waveguides (leads). Incoming electrons from one lead undergo scattering in the dot region and become outgoing in all leads. For quantum dots a fundamental phenomenon is universal conductance fluctuations [6, 51–54] with respect to variations in parameters such as the Fermi energy or the strength of an external magnetic field. In particular, for mesoscopic systems in the ballistic transport regime, at low temperatures the conductance fluctuations tend to be independent of the sample size and impurities [51] and thus can serve as a probe of quantum chaos [6], a field aiming to uncover and understand the quantum manifestations of classical chaos [2]. For over two decades quantum dot systems have become a paradigm to study quantum chaotic scattering [5, 55], and there has been a large body of literature on the effects of distinct types of classical dynamics on conductance fluctuations [7, 8, 12–15, 56–60]. A basic result is that, for systems with integrable or mixed classical dynamics, the conductance curves typically contain a large number of Fano resonances [42, 61–64], leading to sharp conductance fluctuations. But if the system has fully developed
classical chaos, conductance fluctuations will be smooth. This result enables conductance fluctuations to be modulated through the control of the underlying classical dynamics [35, 65].

To address the problem of device stability with respect to random impurities, in this paper we shall not be concerned with conductance fluctuations. Instead, we consider ensemble of random impurities of systematically varying strength and investigate their effects on some appropriately averaged value of the conductance. For this purpose we consider quantum-dot systems of two semi-infinite leads, each supporting a single transverse mode, and focus on the average conductance over the corresponding single-mode Fermi-energy range. This energy range is classically small but quantum mechanically large, rendering applicable semiclassical treatment of the scattering dynamics [17]. To contrast the role of classical dynamics, we choose two types of geometric domains for the dot region: stadium and rectangle, which generate classical chaotic and integrable dynamics, respectively. As the strength of the random impurities is increased from zero, the average conductance will decrease due to localization of wavefunctions. However, we find that the integrable dot system exhibits a much faster decrease in the average conductance than that for the chaotic dot system, implying a stronger conductance stability for the latter. We develop a semiclassical theory to qualitatively explain this phenomenon, and also provide an understanding based on the random matrix theory through analyzing the local density of states in the dot region and the energy level statistics in the corresponding closed system. Our finding strongly advocates the use of chaotic geometry in quantum dot structures, which is consistent with previous results on smooth conductance fluctuations in classically chaotic systems. In fact, we generally believe that classical chaos has the benefit of bringing in greater stability for quantum devices.

Due to the recent interest in two-dimensional Dirac materials [66], we choose to study quantum dot systems made of graphene [23, 67–72]. There were previous experimental [73–75] and
theoretical [76] studies of universal conductance fluctuations in graphene systems. Theoretically and computationally, the effects of disorders were also studied [77–81]. In general, investigating the role of classical chaos in such systems belongs to the emergent field of relativistic quantum chaos [16, 48, 82–87].

In Sec. 2.2, we describe our graphene quantum dot systems and the computational method. In Sec. 2.3, we present results of the average conductance versus the impurity strength and contrast the cases of classically chaotic and integrable dot systems. In Sec. 2.4, we derive a semiclassical theory to explain, qualitatively, the numerical finding that the chaotic dot exhibits a pronouncedly slower decrease in the average conductance with the impurity strength. In Sec. 2.5, we develop an understanding based on the random matrix theory. In Sec. 2.6, we present conclusions.

2.2. Model and Computational Method

Quantum-dot structure with distinct classical dynamics. In order to investigate the effects of classical dynamics on the conductance of the device in the presence of random impurities, we use the tight-binding approximation and the Landauer formalism [24] in combination with the standard Green’s function (GF) method [25], which enables a systematic calculation of the conductances for quantum dots of arbitrary geometry. To be concrete, we choose two standard geometrical shapes for the junction region of the dot structure: one of the stadium shape with chaotic dynamics in the classical limit, and another of the rectangular shape with classical integrable dynamics, as shown in Figs. 7(a) and 7(b), respectively. In each case there are random impurities in the dot region. For simplicity, we assume that, in both devices, the semi-infinite leads that are connected to the dot region are made up of perfect ribbons without any disorder.

Hamiltonian. The tight-binding Hamiltonian of the graphene quantum dot system is

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

(2.1)
Fig. 7. Geometrical dimensions of the quantum dots. (a) Stadium with classical chaotic dynamics and (b) rectangle with classical integrable dynamics.
where \( t_{ij} = t \) is the electronic hopping energy between two nearest neighboring sites in the lattice, \( \langle i, j \rangle \) signifies that the summation is with respect to all nearest-neighbor pairs, \( c_i^\dagger \) and \( c_i \) are the creation and annihilation operators at the \( i \)th site, respectively. The last term in Eq. (2.1) describes the effects of impurities of strength \( V_i \) on the \( i \)th site, where \( V_i \) is uniformly distributed in the range \([-W/2, W/2]\), with \( W \) being the overall impurity strength.

Green’s function formalism. We use the standard Green’s function (GF) formalism [25] to calculate the conductance of the quantum-dot system. We calculate the surface retarded Green’s functions of the leads and their self-energy functions [26, 88]: \( \Sigma_{L,\alpha}(E) \), where \( \alpha = 1, 2 \) denote the left and right leads, respectively. The GF of the device can be obtained through

\[
G_D(E) = [EI - H - \Sigma_{L,1}(E) - \Sigma_{L,2}(E)]^{-1}.
\] (2.2)

The quantum transmission of the system is given by \( T_{\alpha\beta}(E) = Tr[\Gamma_{L,\alpha}G_D\Gamma_{L,\beta}G_D^\dagger] \), where \( \Gamma_{L,\alpha} = i[\Sigma_{L,\alpha} - \Sigma_{L,\alpha}^\dagger] \) and the subscript \( \alpha\beta \) indicates that the transmission is from the \( \beta \)th lead to the \( \alpha \)th lead. The conductance can be obtained by the classic Landauer formula:

\[
G_{\alpha\beta}(E) = \frac{2e^2}{h} T_{\alpha\beta}(E).
\] (2.3)

The local density of states (LDOS) at the \( i \)th site can be obtained as \( n_i = -(1/\pi)\text{Im}[G_D(i, i)] \), where \( G_D(i, i) \) is the diagonal matrix element of the Green’s function at the \( i \)th site. The local current element within the linear response regime is given by [89]

\[
I_{i\rightarrow j}(E_f) = \frac{4e}{h} \text{Im}[H_{ij}G_{ji}^n(E_f)],
\] (2.4)

where \( G_{ji}^n(E_f) \) is the \( (j, i) \)th element of the matrix

\[
G^n(E_f) = G_D^r(E_f)[\Gamma_{L,1}f(\mu_{L,1}) + \Gamma_{L,2}f(\mu_{L,2})]G_D^a(E_f),
\]
with $G^r_D$ and $G^a_D$, being the retarded and advanced Green’s functions, respectively. Here we assume zero temperature so that the Fermi distribution $f(\mu_{L(2)})$ is a step function. The quantity $\mu_{L(2)}$ is the chemical potential of the left (right) lead. To ensure linear response, the chemical potentials of both sides are chosen to be close to the Fermi energy of the device. To be concrete we use a slightly higher potential in the left lead than the right lead.

To obtain statistically reliable results for quantum transmission (conductance), for each fixed Fermi energy and impurity strength, we average the conductance using 1000 random realizations of the impurity configuration, making the computation quite demanding. To be feasible, we simulate relatively small devices, with the following geometric parameters: lead width $w \approx 36.92\text{Å}$ and $15.62\text{Å}$, device width $d \approx 78.7\text{Å}$, and device length $l \approx 151.94\text{Å}$, as shown in Fig. 7. The areas of the stadium and rectangular devices are approximately equal. In order to speed up the computation, we use the recursive Green’s function (RGF) method to calculate the conductance by dividing the device into many small layers and calculating the Green’s function of each layer under the self energies of all other layers and leads. This way, we replace the inverse of a large matrix by the inverses of many small matrices, leading to a remarkable improvement in the computational efficiency.

In our computations, for the integrable device, the top and bottom boundaries have the zigzag orientation. The chaotic dot shape is cut from the rectangular device with the same boundary orientation. While the orientation of the graphene lattice, i.e., zigzag or armchair, can affect the band structure and the conductance, the lattice orientation is unimportant in our setting because of the random disorders. A previous work showed that, for a graphene nanoribbon, although the effect of orientation can be quite significant, when strong short-range disorders are present there is little difference in the average conductances associated with the zigzag and armchair orientations [90]. For the case of weak short-range disorers, the differences between these two orientations can also
be neglected for nanoscale devices. The geometrical shapes of the graphene systems in our study are more complicated than nanoribbons. For example, for a chaotic dot structure, different segments of the boundary can have different lattice orientations. The lattice orientation thus will have little effect on our results.

2.3. Results

The typical behaviors of the ensemble-average conductance versus the Fermi energy and the impurity strength are shown in Figs. 8(a) and 8(b), for classically chaotic and integrable geometries, respectively. The corresponding contour plots are shown in Figs. 8(c) and 8(d). For fixed energy values, two types of behaviors arise in the variation of the conductance with the impurity strength: (1) the conductance increases first as the impurities become stronger, reaches a maximum, and then decreases, and (2) the conductance decreases monotonically with the impurity strength. The first case is somewhat counterintuitive, as exemplified in Fig. 8(e) for $E/t \approx 0.115, 0.233$ for the chaotic dot and in Fig. 8(f) for $E/t \approx 0.185$ for the integrable geometry. This resonance-like phenomenon was reported previously [81], where the initial conductance enhancement can be attributed to the breakdown of the edge states in graphene by weak impurities. However, for strong impurity the quantum states are localized, reducing the conductance. Here we find, for all cases where such a resonance phenomenon occurs, the conductance value for the zero impurity case must be close to zero. That is, when the system is free of any random impurity, the system is already in some pointer state, providing a “room” for impurity to break the state and consequently to enhance the conductance. Two examples of the pointer states in the absence of any impurity are shown in Figs. 8(g) and 8(h), respectively, for the chaotic and integrable dots. If, for certain Fermi energy, in the absence of any impurity the quantum state is not a pointer state so that the conductance
has a relatively large value, introducing impurities into the system can only serve to reduce the conductance, ruling out any possible increase in the conductance and consequently resonance.

To address the conductance stability and to better understand the effect of the interplay between random impurities and classical dynamics on conductance, we examine the average conductance as a function of the impurity strength. In particular, for a fixed value of the impurity strength, we average the conductance over the Fermi energy in the range defined by the first transmission mode of the graphene device, which is about $0.24t$ in our cases. For the dot parameters as in Fig. 8, the normalized average conductance behaviors are shown in Fig. 9(a), where the blue (dash) and red (solid) curves correspond to the integrable and chaotic cases, respectively. We see that, as the impurity strength is increased, the average (or overall) conductance decreases monotonically for both cases. However, for the chaotic dot, the slope of the decreasing trend is smaller than that for the integrable dot. This behavior persists with respect to variations in the device parameters. For example, Fig. 9(b) shows a case with the lead width reduced to $w \approx 15.62\AA$. These results indicate that the conductance of the chaotic dot is more “stable” with respect to variations in the strength of random impurities.

2.4. Semiclassical Understanding of the Interplay Between Random Impurities and Classical Dynamics

Our main numerical result is that classical chaos makes the average conductance of the quantum dot less sensitive to random impurities than integrable dynamics. In particular, as demonstrated in Fig. 9, the derivative of the average conductance with respect to the impurity strength, $d\langle G \rangle(W)/dW$, is negative but its absolute value is small for the chaotic dot and relatively large for the integrable dot. It is possible to obtain a qualitative understanding of the behavior of the derivatives using a semiclassical argument.
Fig. 8. Dependence of the average conductance on the Fermi energy and impurity strength. (a,b) Three-dimensional plot of the conductance versus the Fermi energy and the impurity strength for classically chaotic and integrable dots, respectively. (c,d) The corresponding contour plots. (e) Two cases of resonance-like phenomenon for the chaotic geometry for $E/t \approx 0.115$ (red solid line), 0.233 (blue dash line). (f) Conductance resonance for the integrable geometry for $E/t \approx 0.185$. (g,h) Examples of pointer states in absence of any random impurity for the chaotic and integrable cases, respectively. The device structural parameters are: lead width $w \approx 36.92\text{Å}$, dot width $d \approx 78.7\text{Å}$, and dot length $l \approx 151.94\text{Å}$. (I) Conductances of the chaotic (red solid line) and integrable (blue dash line) devices without impurity. The width of the first transmission mode is about $0.24t$ in both devices. The results are in units of $G_0 = 2e^2/h$. 

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Fig. 9. Effect of lead width on conductance stability. Average conductance over the energy range of the first transmission mode of the lead versus the impurity strength for (a) lead width $w \approx 36.92\text{Å}$ and (b) lead width $w \approx 15.62\text{Å}$. The blue (dash) and red (solid) curves correspond to classically integrable and chaotic dot structures, respectively. We use $\langle G \rangle_0 = \langle G \rangle(W = 0)$ to normalize the average conductance. Note that $\langle G \rangle_0$ should be distinguished from the natural conductance unit $G_0$. 

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For a general open Hamiltonian system, the elements of the quantum $S$-matrix can be expressed via classical quantities through the Miller [17] formula:

$$S_{\mu\nu}(E) = \sum_s [P^{(s)}_{\nu\rightarrow\mu}(E)]^{1/2} \exp \left[ \frac{i}{\hbar} \Phi^{(s)}(E) - \frac{i\pi}{2} \xi^{(s)} \right], \quad (2.5)$$

where $\mu$ and $\nu$ denote quantum states, “$(s)$” denotes a classical path, $P^{(s)}_{\nu\rightarrow\mu}(E)$ is the classical transition probability from state $\nu$ to state $\mu$ along $(s)$, $\xi^{(s)}$ is the Maslov index, and the sum is over all the classical paths connecting states $\nu$ and $\mu$. Let $(I_\nu, \theta_\nu)$ and $(I_\mu, \theta_\mu)$ be the action-angle variables associated with states $\nu$ and $\mu$, respectively. The classical transition probability is given by [17] $P^{(s)}_{\nu\rightarrow\mu}(E) = (1/2\pi)|\partial I_\mu/\partial \theta_\nu|_s^{-1}$. In the study of quantum chaotic scattering, a seminal result [8, 55] is that the energy autocorrelation function of an $S$-matrix element, defined as $C_{\mu\nu}(\varepsilon) \equiv \langle S^*_{\mu\nu}(E)S_{\mu\nu}(E + \varepsilon) \rangle$, can be obtained through Eq. (2.5) as a Fourier transform of the classical particle decay probability:

$$C_{\mu\nu}(\varepsilon) = \int dt \langle P_{\mu\nu}(E,t) \rangle_E \exp (i\varepsilon t/\hbar), \quad (2.6)$$

where $t$ is the time that a classical particle dwells in the scattering (dot) region, $\langle P_{\mu\nu}(E,t) \rangle$ is the classical probability that a $\nu \rightarrow \mu$ transition occurs with the corresponding delay time in the interval $[t, t + dt]$, and the average $\langle \cdot \rangle_E$ is over a classically small but quantum mechanically large energy interval. For our single-mode quantum dot system in the presence of random impurity of strength $W$, we have $\mu = \nu = 1$ so we write $\langle P(t; E, W) \rangle$, which means the probability density for a particle that has a dwell time within the time interval $[t, t + dt]$. The average conductance is given by

$$\langle G \rangle(W) \sim C_{\mu\nu}(0) \quad (2.7)$$

$$\sim |\lim_{\varepsilon \to 0} \int dt \langle P_{\mu\nu}(t; E, W) \rangle_E \exp (i\varepsilon t/\hbar)|.$$
For a chaotic dot, regardless of the presence of random impurities, the particle decay law is exponential: \( \langle P(t; E, W) \rangle_E \sim e^{-t/\tau(W)} \), where \( \tau(W) \) is the average lifetime that a classical particle stays in the dot region. Due to classical chaos, the scattering is random in the dot region. If there are no stable periodic orbits (as in the stadium dot), scattering is already sufficiently random so that the introduction of impurities will enhance the randomness only incrementally, causing insignificant decrease in the average lifetime. It is thus reasonable to assume little dependence of the average lifetime \( \tau \) on \( W \): \( d\tau(W)/dW \leq 0 \). Numerically it may be nontrivial to calculate the particle decay law in the presence of impurities - see Appendix for a detailed description of our procedure and numerical parameters.

Substituting the exponential decay law into Eq. (2.7), we obtain \( \langle G \rangle(W) \sim \tau(W) \) so that

\[
d\langle G \rangle(W)/dW \leq 0,
\]

which explains the slow decrease in the average conductance with the impurity strength for the chaotic dot.

For an integrable dot without random impurities, the classical particle decay is algebraic, as shown in Fig. 10(a). When random impurities are present, the decay law is a mixture of algebraic and exponential behaviors, as shown in Fig. 10(b). Especially, as the impurity strength is increased, random scattering becomes progressively significant so that the “weight” of the exponential decay gradually dominates. A plausible mathematical expression for the decay law is

\[
\langle P(t; E, W) \rangle_E \sim \{ \begin{array}{ll}
at^{-\alpha_c}, & t_0 < t < t_c \\
b \exp[-(t-t_c)/\beta_c], & t > t_c,
\end{array}
\]

(2.9)

where \( a, b, \alpha_c, \) and \( \beta_c \) are all positive constants and \( t_c \) is the “crossover” time, above which there is a transition from algebraic to exponential decay as \( t \) is increased. The relative magnitudes of the
Fig. 10. Classical scattering dynamics for the integrable quantum dot. (a,b) For the integrable dot, particle dwelling time distribution without and with random impurities, i.e., $W/K = 0.0$ and $W/K = 0.2$ (where $K$ is the kinetic energy of the classical particle), respectively, on a double logarithmic scale. We see that the former exhibits an algebraically decaying behavior and the latter shows a mixture of algebraically and exponentially decaying behavior. (c) The probability of having particles with long dwelling time versus the impurity strength. A detailed description of the numerical procedure and the parameters is given in Appendix.
constants can be estimated, as follows. The value of the algebraic decay exponent $\alpha_c$ is typically between 1 and 2 for two degrees of freedom Hamiltonian systems [30, 31, 91, 92]. For relatively weak impurities, the crossover from algebraic to exponential behaviors occurs at some large time $t_c$, which should be much larger than the exponential decay lifetime $\beta_c$ because the particles tend to leave the scattering region fast once the algebraic behavior is over and random scattering from the impurities dominates. It is thus reasonable to assume $\beta_c \ll t_c$. At the crossover time $t_c$, we have $b \approx at_c^{-\alpha_c}$. Since the decay is relatively slow for $t < t_c$, the probability for particle to stay in the dot region can be appreciable for $t = t_c$. We thus have $b \approx at_c^{-\alpha_c} \leq 1$.

As the impurity strength $W$ is increased, we expect $t_c$ to decrease. With the aid of numerical simulation, we can reason that $dt_c(W)/dW < 0$ must hold and $|dt_c(W)/dW|$ is far from being negligible. Specifically, we numerically calculate, for a set of systematically varying values of $W$, the classical probability $P_{t>\bar{t}}(W)$ that a particle stays in the scattering region for $t > \bar{t} > t_c$. As $W$ is increased, we expect $P_{t>\bar{t}}(W)$ to decrease. A typical example is shown in Fig. 10(c), where we observe that $P_{t>\bar{t}}(W)$ decreases rapidly with $W$. Write $P_{t>\bar{t}}(W) = f(W) > 0$, the probability that a particle has a dwell time longer than $\bar{t}$, where $df(W)/dW < 0$ but $|df(W)/dW|$ is large [$f(W)$ can be obtained numerically]. Utilizing Eq. (2.9), we have

$$f(W) = \int_{\bar{t}}^{\infty} b \exp \left\{ - \frac{t - t_c(W)}{\beta_c} \right\} dt$$

$$= a \beta_c [t_c(W)]^{-\alpha_c} \exp \left\{ - \frac{\bar{t} - t_c(W)}{\beta_c} \right\},$$

which gives

$$\frac{dt_c(W)}{dW} = \frac{df(W)/dW}{f(W)} \cdot \frac{1}{1/\beta_c - \alpha_c/t_c(W)}.$$
Since $\alpha_c \sim 1$ and $\beta_c \ll t_c(W)$, we see that the sign of the derivative $dt_c(W)/dW$ is the same as the sign of $df(W)/dW$, which is negative. In addition, we have $|dt_c(W)/dW| \approx |df(W)/dW| \cdot \beta_c/f(W)|$

Substituting Eq. (2.9) into Eq. (2.7), we obtain the average conductance for the integrable dot system in the presence of impurities as

$$\langle G \rangle(W) \sim a \left[ t_c(W) \right]^{1-\alpha_c} \left[ \frac{t_0}{1-\alpha_c} + a \beta_c \left[ t_c(W) \right]^{-\alpha_c} \right],$$

which gives

$$\frac{d\langle G \rangle(W)}{dW} \sim a [t_c(W)]^{-\alpha_c} \left[ 1 - \frac{\alpha_c \beta_c}{t_c(W)} \right] \cdot \frac{dt_c(W)}{dW} \sim e^{[\bar{t} - t_c(W)] / \beta_c} \cdot \left[ 1 - \frac{\alpha_c \beta_c}{t_c(W)} \right] \frac{df(W)}{dW} \equiv A(W) \cdot \frac{dt_c(W)}{dW}.$$ 

Since $\bar{t} > t_c$, $\alpha_c \sim 1$, and $\beta_c \ll t_c(W)$, the factor $A(W)$ in Eq. (2.10) is positive and not negligibly small. We thus have

$$\frac{d\langle G \rangle(W)}{dW} < 0 \text{ and } \left| \frac{d\langle G \rangle(W)}{dW} \right| \sim \left| \frac{dt_c(W)}{dW} \right| \text{ (large).} \quad (2.11)$$

Relations (2.8) and (2.11), for chaotic and integrable quantum dots, respectively, represent a semiclassical understanding of the results in Fig. 9.

2.5. Understanding Based on Random Matrix Theory

In situations where a quantum dot exhibits fully developed chaos in the classical limit and/or has stationary random impurities, electrons injected from the leads will scatter elastically from the dot boundaries and/or from the random impurities. If the mean free path of the electron is much
Fig. 11. Transport statistics for chaotic and integrable graphene quantum dots. The width of the leads is \( w = 6.5a \) with single mode transport in the energy range \( 0 \leq E/t \leq 0.796 \). For both cases, the ratio of the height and width is \( h/d = 1.8 \). For the chaotic (integrable) dot system, there are 12014 (13464) atoms in the scattering region. (a) Transmission coefficient distribution \( P(T) \) for the chaotic (blue circles) and integrable (red squares) dots. The gray solid curves correspond to the RMT prediction [Eq. (2.12)]. (b) Differences in the transmission distribution between the two cases. (c,d) LDS patterns showing the electron distribution in the physical space, where the gray arrows depict the directions of the local currents. The energy values for the chaotic and integrable cases are \( E/t = 0.1048 \) and \( E/t = 0.048 \), respectively.
shorter than the size of the dot, i.e., $l_{MFP} \ll d$, the transport is diffusive and the time of electrons dwelling in the dot region satisfies $\tau_{\text{dwell}} \gg \tau_{\text{erg}}$, where $\tau_{\text{erg}}$ is the time required for a typical classical trajectory to explore the phase space in an ergodic manner [93–95], due to chaos and/or random scattering. The scattering matrix is effectively random, which can be described through the Wigner-Dyson random-matrix theory (RMT). In RMT, the transmission coefficient distribution for a single mode is given by [96–98]

$$P(T) = \frac{\beta_T T^{\beta_T} / 2 - 1}{\beta_T^2 - 1}, \quad (2.12)$$

where the range of the transmission is $0 \leq T \leq 1$ and $\beta_T = 1$ if there is no magnetic field present, and $P(T)$ approaches a circular distribution. A previous work [96] demonstrated that the distribution is highly non-Gaussian, especially for systems where the number of transmission modes is less than three. However, for leads that permit many modes, the transmission distribution approaches Gaussian.

For simplicity, we consider a single-mode quantum-dot system that is fully chaotic in the classical limit. Integrating Eq. (2.12) for transmission in the range $[0, 1]$, we obtain the average conductance as

$$\langle G \rangle_{\text{single}} / G_0 = \langle T \rangle = \frac{\beta_T}{\beta_T + 2} = \frac{1}{2} + \frac{\beta_T - 2}{2\beta_T + 4}, \quad (2.13)$$

where the first term $1/2$ is the “classical” conductance for the chaotic cavity with the physical meaning that a classical particle has equal probability to transmit through and to reflect back from the dot region. The second term is the correction due to quantum interference, also known as the weak localization effect [93] for $\beta_T = 1$, which vanishes when the time-reversal symmetry is broken ($\beta_T = 2$), e.g., when a perpendicular magnetic field is present. If there is spin-orbit coupling
The second term becomes positive and the transmission is enhanced, a phenomenon known as weak anti-localization.

Figure 11(a) shows the numerically obtained statistics of the transmission for the chaotic (red circle) and integrable (blue square) graphene quantum-dot systems. In order to make the effects of chaotic geometry more pronounced, we consider relatively large devices, each having over 10000 atoms, and choose narrow waveguide width so that the coupling between the leads and the dot region is relatively weak. For the chaotic dot system, the transmission distribution agrees well with the prediction in Eq. (2.12), especially in the low transmission regime, as shown in Fig. 11(a). The corresponding average conductance is \( \langle G \rangle_{\beta_T=1}/G_0 = 1/3 \), which is approximately equal to the theoretical prediction \( \langle G \rangle_{\beta_T=1}/G_0 = 1/3 \). For the integrable dot system, the transmission distribution deviates from that for the chaotic case in the low- and high-transmission regimes. However, in the intermediate transmission regime (e.g., \( 0.2 < T < 0.8 \)), there is no apparent difference between the two cases, as shown in Fig. 11(a). The mean conductance of the integrable dot system is \( \langle G \rangle_{rect}/G_0 = 0.4544 \), which is larger than that for the chaotic dot system. From Fig. 11(a), we see that, for the integrable dot system, there are fewer (more) counts of low (high) transmission values as compared with the chaotic dot system. The differences can be seen more clearly in Fig. 11(b). The reason is that, the integrable dot system has a high degree of geometric symmetry, for which quantum pointer states [88, 99] can form, leading to Fano resonances [42, 61, 62, 100, 101] in the transmission (e.g., as a function of the Fermi energy). The resonances contribute to more counts of much higher-than-average transmission values. Symmetry breaking can lead to chaos. For a chaotic dot, the probability for pronounced pointer states to form is significantly lower than that for an integrable dot system so that sharp Fano resonances are much less likely. In this case, the transmission fluctuations tend to be more smooth, giving rise to few counts of extreme transmission values.
The distribution of transmission $P(T)$ in Fig. 5(a) is different from that of the transmission eigenvalues $\rho(T_n)$ obtained from the fixed-energy transmission coefficient between different modes [102]. A transmission matrix can then be constructed with elements $t_{mn}$ and $T_n$ being the eigenvalue of the matrix $t^\dagger t$ for a fixed Fermi energy, where $m$ and $n$ are mode indices. Since we focus on the single-mode case ($N_{channel} = 1$), the matrix is reduced to a number.

We observe, however, that for the stadium dot system, there are more counts of very high transmission values than predicted, which can be understood again by resorting to the consideration of symmetry. In particular, the theoretical curve describes the situation of fully developed classical chaos [98] without any geometric symmetry. The chaotic (stadium) dot used in our computation does in fact possess certain geometry. The finite width of the leads and their symmetric locations on both sides of the device allows ballistic transport channels [103, 104] to be bridged, leading to nearly unity maximum transmission.

Figures 11(c) and 11(d) show, for the chaotic and integrable dot systems, respectively, a set of typical patterns of LDOS and local currents. For the integrable system, there are current channels of direct transport through which electrons transmit with little scattering [50, 87, 105, 106], as indicated by the current direction in Fig. 11(d). In the absence of random impurities, the average transmission value is thus higher for the integrable system. As impurities are introduced into the system, even in the integrable system there are random scatterings. As the impurity strength is increased, the average transmission value decreases. For sufficiently strong impurities, the difference between the chaotic and integrable geometries diminishes, leading to approximately the same average transmission value. An example of this behavior is shown in Fig. 12. Thus, in the same range of variation of the impurity strength, the average transmission for the integrable system needs to decrease by
Fig. 12. Behaviors of unnormalized conductance. For lead width $w \approx 36.92\text{Å}$, unnormalized average transmission over the energy range of the first transmission mode of the graphene lead versus the impurity strength, for the chaotic (red solid line) and integrable (blue dash line) dot systems. For sufficiently strong disorder, the difference in the average transmission values for the two cases diminishes.
a larger amount, leading to a larger slope of decrease in the average normalized transmission, as exemplified in Fig. 9.

To gain further insights, we investigate the integrable and chaotic dot structures from the angle of energy level-spacing statistics. For the corresponding closed systems (e.g., by making the lead width tend to zero), we can calculate a large number of energy levels. In the absence of any random impurity, the level-spacing distributions for the underlying systems are GOE [Gaussian orthogonal ensemble, \( P(S) = (\pi/2)Se^{-\pi S^2/4} \)] and Poisson (\( P(S) = e^{-S} \)) for chaotic and integrable geometries [83], respectively, where \( S \) stands for the normalized nearest-neighbor level spacing. When there are random impurities and as the impurity strength is increased, we expect the difference in the level spacing statistics for the two cases to diminish. Figures 13(a) and 13(b) show \( P(S) \) for the chaotic and integrable dot systems, respectively. In each panel, the blue circles and the red crosses are for the cases where random impurities are absent and present, respectively, where the results are obtained using 100 random impurity configurations. We see that, even in the presence of relatively weak impurities (\( W = 0.2t \)), the level-spacing statistics of both the chaotic and integrable systems are GOE. This convergence to GOE statistics can be more clearly seen through the spectral rigidity, as shown in Figs. 13(c) and 13(d). These results suggest the equivalent effects of classical chaos and impurities: both generating random scattering in both classical and quantum regimes. For an integrable dot system, there is thus a dramatic change in the underlying quantum scattering as impurity is introduced and its strength is increased: from little to significant random scattering. As a result, the average transmission and other device properties tend to exhibit significant changes. However, for a chaotic dot system, the presence of impurities hardly changes the quantum scattering dynamics. From this perspective, chaotic dot systems possess a higher degree of stability against random impurities than integrable dot systems.
Fig. 13. Energy level statistics of chaotic and integrable quantum dots as predicted by the random matrix theory. Level spacing statistics for (a,c) chaotic and (b,d) integrable closed billiard systems. The ratio of the height and the width for both geometries in (a,b) is the same as that of the geometries used to calculate the transmission in Fig. 11. There are 11777 carbon atoms in the unfolded stadium system and 13340 atoms in the rectangular system. In (a,b), the unfolded level-spacing distributions \( P(S) \) are shown, with the corresponding spectral rigidity \( \Delta_3 \) for energy levels in the range of \( 0.1 < E_n/t < 1 \) shown in (c,d). The impurity strength is \( W = 0.2t \). Each data point is the result of averaging over 100 random impurity configurations.
We note that, the quantum pointer states are localized states with long lifetimes and less interactions with the environment. They are related to the stable classical periodic orbits and eigenstates of a closed dot [60]. Previous works showed that change in the geometry of the device, e.g., from integrable to chaotic, can lead to a reduction of the number of quantum pointer states [35]. Random disorders can also reduce the number of quantum pointer states. However, if a strong magnetic field is present, the nature of the classical dynamics and/or random disorders will have less pronounced effects on quantum transport [50, 58, 59]. One set of the quantum pointer states are associated with the stable orbits within the KAM islands in the classical phase space. The probability that these states can be affected significantly by random disorders is small. The corresponding quantum pointer states can then be quite persistent.

2.6. Conclusion

The role of classical chaos in suppressing quantum fluctuations has been recognized in the contexts of quantum chaotic scattering [5, 8, 55] and transport through quantum dots [35, 65] for more than two decades. For integrable or mixed classical dynamics, there are stable periodic orbits in the phase space. The corresponding bounded states typically have little interactions with the leads, giving rise to sharp Fano resonances in the dependence of the conductance on the Fermi energy [61–64, 99]. However, fully developed chaos gives rise to strong ergodicity of classical orbits, enabling strong interaction between the quantum states in the scattering regions and in the leads. It is then difficult for long-lived quantum states to form in the dot region, leading to near-zero probability for pointer states and Fano resonance. As a result, conductance fluctuations tend to be much more smooth then those in integrable or mixed quantum dots. In this sense, while chaos usually generates random dynamical behaviors classically, quantum mechanically it can lead to
suppressed fluctuations. A similar phenomenon arises in the context of quantum resonant tunneling, both non-relativistically [107, 108] and relativistically [84].

This paper deals with the interplay between chaos, random impurities, and quantum behaviors. The main finding is that chaos can be exploited to stabilize quantum behaviors in the presence of impurities, which is consistent with previous works on conductance fluctuations and resonant tunneling. Especially, we focus on the average conductance and ask how it may be affected by random impurities for two cases where the corresponding classical dynamics are chaotic and integrable, respectively. In general, as the impurity strength is increased, the average conductance will decrease, and we find that the decreasing behavior tends to be much less pronounced for the chaotic quantum dot. That is, for a wide range of the impurity strength, the average conductance changes only a little if there is chaos in the classical limit. We develop a physical understanding of this phenomenon using both semiclassical and random-matrix theories. Our work provides a further case where chaos can be advantageous from the standpoint of making stable quantum devices.

2.7. Appendix: Classical Simulation of Scattering Dynamics in the Presence of Random Impurities

We simulate the dynamics of the classical particles in the quantum dot system in the presence of impurities that are modeled by Gaussian random potentials, using the standard leap-frog method for numerically solving Hamiltonian systems [109]. The method is able to maintain the time reversibility of the system and conserve the energy during the simulation. The Hamiltonian of the classical system can be written as

\[ H_{LF} = K(v_x, v_y) + U(x, y), \]

where
\[ K(v_x, v_y) = \frac{1}{2} m(v_x^2 + v_y^2), \]
\[ U(x, y) = \sum_i V'_i \exp \left[ -\frac{(x - x_i)^2 + (y - y_i)^2}{2\sigma_i^2} \right], \]

\( x_i \) and \( y_i \) are the coordinates of the center of the \( i \)th Gaussian potential, \( V'_i \) is its strength uniformly distributed within \([-W/2, W/2]\), and \( \sigma_i \) characterizes the range of the \( i \)th potential.

In our simulations, we use the width of the device to rescale the length. For example, if in the quantum simulations there are about 4000 atoms in the dot, classically we distribute \( N' = 4000 \) random Gaussian potentials throughout the scattering region. We set \( d' = 1.0 \) and \( l' = 1.8 \). We assume the range of each potential to be the same and \( \sigma_i = \sigma \) can be approximately calculated from \( \sqrt{d' \cdot l'/(2\pi N')} = 0.0085 \). Without loss of generality, we use \( \sigma = 10^{-3} \) in our simulations. We keep the kinetic energy \( K \) of the particles to be the same for all cases and change the ratio of \( W/K \) to simulate the particle dynamics in the presence of random impurities of systematically varying strength. In particular, in the interior of the dot region, the classical evolution is obtained by solving the Hamilton’s equations of motion using the leap-frog method. The boundaries are assumed to be hard so that at any boundary point of collision the particle trajectory is simply reflected.
3. NONLINEAR DYNAMICS AND QUANTUM ENTANGLEMENT IN OPTOMECHANICAL SYSTEMS

The uncovering and exploitation of the quantum manifestations of classical nonlinear dynamics is one of the most fundamental problems in physics. Using optomechanical systems as a paradigm, we address this problem from the perspective and advances of quantum entanglement. We uncover strong fingerprints in quantum entanglement of two common types of classical nonlinear dynamical behaviors: periodic oscillations and quasiperiodic motion. There is a transition from the former to the latter as an experimentally adjustable parameter is changed through a critical value. Accompanying this process, except for a small region about the critical value, the degree of quantum entanglement shows a trend of continuous increase. The time evolution of the entanglement measure, e.g., logarithmic negativity, exhibits a strong dependence on the nature of classical nonlinear dynamics, constituting its signature.

3.1. Introduction

When a quantum system contains several degrees of freedom, entanglement among them can arise. Quantum entanglement is a form of quantum superposition, which can be best understood by considering a pair of particles such as electrons. When two such particles are entangled, each particle cannot be fully described without considering the other because they both belong to a single quantum superposition state. Without external disturbance, e.g., a measurement, the particles remain in the entangled state. In order to determine the value of some physical quantity associated with one particle in the entangled state, it is necessary to apply perturbation to the system, after which the state of the particle takes on a definite value. However, the other particle in the originally entangled pair will have the corresponding correlated value for any subsequent time [110], regardless of the physical distance between the two particles [111].
of quantum entanglement has been observed in experiments of large molecules [112] and even small diamonds [113], and it is the foundation of modern quantum computing and information science [114].

While the principle of superposition is defined with respect to linear systems, our physical world, when viewed classically, is nonlinear. A nonlinear dynamical system can exhibit all kinds of interesting phenomena such as periodic oscillations, quasiperiodicity and chaos [115], and they can have distinct fingerprints or manifestations when the system is treated quantum-mechanically. Especially, the studies of quantum manifestations of classical chaos constitute the field of quantum chaos, and there have been tremendous efforts in the past four decades [2] in this field. Some literatures in this field have proven that the transition from integrability, which is characterized by a Poissonian energy level distribution, to quantum chaos, which is characterized by a Wigner-Dyson distribution, can correspond to a quantum phase transition (QPT), e.g., in the Dicke model [116,117]. This QPT also is accompanied by an entanglement singularity which is related to the transition around the bifurcating fixed point in the quantum cusp catastrophe model [118, 119]. While there is no classical correspondence of quantum entanglement in the strict sense, as the measurement of a physical state at one place immediately influences the measurement at the other. In view of the ubiquity of nonlinear dynamics in physical systems and of the fundamental importance of quantum entanglement, curiosity demands that we ask the following question: What is the interplay between nonlinear dynamics and quantum entanglement? Or more explicitly, when the corresponding classical system is nonlinear, what are the signatures on quantum entanglement? This issue may have significant practical implications in the development of devices and systems for quantum computing and quantum information processing.
In this Letter, we address the nonlinear-dynamics/quantum-entanglement issue by using optomechanical systems, a field of intense recent investigation [120–133]. An optomechanical system consists of an optical cavity and a nanoscale mechanical oscillator, such as a cantilever. When a laser beam is introduced into the cavity, a resonant optical field is established that exerts a radiation force on the mechanical cantilever, causing it to oscillate. The mechanical oscillations in turn modulate the length of the optical cavity, hence its resonant frequency. There is thus coupling between the optical and the mechanical degrees of freedom. This coupling, or interaction, can lead to cooling of the mechanical oscillator toward the quantum ground state, a topic of great interest [134, 135]. The optomechanical coupling thus provides a straightforward way to entangle the optical with the mechanical modes, and this can have profound implications to optical information science and quantum computing [136,137]. Existing theoretical works on quantum entanglement in optomechanical systems focused on the situations where the classical dynamics are either steady-state [138, 139] or periodic oscillations [140]. However, very little attentions have been paid on the quasiperiodic and chaotic situations regardless of the fact that the chaotic motion in optomechanical systems has been observed early in experiment [141]. Our goal is to search for nonlinear dynamical behaviors beyond steady-state solutions and periodic oscillations, and to investigate the effects of such behaviors on quantum entanglement. Our main findings are the following. In an experimentally realizable parameter regime, as the power of the driving laser is increased, there is a transition from periodic to quasiperiodic motions, where in the latter, the system is strongly nonlinear with two incommensurate frequencies. The entanglement is enhanced towards the transition, vanishes as the transition point is being reached, but is restored abruptly after the transition and continues to be enhanced as the system evolves deeply into the quasiperiodic regime. A surprising result is that, with respect to time evolution, there is a direct consequence of classical nonlinear dynamics
in quantum entanglement. In particular, for classically periodic dynamics, the time evolution of the entanglement measure is also periodic, but when the classical system enters into the quasiperiodic regime, the quantum entanglement measure exhibits a beats-like behavior with two distinct frequencies. The entanglement, especially when the classical system is quasiperiodic, is robust with respect to temperature variations. Thus, from the perspective of entanglement, there is a clear quantum manifestation and signature of nonlinear dynamics in optomechanical systems.

3.2. Model

We consider a generic type of optomechanical systems, as shown in Fig. 14(a). Such a system is essentially a Fabry-Perot cavity with a fixed, partially reflecting mirror at the left side and a movable, perfectly reflecting end mirror on the right side. The cavity has equilibrium length $l_0$ and fitness $F$. The movable mirror is attached to a mechanical oscillator of mass $m$, characteristic frequency $\omega_M$, and dissipation rate $\Gamma_M$. The fixed end of the cavity has the optical decay rate $\kappa = \pi c/(2Fl_0)$. We assume that a single optical mode of frequency $\omega_c$ is excited by an external laser field of frequency $\omega_0$, where $\omega_c \sim \omega_0$ so that the detuning is on the order of the mechanical frequency $\omega_M$. The Hamiltonian of the system can be written as 

$$\hat{H} = \hbar \omega_c \hat{a}^\dagger \hat{a} + \hbar \omega_M \hat{b}^\dagger \hat{b} - \hbar g_0 \hat{a}^\dagger \hat{a} (\hat{b}^\dagger + \hat{b}) + i\hbar (E e^{-i\omega_0 t} \hat{a}^\dagger - E^* e^{i\omega_0 t} \hat{a}) + \hat{H}_\kappa + \hat{H}_{\Gamma_M},$$

where $\hat{a}(\hat{a}^\dagger)$ and $\hat{b}(\hat{b}^\dagger)$ are the annihilation and creation operators associated with the optical and mechanical modes, respectively. The first two terms in the Hamiltonian describe the free energies of the optical and mechanical components, respectively, and the third term represents the change in the characteristic frequency of the optical mode as a result of the mirror movement. The quantity $g_0 = G \sqrt{\hbar/(2m\omega_M)}$ is the vacuum optomechanical coupling strength characterizing the interaction between one single photon and one single phonon (see Sec. S1 in Supporting Information). The quantity $\sqrt{\hbar/(2m\omega_M)}$ is the mechanical zero-point fluctuation with effective mass $m$, and $G \simeq \omega_c/l_0$. The fourth term describes
Fig. 14. (a) Schematic illustration of a typical optomechanical system driven by a single-mode laser. The laser beam enters the optical cavity through the fixed mirror but photons inside the cavity can also decay through the mirror. The movable mirror is totally reflecting and linked to a frictional mechanical oscillator. (b,c) Time series of the dimensionless canonical coordinate $\tilde{q}$ for the situations where the classical dynamics are periodic and quasiperiodic, respectively.
the interaction between the cavity field and the driving laser field of complex amplitude $E$, where the input laser power is $|E|^2 = 2\kappa P/h\omega_0$. The last two terms in the Hamiltonian represent the dissipation resulting from the cavity decay and mechanical friction, respectively.

### 3.3. Methods

To explore and exploit nonlinear behaviors in the optomechanical system, we study the dynamics of the system by using the Heisenberg equations of motion [144]. The dynamics of the optical-cavity field can be described by its corresponding complex amplitude, and the motion of the mechanical mode can be characterized by a pair of canonical coordinates $q$ and $p$. By replacing the photon annihilation/creation operators by the complex light amplitude and the position operator of the cantilever by its classical counterpart in the Heisenberg equations and neglecting any noise and fluctuations, we can obtain its classical motion of equations [144]. This can effectively be regarded as a classical system described by four independent variables, two associated with the optical mode and two with the mechanical mode. In the language of nonlinear dynamics, the optomechanical system in Fig. 14 has a four-dimensional phase space.

The degree of quantum entanglement can be quantitatively assessed by using the corresponding quantum Langevin equations. Following the standard input-output theory [145] and making use of the reference frame rotating at the laser frequency, we can get the following nonlinear quantum Langevin equations [138, 140]:

$$
\dot{q} = \omega_m p, \quad \dot{p} = -\omega_m q - \Gamma_M p + \sqrt{2}g_0 a^\dagger a + \xi
$$

$$
\dot{a} = -(\kappa + i\Delta_0) a + i\sqrt{2}g_0 a q + E + \sqrt{2\kappa} a^{in},
$$

where $\Delta_0 = \omega_c - \omega_0$ is the cavity detuning. Here we assume that the optical bath is in thermal equilibrium, i.e., in some incoherent state, so that $a^{in}$ can be interpreted as a noise term [145]. The vacuum noise-input term can be described by a zero-mean Gaussian random process. The
autocorrelation function of the vacuum noise is $\langle a^\dagger(t) a(t') \rangle = \delta(t - t')$. The mechanical mode is under the influence of stochastic Brownian noise that satisfies the non-Markovian autocorrelation relation [138, 146, 147]:

$$
\langle \xi(t) \xi(t') \rangle = \frac{\Gamma_M}{\omega_M} \int \frac{d\omega}{2\pi} e^{-i\omega(t-t')} \omega \left[ \coth \left( \frac{\hbar \omega}{2k_B T} \right) + 1 \right].
$$

(3.2)

For the quantum effect of the mechanical mode to be important, the quality factor of the mechanical oscillator must be sufficiently high: $Q = \omega_M / \Gamma_M \gg 1$. In this regime, we have the following Markovian delta-correlated relation: $\langle \xi(t) \xi(t') + \xi(t') \xi(t) \rangle / 2 = \Gamma_M (2\bar{n} + 1) \delta(t - t')$, where $\bar{n} = 1/(\exp[\hbar \omega_M/(k_B T)] - 1)$ is the mean mechanical phonon number and $T$ is the temperature of the mechanical bath. Equation (3.1) is a set of quantum stochastic equations that can be simulated numerically (c.f., Sec. S3 in Supporting Information), and the standard ensemble method can be used to calculate the degree of quantum entanglement. Another method was introduced in Ref. [140], where certain time-dependent covariance matrix is calculated to fully characterize the evolution of the Gaussian state. We use both methods and set the system in the weakly coupling regime so that the magnitudes of noise are small compared to the zeroth-order effects (c.f., Sec. S2 in Supporting Information).

In the Gaussian-evolution method, we assume small fluctuations so that the relevant quantum operators can be expanded about their respective mean values: $O(t) = \langle O \rangle(t) + \delta O(t)$, where $O = q, p, a, a^\dagger$, yielding a set of inhomogeneous equations governing the time evolution of the fluctuations: $\dot{u}(t) = A(t) u(t) + n(t)$, where $A(t)$ is a $4 \times 4$ matrix (see Sec. S4 in Supporting Information). We can also obtain a set of equations for the mean values of the operators but they have the same forms as the corresponding classical equations of motion. Whereas the original Eq. (3.1) is nonlinear, $\dot{u}(t)$ is a set of stochastic linear equations, meaning that the fluctuations will evolve asymptotically into zero-mean Gaussian states but only when none of the Lyapunov
exponents in the corresponding classical system is positive. The covariance-matrix approach is thus not applicable to situations where the classical dynamics are chaotic. For a non-chaotic dynamical process, the properties of the quantum fluctuations can be determined from the $4 \times 4$ covariance matrix that obeys [140, 146]

$$\dot{V}(t) = A(t)V(t) + V(t)A^T(t) + D,$$

(3.3)

where the element of the covariance matrix is defined as $V_{ij} = \langle u_i u_j + u_j u_i \rangle / 2$, and $D = \text{diag}(0, \gamma_M(2n + 1), \kappa, \kappa)$. This comes from $\langle n_i(t)n_j(t') + n_j(t')n_i(t) \rangle / 2 = \delta(t - t')D_{ij}$, characterizing the magnitudes of the noisy terms. For convenience, we can express $V$ as

$$V = \begin{bmatrix} V_A & V_C \\ V_C^T & V_B \end{bmatrix},$$

(3.4)

where $V_A$, $V_B$ and $V_C$ are $2 \times 2$ matrices associated with the mechanical mode, the optical mode, and the optomechanical correlation, respectively. The degree of quantum entanglement between the mechanical and optical modes can thus be assessed by calculating the so-called logarithmic negativity, defined as [148] (c.f., Sec. S5 in Supporting Information),

$$E_N \equiv \max[0, -\ln(2\eta^-)],$$

(3.5)

where $\eta^- \equiv (1/\sqrt{2})[\Sigma(V) - \sqrt{\Sigma(V)^2 - 4\det V}]^{1/2}$, and $\Sigma(V) = \det(V_A) + \det(V_B) - 2\det(V_C)$.

We define $E_p \equiv -\ln(2\eta^-)$ as the pseudo-entanglement measure so that $E_N = \max(0, E_p)$.

For the ensemble method, we simulate Eq. (3.1) a large number of times to obtain an ensemble of time series of the fluctuations. We can then obtain the time series of the covariance matrix from its definition, i.e., $V_{ij} = \langle u_i u_j + u_j u_i \rangle / 2$. The entanglement degree can be calculated from Eq. (3.5).

3.4. Results

We find that there are wide parameter regimes in which the optomechanical system exhibits periodic and quasiperiodic motions, the representative time series of which are shown in Figs. 14(b) and
Fig. 15. (a) Typical bifurcation diagram of the generic optomechanical system in Fig. 14(a), where the asymptotic values of the dimensionless canonical coordinate $\tilde{q}$ are plotted versus the normalized external laser power $\tilde{P}$. The purple dashed line indicates the threshold driving power, $\tilde{P}_c = 0.05842$, at which a transition from periodic to quasiperiodic motions occur. The cavity length is $l_0 = 25\,mm$ with finesse $F = 6 \times 10^4$. (b) The entire spectrum of the Lyapunov exponents versus $\tilde{P}$, and (c) the maximum of the pseudo-entanglement measure $\bar{E}_p$ versus $\tilde{P}$. The red vertical dashed lines at $\tilde{P} = 0.0400, 0.0567, 0.0589$ and $0.0800$ indicate the specific values of $\tilde{P}$ at which the time evolution of $\bar{E}_p$ is to be examined (see Fig. 16).
14(c), respectively. While quasiperiodic motions and even chaos have been discovered recently in a coupled BEC (Bose-Einstein condensation) type of hybrid optomechanical systems [149], to our knowledge there were no previous reports of quasiperiodic motions in the generic optomechanical systems as in Fig. 14, which typically occur for low values of the cavity-decay rate, e.g., $\kappa < 0.2\omega_M$, and for moderate values of the detuning, e.g., for $\Delta_0 \approx -0.8\omega_M$. The dissipation rate of the mechanical oscillator can take on values from a large range, e.g., $10^{-5}\omega_M \sim 10^{-3}\omega_M$. For computational convenience, we rescale the dynamical variables: $\tilde{q} = \sqrt{2g_0q}/\omega_M$ and $\tilde{P} = 8g_0^2E^2/\omega_M^4$. Using the classical Heisenberg equations, we calculate the bifurcation diagram of the system, i.e., the asymptotic value of the dynamical variables as a function of the power of the driving laser, as exemplified in Fig. 15(a), for the experimentally reasonable parameter setting of $\omega_M = 2\pi\text{MHz}$, $Q = 25000$, and $m = 10.67\text{ng}$. For this diagram, the cavity is assumed to be driven by a blue detuned laser with value of the detuning $\Delta_0 = -0.81\omega_M$ and wavelength $\lambda = 1064\text{nm}$. The damping of the mechanical mode is related to the quality factor $Q$ by $\Gamma_M = \omega_M/Q$. To double check the validity of the photon-pressure Hamiltonian, we estimate $x/l = \tilde{q}\omega_M/\omega_c \sim 10^{-8}$ which means that the small displacement assumption is well satisfied [142,144]. As the normalized laser power is increased through a threshold value $\tilde{P}_c$, a transition from periodic oscillation to quasiperiodic motion occurs. Figure 15(b) shows the Lyapunov spectrum versus $\tilde{P}$. We observe that for $\tilde{P} < \tilde{P}_c$, the maximum Lyapunov exponent is zero but there is only one zero exponent, signifying the existence of a periodic attractor. For $\tilde{P} > \tilde{P}_c$, the maximum Lyapunov exponent remains to be zero but there are two such exponents. In particular, the second largest Lyapunov exponent [green (light-gray) line] is negative for $\tilde{P} < \tilde{P}_c$ but it becomes zero for $\tilde{P} > \tilde{P}_c$, a feature characteristic of the transition from periodicity to quasiperiodicity. In the range of $\tilde{P}$ values shown, the third and the fourth Lyapunov exponents are all negative. The feature that there is no positive Lyapunov exponent renders
applicable the use of the quantum Langevin equation to calculate the degree of quantum entangle-
ment, because zero-mean Gaussian random inputs only lead to fluctuation patterns that remain to
be Gaussian. This preservation of the Gaussian distribution means that the fluctuations can be fully
determined by the covariance matrix. Figure 15(c) shows the pseudo-entanglement maximum $E_{p,m}$
as a function of $\tilde{P}$.

Note that, there is quantum entanglement when the value of $E_p$ lies between
0 and $E_{p,m}$, so the shaded region in which the values of $E_{p,m}$ fall below zero indicates a lack of
entanglement. The surprising phenomenon is that, as the system evolves towards the transition
point, the value of $E_{p,m}$ continues to increase but drops to zero rather abruptly as the transition
is reached. In the vicinity of the transition, quantum entanglement disappears. As the classical
dynamics becomes quasiperiodic, entanglement is restored immediately, as the value of $E_{p,m}$ is
recovered and continues to increase as the laser power is increased further. The basic observation
is that strongly nonlinear behavior can lead to enhancement of quantum entanglement between the
optical and mechanical modes.

To probe further into the dynamics of quantum entanglement through the classical transition
point, we calculate the time evolution of the pseudo-entanglement measure, $E_p(t)$, for representa-
tive values of the driving laser power, as shown in Figs. 16 for four cases. Results from the ensemble
approach by simulating the quantum Langevin equations with 3000 realizations are also included.
We observe a strong correlation between $E_p(t)$ and the evolution of the classical dynamics, in that
$E_p(t)$, after a short transient, exhibits periodic (quasiperiodic) behavior if the classical dynamics is
periodic (quasiperiodic). In all cases of $E_p > 0$ so that there is entanglement, the phenomenon of
death and rebirth of entanglement [150, 151] with time occurs, in which $E_p(t)$ becomes negative
suddenly and then restores to some positive value after a time interval. From the prospective of
application, the entanglement duration time is of the order of microsecond so the oscillation could
Fig. 16. (a-d) Time evolution of $E_p$ for four values of the laser driving power $\tilde{P}$ as specified by the vertical red (gray) dotted lines in Fig. 15(a). Insets show the respective zoom-in regions indicated by the black dashed boxes. The thin red dashed lines represent the results from the ensemble approach. The shaded regions correspond to non-physical results and $E_N = \max[0, E_p]$. 
be ignored when the desirable quantum operations can be manipulated at sufficiently high speed. The remarkable phenomenon is that, when quasiperiodicity sets in so that the classical dynamics possesses two incommensurate frequencies, the corresponding quantum pseudo-entanglement dynamics, after its “rebirth,” exhibits a surprising “beats” or temporal modulation phenomenon. There is thus a direct consequence of classical nonlinear characteristics in quantum entanglement. According to the proposal of D. Vitali et al., [138, 152, 153], with the help of an ancillary cavity, we can construct the covariance matrix through homodyne detection and then calculate the logarithmic negativity which provides us a way to observe this nonlinear characteristics experimentally.

To summarize, using optomechanical systems as a paradigm, we have addressed the manifestations of classical nonlinear dynamics in quantum entanglement, with a focus on two common types of classical dynamics: periodic and quasiperiodic motions. Our result is that strong signatures of the classical dynamics exist in the respective quantum entanglement dynamics. For example, when the classical dynamics is quasiperiodic, the corresponding quantum entanglement exhibits a surprising “beating” behavior in its time evolution. Not only is the degree of entanglement enhanced as the classical dynamics transits from periodic to quasiperiodic motions, the entanglement corresponding to the latter is also more temperature robust (c.f., Sec. S6 in Supporting Information). Pushing the classical system into a highly nonlinear regime so that it exhibits more complicated motion than periodic oscillation can thus be beneficial for achieving quantum entanglement.

3.5. Photon-Phonon Coupling

The photon-phonon coupling can be transformed to the photon-photon coupling by applying the so-called polaron transformation [154]: $\hat{H} = \hat{U}^\dagger \hat{H} \hat{U}$, in the absence of any driving and dissipation. The resulting Hamiltonian

$$\hat{H} = \hbar \omega_c \hat{a}^\dagger \hat{a} + \hbar \omega_M \hat{b}^\dagger \hat{b} - \hbar \frac{g^2}{\omega_M} (\hat{a}^\dagger \hat{a})^2$$

(3.6)
has the eigenvalue $E_{nj} = \hbar \omega_c n - \hbar g_0^2 n^2 / \omega_M + \hbar \omega_M j$, where $n$ and $j$ are the photon and phonon numbers, respectively. The effective photon-photon coupling term makes the photon level spectrum anharmonic, leading to many interesting physical phenomena such as photon block effect and photon-induced tunneling [154, 155].

3.6. Relevance of Weak Coupling Regime

In order to understand the dynamics of fluctuations in the optomechanical system as described by the quantum Langevin equations, we consider the corresponding variational equations. For example, a dynamical variable $x$ can be written as $x(t) = x_0(t) + \delta x(t)$, where $x_0(t)$ is the corresponding variable in the zeroth-order system and $\delta x(t)$ characterizes the fluctuations. For the full system described by Eq. (1) in the main text, the zeroth-order system is given by

$$\ddot{q}_0 = -\omega_m^2 q_0 - \Gamma_M \dot{q}_0 + \sqrt{2} g_0 \omega_m |a_0|^2$$

$$\dot{a}_0 = -\left(\frac{\kappa}{2} + i \Delta_0\right) a_0 + i \sqrt{2} g_0 a_0 q_0 + E.$$ (3.7a, 3.7b)

Letting $x_0 = g_0 q_0$ and $\alpha_0 = \frac{a_0}{E}$, we can write Eq. (3.7) as

$$\ddot{x}_0 = -\omega_m^2 x_0 - \Gamma_M \dot{x}_0 + \sqrt{2} g_0^2 E^2 \omega_m |\alpha_0|^2$$

$$\dot{\alpha}_0 = -\left(\frac{\kappa}{2} + i \Delta_0\right) \alpha_0 + i \sqrt{2} \alpha_0 x_0 + 1,$$ (3.8a, 3.8b)

where the parameters $g_0$ and $E$ appear as a product, indicating that the zeroth-order properties of the system are determined by this product as well as other system parameters. To study how the system dynamical behaviors depend on $g_0$ and $E$, we can conveniently fix their product $g_0^2 E^2$ and change one of them systematically, say $g_0$.

As described in the main text, quasiperiodic motion emerges in the weak optomechanical coupling regime, i.e., $g_0 \ll \kappa$, and it can enhance quantum entanglement. This remarkable phenomenon, however, cannot be guaranteed to occur in the strong coupling regime $g_0 \sim \kappa$, due to
the fact that the magnitude of the input noise behaves as $\xi \rightarrow g_0 \xi$ and $\sqrt{\kappa a_{in}} \rightarrow \sqrt{\kappa a_{in}}/E$. As we increase $g_0$ towards the strong coupling region, the amplitude of the input noise will be enhanced by a factor of the the same order of magnitude. In this case, noise and the zeroth-order terms will have comparable magnitude. Classically, the system dynamics will then be affected strongly by noise, making it difficult to assess the interplay between nonlinear dynamics and quantum entanglement.

### 3.7. Numerical Simulation of the Quantum Langevin Equations

In order to gain insights into the dynamics of the optomechanical system and to validate the time-dependent covariant matrix method for quantifying quantum entanglement, we use a stochastic fourth-order Runge-Kutta (RK4) method to simulate the evolution of the quantum Langevin equations [156]. The stochastic RK4 method can yield accurate and stable solutions even when using step size $\Delta$ of two orders of magnitude larger than that in the widely used Heun’s method [157].

The quantum Langevin equations can generally be written as

$$\frac{d\mathbf{X}}{dt} = \mathbf{F} + \mathbf{G} \cdot \mathbf{z}, \quad (3.9)$$

where $\mathbf{G} \cdot \mathbf{z} = [G_1 z_1, G_2 z_2, \ldots, G_n z_n]^T$, $G_i$ is the autocorrelation of the $i$th noise input, and $z_i$ is the Gaussian white noise with the normal distribution $N(0, 1)$. The Stochastic RK4 method can be explicitly expressed as

$$\mathbf{X}(t + \Delta) = \mathbf{X}(t) + \sum_{j=0}^{3} p_j \mathbf{K}_j \Delta + \sum_{j=0}^{3} q_j \mathbf{M}_j \cdot \mathbf{z} \quad (3.10)$$
where

\[
\begin{align*}
K_0 &= F(X(t), t) \\
M_0 &= G(X(t), t) \\
X^{(1)} &= X(t) + \frac{1}{2}K_0\Delta + \frac{1}{2}M_0 \cdot z \\
K_1 &= F(X(t)^{(1)}, t + \frac{1}{2}\Delta) \\
M_1 &= G(X(t)^{(1)}, t + \frac{1}{2}\Delta) \\
X^{(2)} &= X(t) + \frac{1}{2}K_1\Delta + \frac{1}{2}M_1 \cdot z \\
K_2 &= F(X(t)^{(2)}, t + \frac{1}{2}\Delta) \\
M_2 &= G(X(t)^{(2)}, t + \frac{1}{2}\Delta) \\
X^{(3)} &= X(t) + K_2\Delta + M_2 \cdot z \\
K_3 &= F(X(t)^{(3)}, t + \Delta) \\
M_3 &= G(X(t)^{(3)}, t + \Delta)
\end{align*}
\]

The stochastic RK4 algorithm converges to that based on the Stratonovich calculus [156]. For our optomechanical system, \(G\) is a constant, facilitating greatly numerical integration. Note that \(M \cdot z\) has the same meaning as \(G \cdot z\). We simulate the quantum Langevin equations a large number (e.g., 3000) of times to obtain well converged ensemble-averaged quantities, as exemplified in Fig. 3 in the main text.

### 3.8. Time Evolution of Fluctuations

As described in the main text, the time evolution of the fluctuations in the optomechanical systems is governed by

\[
\dot{u}(t) = A(t)u(t) + n(t),
\]  

(3.11)
where $A(t)$ is a $4 \times 4$ matrix given by

$$
A(t) = \begin{bmatrix}
0 & \omega M & 0 & 0 \\
-\omega M & -\Gamma_M & g_x(t) & g_y(t) \\
-g_y(t) & 0 & -\kappa & \Delta(t) \\
g_x(t) & 0 & -\Delta(t) & -\kappa
\end{bmatrix}.
$$

Here we have made the following substitutions: $\delta x = (\delta a + \delta a^\dagger) / \sqrt{2}$ and $\delta y = -i(\delta a - \delta a^\dagger) / \sqrt{2}$, so that $u = (\delta q, \delta p, \delta x, \delta y)^T$ and $n = (0, \xi, \sqrt{\kappa x^0}, \sqrt{\kappa y^0})^T$. Other variables are defined as $g_x(t) = g_0 \langle x(t) \rangle$, $g_y(t) = g_0 \langle y(t) \rangle$ and $\Delta(t) = \Delta_0 - g_0 \langle q(t) \rangle$.

### 3.9. Logarithmic Negativity

There has been no universal definition of quantum entanglement that can be applied to different situations of physical interest, nor any general quantitative measure that can be used to characterize the degree of quantum entanglement. Only special cases can be dealt with where, for example, the density operators are relatively simple. In a canonical bipartite system described by continuous variables, quantum entanglement can be quantified by the so-called measure of logarithmic negativity, defined for Gaussian quantum state as well as pure and symmetric states. In particular, say the quantum system has the density operator $\rho$ and has a subsystem $A$. The logarithmic negativity is defined as [158]

$$
E_N(\rho) \equiv \log_2 \|\rho^{T_A}\|_1,
$$

where $\rho^{T_A}$ is the partial transpose of the bipartite mixed state $\rho$ for its subsystem $A$. $\| \cdot \|_1$ means its trace norm and is expressed as

$$
\|\rho^{T_A}\|_1 = 1 + 2 \sum_i |\mu_i|,
$$

where $\mu_i$’s are the negative eigenvalues of $\rho^{T_A}$. For a general mixed state of infinite dimension without any symmetry, it is extremely difficult to calculate the trace norm. However, for a Gaussian
state, the method of symplectic diagonalization or normal-mode decomposition can be employed, in which the state is transformed into a tensor product of independent thermal oscillator states fully specified by their energies. Note that the quantum properties a Gaussian state can be completely characterized by its covariance matrix. The normal-mode decomposition then enables us to diagonalize the covariance matrix as \( \text{diag}(c_1, c_1, c_2, c_2, ..., c_n, c_n) \), where \( c_i \) is the energy of the \( i \)th thermal oscillator state. For a state at thermal equilibrium, we have \[ \rho = \frac{e^{-\beta a^\dagger a}}{\text{Tr}[e^{-\beta a^\dagger a}]} = (1 - z) \sum_{n=0} z^n |n\rangle \langle n|, \tag{3.15} \]
where \( z = e^{-\beta} \) and \( \beta \propto 1/(k_B T) \). In general, for a physical density operator, we have \( z \geq 0 \). However, the operator under consideration here is a partially transposed operator for which the uncertainty relation is not preserved. There can then be states with \(-1 < z < 0\). Nonetheless, a connection between \( ||\rho^{T_A}||_1 \) and \( c_i \) can be established via the quantity \( z \) through the definition of trace norm as well as the energy relation. Particularly, for a Gaussian state with diagonal covariance matrix \( \text{diag}(c, c) \), its trace norm is
\[ F(c) = \begin{cases} 0, & \text{for } 2c \geq 1 \\ - \log_2 (2c), & \text{for } 2c \leq 1 \end{cases} \tag{3.16} \]
and the logarithmic negativity is the sum of different trace norms of \( c \). The physical meaning is that, for \( 2c \geq 1 \), i.e., \( z \geq 0 \), the state corresponds to a normal thermal state, indicating that energy is characterized by \( c \). As the trace norm of this state is 1, it has no contribution to the entanglement of the total system. However, for \( 2c \leq 1 \), i.e., \(-1 < z < 0\), a negative density operator arises with a non-trivial trace norm, which contributes to entanglement.

The quantum states in an optomechanical system are naturally bipartite state: any such state is composed of the entangled sub-states associated with the optical and mechanical degrees of free-
dom, respectively. In this case, the quantities \( c_1 \) and \( c_2 \) can be calculated from

\[(ic)^4 + [(\det(A) + \det(B) - 2\det(C))(ic)^2 + \det\gamma = 0, \tag{3.17}\]

where \( A, B, \) and \( C \) are the \( 2 \times 2 \) block matrices comprising the covariant matrix

\[
\gamma = \begin{pmatrix}
    A & C \\
    C^T & B
\end{pmatrix}.
\tag{3.18}
\]

It can be seen that \( \det(A), \det(B), \det(C) \) and \( \det(\gamma) \) are four invariants under the symplectic transformation \( S_A \oplus S_B \), where \( S_A, S_B \in Sp(2, \mathbb{R}) \). The conditions of \( c \) for the entangled states can be obtained directly from the PHS criterion [160] associated with the uncertainty relation [161].

We then have

\[
E_N = -\sum_{i=1}^{2} \min(0, \log(c_i)). \tag{3.19}
\]

3.10. Temperature Dependence

How robust is quantum entanglement against thermal fluctuations? To address this question, we calculate the dependence of maximum entanglement measure \( E_N \) on temperature for a large number of values of the laser driving power. In the system of quantum Langevin equations, a convenient way to incorporate the temperature effect is through the input noise. There are two sources of noise: vacuum radiation input noise \( a_{in}(t) \) for the optical subsystem and the viscous force to the mechanical subsystem through the Brownian stochastic process \( \xi(t) \). For the vacuum radiation input noise, at high optical frequency, the equilibrium mean thermal photon number

\[
N(\omega_c) = \left[\exp(h\omega_c/k_B T) - 1\right]^{-1}
\tag{3.20}
\]

tends to zero [162]. This leads to the correlation functions

\[
\langle a_{in}^\dagger(t)a_{in}(t')\rangle = [N(\omega_c) + 1]\delta(t - t') \rightarrow \delta(t - t') \tag{3.21a}
\]

\[
\langle a_{in}^\dagger(t)a_{in}(t')\rangle = N(\omega_c)\delta(t - t') \rightarrow 0 \tag{3.21b}
\]
Fig. 17. For three values of the driving power, dependence of the entanglement maximum $E_N$ on the environmental temperature $T$. In all cases, robust entanglement exists for $T$ in the range of tens of millikelvin. Inset: rescaled average entanglement.
which do not depend on the temperature. For the case of Brownian noise, as its frequency has the same order of magnitude as the mechanical frequency, the equilibrium mean thermal phonon number can remain finite even at relative low temperature. As a result, the temperature of the mechanical reservoir can affect the dynamics of the system through

\[
\bar{n} = \frac{1}{\exp \left[ \frac{\hbar \omega_M}{k_B T} \right] - 1}.
\]

(3.22)

Three representative cases are shown in Fig. 17. We plot the maximum of entanglement as well as the rescaled average entanglement within the stable periodic or quasiperiodic regime when the transient behaviour has died out. In general, we find that, for low mechanical dissipation rate \( \Gamma_M \) and high mechanical frequency, entanglement can persist in the temperature range up to tens of millikevins, which is experimentally readily achievable. This is reasonable as the magnitude of the autocorrelation of the mechanical Brownian noise is \( \Gamma_M (2\bar{n} + 1) \). Insofar as the mechanical mode has a high-Q factor, the effect of the stochastic mechanical effect is small. Especially, for high frequency, the thermal occupation number of the mechanical mode is small, leading to a robust entanglement. A rather surprising phenomenon is that quantum entanglement corresponding to classical quasiperiodic motion is more temperature-robust than that associated with periodic motion.
4. TRANSIENT CHAOS - A RESOLUTION OF BREAKDOWN OF QUANTUM-CLASSICAL CORRESPONDENCE IN OPTOMECHANICS

Recently, the phenomenon of quantum-classical correspondence breakdown was uncovered in optomechanics, where in the classical regime the system exhibits chaos but in the corresponding quantum regime the motion is regular - there appears to be no signature of classical chaos whatsoever in the corresponding quantum system, generating a paradox. We find that transient chaos, besides being a physically meaningful phenomenon by itself, provides a resolution. Using the method of quantum state diffusion to simulate the system dynamics subject to continuous homodyne detection, we uncover transient chaos associated with quantum trajectories. The transient behavior is consistent with chaos in the classical limit, while the long term evolution of the quantum system is regular. Transient chaos thus serves as a bridge for the quantum-classical transition (QCT). Strikingly, as the system transitions from the quantum to the classical regime, the average chaotic transient lifetime increases dramatically (faster than the Ehrenfest time characterizing the QCT for isolated quantum systems). We develop a physical theory to explain the scaling law.

4.1. Introduction

The quantum-classical correspondence is a fundamental and fascinating problem in physics. For a specific physical process in a quantum system, if a large number of energy levels are involved (e.g., in the high energy regime), the evolution of the expected values of the observables will be governed by the classical Newtonian dynamics. This is the usual quantum-classical correspondence. Exceptions can occur when only a few lower energy levels are involved, e.g., at low temperatures, such that the quantum features of the ground state are manifested on a macroscopic scale [163], leading to fascinating phenomena such as Bose-Einstein condensation, superconductivity, and superfluids.
In this paper, we report our discovery of transient chaos as a natural paradigm to explain the recently discovered phenomenon of the breakdown of quantum-classical correspondence in optomechanics.

A prototypical optomechanical system consists of an optical cavity with a fixed mirror and a nanoscale, mechanically movable cantilever, as shown schematically in Fig. 18. The basic physics is that the radiation pressure from the optical field changes the position of the movable mirror, which in return modulates the resonance frequency of the optical cavity, leading to a coupling between the optical and mechanical degrees of freedom [122, 164]. In addition to this prototypical setting, alternative configurations for realizing the optical-mechanical coupling exist, such as those based on the whispering-gallery modes [165], microtoroid [166] and microsphere [164] resonators. Optomechanics is thus not only fundamentally important, as it provides a setting to understand the physics of optical-mechanical interactions [121, 130, 164], but also practically significant with applications ranging from ultra-precision measurements [122, 167, 168], light-matter entanglement [138, 140, 169], mechanical memory [170], tunable optical coupler [171], classical state preparation through squeezing [172, 173], optical transparency [174], and photon shuttling [175] to creation of nonclassical light [143, 176] and cooling of microscopic or mesoscopic objects [177, 178]. The classical equations of motion of an optomechanical system are nonlinear, rendering possible chaotic behaviors [141, 179].

In a recent work [180], it was demonstrated that, in the classical regime where the system exhibits chaos, in the corresponding quantum regime the motion becomes regular and no signatures of chaos appear to exist. This is the so-called quantum-classical correspondence breakdown in optomechanics. A conventional approach to studying the correspondence is to compare the quantum Wigner function distribution with the classical phase space distribution [143, 181, 182], both being average quantities. However, a recent work [183] demonstrated an optimal state estimation for
cavity optomechanical systems through Kalman filtering, which allows us to obtain the conditional system state in the presence of experimental noise. In addition, observation of quantum trajectories obeying quantum state diffusion through heterodyne detection in a coupled system between a superconducting qubit and an off-resonant cavity was reported [184], as well as other types of quantum trajectories [185–195]. Thus, rather than focusing on the average properties of the system, we study the individual quantum trajectories of the system as related to the continuous weak measurement to probe into the quantum-classical correspondence breakdown.

Our aim is to uncover, through systematic classical and quantum simulations, the dynamical and physical mechanisms responsible for the breakdown phenomenon. The standard treatment [164] of an optomechanical system consists of quantizing the cavity optical field and the oscillations of the cantilever as two mutually interacting quantum boson fields while treating the driving laser field classically. Dissipation associated with the optical and mechanical fields can be incorporated into the quantum Langevin equations from the quantum input-output theory [196] or by solving the quantum Master equation with the Lindblad operators. When chaos occurs in the classical limit, the system is typically in a high energy state with hundreds of photons and phonons, rendering infeasible direct simulation of the quantum Master equation. An effective framework is the method of quantum state diffusion (QSD), which generates quantum trajectories to approximate the time evolution as governed by the quantum Master equation [197–199]. The QSD method has been instrumental to homodyne detection and the study of quantum-classical correspondence in dissipative quantum chaos [200–202]. Here, using the QSD method, we calculate the dynamical trajectories of the system in the quantum regime. Our computations extending to the long time scales (which were not attempted in previous works) suggest that transient chaos [4] associated with quantum trajectories is ubiquitous. (To our knowledge, in spite of reports of chaos [141, 164, 179], there were
no prior results of transient chaos in optomechanical systems.) In particular, before approaching a regular final state, the quantum system exhibits a behavior that is consistent with the classical chaotic behavior. Thus, in short and in long time scales, the time evolutions of the system in the quantum regime would appear to be chaotic and regular, respectively. This means that, in short time scales a quantum-classical correspondence does exist, but its breakdown occurs in the long time limit. A striking finding is that, as the classical regime is approached, the average transient lifetime increases dramatically (faster than the Ehrenfest time - see Discussion). As the quantum system becomes “more classical,” the quantum-classical correspondence holds significantly longer, providing a natural resolution for the breakdown phenomenon.

4.2. Results

4.2.1. Hamiltonian.

In the rotating frame of the driving laser field, the Hamiltonian of a generic optomechanical system is [164]:

\[ H = \hbar \left[ -\Delta_0 + g_0 (b^\dagger + b) a^\dagger a + \hbar \omega_m b^\dagger b + \hbar \alpha_L (a^\dagger + a) \right], \tag{4.1} \]

where \( a^\dagger \) and \( a \) are the creation and annihilation operators for the optical field, \( b^\dagger \) and \( b \) are the corresponding phonon operators for the mechanical cantilever, \( \Delta_0 = \omega_d - \omega_{\text{cav}} \) is the detuning between the driving laser and the optical cavity field, and \( \omega_m \) is the resonant frequency of the mechanical mode. The quantity \( \alpha_L \) is the classical amplitude of the driving laser field, which is related to its power \( P \) through \( |\alpha_L|^2 = 2\kappa P / (\hbar \omega_d) \), where \( \kappa \) is the quality factor of the optical cavity. The basic physics behind the optomechanical coupling [203] is that a change in the position of the cantilever, which is proportional to \( (b^\dagger + b) \), can lead to a change in the resonant frequency of the optical field with a strength factor \( g_0 \), where \( g_0 \approx (\omega_{\text{cav}} / l_0) \sqrt{\hbar / (2m\omega_m)} \), with \( l_0 \) being the nominal cavity length.
4.2.2. Calculation of Classical Trajectories.

A conventional approach to investigating the dynamics of an optomechanical system is to use the quantum input-output theory [196] to obtain the standard quantum Langevin equations in the Heisenberg picture. While dissipation and fluctuations of the photon and phonon fields have been taken into account, these are operator equations with stochastic fluctuations. In the classical limit \( (\hbar \to 0) \), i.e., bad cavity limit, the quantum correlations between the operators are negligible as compared with their averages, so we have \([140]\) \( \langle (b^\dagger + b)a \rangle \approx \langle b^\dagger + b \rangle \langle a \rangle \). Under this approximation, the operator equations can be replaced by those for the corresponding mean values, leading to the semiclassical Langevin equations. The deterministic dynamics of the system can be assessed by neglecting the small fluctuations in the photon and phonon fields. The resulting deterministic equations are:

\[
\begin{align*}
\frac{d\langle a \rangle}{dt} &= i(\Delta_0 \langle a \rangle + g_0 \langle a \rangle \langle b^\dagger + b \rangle - \alpha_L) - \frac{1}{2} \kappa \langle a \rangle \\
\frac{d\langle b \rangle}{dt} &= -i(g_0 |\langle a \rangle|^2 + \omega_m \langle b \rangle) - \frac{\Gamma_m}{2} \langle b \rangle,
\end{align*}
\]

where \( \Gamma_m \) is the dissipation rate. A property of the classical equations is that, if \( b \) and \( a \) are replaced by \( g_0 b \) and \( a/\alpha_L \), respectively, the resulting equations contain the parameter \( P \propto g_0^2 \alpha_L^2 \), where \( g_0 \) and \( \alpha_L \) no longer appear as individual parameters. If other parameters are kept constant, the dynamics of the classical system is solely determined by the power of the driving laser field, i.e., \( P \), with \( g_0 \) and \( \alpha_L \) as scaling factors. Intuitively, this can be understood by noting that, when a quantum system approaches its classical limit, \( \hbar \) vanishes so that the quantum strength factors \( g_0 \propto \sqrt{\hbar} \) and \( \alpha_L \propto 1/\sqrt{\hbar} \) (both containing \( \hbar \)) are degenerate into a single parameter \( P \) that does not contain \( \hbar \). However, in the stochastic Langevin equations, the strengths of the quantum fluctuations associated with the photon and phonon fields are proportional to \( g_0 \) and \( 1/\alpha_L \), respectively. In the moderate and deep quantum regimes away from the classical limit, as \( g_0 \) is increased, the deterministic Langevin equations are less meaningful due to the more pronounced quantum fluctuations.
The classical equations are nonlinear, so chaos can arise, as uncovered in previous experimental [141, 179] and theoretical [180, 204, 205] works. To demonstrate the chaotic behavior, we use the same parameter setting as in the recent work of Bakemeier et al. [180]: $\kappa/\omega_m = 1.0$, $\Gamma_m/\omega_m = 10^{-3}$, $\Delta_0/\omega_m = -0.7$, and $\tilde{P} = 8\alpha_f^2 g_{0}^2/\omega_m^4 = 1.5$. Figure 19(a) shows a representative chaotic orbit in the two-dimensional subspace of the variables $q = (g_0/\sqrt{2}\omega_m)(\hat{b} + b)$ and $p = (-ig_0/\sqrt{2}\omega_m)(\hat{b} - b)$, where the evolution time $\tau$ is made dimensionless through $\tau \equiv \omega_m t$.

The corresponding chaotic time series is shown in Fig. 19(b-c).

4.2.3. Calculation of Quantum Trajectories.

The quantum evolution of the optomechanical system can be calculated by using the quantum Master equation, which incorporates the effects of photon and phonon dissipation through the Lindblad operators. In particular, at zero temperature the quantum Master equation is [144, 164]

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H, \rho] + \Gamma_m \mathcal{D}[b, \rho] + \kappa \mathcal{D}[a, \rho]$$

(4.3)

where the Lindblad operator is given by

$$\mathcal{D}[L, \rho] = L\rho L^\dagger - (L^\dagger L\rho + \rho L^\dagger L)/2,$$

(4.4)

and $L$ stands for either $a$ or $b$. The quantum Master equation describes the time evolution of an ensemble of identical quantum systems. The dimension of the optomechanical system is $(N_a N_b)^2$, where $N_a$ and $N_b$ denote the highest photon and phonon Fock states, respectively. An approach to reducing the dimension to $(N_a N_b)$ is to “unravel” the deterministic quantum Master equation through the stochastic wavefunction equation for quantum trajectories [197–199, 206]. The deterministic property is retained through the ensemble average of many realizations of the system starting from the same initial condition. Among the many unraveling schemes for generating quantum trajectories, the QSD approach is convenient and efficient with results that can be related to the
record of homodyne detection, an important measurement tool in optomechanics [183]. The QSD equation is given by [207, 208]

\[
|d\psi\rangle = -(i/\hbar)H|\psi\rangle dt + \sqrt{\kappa}(a - \langle a \rangle)|\psi\rangle \circ (d\xi_1 + \sqrt{\kappa}\langle a^\dagger \rangle dt) - (1/2)\kappa(a^\dagger a - \langle a^\dagger a \rangle)|\psi\rangle dt \\
+ \sqrt{\Gamma_M}(b - \langle b \rangle)|\psi\rangle \circ (d\xi_2 + \sqrt{\Gamma_M}\langle b^\dagger \rangle dt) - (1/2)\Gamma_M(b^\dagger b - \langle b^\dagger b \rangle)|\psi\rangle dt,
\]

(4.5)

where \( \langle O \rangle = \langle \psi | O | \psi \rangle \) is the expectation value of operator \( O \) for the specific wave function \( |\psi\rangle \).

The QSD equation (4.5) is in fact a Stratonovich type of stochastic equations. (The Ito form of QSD has also been established and widely used [197–200, 209].) In the QSD equation, the terms \( d\xi_j \) \((j = 1, 2)\) are complex Gaussian white noise for the photon and phonon fluctuations, which satisfy

\[
Md\xi_j = Md\xi_i d\xi_j = 0 \quad \text{and} \quad Md\xi_i^* d\xi_j = \delta_{ij} dt,
\]

where \( M \) stands for the ensemble average. The density operator can be reconstructed through the mean over the projectors of the ensemble quantum states

\[
\hat{\rho} = M|\psi\rangle \langle \psi|.
\]

(4.6)

In an optomechanical system, the quantum effects can be characterized by the parameters \( g_0 \propto \sqrt{\hbar} \) and \( \alpha_L \propto 1/\sqrt{\hbar} \). Figure 20(a) shows, for \( g_0/\omega_m = 0.1 \), a typical quantum trajectory calculated from the QSD equation in the \((q, p)\) plane. This is a periodic, limit-cycle trajectory, despite being noisy due to the quantum fluctuations. The corresponding time series \( q(2\pi \tau) \) is shown in Fig. 20(c).

Since the value of the laser power \( P \) is fixed, the corresponding classical behavior is that shown in Fig. 19, which is chaotic. The remarkable phenomenon is that, the quantum trajectory in Fig. 20(a) is characteristically different from the classical trajectory in Fig. 19(a): the former is regular while the latter is chaotic! This is the recently discovered phenomenon of quantum-classical correspondence breakdown in optomechanical systems [180].
4.2.4. Transient Chaos in the Quantum Regime.

We find that the breakdown can be naturally viewed as a manifestation of transient chaos. We note from Fig. 20(c) that, before the periodic quantum state is reached, there is a relatively short time interval during which the quantum evolution is characteristically different, which is a transient phase. The quantum trajectory of the system in the transient phase is shown in Fig. 20(b), which appears chaotic. The striking finding is that, the transient quantum trajectory is remarkably consistent (in fact coincides) with the corresponding classical trajectory (the red background trajectory in Fig. 20(b), which overlaps with the quantum trajectory almost completely). As we tune the parameter $g_0/\omega_m$ towards the classical regime, the duration of the transient phase increases. The extreme situation is that the transient time becomes so long that the system stays in a chaotic state for any practical time. An example is shown in Fig. 20(d) for $g_0/\omega_m = 0.05$.

How does the average chaotic transient lifetime $\langle T \rangle$ depend on the quantum strength parameter $g_0$? Here the chaotic transient lifetime is defined as the length of the time for each trajectory stays near the classical chaotic orbit, and the average is all for realizations. As shown in Fig. 21, as $g_0$ is decreased so that the quantum effect becomes progressively weaker, $\langle T \rangle$ increases dramatically. A qualitative explanation for Fig. 21 is the following. The classical trajectories are calculated from the deterministic, semiclassical Langevin equation in the Heisenberg picture with dissipation, where quantum fluctuations are neglected. The quantum trajectories are obtained from the QSD method, an unraveling of the general quantum Master equation in the Schrödinger picture using the Lindblad operators. The quantum fluctuations in QSD not only play the role of noise in the classical deterministic system, but more importantly, they can induce characteristic changes in the system dynamics. Say we fix the laser power so that the classical dynamics remains chaotic. What will happen when the quantum effects (fluctuations) become increasingly pronounced? Mathematically,
as $g_0$ is increased, it is necessary to decrease $\alpha_L$ to keep the driving laser power constant. This effectively enhances the ratios $\sqrt{\kappa}/\alpha_L$ and $\sqrt{\Gamma_m}/\alpha_L$ in the QSD equation, which are the relative noise-to-driving ratios. As noise becomes more pronounced, the probability that the system can stay in the deterministic chaotic set is decreased, reducing the chaotic transient lifetime.

To further test the proposition that noise or quantum fluctuations can drive the quantum system away from the classical chaotic invariant set, we calculate the quantum trajectories but with the noise term excluded. We find that, without random fluctuations, the quantum trajectories follow the classical chaotic set all the time. This result confirms that it is the quantum fluctuations which eventually drive the quantum trajectories out of the classical chaotic set, generating transient chaos. The weaker the quantum fluctuations, the longer the average transient lifetime will be. The quantum-classical transition is thus induced by quantum fluctuations, which resembles the phenomenon of noise-induced transition in classical systems that can be treated using the classical Kramer rate theory [210]. The transient chaos associated with quantum-classical transition is also relevant to the quantum activation process [211], a transition process induced by noise between coexisting asymptotic states in a quantum system. Also we notice that our idea is tightly connected with the work of G. G. Carlo [212], which reported that the quantum isoperiodic stable structures can be retained by the information from the classical isoperiodic stable structures plus disturb of noise.

4.2.5. Scaling of Transient Lifetime and Physical Understanding.

The Kramer theory or the quantum activation theory stipulates that the escape rate $\kappa$ generally follows the scaling as

$$\kappa = \nu \exp(-E_b/E_{\text{noise}}),$$

where $E_b$ denotes the threshold energy for activation, $\nu$ is a prefactor, and $E_{\text{noise}}$ is the strength of the fluctuation, e.g., on the order of $k_B\tilde{T}$ due to the thermal environment or $h\omega$ in the deep
quantum regime, where $\tilde{T}$ represents temperature. At low temperatures, the quantum fluctuations are dominated by the zero-point energy.

Figure 21 shows the relation between the average chaotic transient lifetime $\langle T \rangle$ and the magnitude $g_0$ of the quantum fluctuations on a double logarithmic scale. The relation can be well fitted by a straight line, as shown in the inset of Fig. 21, which indicates the scaling law:

$$\ln \langle T \rangle \sim \left( \frac{g_0}{\kappa} \right)^{-s},$$

where $-s$ ($s > 0$) is the slope of the linear fit. The scaling law is characteristic of superpersistent chaotic transients in nonlinear dynamical systems [213–217]. The physical meaning is that, as the quantum fluctuations are reduced so that the classical description becomes more accurate, the chaotic behavior becomes significantly more persistent in that its lifetime increases faster than the Ehrenfest time.

To better understand the scaling behavior of the average transient lifetime, we exploit the quantum Langevin equations:

$$\frac{dq}{d\tau} = p,$$

$$\frac{dp}{d\tau} = \left( \frac{\sqrt{2}}{8} \right) \tilde{P} |\alpha|^2 - q - \Gamma_M p + g_0 \xi,$$

$$\frac{d\alpha}{d\tau} = i(\Delta_0 \alpha + \sqrt{2} \alpha q - 1) - \kappa \alpha / 2 + \left( \sqrt{\kappa / 2} / \alpha_L \right) \alpha_{in}.$$  

In general, a Langevin equation can be analyzed using the corresponding Fokker-Planck equation, where the stochastic component of the former contributes to the diffusion term in the evolution of the probability distribution of the latter. For the Fokker-Planck equation, a general solution cannot be written down explicitly except for one-dimensional systems. In this case, the steady state distribution has the form $W_s(x) = \mathcal{N} \exp [-U(x)/D]$, where $U(x)$ is the effective potential, $D$ is the noise amplitude proportional to $g_0^2$, and $\mathcal{N}$ is a normalization constant. The mean first passage time over a barrier, i.e., the diffusion time from a local minimum $U(a)$ over a saddle point $U(b)$,
obeys the following scaling law [218] with \( D \): 
\[ T_{\text{MFP}} \propto e^{[U(b)-U(a)]/D} \]. However, to predict the exact form of the scaling law from the general multivariable Fokker-Plack equation is difficult. An alternative is to calculate the average chaotic transition lifetime (or the mean first passage time) from the Langevin equations. The results are shown in Fig. 22. Due to the relative simplicity of the Langevin equation as compared with the QSD equation, it is possible to probe more deeply into the classical regime with much longer transition lifetime. We find that, in the \( g_0 \) regime where both types of results are available, the agreement is excellent. In particular, solutions of the Langevin equation gives

\[
\ln \ln \langle T \rangle / \ln g_0 \approx -1.
\]

In Fig. 22(a), we show the fitting curve of the Ehrenfest scaling (red dash) as well as the superpersistent chaotic transition behavior (magenta dash-dot). For the Ehrenfest scaling, we use the least-squares method to fit \( \langle T \rangle = C_0 \cdot g^{-\delta} \) on a double logarithmic scale. For the superpersistent scaling, it is not straightforward to fit the relation \( \langle T \rangle = C_1 \cdot e^{C_2/g^s} \). We thus set \( C_1 = 1 \) and fit the simulation results in terms of \( \log \log (\langle T \rangle) \) versus \( \log g_0 \). We see that the magenta curve fits better than the red curve, especially in the middle region. For small values of \( g_0/\omega_0 \), the Ehrenfest scaling exhibits larger deviations from the simulation results as compared with the superpersistent transient scaling.

For the QSD results (Fig. 21), we estimate the slope of the fitting line of \( \ln \ln (\langle T \rangle) \) with \( \ln g_0 \) and obtain the absolute value of about 0.7, which is smaller than the result from the Langevin equation. There can be multiple reasons for the difference. For example, for a large value of \( g_0/\omega_0 \), the trajectories tend to approach the periodic attractor from the beginning. However, the transition process takes time, so the state at an arbitrary instant of time during the transition is actually recorded. When the transition time is comparable with the transient time, error can occur.
Considering that our system is higher than one dimensional and the simulations were done with the full quantum state diffusion equation, the difference in the slope may not be unreasonable. In particular, in high dimensions the slope should have a smaller absolute value because of the existence of more “paths” to cross the saddle point (there is only one route in one dimension), facilitating the transition.

A natural question is whether the reverse process, i.e., transition from the periodic orbit to the chaotic orbit, can happen. In nonlinear dynamics, periodic attractors are usually more stable than chaotic attractors. Heuristically, a system in which a periodic and a chaotic attractors coexist can be viewed as particle motion in a mechanical system with two asymmetric potential wells subject to unbounded (e.g., Gaussian) noise, where the periodic attractor corresponds to the deep well and the chaotic attractor is associated with the shallow well, as schematically shown in Fig. 23(a). The probability for the particle to “hop” into the shallow well from the deep well is considerably smaller than that in the opposite direction. In optomechanical systems, this kind of backward transition can occur but it is rare. One such case is shown in Figs. 23(b) and 23(c), where the transition occurs at $g_0/\omega_0 = 0.056$. For smaller values of $g_0$, it is highly unlikely that the trajectory can switch into the periodic attractor. Even if this occurs, the probability for the trajectory to escape the periodic attractor will be exponentially small due to the higher potential barrier. For large values of $g_0$, transition in both directions can occur, as shown in Fig. 23(c). We notice that there are some recent works observing the emergence of quantum chaos in a regular classical limit system as well as control of this emergence through different measurement technicals [219,220]. Here we restrict our system to be of chaotic classical limit and only consider QSD. And we expect our understanding, i.e., the transition process between different attractors, might prove some helps insights about the emergency of quantum chaos in regular classical limit system.
Our reasoning based on separating the deterministic and stochastic components of the Langevin equation does not depend on the specific details of the system, suggesting that the fast growing behavior in the average transient lifetime and the associated scaling law are \textit{generic}.

4.3. Discussion

To summarize, we investigate the fundamental problem of quantum-classical correspondence in optomechanical systems from the perspective of dynamical evolution. When the classical system exhibits chaos, the evolution of the quantum system contains two phases: chaotic motion in the (relatively) short time scale and regular motion in the long time scale. The transient chaotic behavior of the quantum system corresponds precisely to that in the classical limit - in this sense there is a well-defined quantum-classical correspondence. The long term behavior of the quantum system, however, is characteristically different from the classical behavior - in this sense there is a breakdown [180] of the quantum-classical correspondence. As the classical regime is approached, the chaotic transient lifetime increases dramatically (faster than the Ehrenfest time for isolated systems - see below). Our finding of transient chaos in optomechanical systems, besides being a remarkable phenomenon by itself, provides a natural resolution for the paradoxical breakdown of quantum-classical correspondence. Here we would like to emphasis that our notations of “classical limits” and “quantum regime” are used in a relatively way. The real classical limit results should be obtained when $g_0 \to 0$, and the most classical case we simulated is $g_0/\kappa = 0.045$, which we think is good enough to proof our statement. This means that our system does not loss its quantum properties and does not chanllenge the results of previous works that chaos can emergence in the quantum regime [200–202, 221, 222].

In general, the problem of quantum-classical correspondence can be addressed through the approach of quantum-classical transition (QCT). It is known that, unlike special relativity where Ein-
stein’s theory can be smoothly transformed to Newtonian mechanics in the limit \( v/c \to 0 \), the approach of a quantum system to the classical limit \( \hbar \to 0 \) is singular. In the classical world, chaos exists in both dissipative and Hamiltonian systems, and chaotic dynamics are often studied in the phase space. However, to our knowledge, attempts to find chaos in the Schrödinger equation or in the quantum Liouville equation have not been convincingly successful. One reason is that isolated quantum systems are fundamentally linear. Another reason is that, the uncertainty principle forbids arbitrarily fine scale structures in the phase space. Indeed, in bounded and isolated (or closed) quantum systems the most complicated dynamics are quasiperiodic. Even though the transient behavior of a quantum system can be similar to that in the corresponding classical system, any classical features will be lost after a time scale called the Ehrenfest time: \( t_E \propto \hbar^{-\delta} \), where \( \delta \) is determined by the details of the system. Strictly, the Ehrenfest time holds for the idealized situation where the underlying system is fully closed. With the development of the quantum theory and advances in experimental techniques, the quantum dynamics of other types of situations have been considered, such as unconditioned open and conditioned open systems [223,224]. In the former case, the system is coupled to the environment but no information about the system is extracted, while for the latter information about the state of the system is extracted from it. For an unconditioned open system, the dynamical evolution is governed by the quantum Master equation, which is still linear. However, for a conditioned open system, its dynamical evolution follows a stochastic quantum equation that contains a nonlinear term representing the conditioning due to the measurement.

In the study of QCT, there are two general approaches to addressing the quantum-classical correspondence. The first is to focus on the agreement between the distribution functions, i.e., the quantum Wigner and the classical distribution functions - the weak form of QCT [181, 182]. The second approach, the strong form of the QCT [221,224], is to examine the localization of the
quantum trajectory on the classical orbits, in which chaos can emerge naturally. To assess the degree of localization, continuous measurements of the system are required, introducing a nonlinear term in the quantum equation, so this approach is applicable only to conditioned open systems.

Table 1 presents an overview of the status of the knowledge about QCT, with knowns and unknowns specified. An outstanding issue concerns the scaling of the transition time in the strong QCT regime. In particular, the question is whether the QCT time follows the same scaling law as the Ehrenfest time. We address this issue in this paper by exploiting optomechanical systems subject to continuous heterodyne detection, which fundamentally exhibits a strong form of QCT. Qualitatively, our main finding is that transient chaos effectively serves as a bridge for the QCT. Quantitatively, we uncover a scaling law for the transition time which is different from that for the Ehrenfest time associated with the conventional QCT for isolated systems. With the advances in experimental techniques, there is now ability to observe quantum trajectories [180, 184]. We expect the main results of this paper to be experimentally testable.

We make a few further remarks pertinent to our results.

4.3.1. Remark 1: Transient Chaos in Quantum Systems - What Does It Mean?

A quantum system is fundamentally linear. How can then a quantum trajectory be chaotic, even transiently? This paradox can be resolved, as follows. The Schrödinger (quantum Master) equation describes the time evolution of an individual system in an ensemble of identical systems, from which the mean value of any physical quantity, \( \langle \psi | \hat{O} | \phi \rangle \) \[ \text{Tr}(\hat{O} \rho) \] for an operator \( \hat{O} \), can be obtained. This is an ideal evolution process during which no further disturbance or measurement should be made; for otherwise the wavefunction will collapse into an eigenstate determined by the whole system, including the measurement apparatus. Based on the quantum trajectory theory, the time evolution of the mean value can also be produced from the QSD calculations through the
ensemble average. When there is chaos in the classical limit, the ensemble averaging process can make the time evolution of the mean value periodic. That is, even when QSD calculation gives that a single quantum trajectory is chaotic in the transient phase, the ensemble average of many such trajectories can still be regular.

4.3.2. Remark 2: Effect of Measurement.

A single quantum trajectory, however, is not physically meaningless. For a dissipative quantum system, the Master equation can yield the best prediction about the dynamical evolution of an ensemble of the system in absence of any measurement. The single trajectory calculated from quantum methods, such as QSD and quantum jump theory, has the physical meaning of conditioned realization of an individual system under a particular observation record, through homodyne/heterodyne detection and photodetector [225,226]. This makes the quantum trajectories subjectively real [226]. In the continuously conditioned measurement theory, any measurement introduces a factor called the detector efficiency, $0 \leq \eta \leq 1$, into the QSD simulation [227–230], which models the situation where the beam-splitter transmittivity is less than unity [227]. Mathematically, this factor can be taken into account by decomposing the photon fluctuation term into two uncorrelated terms of strength $\sqrt{\eta}$ and $\sqrt{1-\eta}$, respectively [227, 230]. In the limit $\eta \rightarrow 1$, this form of stochastic equation is reduced to the equation simulated in our work, which corresponds to perfect detection.

4.3.3. Remark 3: Effect of Temperature.

Our treatment of the breakdown of quantum-classical correspondence in optomechanical systems as a problem of strong QCT assumes the low temperature limit. As we argue and demonstrate, the transition from chaos to a regular state is mediated by quantum fluctuations or noise. Naturally we expect that thermal noise would play a similar role. In particular, if we focus on the classical
system subject to thermal noise, a transition from a chaotic attractor to a periodic one can occur, accompanied by transient chaos.

In an optomechanical system, the fundamental physical constant $\hbar$ cannot be changed in experiments. The degree of quantum fluctuations can be controlled by adjusting or engineering other parameters, e.g., the mass of the cantilever, while keeping the system at low temperature. Weaker quantum fluctuations corresponding to smaller values of $g_0$ can be realized using a heavier cantilever. In this case, the quantum system would behave chaotically for a relatively long time, due to the exponentially long transient lifetime. We note that, in the high temperature regime, the strength of the quantum fluctuations scales as $\sim g_0^2(2\bar{n} + 1)$, where $\bar{n} \sim k_B T / \hbar \omega_m$. This indicates a counterbalancing effect between temperature $T$ and mass $m$ as $\sim T/m$. Consequently, at high temperatures a system of relatively large mass can still behave chaotically for a long time.

4.4. Methods

Historically, the method of quantum trajectory represented an efficient way to solve the master equation, and certain types of quantum trajectories can correspond to the result of conditioned measurement [184–195]. Mathematically, an ensemble of quantum systems whose state vectors are governed by a stochastic differential equation can have a density operator that satisfies a unique deterministic master equation. In contrast, a specific master equation can correspond to many different stochastic equations or different unravellings such as the QSD equation, the quantum jump equation, or the orthogonal jump equation [231]. While all the unravellings can be used to simulate the master equation, they have a different physical meaning. The most commonly calculated quantum trajectories are those from the QSD equation and the quantum jump equation, corresponding to homodyne and photon counting detection, respectively.
For a general Lindblad form of the master equation:

$$\frac{d}{dt}\hat{\rho} = -\frac{i}{\hbar}[\hat{H}, \hat{\rho}] + \sum_j (\hat{L}_j \hat{\rho} \hat{L}_j^\dagger - \frac{1}{2} \hat{L}_j^\dagger \hat{L}_j \hat{\rho} - \frac{1}{2} \hat{L}_j \hat{L}_j^\dagger \hat{\rho}),$$

the QSD equation is [206, 231]:

$$|\psi\rangle = -\frac{i}{\hbar} \hat{H} |\psi\rangle dt + \sum_j (\langle \hat{L}_j^\dagger \rangle \psi \hat{L}_j - \frac{1}{2} \hat{L}_j^\dagger \hat{L}_j \langle \psi \rangle) dt + \sum_j (\hat{L}_j - \langle \hat{L}_j \rangle \psi) d\xi_j, \quad (4.9)$$

and the quantum jump equation is:

$$|\psi\rangle = -\frac{i}{\hbar} \hat{H} |\psi\rangle dt + \sum_j (\frac{1}{2} \langle \hat{L}_j^\dagger \hat{L}_j \rangle \psi) dt + \sum_j (\frac{\hat{L}_j}{\sqrt{\langle \hat{L}_j^\dagger \hat{L}_j \rangle}} - 1) |\psi\rangle dN_j. \quad (4.10)$$

The QSD equation Eq. (4.9) is in the Ito form, which historically was called the nonlinear stochastic Langevin-Ito equation. Generally, for the Langevin equations of $N$ variables of the form

$$\dot{q}_i = h_i(q, t) + g_{ij}(q, t)\xi_j(t),$$

where $\{q\} = q_1, q_2, \ldots, q_N$ and $\langle \xi_i(t) \rangle = 0, \langle \xi_i(t) \xi_j(t') \rangle = 2\delta_{ij}\delta(t - t')$, the corresponding probability density function $W(x, t)$ satisfies the Fokker-Planck equation [232]

$$\frac{\partial W(x, t)}{\partial t} = (-\frac{\partial}{\partial x_i} D_i(x, t) + \frac{\partial^2}{\partial x_i \partial x_j} D_{ij}(x, t))W,$$

where the drift and diffusion coefficients are defined as

$$D_i(x, t) \equiv D_{i}^{(1)}(x, t) = \lim_{\tau \to 0} \frac{1}{\tau} \langle q_i(t + \tau) - x_i \rangle_{q_k(t) = x_k} = h_i(x, t) + g_{ik}(x, t) \frac{\partial}{\partial x_k} g_{ij}(x, t),$$

$$D_{ij}(x, t) \equiv D_{ij}^{(2)}(x, t) = \frac{1}{2} \lim_{\tau \to 0} \frac{1}{\tau} \langle [q_i(t + \tau) - x_i][q_j(t + \tau) - x_j] \rangle_{q_k(t) = x_k} = g_{ik}(x, t) g_{jk}(x, t).$$

Note that $q_i(t + \tau) (\tau > 0)$ is a solution of the Langevin equation, which has the sharp value $q_k(t) = x_k (k = 1, 2, \ldots, N)$ at time $t$. The quantity $D_{i}^{(n)}(x, t) \equiv \lim_{\tau \to 0} \frac{1}{\tau} \langle [q(t + \tau) - x]^n \rangle_{q_k(t) = x_k}$ is the Kramers-Moyal expansion coefficients. For a process described by the Langevin equation with $\delta$-correlated Gaussian noise, all the Kramers-Moyal coefficients $D^{(n)}$ with $n \geq 3$ vanish [232]. The physical significance is that the deterministic component of the Langevin equations contributes to
the drift part in the evolution of the probability distribution while the stochastic component contributes to both the drift and diffusion evolution of the probability distribution.

In general, QSD represents a conditioned measurement experiment and the wave functions that it generates are normally localized about a point in the phase space. This fact can be exploited to improve the computational efficiency [233]. Say a wave function is localized about the point \((q, p)\). We can represent it using the so-called excited coherent basis states, \(|q, p, n⟩ = D(q, p)|n⟩\), instead of a large number of Fock states. Physically, this means that we exploit a moving basis that separates the wavefunction representation into a classical part \((q, p)\) and a quantum part \(|q, p, n⟩\), which is effectively a mixed representation. The excited coherent states are defined through the coherent state displacement operator:

\[
D(q, p) = \exp \frac{i}{\hbar}(p\hat{Q} - q\hat{P}).
\]

where \(\hat{Q}\) and \(\hat{P}\) are the position and momentum operators. The displacement operator can be defined using the creation/annihilation operator as

\[
D(\alpha) = e^{\alpha^*\hat{a} - \alpha\hat{a}^*},
\]

and the matrix element in Fock state is

\[
⟨m|D(\alpha)|n⟩ = e^{\frac{1}{2}|\alpha|^2} \sqrt{\frac{m!}{n!}} (-\alpha^*)^{n-m} L_{m}^{n-m}(|\alpha|^2),
\]

where \(L_{m}^{n-m}(|\alpha|^2)\) is the associate Laguerre polynomials.

Suppose at \(t = t_0\) the state of the system is localized about \((q_0, p_0)\), i.e.,

\[
(q_0, p_0) = (⟨\psi(t_0)|\hat{Q}|\psi(t_0)⟩, ⟨\psi(t_0)|\hat{P}|\psi(t_0)⟩).
\]

After one time step, we have

\[
(q_1, p_1) = (⟨\psi(t_0 + \delta t)|\hat{Q}|\psi(t_0 + \delta t)⟩, ⟨\psi(t_0 + \delta t)|\hat{P}|\psi(t_0 + \delta t)⟩) \neq (q_0, p_0).
\]
We then shift the basis from \((q_0, p_0)\) to \((q_1, p_1)\), which can be done through

\[
|\psi(t_0 + \delta t)\rangle = D(-\delta q, -\delta p)|\psi(t_0)\rangle.
\]

Besides the wavefunction, we need to transform the operators into the new basis as well. The procedure is straightforward due to certain properties of the displacement operator:

\[
D^{\dagger}(\alpha)\hat{a}D(\alpha) = \hat{a} + \alpha
\]

\[
D^{\dagger}(\alpha)\hat{a}^{\dagger}D(\alpha) = \hat{a}^{\dagger} + \alpha^*\]

which changes the transformation of the Hamiltonian and the operators from two matrix multiplications to one matrix addition. In spite of the need to perform base transformation at each time step, the overall computational speed is faster than that with the Fock state calculation.
Fig. 18. A schematic figure of the optomechanical system.

Fig. 19. From the deterministic classical equation, (a) a representative chaotic trajectory and (b,c) the corresponding time series for $q$ and $p$. The dashed circle in (a) indicates a coexisting periodic attractor.
Fig. 20. For $g_0/\omega_m = 0.1$, (a) an asymptotic quantum trajectory calculated from the QSD method, (b) the quantum trajectory in the transient phase, overlapped with the corresponding classical trajectory, (c) the corresponding time series. The asymptotic quantum trajectory is regular, in spite of the quantum fluctuations. However, the transient quantum trajectory is chaotic and coincides well with the classical trajectory (gray). (d) An example of a very long chaotic transient in the quantum regime for $g_0/\omega_m = 0.05$. 

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Fig. 21. QSD Results: Dependence of average chaotic transient lifetime, $\langle T \rangle$, on $g_0$ on a linear-linear plot and on a double logarithmic versus logarithmic scale (inset). All points are result of averaging 100 QSD realizations.

Fig. 22. Results from classical Langevin equation: (a) Dependence of the average chaotic transient lifetime, $\langle T \rangle$, on $g_0$ on a linear-linear plot. Inset: the same plot but on a double logarithmic versus logarithmic scale. The magenta dash-dot curve is a fit of the superpersistent chaotic transients behavior while the red dash curve is a fit of the Ehrenfest scaling. In the inset the red straight curve shows the slope of the supperpersistent chaotic transients behavior is about $-s_c \approx -0.96$. All points are result of averaging 10000 Langevin equation realizations.
Fig. 23. (a) A mechanical picture illustrating the noise-induced transition between chaotic and periodic attractors, where the periodic attractor is more stable than the chaotic attractor. For $g_0/\omega_m = 0.056$, representation in the $q-p$ space (b), where the red stars represent the transition process from the inner chaotic attractor to the outer periodic attractor while the magenta circles represent the transition in the opposite direction. (c) The corresponding time series, where the blue and red colors are for $q$ and $p$, respectively.

### TABLE 1

An overview of distinct QCT regimes.

<table>
<thead>
<tr>
<th></th>
<th>Conventional QCT</th>
<th>Weak QCT</th>
<th>Strong QCT</th>
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<tbody>
<tr>
<td>System</td>
<td>Isolated</td>
<td>Unconditioned Open</td>
<td>Conditioned Open</td>
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<tr>
<td>Equation</td>
<td>Schrödinger</td>
<td>Master</td>
<td>Quantum Trajectory</td>
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<tr>
<td>Dynamics</td>
<td>Linear</td>
<td>Linear</td>
<td>Stochastic Nonlinear</td>
</tr>
<tr>
<td>Characteristic Time</td>
<td>Ehrenfest time $\sim \hbar^{-s}$</td>
<td>Unknown at present</td>
<td>$Eq. (4.7)$ discovered in this paper</td>
</tr>
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</table>

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Zitterbewegung (ZB) is a phenomenon in relativistic quantum systems where the electron wave packet exhibits a trembling or oscillating behavior during its motion, caused by its interaction or coupling with the negative energy state. To directly observe ZB in electronic systems is difficult, due to the challenges associated with the atomic scale wavelength of the electron. Photonic systems offer an alternative paradigm. We exploit the concept of pseudo parity-time (pseudo PT) symmetry to study ZB in non-Hermitian quantum systems implemented as an experimentally feasible optical waveguide array. In particular, the non-Hermitian Hamiltonian is realized through evanescent coupling among the waveguides to form a one-dimensional lattice with periodic modulations in gain and loss along the guiding direction. As the modulation frequency is changed, we obtain a number of phenomena including periodically suppressed ZB trembling, spatial energy localization, and Hermitian-like ZB oscillations. We calculate phase diagrams indicating the emergence of different types of dynamical behaviors of the relativistic non-Hermitian quantum system in an experimentally justified parameter space. We provide numerical results and a physical analysis to explain the distinct dynamical behaviors revealed by the phase diagrams. Our findings provide a deeper understanding of both the relativistic ZB phenomenon and non-Hermitian pseudo-PT systems, with potential applications in controlling/harnessing light propagation in waveguide-based optical systems.

5.1. Introduction

There has been a great deal of recent interest in investigating the role of parity-time reversal (PT) symmetry in wave propagation at different scales with the discoveries of phenomena such as non-reciprocal beam propagation [234–238], and uni-directionally transparent invisibil-
ity [239–241]. The phenomenon of topologically protected states [242, 243] was originally discovered in condensed matter physics associated with electronic transport, but recently it has been demonstrated in optics [244–250], due naturally to the correspondence between matter and optical waves. For example, topological photonics/acoustics were demonstrated by exploiting the analogy between electronic and synthetic photonic crystals, where tunable and topologically protected excitations were observed [251,252]. There were also efforts in exploring new wave features in artificial photonic crystals with/without the $\mathcal{PT}$-symmetry [253–260]. All these have led to the emergence of a forefront area of research in optics: light propagation in non-Hermitian $\mathcal{PT}$-symmetric media with balanced loss and gain profiles. The new field offers the possibility to engineer light propagation, potentially revolutionizing optics with unconventional applications.

In conventional quantum mechanics, the observable operators are required to be Hermitian to ensure real eigenvalues. This requirement is the result of one of the fundamental postulates in quantum mechanics: the physically observable or measurable quantities are the eigenvalues of the corresponding operators. However, the seminal works of Bender et al. [261–263] demonstrated that non-Hermitian Hamiltonians are also capable of generating a purely real eigenvalue spectrum and therefore are physically meaningful, if the underlying system possesses a $\mathcal{PT}$ symmetry. This opened a new research field called non-Hermitian $\mathcal{PT}$ symmetric quantum mechanics. In fact, in physical systems, non-Hermitian Hamiltonians exist in contexts such as electronic transport (in open Hamiltonian systems) and gain/loss materials in optics [264]. Especially, in optics, materials with a complex index of refraction can effectively be a non-Hermitian $\mathcal{PT}$ symmetric system [265]. However, in such a case, the $\mathcal{PT}$ symmetry constrictions require that the real and the imaginary parts of the refractive index be an even and odd function in space, respectively [266–268], which may be challenging to be fabricated for experimental study. An alternative configuration that does
not require even/odd spatial functions is the pseudo-$\mathcal{PT}$ symmetric system with periodic modulations [269]. While such a system does not conserve the energy at any given instant of time because of gain/loss, the energy does not diverge within any practically long time.

An outstanding problem is how relativistic quantum effects manifest themselves in non-Hermitian photonic systems with full or pseudo $\mathcal{PT}$ symmetry. This is motivated by the tremendous development of 2D Dirac materials in the past decade such as graphene [23, 67–72], topological insulators [242, 243], molybdenum disulfide (MoS$_2$) [270, 271], HITEP [Ni$_3$(HITP)$_2$] [272], and topological Dirac semimetals [273, 274], where the underlying quantum physics is governed by the relativistic Dirac equation. It is thus of interest to investigate experimentally more realizable optical systems hosting relativistic excitations and to study the manifestations of the fundamental phenomena [275] such as the Klein tunneling, Zitterbewegung (ZB), and pseudo spin to exploit their topological origin. In this regard, including gain/loss in synthetic optical systems can generate non-Hermitian relativistic $\mathcal{PT}$-symmetric excitations through engineering the gain and loss in a balanced manner. For example, arranging $\mathcal{PT}$-symmetric couplers periodically provides a unique platform to realize the analogy of the non-Hermitian relativistic quantum systems in optics [276–279].

In this paper, we focus on a fundamental phenomenon in relativistic quantum mechanics - ZB oscillations. While the optical analog of the relativistic ZB effect in Hermitian quantum systems was previously observed [280], we investigate the manifestations of ZB in non-Hermitian photonic systems. In particular, we consider a binary waveguide array with periodically modulated imaginary refraction index in the guiding direction, which is experimentally realizable. The optical waveguide array system, due to its controllable degrees of freedom, has been a paradigm to study a host of fundamental physical phenomena [281] such as the neutrino oscillations [282], Bloch oscillation [283], Zener tunneling [284, 285], and Klein tunneling [286]. We configure the system to have
a pseudo-$\mathcal{PT}$ symmetry, so that it exhibits quasi-stationary light propagation with slowly varying time-averaged total intensity [269]. By calculating a detailed phase diagram in an experimentally meaningful parameter space, we uncover a number of phenomena in the system. In particular, we find that, in certain parameter regime, the wave amplitude tends to diverge. A remarkable phenomenon is that there are parameter regimes in which the dependence of ZB oscillations on the modulation frequency is non-monotonic, where the system exhibits a striking, periodically suppressed ZB effect with revival or intermittent ZB oscillations for low frequencies and a Hermitian-like ZB effect in the high frequency regime. In the intermediate frequency regime, a surprising spatial energy localization behavior emerges. By solving the corresponding time-dependent Dirac equation, we obtain analytic results that provide explanations for the numerically observed, ZB manifested phenomena. The findings have implications. For example, the wave divergence phenomenon may be exploited for applications in optical amplifier and lasing. Intermittent BZ oscillations can potentially lead to a new mechanism to manipulate/control light propagation.

Before describing our results in detail, we remark on the two unique aspects of our work. First, what results can be considered as constituting a highly nontrivial or unexpected general fundamental insight into the ZB phenomenon for researchers working in this field? Photonic crystals allow researchers to build up classical simulators of quantum systems. For example, through engineering the gain/loss media, non-Hermitian, PT-symmetric and non-relativistic quantum physics has been analogously realized using two sets of evanescently coupled waveguides [265] through non-reciprocal beam dynamics. Most previous studies on the optical analogies of non-Hermitian PT-symmetric quantum systems are nonrelativistic. Quite recently, optical analogies of the Hermitian relativistic Dirac equation have been articulated, such as synthetic photonic graphene and photonic topological insulators. An outstanding issue concerns the PT-symmetry and the related
physical effects in synthetic relativistic quantum systems. Existing theoretical proposals [276, 278] rely on an exact design of the gain-loss profile or a sophisticated strain-based control scheme for the given gain-loss configuration, leading to stationary, non-Hermitian PT-symmetric systems. Distinct from the existing works, our work reports a dynamical scheme to optically realize time-dependent, pseudo-PT symmetric relativistic Dirac equation, and we find the striking phenomenon of periodically suppressed and revival ZB oscillations. This “intermittent” ZB phenomenon is in sharp contrast to conventional ZB oscillations with a constant amplitude. Another novel aspect of our work lies in uncovering a resonance boundary between the pseudo-PT and PT-breaking regions, due to the interplay between two frequencies: the intrinsic ZB frequency and the external modulation frequency used to realize the pseudo-PT symmetry.

Second, are there potentially feasible experimental schemes? The answer is affirmative. Experimentally, conventional non-Hermitian PT-symmetry systems require that the real part of the effective potential to be an exactly even while the imaginary part be an exactly odd function in space. Our system design relaxes these requirements and significantly expands the configuration range of the non-Hermitian systems through introducing spatial modulation. The width of ZB trembling is on the order of micrometer and the length of the waveguides is millimeters. Concretely, our system can be realized in a waveguide array configuration similar to that in Ref. [280], where the gain effect can be realized, for example, through doping of dye molecules such as Rhodamine B (emission at 627 nm, excitation at 554 nm - green laser). Loss can be introduced using metals evaporated into the waveguides during the fabrication process.

In Sec. 5.2, we provide a detailed description of our photonic waveguide array system with pseudo $\mathcal{PT}$ symmetry, and derive the underlying Dirac equation. In Sec. 5.3, we present our main results: phase diagrams, amplitude divergence, regular and revival ZB oscillations, and spatial en-
ergy localization. In Sec. 5.4, we summarize the main results and offer a discussion. Certain details of the analytical derivation based on the relativistic quantum Dirac equation are given in Appendix.

5.2. Optical Waveguide System with Pseudo $\mathcal{PT}$ Symmetry and Description in Terms of the Dirac Equation

We consider a two-dimensional binary photonic superlattice consisting of two kinds of interleaved waveguides, $A$ and $B$, as shown in Fig. 24. The distance between two adjacent waveguides is $a$ and the coupling strength between them in the effective tight-binding Hamiltonian is $\kappa$. Due to the similarity between the optical and electronic waves, an optical waveguide system can simulate the time evolution of the electronic wavefunction subject to an equivalent potential. If the real parts of the refractive index of the nearest neighboring waveguides have the same mismatch, the waveguide superlattice can simulate the behaviors of the finite-mass Dirac equation. In particular, the dispersion relation of the lattice is a hyperbola about the edge of the first Brillouin zone [280, 286], and the $A$ and $B$ sublattices can be regarded as corresponding to the two components of the spinor wavefunction underlying the Dirac equation. When the incident angle of a wave packet is approximately the first Bragg angle, for an initial group velocity close to that of the edge of the first Brillouin zone, the optical system obeys the relativistic Dirac equation. Experimentally, it is difficult to realize a waveguide system with time-dependent refractive index. However, the $z$ direction represents effectively the time dimension. The two-dimensional binary photonic superlattice system is then completely equivalent to a time dependent, one-dimensional relativistic Dirac system, making possible experimental studies of various relativistic quantum effects.

We employ the tight-binding approximation to analyze the waveguide superlattice. The amplitude of the optical field is described by

$$ i \frac{da_n}{dz} = -\kappa (a_{n+1} + a_{n-1}) + (-1)^n \sigma(z) a_n, $$

(5.1)
Fig. 24. Schematic illustration of the system configuration. Two sets of waveguides, marked as $A$ and $B$, are interleaved with each other. The real parts of the refractive index for $A$ and $B$ are different, and their imaginary parts are small but have opposite signs. The distance between two adjacent waveguides is $a$ and they are coupled through constant strength $\kappa$. The imaginary part of the refractive index changes along the $z$ direction, mimicking a time dependent non-Hermitian potential.
where \( a_n \) is the amplitude of the optical field in the \( n \)th waveguide, \( \kappa \) is the effective coupling constant, and \( \sigma \) is the propagation mismatch. We assume that the real part of the mismatch \( \sigma_r \) between the nearest neighboring waveguides is constant. The space dependence of \( \sigma(z) \) is embedded in its imaginary part: \( \sigma_i(z) = r \sigma_r \sin(\omega z) \), where \( \sigma_r \) and \( \sigma_i \) denote its real and imaginary parts, respectively, with \( r \) being the ratio between them that characterizes the strength of gain/loss. The quantity \( \omega \) is the frequency of spatial gain/loss modulation in the \( z \)-direction. Equivalently, \( \omega \) can be regarded as the frequency of the imaginary part of the time-varying potential for the corresponding quantum system that is fundamentally non-Hermitian due to the imaginary potential. We note that, for a Hermitian system, i.e., a superlattice system with a purely real refractive index, previous works \([280, 286]\) showed the emergence of two minibands with the dispersion relation given by

\[
\omega_{\pm}(q) = \pm \sqrt{\sigma^2 + 4\kappa^2 \cos^2 \left( qa \right)}.
\]

For the wavevector along the \( x \)-direction, \( q \) is close to \( \pi / (2a) \) and the quantities \( \omega_{\pm}(q) \) exhibit a hyperbola-like behavior with a gap of \( 2\sigma \), which is similar to the electron and positron dispersion curves from the finite-mass Dirac equation. For a general non-Hermitian system, it is straightforward to show that the dispersion relation has the same form as that for a Hermitian system (see Appendix), but there are two differences: (a) the quantity \( \sigma \) becomes complex and (b) the system is time dependent due to the external driving. In the limit of small imaginary part, the complex frequency in the dispersion relation possesses the following real part

\[
\pm \sqrt{(\sigma_r^2 - \sigma_i^2(z)) + 4\kappa^2 \cos^2 \left( qa \right)},
\]

guaranteeing that our non-Hermitian system can still retain the equivalence to the relativistic quantum system for a massive particle at the boundaries of the Brillouin zone. This condition constrains the incident angle of the wave packet to be about \( \theta_B \approx \lambda / (4n_s a) \), where \( \lambda \) is the wavelength and \( n_s \) is the refractive index of the substrate. We emphasize that this analogy holds only when the wave packet is located near the Brillouin zone boundary. Analogy in other regions would be affected by
the dispersive effect of the waveguides. In fact, many experiments have shown that the analogy can hold up to hundred millimeters [286–288].

To demonstrate the equivalence of the waveguide equation to the Dirac equation, we make the following substitutions [280, 286, 288]:

\[
[\psi_1, \psi_2]^T = [(-1)^n a_{2n}, i(-1)^n a_{2n-1}].
\] (5.2)

From the periodicity and symmetry of the system, we see that a unit cell from sublattice \(A\) combining with one from sublattice \(B\) is effectively a unit cell that forms a Dirac spinor. It is necessary to use the dimensionless continuous transverse coordinate \(\xi \leftrightarrow n = x/(2a)\) to form a spatial derivative operator. With these considerations, we obtain the following equivalent one-dimensional Dirac equation

\[
i \frac{\partial \psi}{\partial z} = -i\kappa \alpha_1 \frac{\partial \psi}{\partial \xi} + \sigma(z) \alpha_3 \psi,
\] (5.3)

where

\[
\alpha_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \alpha_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},
\] (5.4)

are the Pauli matrices. These considerations hold when \(\sigma\) is complex. Comparing with the standard Dirac equation, we note the following equivalence:

\[
\kappa \leftrightarrow c, \ \sigma \leftrightarrow mc^2/h,
\] (5.5)

i.e., the coupling constant between the waveguides corresponds to the speed of light while the mismatch between the waveguides is equivalent to the mass of the underlying particle. Indeed, as we can see from the dispersion relation of the superlattice, the band gap for the Brillouin zone is also proportional to \(\sigma\), corresponding to the dispersion relation of a massive relativistic quantum particle.
In our simulations, we assume that the initial optical field has the form \( E(x,0) = G(x)e^{2\pi i x n_0 \theta_B}/\lambda \), where \( G(x) \) is a Gaussian beam envelope. The superlattice is made of 200 waveguides separated from each other with the distance \( a = 16 \mu m \), and the effective coupling rate is \( \kappa = 0.14 \text{mm}^{-1} \). The Gaussian beam has the wavelength of \( \lambda = 633 \text{nm} \) with a spot size about \( 105 \mu m \). The modulation frequency is scaled by the factor \( \omega_0 = 1/a \) and the lengths are normalized by \( a \).

5.3. Results

5.3.1. Emergence of Pseudo-\( \mathcal{PT} \) Symmetry

To ascertain the emergence of the pseudo-\( \mathcal{PT} \) symmetry, we probe into the parameter space of the photonic superlattice system systematically by calculating the phase diagrams. The results are shown in Fig. 25, where the same initial wave packet with a group velocity determined by the relativistic Dirac point is used for different parameter combinations. The evolution is simulated for a relatively long time to ensure that the system has settled into a steady state. Figures 25(a) and 25(b) show the phase diagrams in the \( r - \omega \) and \( \sigma_r - \omega \) parameter planes, respectively. The color is coded in terms of the maximum value of the intensity of the optical field for the corresponding parameters. Considering the fact that, in the pure gain regime, the intensity grows exponentially, we use a logarithmic function to rescale the intensity for better visualization. We set a cut-off intensity level beyond which the optical field is deemed to have diverged, corresponding to the \( \mathcal{PT} \) breaking case. The cut-off criterion we used is \( E_{\text{tot}}/E_{\text{tot}}^0 \sim 10^9 \), where \( E_{\text{tot}} \) is the maximum of the total intensity and \( E_{\text{tot}}^0 \) is the total intensity when there is no modulation. Even for this relatively high cut-off intensity, there is little change in the shape of the boundary. In most parts of the boundary of the \( \mathcal{PT} \) breaking phase and the pseudo-\( \mathcal{PT} \) phase, the change in the color from red to blue are quite rapid. In Figs. 25(a) and 25(b), the divergent regions are coded as dark red. For a small modulation
Fig. 25. Phase diagrams of relativistic quantum photonic superlattice system. The dark red region indicates the pseudo-$\mathcal{PT}$ breaking phase, and the other region corresponds to the pseudo-$\mathcal{PT}$ phase. (a,b) Phase diagrams in the $r - \omega$ and $\sigma_r - \omega$ parameter plane, respectively. The color is coded in terms of the logarithm of the maximum intensity in the specific parameter region. The white lines in (a) denote the positions of the valleys in the oscillatory variations of the boundary. The first two vertical lines, counted from right to left, correspond to the two sets of parameters shown in Fig. 26. The red stars in (a) specify the positions of the parameters shown in Fig. 27. For each phase diagram, the computational grid in the corresponding parameter plane has the size $512 \times 512$. The parameters are $\sigma_r/\kappa = 2.1$ (a) and $\sigma_i/\kappa = 0.5$ (b).
frequency, a number of waveguides absorb energy within the simulation time so that their intensity can exceed the cut-off value. For such waveguides, a pseudo-$\mathcal{PT}$ behavior cannot be numerically detected. Because of this, there is a persistently red region in the phase diagrams when the modulation frequency is close to zero. From Fig. 25(a), we see that a pseudo-$\mathcal{PT}$ behavior exists either in the parameter region with small gain/loss strength or in the region with a high modulation frequency. The reason is that, when the gain/loss of the waveguides is small, energy absorption is insignificant so that the waveguides will have sufficient time to transfer the energy within the superlattice and dissipate the absorbed energy into the adjacent waveguides. When the modulation frequency is high, the period becomes small so that the waveguides are able to dissipate the absorbed energy through itself when the imaginary part of the refractive index changes its sign during light propagation. In general, the stronger the gain/loss strength, the higher the modulation frequency is needed to balance the gain and loss, providing an explanation for the shape of the boundary of the two regions in the high modulation frequency regime in the phase diagrams. Figure 25(b) exhibits a similar behavior, i.e., the pseudo-$\mathcal{PT}$ behavior exists in the larger real refractive index (corresponding to weaker gain and loss effects) and higher modulation frequency regions. A general feature is that higher modulation frequency is favorable for the emergence of the pseudo-$\mathcal{PT}$ symmetry.

A phenomenon present in both Figs. 25(a,b) is that the boundary of the pseudo-$\mathcal{PT}$ symmetric and the non pseudo-$\mathcal{PT}$ regions exhibits oscillatory variations as the modulation frequency is changed. For $\omega/\omega_0 \sim 4 - 6$, the system exhibits a divergent behavior even for the small gain/loss strength. To understand the origin of the boundary variations, we examine the details of the time evolutions of the system. In Fig. 25(a), we mark the positions of the valleys in the variation with white lines, which are $\omega/\omega_0 = 0.6, 0.9, 1.5$ and 4.2, leading to the ratio of the period, i.e., $1/\omega$, to be about $7 : 5 : 3 : 1$, indicating that the system tends to diverge when the modulation period is odd
times of the rightmost line. When the ratio is even, the system tends to stay in the pseudo-\(PT\) phase. However, when the ratio becomes large, it is hard to observe the oscillatory behavior, due mainly to the finite resolution of the simulation. Another reason is that the system tends to shift into the high energy regime when the modulation frequency is low, so the oscillations are buried in the regime that does not correspond to \(PT\) breaking. The boundary in Fig. 25(b) exhibits a similar variational behavior. Particularly, as \(\sigma_r\) becomes larger, the imaginary part becomes relatively less significant. As a result, the band gap and thus the ZB trembling frequency is given by \(2\sigma_r\) (to be described in Sec. 5.3.2). When the modulation frequency is equal to the ZB trembling frequency, a resonant effect appears, forming a pseudo-\(PT\) phase boundary that starts from \(\omega/\omega_0 = 2\) in Fig. 25(b). The specific ratio relation suggests the occurrence of resonances in the system that can enhance or suppress the gain and loss of the superlattice. A more detailed understanding can be obtained through the dynamical oscillations in the system, i.e., the ZB effect.

### 5.3.2. Relativistic Zitterbewegung in Photonic Superlattice

ZB is a purely relativistic quantum effect resulting from the interference between the positive and negative energy states of the Dirac fermion. To experimentally observe ZB in electronic systems is challenging due to the small wavelength and the extremely high oscillating frequency. Photonic superlattice systems with the underlying equation having the same mathematical form as the Dirac equation provide an alternative paradigm for detecting and characterizing the ZB phenomenon [280]. Our goal is to investigate whether ZB can emerge in pseudo-\(PT\) symmetric photonic systems. Figure 27 shows a number of representative time series of the beam center of mass of the wave packet for different parameters. There are apparent oscillations in the time series. Since oscillations are a generic feature of the wave equations, the issue is whether these oscillations are true manifestations of ZB. We address this issue by analyzing the equivalent Dirac equation to de-
termine if the oscillations have a relativistic quantum origin. The basic idea is to write the Dirac equation in the momentum space to obtain the time evolution of the wavefunction [289]. In order to arrive at an analytical form, we make the assumption that the total Hamiltonian at any two given instants of times are commutative so that a sophisticated treatment of the time ordering operator is not necessary. Note that, while for time independent quantum systems time ordering is not necessary, for a time dependent Hamiltonian this may not be the case. Nonetheless, we expect that, in the parameter regime where the non-Hermitian effect is weak, i.e., small $\sigma_i$, our analytic results would agree with the direct simulations results.

The main results of our analysis can be summarized by dividing the time evolution of the expectation value of the position operator into three components: the drift $\xi_d(t)$, the ZB trembling component $\xi_{ZB}(t)$, and the purely imaginary component $\xi_{Im}(t)$. We have (detailed derivation can be found in Appendix)

\[
\langle \xi \rangle(t) = [\xi_d(t) + \xi_{ZB}(t) + \xi_{Im}(t)] / |\psi(t)|^2,
\]

\[
\xi_d(t) = 4\pi \int_{-\infty}^{\infty} dk G^2(k) \kappa^2 k^2 \left[ \cos(A)^2 A^* + |\sin(A)|^2 A^3 \right], \tag{5.6}
\]

\[
\xi_{ZB}(t) = 4\pi \int_{-\infty}^{\infty} dk G^2(k) \sin(A) \cos^*(A) \kappa (-\sigma_r t + i \sigma_i (\cos(\omega t) - 1)/\omega)^2 t, \n\]

\[
\xi_{Im}(t) = 8\pi i \int_{-\infty}^{\infty} dk G(k) \partial_k G(k) \kappa k \text{Im} \left( \frac{\sin(A) \cos^*(A)}{A} \right) t,
\]

where

\[
A(t) = \sqrt{\kappa^2 k^2 t^2 + (\sigma_r t - i \sigma_i \frac{\cos(\omega t) - 1}{\omega})^2}
\]

is the normalization constant associated with the Euler formula for the Pauli matrices, and

\[
G(k) = (1/2\pi) \int_{-\infty}^{\infty} d\xi G(2d\xi) e^{-ik\xi}
\]
is the angular spectrum of the Gaussian beam envelop. The modulus of the wavefunction is

$$|\psi(t)|^2 = 4\pi \int_{-\infty}^{\infty} dk G(k)^2 [|\cos(A)|^2$$

$$+ |\frac{\sin(A)}{A}|^2 (\kappa^2 k^2 t^2 + \sigma^2 \tau^2 + \frac{\cos(\omega t) - 1}{\omega} \sigma_i^2)],$$

(5.7)

We note that, for a relativistic quantum system described by the Dirac equation, the time evolution of the expectation value of the position operator contains the drift and the ZB trembling components only. For a stationary Hermitian system, we have $A = A^* \propto t$, the drift component can be simplified as

$$\xi_d(t) \propto A \cos^2(A) + A \sin^2(A) t^3 \propto t,$$

which describes the motion of the wave packet at constant velocity. The ZB trembling component $\xi_{ZB}(t)$ can be simplified as an oscillatory term described by $\sin(A) \cos(A) \propto \sin(2A)$, and the purely imaginary component $\xi_{Im}(t)$ is simply zero.

The analytical results can be used to interpret the numerically observed dynamical behaviors of the system associated with the boundary variations in the phase diagrams in Fig. 25. Specifically, Fig. 26 shows the analytical results for $r = 0.5$ and $\omega/\omega_0 = 4.2, 1.5$ (the blue solid and red dashed curves, respectively), which correspond to the two rightmost white lines marked in Fig. 25(a). Figure 26(a) shows the time evolution of the normalized modulus of the two sublattices $A$ and $B$. As expected, the modulus of the red dashed curve is about three times slower than that of the blue solid curve, which is the ratio between the modulation frequencies. However, the time evolution of the ZB trembling term $\xi_{ZB}(t)$ has the same frequency for the two sublattices, as shown in Fig. 26(b), indicating that ZB trembling has little dependence on the modulation frequency. A comparison of the time series in Figs. 26(a,b) indicates that the frequency of ZB oscillations is close to that of the modulus oscillation for $\omega/\omega_0 = 4.2$. 

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Fig. 26. Oscillatory behaviors in the wave packet. Time series (equivalently, propagation along the $z$ direction) of the photonic superlattice system for the parameters corresponding to the valleys of the boundary variations in the phase diagram (Fig. 25). (a-c) Time series of the modulus of the Dirac spinor of the two sublattices, of ZB trembling, and of the oscillation term $\sin(A)\cos^*(A)$ in $\xi_{ZB}$, respectively. The parameter setting is $\sigma_r/\kappa = 2.1$, $r = 0.5$, $\omega/\omega_0 = 4.2$ (blue solid curves), and $\omega/\omega_0 = 1.5$ (red dashed curves).
Note that, for \( r = 0 \) the band gap is \( 2\sigma_r = 4.2 \). These results imply that the variations in the boundary between the pseudo-\( PT \) symmetric and the pseudo-\( PT \) symmetry breaking regions are due to the resonant interaction between the modulation to the waveguides and ZB trembling. The energy absorption process is enhanced when the ratio between the modulation period and the ZB trembling period is an odd integer. For the high frequency region where the modulation period is smaller than the ZB trembling period, the system exhibits a relatively simple behavior, where the boundary can be described by a linear relation between \( r \) and \( \omega/\omega_0 \).

Figure 27 shows the simulation (blue) and analytic (red) results for the ZB effect, where the behavior of the real part of the quantity \( (\xi_d(t) + \xi_{\text{ZB}}(t))/|\psi(t)|^2 \) is illustrated for six different parameter combinations indicated by the red stars in Fig. 25(a). When the imaginary part of the refractive index is relatively small, i.e., when the system is only weakly non-Hermitian, the analytical and simulation results agree well with each other, as shown in Figs. 27(a-c) for \( r = 0.2 \). Note that the scale of the \( x \) axis in Fig. 27(a) is about three times of that in Fig. 27(b-c), and the periods of the oscillations for these cases are the same, indicating that the oscillation periods have little dependence on the modulation frequency. Our analytical results provide a base to attribute the oscillations as resulting from the ZB trembling term \( \xi_{\text{ZB}}(t) \), demonstrating their relativistic quantum origin. We note that, for a Hermitian system, the dynamical evolution of the wave packet can be represented as the superposition of a constant drift behavior and simple sinusoidal oscillations, but the dynamics of ZB oscillations in the relativistic non-Hermitian system are richer. Specifically, from Fig. 27(a), we see that, for low modulation frequencies, ZB oscillations can be enhanced or suppressed in different time intervals. However, for high modulation frequencies [e.g., Fig. 27(c)], ZB oscillations are conventional in the sense that there are no apparent enhancement or reduction effects. An intermediate situation arises between these two cases, e.g., for \( \omega/\omega_0 = 1.0 \). These
Fig. 27. Relativistic Zitterbewegung in non-Hermitian photonic superlattice systems. The six panels correspond to all possible combinations of $r = 0.2, 0.5$ and $\omega/\omega_0 = 0.2, 1.0, 3.0$, as marked by the red stars in Fig. 25(a). (a-c) Mean/expectation values of the position of the wave packet for $r = 0.2$ and $\omega/\omega_0 = 0.2, 1.0, 3.0$, respectively. (d-f) Similar plots but for $r = 0.5$. The blue and red curves correspond to the beam center of mass of the wave packet from the simulation results and the mean expectation value of the position operator from the analytic results, respectively.
results indicate that the modulation frequency of the refractive index can affect the amplitude of ZB oscillations.

The role of the modulation frequency in the amplitude evolution of ZB oscillations can be assessed in a more detailed manner through a close examination of the oscillation term in $\xi_{ZB}(t)$, i.e., $\sin A \cos^* A$, for different values of the modulation frequency, as shown in Figs. 26(b-c), where the oscillating patterns have the same modulation frequency, implying that the frequency of ZB oscillations is entirely determined by its sine and cosine components. Further, the ZB oscillations for the two different values of the modulation frequency are in pace with each other in time, indicating that the modulation frequency has little effect on the frequency of ZB oscillations. This is expected because the quantity $A(t)$ is an integration of $\sigma(t)$ so that the amplitude of $\sigma(t)$ is a key factor. Nonetheless, the modulation frequency does affect the oscillating intensity, as shown in Fig. 26(a). Thus, the envelope behavior of ZB oscillations in Figs. 27(a-c) is determined by the modulation of the periodic refractive index: for high and low modulation frequencies, ZB oscillations are suppressed and enhanced, respectively. A conclusion is that, for high modulation frequency and low modulation intensity, the effect of refractive-index modulation is weak, as exemplified in Fig. 27(c). For $r = 0.5$, the analytically predicted amplitude of the oscillation behavior [Figs. 27(d-f)] deviates from the simulation results (except for the initial phase of the dynamical evolution). In spite of the disagreement, the predicted phase behavior of the oscillations agrees with the simulation results. The failure of the analytic theory to predict correctly the amplitude behavior of ZB oscillations stems from the hypothesis used in our analysis: the Hamiltonians at different times are commutative. This hypothesis is violated when the non-Hermitian effect becomes pronounced, i.e., as the imaginary component of the refractive index and the time dependent modulation are relatively large. Indeed, as we increase the value of $r$ from 0.2 to 0.5, the agreement becomes increasingly worse,
especially for large time. However, for the parameter region on the right side of the phase diagrams in Fig. 25 where the imaginary part of the refractive index is small, a reasonably good agreement between the analytical and simulation results is obtained, due to the relatively weak non-Hermitian effect. For the high modulation frequency region (the rightmost part of Fig. 25), ZB oscillations are similar to those of the conventional case where the modulation in the refractive index is absent. Physically, in the high modulation frequency region, the waveguides do not have time to absorb and dissipate energy, generating a mean-field like effect.

In the intermediate frequency regime, the analytical and simulation results do not agree with each other. Numerically, we find the phenomenon of spatial energy localization, as shown in Fig. 28. In particular, in the parameter space near the boundary of the phase diagram, e.g., for \( r = 0.5 \) and \( \omega/\omega_0 = 4.0 \), spatially the wave energy is localized within a small region about the center of the waveguide array, as shown in Fig. 28(a). This phenomenon of energy localization is sensitive to the value of \( \omega \). Figure 28(b) shows a contrary example for \( \omega/\omega_0 = 3.5 \), where the wave packet spreads after a short time. We find that the wave spread becomes faster as the value of \( \omega \) is reduced. Figures 28(c,d) show the total wave intensity corresponding to the cases in Figs. 28(a,b), respectively. We observe an apparent envelope modulation behavior in the case of energy localization. The strong reduction in the spread of the wave packet is similar to that reported in Ref. [290], where a localization behavior in quantum diffraction was found to result from the linearization of the quasienergy spectrum close to the \( \mathcal{PT} \)-symmetry breaking boundary. Generally, this is a dynamical localization phenomenon in one-dimensional driving systems [291–294]. The width of the localized wave packet depends on the width of the initial wave packet.
Fig. 28. Phenomenon of spatial energy localization in photonic superlattice. Spatial view of the field intensity and time evolution of the modulus of the wave function for $r = 0.5$, (a,c) $\omega/\omega_0 = 4.0$, and (b,d) $\omega/\omega_0 = 3.5$. 

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5.4. Conclusion

Novel electronic materials obeying relativistic quantum mechanics are a current focus of condensed matter physics and materials science, which provide us with a platform to uncover, understand, and exploit unusual physical phenomena. It is of great interest to use optical systems to gain insights into the fundamentals of relativistic quantum solid state devices, and vice versa, i.e., to exploit relativistic quantum electronic behaviors to generate revolutionary ideas/methodologies in manipulating light propagation. The main reason for such an interest is that, electronic materials face many experimental and technological challenges due to the extremely small wavelength issue. The conventional method is to engineer, e.g., through strain, doping and voltage control, some specific materials to realize the desired configuration, constraining researchers to some limited kinds of lattice structures and interactions. Compounded on the small wavelength issue are various kinds of disorders and impurities. Photonic crystals and waveguides can be used to mimic the electronic properties, e.g., the dispersion relations, of solid state materials, with the advantage that the optical wavelength is orders of magnitude larger than the electronic wavelength. Substantially larger optical devices can then be fabricated to investigate a host of electronic behaviors in relativistic quantum solid devices. These are synthetic photonic materials and devices.

This paper is a case study of exploiting the equivalence between coupled wave equations and the Dirac equation to model/simulate relativistic quantum effects in a non-Hermitian setting. Standard quantum mechanics requires observable operators to be Hermitian to ensure real eigenvalues. However, non-Hermitian Hamiltonians are also capable of generating a purely real eigenvalue spectrum insofar as the system has a $\mathcal{PT}$ symmetry. In optics, non-Hermitian Hamiltonian systems can be realized using materials with a complex index of refraction, rendering experimentally feasible such systems [235, 237, 256, 257]. We studied a class of non-Hermitian waveguide systems with
Fig. 29. (a-e), Phase diagrams for $\sigma_r/\kappa = 1.1, 1.5, 2.1, 2.5, 3.1$. $\omega_1$ is the base frequency, i.e., the largest resonance frequency, for $\sigma_r/\kappa = 2.1$. The white dashed lines on (c) correspondent for $\omega_1/\omega = 1, 3, 5, 7, 9$. The rest of the phase diagrams also satisfy the same relation, with the base frequency changes according to $\omega_{\text{base}} \propto \sigma_r/\kappa$.

Periodic modulated imaginary refraction index in order to uncover the optical counterpart of the relativistic ZB effect, which exhibit $\mathcal{PT}$ symmetry breaking at any instant of time but the symmetry is preserved on a larger time scale (herewith the term pseudo $\mathcal{PT}$ symmetry). We generated phase diagrams of the pseudo-$\mathcal{PT}$ behavior, which provide a general picture for controlling and harnessing light propagation in the waveguide system. The phenomenon of oscillatory boundary variations in the phase diagrams is explained. In the low modulation frequency region, we observed periodically enhanced and suppressed ZB oscillations, as predicted by an analysis of the equivalent Dirac equation. The phenomenon that there are time periods where the ZB trembling is absent, interspersed by time intervals where the relativistic quantum oscillations emerge and disappear, a kind of “revival” phenomenon, can potentially lead to a new mechanism to manipulate/control light propagation. In the high frequency regime, a conventional ZB trembling behavior arises due to a mean-field effect. In the intermediate region, the equivalent description based on the Dirac equation no longer holds. However, numerically we uncovered a spatial energy localization phenomenon.
5.5. Appendix

5.5.1. Phase Diagram in $1/\omega$ Axis.

As we can see in our phase diagram Fig. 25, the boundary between the pseudo-$\mathcal{PT}$ breaking phase and the pseudo-$\mathcal{PT}$ phase shows an oscillation. A detailed investigation find that the inverse of the peak frequencies are odd times of the inverse of the rightmost peak frequency. To reveal this behavior better, especially when $\omega \to 0$, we present here several phase diagrams in $1/\omega - r$ planes for different $\sigma_r/\kappa$. In Fig. 29 (c), we use the same parameters as we used in Fig. 25 (a). The $1/\omega$ axis is rescaled to $1/(\omega_1/\omega_0)$, where $\omega_1/\omega_0 = 4.2$ in this case. The rest figures are all scaled using the base frequency of Fig. 29 (c). In Fig. 29 (c), the white dashed lines are $\omega/\omega_1 = 1, 3, 5, 7, 9$, so we can clearly see that the system is tend to be in the pseudo-$\mathcal{PT}$ breaking phase around these lines. As we mentioned, $\omega_1/\omega_0 \sim 2\sigma_r/\kappa$, so when we change $\sigma_r/\kappa$ we expect to see a similar resonance phenomena but with different base frequency, which is what is shown in Fig. 29 (a,b,d,e). Physically, $\sigma_r/\kappa$ is a measure of the band gap of the massive relativistic dispersion relation, and it is well established that in the Hermitian case the ZB trembling frequency is proportional to the band gap. Thus, the modulation frequency which is at resonance with the ZB trembling frequency is also changed, as well as its old times. Several similar results have been reported recently [295–299].

5.5.2. Derivation of the Main Analytical Result.

We start from the Dirac equation in the momentum space:

$$i\hbar \frac{\partial \psi(k,t)}{\partial t} = \hbar[k\kappa\alpha_1 + \sigma(t)\alpha_3]\psi(k,t).$$

The wavefunction at any given time can be written as

$$\psi_k(t) = T e^{-\frac{i}{\hbar} \int_0^t H(t') dt'} \psi_k(0).$$

where $T$ is the time ordering operator. Since our system is a time dependent non-Hermitian system, i.e., $[H(t_1), H(t_2)] \neq 0$, the expansion of the exponential factor under the time ordering operator
can be quite sophisticated. In order to gain analytical insights, we assume 
\[ [H(t_1), H(t_2)] = 0. \] This does not mean that the non-Hermitian property of our system is lost. In fact, non-Hermitian characteristics still exist in \( E_{\pm}(t) \).

First of all, we would like to discuss the validity of our approximations made here. The effective Hamiltonian of our system is 
\[ H(k, t) = \kappa k \alpha_1 + \sigma(t) \alpha_3. \] The time modulation in our system only consists in the imaginary part of \( \sigma(t) = \sigma_r + i \sigma_i \sin(\omega t) \) while the real part of it \( \sigma_r \) is time independent. So in the limit of \( \sigma_i = 0 \), we can see that our system tends to be exactly time independent, which directly leads to the elimination of the time ordering operator. Because 
\[ \lim_{\sigma_i \to 0} [H(t_1), H(t_2)] \propto \kappa k \sigma_i \to 0. \] The time dependent weight on the \( \alpha_1 \) piece actually comes from 
\[ \int_0^t H(t') dt' \], and will only be responsible for the dynamic phase in such a limit. In this case, we do not need to make this approximation. When \( \sigma_i \) is finite, the time ordering operator can be expanded as:

\[
\mathcal{T}[e^{-i \int_0^t H(t') dt'}] = I + \frac{-i}{1!} \int_0^t dt_1 \mathcal{T}[H(t_1)] \\
+ \frac{(-i)^2}{2!} \int_0^t dt_1 \int_0^t dt_2 \mathcal{T}[H(t_1)H(t_2)] \\
+ \ldots \\
+ \frac{(-i)^k}{k!} \int_0^t dt_1 \ldots \int_0^t dt_k \mathcal{T}[H(t_1) \ldots H(t_k)] \\
+ \ldots,
\]

where we have ignored \( \hbar \) for simplicity. We take the second order term for example. The difference induced by the time ordering operator, compared to the one without it, is of the order of 
\[ [H(t_1), H(t_2)] \propto \kappa k \sigma_i, \] while the main part of the second order term is dominated by \( \kappa^2 k^2 + \sigma_r^2 \).

As we mainly consider the excitations around the \( k \sim 0 \) points, i.e., the Brillouin zone boundary in the original waveguides system, the ratio of the two terms \( \frac{\kappa k \sigma_i}{\kappa^2 k^2 + \sigma_r^2} \) can be rather small. Thus, the difference contributed by the time ordering operator is negligible when \( \sigma_i/\sigma_r \) is small. And the
difference will be decreased in the higher order terms. To summary, when $\sigma_r$ is not zero, our results are exact when $\sigma_i = 0$, as our system degrades to a time independent system. When $\sigma_i$ is finite but small compared with $\sigma_r$, our approximation holds as tested by our numerical results in the case of $\sigma_i/\sigma_r = 0.2$.

Since $\sigma(t) = \sigma_r + i\sigma_i \sin(\omega t)$, we have

$$-\frac{1}{\hbar} \int_0^t H(t')dt' = -\kappa kt\alpha_1 + (-\sigma_r t + i\sigma_i \frac{\cos(\omega t) - 1}{\omega})\alpha_3$$

$$\equiv A(\hat{A} \cdot \vec{\alpha}),$$

where

$$\vec{A} = A \cdot \hat{A} = (-\kappa kt, 0, -\sigma_r t + i\sigma_i \frac{\cos(\omega t) - 1}{\omega}),$$

$$A = \sqrt{\kappa^2 k^2 t^2 + (\sigma_r t - i\sigma_i \frac{\cos(\omega t) - 1}{\omega})^2},$$

and

$$\vec{\alpha} = (\alpha_1, \alpha_2, \alpha_3)^T.$$

Using the Euler formula for Pauli matrices,

$$e^{iA(\hat{A} \cdot \vec{\alpha})} = \hat{I} \cos(A) + i(\hat{A} \cdot \vec{\alpha}) \sin(A),$$

we have

$$\psi_k(t) \approx e^{-\frac{i}{\hbar} \int_0^t H(t')dt'} \psi_k(0) = [I \cos(A) + i(\hat{A} \cdot \vec{\alpha}) \sin(A)] \psi_k(0).$$

Next we consider the initial condition. At the input plane $z = 0$, the initial wave packet can be chosen to have the shape of a slowly varying Gaussian form. The initial amplitude of $\psi_{1,2}(\xi, 0)$ is then proportional to $G(2na)$ and $G((2n - 1)a) \approx G(2na)$, so the two components of the Dirac spinor have the same initial condition, i.e., $\psi_k(0) = G(k)[1, 1]^T$. The Pauli matrices operate on the initial Dirac spinor, and we get the time evolution of the two components of the Dirac spinor as

$$\psi_k(t) = G(k) \begin{pmatrix} \cos(A) + \frac{i}{A} \sin(A) \left[ -\kappa kt + (-\sigma_r t + i\frac{\cos(\omega t) - 1}{\omega} \sigma_i) \right] \\ \cos(A) + \frac{i}{A} \sin(A) \left[ -\kappa kt - (-\sigma_r t + i\frac{\cos(\omega t) - 1}{\omega} \sigma_i) \right] \end{pmatrix},$$

(5.9)
The expectation value of the position operator can be calculated through

$$\langle \xi \rangle (t) = 2\pi i \int_{-\infty}^{\infty} \psi_k^*(t) \partial_k \psi(t)$$  \hspace{1cm} (5.10)$$

A lengthy algebra leads to the main analytic result: the formulas in Eq. (5.6) as well as the time evolution of the modulus of the wavefunction. The convergence of the integrals in Eq. (5.6) is guaranteed by the exponential decay of the Gaussian wave spectrum $G(k)$. In particular, for small $t$ values, $|\cos(A)|^2$ is about unity. For large values of $t$, we have $|\psi(t)|^2 \approx |\cos(A)|^2 + |\sin(A)|^2 \geq 1$. Thus, $|\psi(t)|^2$ can never approach 0, so Eq. (6) converges.

### 5.5.3. Derivation of the Dispersion Relation.

We follow Refs. [286,300] to derive the dispersion relation. Specifically, from the coupled mode equation, we obtain, for $a_{2n}$ and $a_{2n+1}$, the following equations:

$$i \frac{da_{2n}}{dz} = -\kappa (a_{2n-1} + a_{2n+1}) + \sigma(z) a_{2n},$$

$$i \frac{da_{2n+1}}{dz} = -\kappa (a_{2n} + a_{2n+2}) - \sigma(z) a_{2n+1},$$

where $\sigma(z)$ is in general complex. As there are two sets of waveguides, we assume $a_{2n} \sim A e^{iq(2n)z - i\omega z}$ and $a_{2n+1} \sim B e^{iq(2n+1)z - i\omega z}$. Substituting these into the equations for $a_{2n}$ and $a_{2n+1}$, after some algebra, we have

$$(\omega - \sigma(z)) A + 2\kappa \cos(qa) B = 0,$$  \hspace{1cm} (5.11)

$$2\kappa \cos(qa) A + (\omega + \sigma(z)) B = 0.$$

The determinant of the above equation needs to be 0, which leads to $\omega = \pm \sqrt{\sigma(z)^2 + 4\kappa^2 \cos^2(qa)}$.

To account for the fact that $\sigma(z)$ is complex, we substitute $\sigma(z) = \sigma_r + i\sigma_i(t)$ into the dispersion
relation and consider the limit of small imaginary part:

\[ \omega = \pm \sqrt{(\sigma_r + i\sigma_i(z))^2 + 4\kappa^2 \cos^2(qa)} \]  \hspace{1cm} (5.12)

\[ = \pm \sqrt{\sigma_r^2 - \sigma_i^2(z) + 4\kappa^2 \cos^2(qa)} \cdot \sqrt{1 + \frac{2i\sigma_r\sigma_i}{\sigma_r^2 - \sigma_i^2(z) + 4\kappa^2 \cos^2(qa)}} \]

\[ \approx \pm \sqrt{\sigma_r^2 - \sigma_i^2(z) + 4\kappa^2 \cos^2(qa)} \cdot (1 + \frac{i\sigma_r\sigma_i}{\sigma_r^2 - \sigma_i^2(z) + 4\kappa^2 \cos^2(qa)}). \]

The real part of the dispersion relation in the limit of small imaginary part is then given by

\[ \pm \sqrt{\sigma_r^2 - \sigma_i^2(z) + 4\kappa^2 \cos^2(qa)}. \]  \hspace{1cm} (5.13)
6. MECHANICAL TOPOLOGICAL SEMIMETAL

Much attention has been paid to mechanical analogs of topological quantum phases, where finite momentum-space Berry curvatures are typically required to render nontrivial dominant topologically invariant quantities, say the Chern number, associated with the underlying bandstructures. It is well known that the finite Berry curvatures can be arised from breaking the inversion symmetry or the time-reversal symmetry (TRS). Conventionally for graphene or graphene-inspired two-dimensional (2D) systems with gapless Dirac cones, such broken symmetries will be inevitable to push the systems into an insulating bulk phase via lifting the degeneracies of the cone. Realizing a robust Dirac cone based semimetal phase in 2D with as well as non-vanishing Berry curvatures is thus very challenging. In this work, a 2D mechanical dice lattice system is proposed, based on which we surprisingly find a novel semimetal phase with a gapless bulk Dirac-like cone and finite momentum-space Berry curvatures associated with it. In addition to represent a solid demonstration of robust 2D semimetal with unusual conical bandstrutures, it is followed from this finding that intrinsic valley Hall effect can arise without hurting/suppressing the carriers’ mobility. Comprehensive numerical evidences are given together with the explanations based on analytical results. When our system is confinement along the zigzag edges, gapless edge states are found. Surprisingly, the gapless edge states are divided into two classes possessing opposite edge polarizations, with one having a finite group velocity while the other has zero group velocity.

6.1. Introduction

Topology initially studied in mathematics has been being a fundamental and powerful concept to understand or characterize exotic phases of matter, by which emerging topological materials e.g. topological insulators, topological superconductors and topological metals are now being successfully indentified and have been frontline research in condensed matter physics [242, 243, 301–303].
The topological invariant which used to characterize the novel topological states is called the Chern number, which is calculated by integrating the Berry curvature within the whole Brillouin zone. Berry curvature, the Berry phase per unit area in the $k$ space, is characterized by the spin and valley degree of freedom, except the details of different materials. Based on the Berry phase supported topological transport theory, Bloch electron will acquire an anomalous term proportional to the mechanical force induced by the finite Berry curvature [303–306]. This is the fundamental mechanism for the anomalous Hall effect [307] and the valley Hall effect [306].

The valley Hall effect has been firstly proposed in graphene [306]. Graphene is a monolayer carbon honeycomb lattice, which possesses extraordinary electronic and mechanic properties [308, 309]. Regardless of its weak intrinsic spin-orbit interaction, it has two large separated inequivalent valleys at the corners of the Brillouin zone. Thus, intervalley scattering is strongly suppressed and the valley index can be used in analog to spin. It has been well established that, a finite Berry curvature can only be obtained in a system with broken inversion symmetry, and a finite Chern number requites a further breaking of TRS. In graphene, or the Haldane model [310], the interactions added to break the inversion symmetry or TRS will inevitably open the degenerate points at its two valleys [306, 311, 312]. In three-dimensional system, people have achieved new topological phases on gapless bulk systems, e.g., Weyl [313] and Dirac [314] semimetals. Recently, G. Palumbo et al. have proposed a two-dimensional Chern semimetals on the Lieb lattice, in which the degenerate point is still opened by the interaction [315]. A natural question is, can we achieve a 2D system which possesses a finite Berry curvature without opening the bulk degenerate points? We try to address this issue exploiting the emerging idea of mechanical analogue of electronic system.

Many novel electronic concepts, e.g., Dirac cones, quantum (anomalous) Hall state and topological protected edge state, have already found their correspondences in the classical mechanical
An emerging field named “topological phononics” has been proposed [318]. Many studies in the photonic and phononic systems have led to the understanding that the nontrivial topological phase is fundamentally a wave phenomenon rather than a quantum effect [317]. Thus, many topological related physics can be explored using a prototype following the classical mechanism. Compared to the electronic system, the Newton’s law governed classical mechanical system has the advantage of superior controllability and much easier experiment realizations.

In this work, we utilize the spring-mass model to construct a mechanical dice lattice system. The dice lattice can be thought of as two sets of honeycomb lattice and is predicted to have a three-band degenerate electronic band structure [321]. Through systematically investigations within the parameter space, we find several interesting phases which possess three-band degeneration and two-band degeneration. Surprisingly, by modifying the spring constant of one subset of the dice lattice, inversion symmetry can be naturally broken while the degeneracy still holds. This leads to a finite Berry curvature and thus the new mechanical topological semimetal phase. Detailed analysis of the phase diagrams are given as well as the Berry curvatures for some specific cases. We also investigate the ribbon band structure of the mechanical topological semimetal state, where gapless edge states are found. A rather interesting discover is that our mechanical dice lattice system possesses a conducting channel in one edge and a non-conducting channel in the other edge.

6.2. Mechanical Lattice Model and Dynamic Matrix

We begin by considering the mechanical dice lattice which is made up of the same components of the previously studied mechanical honeycomb lattice [316, 317], in which atoms are modeled by identical mass points and the connection is made by the spring with spring constant $\kappa$ and natural length $l_0$, as is shown in Fig. 30. However, in the equilibrium situation, the length of spring, $R_0$, does not necessary to be equal to the natural length, thus we use $\eta = l_0/R_0$ as a parameter to characterize
the spring. The static equilibrium of the bulk mass points is guaranteed by the symmetry of the dice lattice while the boundary mass points replies on the boundary condition. Furthermore, we restrict the motion in the 2D plane and consider only the small displacement around the equilibrium points. Thus the dynamical variables are the deviations of mass points from the static equilibrium positions, which is written as $x_r = (x_{r,a}, y_{r,a}, x_{r,b}, y_{r,b}, x_{r,c}, y_{r,c})^T$, where $r$ denotes an unit cell lattice coordinate and $a, b, c$ denote three mass points in one unit cell. In the general case, the two sub honeycomb lattices are of different parameters, so that there are three inequivalent mass points in one unit cell.

The motion of mass points can be well described by the Hamilton mechanism. For one degree of freedom of a given mass point, we have $m\ddot{x} + \frac{\partial H}{\partial x} = 0$. In our system we consider identical mass points so $m = 1$ is assumed for simplicity. Only the nearest neighbor terms in the Hamiltonian $H$ have contributions and the kinetic part becomes zero with respect to the partial derivative of the position. Following previous method [316], we assume the springs are in the linear region, i.e., the elastic potential within one spring is written as $U_s = \frac{\kappa}{2}(l - l_0)^2$, where $l$ is the instant length of the spring. We can linearize the elastic potential by using the assumption that the motion is only around the equilibrium position and expand it up to second order of the derivation. By changing the dynamical variables from real $r$ space into momentum $k$ space, i.e. $z_{r,\nu} = \frac{1}{N} \sum_k e^{ik\cdot r} \mu_{k,z}^{\nu}$ and $\mu_{k,z}^{\nu} = e^{i\omega t} \phi_{z}^{\nu}(k)$, where $z \in \{x, y\}$ and $\nu \in \{a, b, c\}$, we can obtain an eigenfunction defined by the dynamic matrix, from which the frequency spectrum can be obtain:

$$\omega^2 \phi(k) = \Gamma(k)\phi(k),$$

(6.1)
Fig. 30. Schematic illustration of the mechanical dice lattice. The two subsets of honeycomb lattices are colored by black and red. The spring parameters are $\kappa_1, \eta_1$ and $\kappa_2, \eta_2$, respectively. All the mass points are identical but can be physical inequivalent. In the general case, there are three mass points in one unit cell, which are colored by red, blue and green. Inversion symmetry is naturally broken if the spring constants for the two subsets are different.
where $\phi(k) = [\phi^x_a(k), \phi^y_a(k), \phi^x_b(k), \phi^y_b(k), \phi^x_c(k), \phi^y_c(k)]^T$, and

$$
\Gamma(k) = \begin{bmatrix}
    \Lambda_1 & \Gamma_{ab}(k) & 0 \\
    \Gamma_{ab}^\dagger(k) & \Lambda_1 + \Lambda_2 & \Gamma_{bc}(k) \\
    0 & \Gamma_{bc}^\dagger(k) & \Lambda_2
\end{bmatrix}, \quad (6.2)
$$

where

$$
\Lambda_i = 3\kappa_i(1 - \frac{\eta_i}{2})I_2
$$

$$
\Gamma_{ab}(k) = -\kappa_1(\gamma_{R_1}^{xy} e^{ik\cdot a_1} + \gamma_{R_2}^{xy} e^{ik\cdot a_2} + \gamma_{R_3}^{xy})
$$

$$
\Gamma_{bc}(k) = -\kappa_2(\gamma_{R_1}^{xy} + \gamma_{R_2}^{xy} e^{-ik\cdot(a_1-a_2)} + \gamma_{R_3}^{xy} e^{-ik\cdot a_1})
$$

Where $\gamma_{R}^{xy} \equiv [1 - \eta, \eta R_x R_y; \eta R_y R_x, 1 - \eta]$ for $R = (R_x, R_y)$, $a_1 = (\frac{1}{2}, \frac{\sqrt{3}}{2})a$, $a_2 = (\frac{-1}{2}, \frac{\sqrt{3}}{2})a$.

Here $a$ is the length of the primitive basis vectors, and are shown in Fig. 30. Eq. (6.1) is a six-dimensional eigenfunction problem of which the general analytic results are too complex. The frequency $\omega$ is the square root of the eigenvalues of Eq. (6.1). Mathematically speaking, there could exist negative eigenvalues for Eq. (6.1) which leads to a pair of pure imaginary $\omega$. Physically, these solutions correspondence to instable states and ones shall only consider the stable cases. The numerical approach is rather straightforward, ones also try to obtain analytical results by making further approximations.

In our mechanical dice lattice system, as shown in Fig. 30, there are two subsets of honeycomb lattice, which are characterized by $\kappa_1, \eta_1$ (black) and $\kappa_2, \eta_2$ (red), respectively. That makes our parameter space of the system as $\{\kappa_1, \eta_1, \kappa_2, \eta_2\}$. From Eq. (6.2), we can see that $\kappa_1, \kappa_2$ are appeared as the scaling factor for the strength of the two sub lattices. They do not participate in any more complicity interactions. We thus can arbitrarily set $\kappa_1 = 1$ in all the following analysis, which is equivalent to scale $\kappa_2$ as $\kappa_2/\kappa_1$. 

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Fig. 31. Phase diagrams of the mechanical dice lattice system. (a) Phase diagram at $\eta_1 = 0$, the red lines are three-band degenerate phases and the rest area are the two-band degenerate phases. Insets figures are samples of the two-band degenerate phases off the red lines. (b-e) Typical band structures of the three-band degenerate phases, the parameters used are marked by cyan points in (a). (f) Phase diagram at $\eta_1 = 0.5$, the blue lines are two-band degenerate phases. The inset figure is a sample of the non-degenerate phases off the blue lines. (g-j) Typical band structures of the two-band degenerate phases, the parameters used are marked by magenta points.

If one considers more complicated interactions, like the Coriolis force which is widely used to break TRS, one may can not relate the frequency $\omega$ directly to the eigenvalues of an eigenfunction through the above procedure. Y. Liu et al., recently proposed a Schrödinger-like equation of phonons, which overcomes this problem and thus the concepts of wavefunction as well as other topology-related quantities can be naturally introduced.
6.3. Phase Diagrams and High Degenerate States

High degenerate states, as well as the approximate dispersion relation around these points, have always been the focus of study. In Fig. 31, we draw two typical phase diagrams of our mechanical dice lattice system, using the appearances of high degenerate points as a discrimination. As our parameter space is now \( \{ \eta_1, \kappa_2, \eta_2 \} \), we would pin \( \eta_1 \) and show the 2D phase diagram on the \( \kappa_2 - \eta_2 \) parameter space. In Fig. 31 (f), we set \( \eta_1 = 0.5 \) and scan \( \kappa_2 \) from 0 to 3 and \( \eta_2 \) from 0 to 4. We find there are several two-band degenerate phases in this parameter region, as we marked by blue lines. Fig. 31 (g-j) are typical band structures on the four two-band degenerate phases with its parameters marked by magenta dots. As we are only interested in the stable solutions, we ignore the purely imaginary band, which may make the total number of bands fewer than six. In Fig. 31 (i), no explicit degenerate point can be seen as the middle two bands appeared coincidently along all our \( \mathbf{k} \) space route. A typical band structure of the non-degenerate phase is also shown in the inset of Fig. 31 (f). If we compare Fig. 31 (g) with Fig. 31 (j), we can see that the former is more similar to the mechanical graphene results, while the later shows clearly a six band feather. This can be understood that, as \( \kappa_2 \) decreases, the connect between the two sub honeycomb lattices becomes weak. The limit case is \( \kappa_2 = 0 \), which degrades our results to the mechanical graphene results, regardless of the value of \( \eta_2 \).

The most distinct point of the electrical dice lattice is it has the three-band degenerate point, which is made up of a flat band intersecting at the degenerate point of the conventional Dirac cone. Thus, we want to see whether the three-band degenerate point still exists in the mechanical dice lattice. After some numerical and analytical evaluations, we find that the three-band degenerate points could exist when we set \( \eta_1 = 0 \). We show the three-band degenerate phases in Fig. 31 (a), marked by the red lines. The rest areas are characterized by two-degenerate phases. Again, in
Fig. 31 (b-e), we show typical band structures from the four red lines, with the parameters specified by the cyan points. As the same with the case of $\eta_1 = 0.5$, the band structure with a small $\kappa_2$ is rather similar to that of the mechanical graphene, as is shown in Fig. 31 (b). Fig. 31 (c) has a local dispersion behavior which is very similar to the electrical dice lattice, i.e., the green and yellow bands form a Dirac cone at the $K(K')$ point, which intersects with a third flat purple band. Fig. 31 (d) shares the same behaviors with Fig. 31 (i), plus that the orange band touches the two flat bands at the $K(K')$ point. Fig. 31 (3) shows six bands all over the momentum space, and no instable states exist. From Fig. 31 (b-e), we can see that the numbers of band on top of the three degenerate points change gradually, i.e., from zero in Fig. 31 (b) to three in Fig. 31 (e). And the inset figures show the intermediate processes.

To gain further understanding about the phase diagrams, we try to discriminate the band structures analytically. We expand the dynamic matrix $\Gamma(k)$ around the $K = (\frac{2\pi}{3a}, \frac{2\pi}{\sqrt{3}a})$ and $K' = (-\frac{2\pi}{3a}, \frac{2\pi}{\sqrt{3}a})$ points and keep only lower order terms. As $\Gamma(k)$ is a six order matrix, it is still rather difficult to obtain a readable general analytical expressions. However, as most degenerate points are at the $K(K')$ points, we thus can only focus the energy levels on these points. The frequency square at $K$ point is

$$
\omega^2 = \begin{cases}
3 - \frac{3}{2} \eta_1, \\
3\kappa_2 - \frac{3}{2} \eta_2 \kappa_2, \\
\frac{3}{4} [4 - 2\eta_1 - (-2 + \eta_2)\kappa_2 \pm \sqrt{4\eta_1^2 + (-2 + \eta_2)^2 \kappa_2^2}], \\
\frac{3}{4} [2 - \eta_1 - 2(-2 + \eta_2)\kappa_2 \pm \sqrt{(-2 + \eta_1)^2 + 4\eta_2^2 \kappa_2^2}] 
\end{cases}
$$
By setting $\eta_1 = 0$, we can get two bands at $\omega^2 = 3$, regardless of $\kappa_2$ and $\eta_2$. To achieve the three-band degenerate state, we just need to adjust $\kappa_2$ and $\eta_2$ to make another band across the $\omega^2 = 3$ point. Thus, we can get

$$
\eta_2 = \begin{cases} 
2 \rightarrow \text{Band II} \\
2 - \frac{2}{\kappa_2} \rightarrow \text{Band III} \\
1 + \frac{1}{1 - 2\kappa_2} \rightarrow \text{Band I/IV}
\end{cases}
$$

which defines the three-band degenerate phases. In Fig. 31 (a), the top-left red line shares the same $\eta_2(\kappa_2)$ relation with the bottom-right red line, as they correspondence to $\omega^2 = \frac{3}{4}[2 - \eta_1 - 2(-2 + \eta_2)\kappa_2 \pm \sqrt{(-2 + \eta_1)^2 + 4\eta_2^2\kappa_2^2}]$. The physical picture here is that, in the limit of $\eta_1 = 0$, as explained in the Appendix, one of the three inequivalent mass points, i.e., the green mass point in Fig. 30, can be decoupled from the rest two around the $K(K')$ point, up to the first order. The decoupled two bands are degenerate at the $K(K')$ point, and the three-band degenerate states can be achieved as long as on the four bands in the rest crosses $\omega^2 = 3$. The analysis for Fig. 31 (f) follows the same philosophy.

The most direct consequence, which results from the differences of the two sub honeycomb lattices, is the naturally breaking of the inversion symmetry. Next, we are going to investigate the effect of the inversion symmetry breaking from a prospect of topology-related quantities.

### 6.4. Anomalous Valley Hall Effect in Semimetal State

We first consider the Berry curvature associated with the occupied Bloch states. In the presence of an in-plane electric field, an electron will acquire an anomalous velocity proportional to the Berry curvature in the transverse direction [304–306]. This leads to the well known quantum anomalous Hall effect and the anomalous valley Hall effect. From the consideration of symmetry,
in the momentum space, the Berry curvature

$$\Omega(k) = \nabla_k \times \langle \phi_n(k) | i\nabla_k | \phi_n(k) \rangle,$$

is odd in the presence of TRS and even in the presence of inversion symmetry. Here, the subscript $n$ denotes the band index and $\phi(k)$ is the Bloch wave defined in Eq. (6.1). Thus when the system keeps both TRS and inversion symmetry, the Berry curvature is zero over the whole Brillouin zone. As we keep TRS in our system while breaking the inversion symmetry, we expect to obtain an odd finite Berry curvature in our Brillouin zone. The Chern number, which is the integration of Berry curvature within the entire Brillouin zone, should be zero, without breaking TRS. But the local finite Berry curvature should bring anomalous valley Hall effect in our semimetal phases, which is difficult to realize in the conventional electronic system.

Here in Fig. 32, we show the Berry curvature in the three-band degenerate configuration which correspondences to Fig. 31 (e) with six bands. From Fig. 32 (a-f), we can clearly see that there exists a finite Berry curvature across the Brillouin zone, especially around $K(K')$ points. The colorbar is shown in the right of Fig. 32 (g). Also, the Berry curvature possesses odd inversion symmetry with respect to the $\Gamma$ point, which follows the restriction of the TRS. To justify our numerical results, we try to obtain the Berry curvature analytically around the $K(K')$ points. The analytic results is shown as the red dished line, in Fig. 32 (g), in comparison with the numerical results, which is the blue solid line. Here we want to say that as our dimension of the system is six, it is difficult to obtain a general analytical result. We thus reduce our dynamic matrix into a four dimensional matrix. As Berry curvature dependences on the Bloch wave, which is normalized, the reduction of dimension will modify the value of Berry curvature, in a small quantity sense. To better compare with the analytical results, our numerical results in Fig. 32 (g) are also calculated from the reduced four dimensional dynamic matrix. We checked that there is only a small difference with the value.
Fig. 32. Berry curvature: numeric versus analytic. (a-f) Berry curvatures for the six bands of a three-degenerate band configuration. (g) A comparison between the numerical result (blue solid line) and the analytical result (red dished line) at the vicinity of $K(K')$ points. The numerical result is from the green line marked in (b). The parameters used are $\eta_1 = 0, \kappa_2 = 1.5, \eta_2 = 0.5$, which correspondences to Fig. 31 (e).
on the line marked by green in Fig. 32 (b). As the dimension of the system is still high, it is difficult to obtain a universal expression with arguments of system parameters. However, the sign, value as well as the trend of the Berry curvature around the $K(K')$ points are verified. The detail approach is shown in Appendix. The finite Berry curvature will contribute to a mechanical force under the external field, which leads to an anomalous valley Hall effect in our semimetal phases. We also would like to state that, while $\eta_1 = 0$ is a limit case, the case of $\eta_1 = 0.5$ can still possess the same effect, as it is guaranteed by the breaking of the inversion symmetry in our system.

If ones want to obtain a finite Chern number in this system, the well established way is to introduce Coriolis force, as suggested by many recent works. Briefly, when we uniformly rotate the classical system with angular frequency $\Omega_a$, the mass point, with mass $m$ and velocity $v$, will experience a force proportional to $mv \times \Omega_a$. This is equivalent to the Lorentz force for the charged particles under a magnetic field. It is a open question about whether the TRS breaking effect will open the gap in the semimetal phase or not.

6.5. Edge States

Then we investigate edge states in our mechanical dice lattice system. We employ hard walls along the zigzag edges to form a ribbon structure, and consider the periodic boundary along its perpendicular direction. Of particular interest is whether the restriction will induce a gap at the degenerate points. We find that in most cases, the gap will open, as expected from the confinement effect. However, for the cases which lay at the most bottom line of Fig. 31 (a,f), we find gapless states between $K(K')$ projections which localize on the edge of the system.

In Fig. 33 (a,b), we show two ribbon band structures which correspondence to the bulk band structures in Fig. 31 (e,j), respectively. We can see that the density of states are finite along the bulk degenerate energy. The behavior of the bands around the bulk degenerate energy reminds us of the
Fig. 33. Ribbon band structure and edge states in three and two bands degenerate configurations. (a) Ribbon band structure of a three-band degenerate bulk configuration, this is the case of Fig. 31 (e). (b) Ribbon band structure of a two-band degenerate bulk configuration, this is the case of Fig. 31 (j). (c-d) Distribution of the weight of the edge states along the index $i$ of mass points in one unit cell. The corresponding bands are marked by the same color in (a,b). (e) A schematic figure of the polarization of edge states.
gapless edge states in many topological nontrivial materials [242, 243, 302, 311, 315]. These edge states basically have quite distinct trends with the nearby bulk states. To check whether these bands are localized on the edge, we draw the distribution of the weight of the wave function along the confinement direction of one unit cell, in Fig. 33 (c,d). In our simulation, there are 252 mass points within one unit cell, and we mark the index of mass points from one end to the other monotonically. In Fig. 33 (a), we see there are mainly three bands with unique behaviors, which are marked by red, cyan and magenta. We arbitrarily choose a momentum where these strange bands appear and draw its real space distributions in Fig. 33 (c). We can see that these bands are indeed edge states. To verify the level crossing phenomenon between the red and cyan bands, we choose momentums before and after the crossing points and confirm that the localization behavior does not change around the crossing points, i.e., the red band edge states localize on one edge and the cyan edge states localize on the other edge. A schematic figure is shown in Fig. 33 (e). Also, if we zoom in the flat band around $\omega = \sqrt{3}$ in Fig. 33 (a), we find that there are actually two degenerate flat bands. One is already marked by cyan and the other is kept blue. Furthermore, the two degenerate bands are localized on the same edge, i.e., the opposite side of the red and magenta edge states. One may say the $\eta_1 = 0$ case is in a limit, we also find similar behaviors at $\eta_1 = 0.5$. In Fig. 33 (b), we show the ribbon band structure of a two-band degenerate state. Its bulk band structure is shown in Fig. 31 (j), which is also from the most bottom line of the phase diagram. In Fig. 33 (d) we show the real space distributions of the edge states.

The slope of the red edge states makes sure that there is at least one conducting channel around the bulk degenerate energy. Interestingly, as the conducting channels are at the opposite side of the non-conducting channels for the edge states, this makes our system possess a real space one side conducting property. As can be seen from Fig. 30, there is even no inversion symmetry along
the vertical direction, which makes the asymmetry edge states possible. Here we also want to mention that the level crossing behavior shown here can happen within a finite parameter regions. For example, in the case of \( \eta_1 = 0 \), if we check the ribbon band structure along the most bottom line, this level crossing behavior can happen between \( \eta_2 \). When \( \eta_2 \) is larger than that, the red state will be flat and coincide with the blue band, leading to two edge states with the same frequency but localize on different edges. For other high degenerate phases, the confinement effect will open a gap in the ribbon band structure. But edge states, which possess bands connecting the projections if \( K \) and \( K' \) valleys can exist.

6.6. Conclusion

Summarizing, we systematically investigate the band structure of the mechanical dice lattice system. Inversion symmetry can be naturally broken in the general case of our system while time reversal symmetry is kept all the time. We find three-band and two-band degenerate phases and give analytical expressions for the appearances of these high degenerate points. As the breaking of the inversion symmetry, finite Berry curvatures are found within the momentum space, especially around the \( K \) and \( K' \) valleys, which demonstrate a topological nontrivial band structure and indicate the existence of the anomalous valley Hall effect. As the degenerate points do not need to be opened by the inversion symmetry breaking effect, this makes our system a mechanical topological semimetal. We also consider the confinement effect and find gapless edge states around the degenerate energy. Within certain range of the parameter space, we find conducting edge channels associated with a particular edge and non-conducting edge channels in the other side, between the projections of \( K \) and \( K' \) valleys. A direct extension of our work is to study the mechanical dice lattice under a uniformly rotating frame, which would break the time reversal symmetry which might lead to a finite Chern number and topological protected edge states might be found. Within such circumstances,
one could investigate whether high degenerate phases could still be found. And whether the well
established bulk edge correspondence is still held.

6.7. Appendix

In this Appendix we will show the procedures to our analytical results and here we have already
assumed $\kappa_1 = 1$. The starting point is Eq. (6.1, 6.2). As we mainly focus on the band structure
around the $K(K')$ points, we set the momentum at the $K$ point to obtain the six energy levels
at this specific point. Generally speaking, the six energy levels are determined by $\kappa_2, \eta_1, \eta_2$. By
setting $\eta_1 = 0$ and letting three of the six energy levels to have the same energy, we can obtain
the expression for the three-band degenerate phases. The expression for the two-band degenerate
phases can be gained through the similar approach, after specifying $\eta_1$. However, to analyze the
quantities that need the information around the degenerate points, we can not obtain a general simple
expression. To try our best to verify the numerical results. We first expand the dynamic matrix, Eq.
(6.2), around the $K = \left(\frac{2\pi}{3a}, \frac{2\pi}{\sqrt{3}a}\right)$ point, and introduce $(dk_x, dk_y)$ through $k_x = \frac{2\pi}{3a} + dk_x, k_y = \frac{2\pi}{\sqrt{3}a} + dk_y$. Neglecting higher order terms of $(dk_x, dk_y)$, the off diagonal parts of the dynamic
matrix are changed to:

$$
\Gamma_{ab}(dk_x, dk_y) = \begin{pmatrix}
3\eta_1 - i\frac{\sqrt{3}(\eta_1-4)}{8}dk_y + \frac{\sqrt{3}(\eta_1-4)}{8}dk_x & i\frac{3\eta_1}{8} - 3\frac{\sqrt{3}\eta_1}{8}dk_y + i\frac{\sqrt{3}\eta_1}{8}dk_x \\
\frac{3\eta_1}{4} - 3\frac{3\sqrt{3}\eta_1}{8}dk_y + i\frac{\sqrt{3}\eta_1}{8}dk_x & \frac{3\eta_1}{4} - i\frac{3\sqrt{3}(\eta_1-4)}{8}dk_y + \frac{\sqrt{3}(\eta_1-4)}{8}dk_x
\end{pmatrix}
$$

From the expressions of $\Gamma_{ab}$ and $\Gamma_{bc}$, we can see that each matrix element contains a $O(1)$
term, which is proportional to $\eta_1$ and $\eta_2$, plus the $O(dk)$ terms. The physical meaning of $\Gamma_{ab}$
and $\Gamma_{bc}$ is the coupling between the inequivalent mass points. This indicates that in the limit of
$\eta_1 = 0$, the coupling between the mass points $a$ and $b$ is at best the first order term. As argued
by T. Kariyado et al., $\eta$ controls the relation between the longitudinal and the transverse wave
modes. In the mechanical graphene system, at the limit of $\eta = 0$, there is no distinction between the
longitudinal and transverse waves, so that the system possesses a two-fold degenerate dispersion relation of the nearest neighbor tight-binding graphene system. In our mechanical dice lattice, however, even we set \( \eta_1 = 0 \), the blue mass points in Fig. 30 still couples with the red mass points through \( \kappa_2, \eta_2 \), thus possesses much more rich dynamics. Mathematically, as long as \( \eta_2 \neq 0 \), \( \Gamma_{bc} \) can always contribute a \( O(1) \) order coupling between the blue mass points (b) and the red mass points (c). Indeed, to degrade our mechanical dice lattice down to the mechanical graphene system, we just need to set \( \kappa_2 = 0 \).

To calculate the Berry curvature around the \( K \) point, we need to get the Bloch wave first. This is difficult for a six dimensional matrix. However, when \( \eta_1 = 0 \), we can boldly ignore the influence of mass points \( a \) on the mass points \( b, c \), as \( \Gamma_{ab} \sim O(dk) \). We then deal with:

\[
\tilde{\Gamma}(dk) = \begin{bmatrix}
\Lambda_1 + \Lambda_2 & \Gamma_{bc}(dk) \\
\Gamma_{bc}^\dagger(dk) & \Lambda_2
\end{bmatrix}.
\]

For this four dimensional reduced dynamic matrix, we can obtain analytical expressions for the eigenfunctions, after plugging in the values of \( \kappa_2, \eta_2 \), from which the Berry curvature can be obtained. In Fig. 32 (g), we plot the Berry curvature along \( k_y = \frac{2\pi}{\sqrt{3}a} \). The parameters we used are \( \kappa_2 = \frac{3}{2}, \eta_2 = \frac{1}{2} \). The Berry curvature expression is:

\[
\Omega(dk_x) = \tau_z(1.2 - 7.43dk_x^2),
\]

where \( \tau_z = 1(-1) \) for \( K(K') \) point.
7. NONLINEAR DYNAMICS INDUCED ANOMALOUS HALL EFFECT IN TOPOLOGICAL INSULATORS

We uncover an alternative mechanism for anomalous Hall effect. In particular, we investigate the magnetization dynamics in an insulating ferromagnet (FM) deposited on the surface of a three-dimensional topological insulator (TI), subject to an external electrical driving signal. The spin-polarized current on the TI surface induces a spin-transfer torque on the magnetization of the top FM while the associated magnetization dynamics can change the transmission probability of the surface electrons through the exchange coupling and hence the current. We find a host of nonlinear dynamical behaviors including multistability, chaos, and phase synchronization. Strikingly, a dynamics mediated Hall-like current can arise, which exhibits a nontrivial dependence on the channel conductance. We develop a physical theory to elucidate the mechanism that leads to the anomalous Hall effect. The nonlinear dynamical origin of the effect stipulates that a rich variety of final states exist, implying that the associated Hall current can be controlled to yield desirable features. The phenomenon can find applications in spintronics.

7.1. Introduction

Hall effect is one of the most striking and widely investigated phenomena in contemporary physics. The classical Hall effect is simply due to the Lorentz force, the quantum Hall effect can be attributed to the emergence of surface states due to the formation of Landau levels in a magnetic field, and the fractional quantum Hall effect results from many body interactions [322]. In certain materials, in absence of a magnetic field, the spin-orbit interaction can lead to spin Hall effect, the physical base for topological insulators (TIs) [242,243,323], a subfield of tremendous recent interest in condensed matter physics. In this paper, we report our finding of an alternative mechanism,
a mechanism that is essentially dynamics based, which can result in anomalous Hall effect. The underlying physics is the spin-transfer torque (STT).

STT originates from the exchange coupling between the magnetization in a ferromagnet and a polarized spin current. When such a current flows close to a ferromagnet, a finite torque will be exerted on the magnetization of the ferromagnet, provided that the magnetization is not aligned with the direction of spin polarization. Semiclassically, the dynamical evolution of the magnetization can be described by the Landau-Lifshitz-Gilbert (LLG) equation [324]. In spintronics applications, STT is interesting as it provides a way to manipulate or even switch, electronically, the magnetization in the ferromagnet, which can lead to reduced dimensions and efficient energy consumption as compared to with the conventional magnetic schemes [325]. Previous studies on STT focused on heavy metals with strong spin-orbit coupling (SOC) which can generate strong enough spin-polarized current through the spin Hall effect (SHE) [326–328] or in materials with strong Rashba SOC effect at the interfaces [329–332]. Another promising material is TIs that possess a bulk band gap but with metallic massless Dirac surface states [242, 243, 323]. The strong Rashba-type SOC guarantees that the momentum of the surface electron is interlocked to its spin. When a TI is coated with a thin film of insulating ferromagnet, a host of novel magnetoelectric effects can occur. In this configuration, phenomena that have been predicted theoretically include the inverse Spin-Galvanic effect [333], current-induced magnetization reversal [334], anomalous magnetoresistance of a two-dimensional ferromagnet/ferromagnet junction [335], and auto-oscillation of magnetization [336].

In this paper, we focus on the dynamics of magnetization in an insulating ferromagnet as well as the spin-polarized current on the surface of TI. When the system is subject to a periodic electric driving signal with a $dc$ offset applied to the the TI surface, rich nonlinear dynamical phenomena in magnetization can arise in the upper insulating ferromagnet via the induced STT, which include
multistability, chaos, and phase synchronization. In certain range of the ratio of the $dc$ and $ac$ amplitudes, e.g., $[-1, 1]$, there are critical points at which the magnetization dynamics in the ferromagnet can change abruptly between two stable states (attractors), leading to interesting (adiabatic) dynamical transport of the surface electrons in the 3D TI via the exchange coupling (i.e., the proximity effect). Our main finding is the emergence of an unconventional Hall-like current results from the STT-induced magnetization, which exhibits an anomalous physical relation between the longitudinal and transversal conductance. To our knowledge, the nonlinear dynamical mechanism uncovered in this paper represents an alternative route to Hall effect, which has not been noted previously. The dynamics-induced anomalous Hall effect can have potential applications in spintronics.

7.2. Model

We consider a coupled system consisting of a ferromagnet and a 3D TI, as shown in Fig. 34, where the former sits on the top surface of the latter. When a voltage is applied to the surface, a spin-polarized current will be induced along the direction of the voltage drop, i.e., the $+x$ direction, which is the easy axis of the upper ferromagnet (an energetically favorable direction of spontaneous magnetization). As the spin-polarized current flows through the region of the ferromagnet, the net spin will exert a torque, i.e., spin-transfer torque, on the magnetization of the ferromagnet, the dynamics of which is governed by the LLG equation. The exchange coupling between the two materials will change the transport behaviors of the TI, leading to a redistribution of the spin-polarized current. The typical time scale of the dynamical evolution of magnetization is on the order of $1\text{ns}$, which is quite slow as compared to the surface electron response time. It is thus reasonable to apply the adiabatic approximation to modeling the dynamical behavior of the surface electrons. In particular, the transmission coefficient of the surface electron of the TI can be solved using the time-independent Schrödinger equation with a constant exchange coupling term at any
specific time \[334,336\]. The low energy effective surface state Hamiltonian of the TI is given by

\[
H = \hbar v_F (\mathbf{\sigma} \times \mathbf{k}) \cdot \hat{z} + \mathbf{m} \cdot \mathbf{\sigma} \Theta(x)\Theta(L-x),
\]

(7.1)

where \(\mathbf{\sigma} = (\sigma_x, \sigma_y, \sigma_z)\) are the Pauli matrices describing the spin of the surface electron, \(\Theta(x)\) is a step function to ensure only the ferromagnet region \((0 < x < L)\) has the exchange coupling, \(\hbar k = -i\hbar(\partial_x, \partial_y, 0)\) is the momentum operator for the surface electron, \(v_F\) is the Fermi velocity, and \(\mathbf{m}\) is the magnetization in the upper ferromagnetic layer. We assume the surface of the TI is within the \(x-y\) plane so that the \(z\) component of the surface electron momentum is zero, as shown in Fig. 34a. The first term of the effective Hamiltonian describes the conventional spin-orbit coupled TI surface state while the second term introduces the electron exchange interaction with the proximate ferromagnet. Let \(\xi \equiv |\mathbf{m}|\) be the magnitude of the vector \(\mathbf{m}\) so that \(\mathbf{n} = \frac{1}{\xi} \mathbf{m}\) is the unit vector of magnetization. A typical evolution of \(\mathbf{n}\) is shown in Fig. 34b.

From the Hamiltonian (7.1), we can calculate the transmission coefficient of the ferromagnet region. The procedure is to write down the wavefunctions before entering, within, and after exiting the ferromagnet region, and then to apply the boundary conditions at the interfaces of the three regions. The result is \[334\]

\[
t = \frac{-4 \cos \theta \hbar v_F \tilde{k}_x}{\alpha(A + ie^{i\theta}B)},
\]

(7.2)

where

\[
A = \{ \alpha_2 [ie^{-i\theta} \hbar v_F (\tilde{k}_y + i\tilde{k}_x) - E - m_z] \\
- \alpha_1 [ie^{-i\theta} \hbar v_F (\tilde{k}_y - i\tilde{k}_x) - E - m_z] \},
\]

(7.3)

\[
B = \{ \alpha_2 [ie^{-i\theta} (E - m_z) - \hbar v_F (\tilde{k}_y - i\tilde{k}_x)] \\
- \alpha_1 [ie^{-i\theta} (E - m_z) - \hbar v_F (\tilde{k}_y + i\tilde{k}_x)] \},
\]

and \(E = \hbar v_F k_F, k_x = k_F \cos \theta, k_y = k_F \sin \theta, \hbar v_F \tilde{k}_x = \sqrt{E^2 - m_z^2 - (\hbar v_F \tilde{k}_y)^2}, \hbar v_F \tilde{k}_y = \hbar v_F k_y + m_x, \alpha = e^{i k_F L \cos \theta}, \alpha_1 = e^{i(\tilde{k}_x + m_y)L}, \text{ and } \alpha_2 = e^{i(-\tilde{k}_x + m_y)L}.\) Here \(k_F\) is the Fermi wave
vector and $\theta$ is the incident angle of the electron to the ferromagnet region. From the transmission coefficient $t$ we can get the current densities along both $x$ and $y$ directions as

$$j_x = -\frac{k_F e^2}{2\pi \hbar} V \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} d\theta |t|^2 \cos \theta,$$

$$j_y = -\frac{k_F e^2}{2\pi \hbar} V \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} d\theta |t|^2 \sin \theta,$$

where $V = V_{dc} + V_{ac} \cos \Omega t$ is the driving voltage along the $x$ direction. On the surface of a TI, the spin density of the electrons can be written as

$$\langle \sigma \rangle = -\frac{1}{e v_F} \langle j \times \hat{z} \rangle = \frac{1}{e v_F} \cdot (-j_y, j_x, 0) = \frac{j_x}{e v_F} \cdot \eta,$$

where $\eta = (\eta_x, 1, 0)$. The quantity $|\eta_x| = |j_y/j_x| = |\sigma_{xy}/\sigma_{xx}|$ is the ratio of the Hall conductance to the channel conductance [307, 336]. Indeed, when the surface current is outside the ferromagnet regime, we have

$$|t|^2 = \frac{\cos^4 \theta}{\cos^4 \theta \cos^2 (k_x L) + (\sin^2 \theta - 1)^2 \sin^2 (k_x L)},$$

which is an even function of $\theta$ so that $j_y = 0$. However, under the influence of the magnetization, $|t|^2$ is no longer an even function of $\theta$, which leads to a finite $j_y$. Physically, this is because the $y$ components of the current contributed by the electrons with incident angles $\theta$ and $-\theta$ do not have the same magnitude so that a net $j_y$ component appears. The situation can be seen schematically through Fig. 34c, where the central dashed circle is electron’s Fermi surface in the momentum space without the effect of the magnetization. However, when a current flows through the ferromagnet, the magnetization evolves [Fig. 34b] and the position of the Fermi surface will shift, as shown in Fig. 34c. Since there is no external voltage applied along the $y$ direction and there is no external magnetic field neither, $j_y$ originates entirely from its interplay with $j_x$ through the exchange coupling, giving rise to an anomalous Hall effect.
When a spin-polarized current flows under the ferromagnet, the dynamics of the magnetization is governed by the following LLG equation:

\[
\dot{n} = -\frac{D}{\hbar} n \times \hat{x} + \alpha_G n \times \dot{n} + \frac{1}{\hbar} T,
\]

where the first term describes the procession along the easy axis \(\hat{x}\) and \(D\) represents the anisotropy energy of the ferromagnet. The second term characterizes the damping of the magnetization with \(\alpha_G\) being the Gilbert damping constant. The last term represents the spin-transfer torque \(T = \langle \sigma \rangle \times m = \xi \langle \sigma \rangle \times n\), which comes from the effective exchange coupling averaged over the entire ferromagnet region.

In our simulations, we set the initial direction of the magnetization to be along the easy axis, i.e., \(n(t = 0) = (1, 0, 0)\). We then calculate the electron transmission coefficient and the average spin density. The magnetization at the next time step can be obtained through the updated spin-transfer torque.

### 7.3. Results

#### 7.3.1. Bifurcation Diagram and Anomalous Hall Currents.

The coupling term in Eq. (7.6) is nonlinear, rendering possible complex dynamical behaviors including chaos. These behaviors can be uncovered through a systematic computation of the bifurcation diagram. Specifically, we set \(\Omega/\omega_F = \Omega/(D/\hbar) = 10\), \(\xi/E = 0.1\), \(k_F L = 100\), \(E^2 e V_{ac}/(2\pi \hbar^3 \omega_F v_F^2) = 100\), and use the ratio \(V_{dc}/V_{ac}\) as a convenient bifurcation parameter (in the range \([-4, 4]\)). The resulting bifurcation diagram is shown in Fig. 35a. We observe a rich variety of dynamical behaviors, e.g., a chaotic region (marked with purple stripe) and a phase-synchronization region (marked with yellow stripe). Representative time series in the chaotic regime are shown in Figs. 35c and 35d, and those from the phase synchronization regime are shown in
Figs. 35e and 35f. Considering that the driving frequency $\Omega$ is ten times larger than the intrinsic procession frequency of magnetization, it is remarkable that phase synchronization can occur. From the behavior of $n_y$ in Fig. 35e, we see that it undergoes periodic oscillations of period about $T = 2\pi/\Omega = 2\pi/(10\omega_F) \approx 0.6/\omega_F$.

The time series shown in Figs. 35d and 35f are in fact the time evolutions of the anomalous Hall current density $j_y(t)$. For Fig. 35d, the behavior is chaotic, which can be seen by noting, e.g., that the occurrences of the local minima and their values are irregular. For Fig. 35f, the current density exhibits a period-2 behavior. In both cases, the rms (root mean square) value of the Hall current density is finite. The Hall effect is anomalous because it arises without any external magnetic field. As we argue later, it has a dynamical origin, i.e., it is induced by the nonlinear, dynamical interactions due to spin-transfer torque between the FM and TI.

7.3.2. Multistability.

From the bifurcation diagram in Fig. 35, we see that there are a number of transition regimes, in which the dynamics of the system change characteristically. In Fig. 35b, we show a zoom in figure of the transition region, which is marked by the cyan strip in Fig. 35a and starts from $V_{dc}/V_{ac} = 0.45$ to $V_{dc}/V_{ac} = 0.55$. We can see there exists a rather abrupt change of the bifurcation around $V_{dc}/V_{ac} \approx 0.517$. Generally, a transition region along the parameter axis is one in which there is multistability. Preceding the transition, there is one final state (attractor). At the onset of transition, a new attractor is born, leading to coexistence of two attractors, each with its own basin. As the parameter is varied (e.g., increased) in the transition region, the basin of the new attractor grows while that of the “old” attractor, the continuation of the attractor before the transition, shrinks. The disappearance of the basin of the “old” attractor marks the end of the transition regime. Thus, before and after the transition, the final states of the system are typically characteristically distinct.
To investigate the detail evolution along the transition region, we systematically simulate the system under different initial conditions and the results are shown in Fig. 36. For our TI-FM coupled system, since \( \mathbf{n} \) is a unit vector, the phase space is effectively the surface of a sphere in which all possible initial conditions and final states lie. On the unit sphere of the magnetization vector, the initial conditions can be represented as
\[
\mathbf{n} = (\sin \beta \cos \phi, \sin \beta \sin \phi, \cos \beta).
\]
Choosing a uniform, 100 \( \times \) 100 grid for \( \beta \in [0, \pi] \) and \( \phi \in [0, 2\pi] \), we obtain \( 10^4 \) different initial conditions and then calculate the final attractor for each initial condition. To quantify the final states under different initial conditions, we calculate the mean value of \( n_y \) after a relative long evolution time. In Fig. 36c, we show a typical basin of the system under multistable state, e.g., \( V_{dc}/V_{ac} = 0.5179 \). The upper-half figure is an aerial view of the unit sphere while the bottom-half figure is a ground view of the unit sphere. Compared with the colorbar we can see there are clearly two distinct states, i.e., one is the red state, which \( n_y \approx 0 \), and the other is the blue state, which \( n_y \approx -1 \). In Fig. 36a, we make a statistics about the ratio of the red/blue states versus the system parameter. We can see that there is a gradual monotone change of the percentage of both states. In Fig. 36b–e, we show four basins under \( V_{dc}/V_{ac} = 0.5, 0.5179, 0.5228 \) and \( 0.525 \), respectively. The shrink of the old attractor and the growth of the new attractor are clearly shown.

We now investigate the physical signatures of the multistability in the transition region for the TI-FM coupled system. (Multistability is a common phenomenon in nonlinear dynamical systems [4, 337–341].) Figure 37a shows, for \( V_{dc}/V_{ac} = 0.5179 \), two distinct trajectories, projected in the \( n_x - n_z \) plane, which correspond to two different final states (colored according to the mean value of \( n_y \)) after disregarding reasonably long transients. Fig. 37b shows the corresponding basins of attraction, and Fig. 37c shows a two-dimensional view of Fig. 37b, where the upper panel is an aerial view and the lower panel is a ground view (the same as Fig. 36c). Specifically, one final attractor has
near zero mean $n_y$ values, which are colored as red. For this attractor, the magnetization oscillates in
the vicinity of the $x-z$ plane and both $n_x$ and $n_z$ exhibit a dramatic switching behavior between the
extreme values $-1$ and $1$, as shown in Fig. 37d. (The corresponding time series of distinct current
densities are shown in Fig. 37e - to be discussed below.) For the blue attractor, the mean $n_y$ value is
close to unity, which hence fixes the magnetization vector around $n_y = -1$ with small oscillations in
$n_x$ and $n_z$: the corresponding magnetization vector is oriented close to the $-y$ direction, as shown
in Fig. 37f. Depending on the initial condition, the system settles into either the red or the blue
attractor, signifying multistability.

7.3.3. Anomalous Hall Effect.

A remarkable phenomenon is that, about the transition regime, there is current in the direction
transverse to the channel, i.e., $j_y(t) \neq 0$. This is essentially the Hall current density. Since there
is no external magnetic field, the Hall effect is anomalous - it is induced by the coupling dynamics
between FM and TI. The anomalous Hall current is persistent in that it exists prior to, during, and
after the transition. As the transition regime is swept through, there is a phase change associated
with the Hall current. In particular, for $V_{dc}/V_{ac} = 0.5$ (before transition), the oscillations of the
Hall current density are in phase with the external electrical driving, as shown in Fig. 36c. For
$V_{dc}/V_{ac} = 0.525$ (after transition), the Hall current is $180^\circ$ out of phase with the driving, as shown
in Fig. 36f. During the transition, the two coexisting states (attractors) retain the respective phase
relations with the driving. For example, as shown in Fig. 37e, for $V_{dc}/V_{ac} = 0.5179$, the red
attractor has the same phase as the external driving, which is the continuation of the attractor before
the transition. However, as shown in Fig. 37g, the blue attractor, which evolves to become the
attractor after the transition, has the opposite phase to that of the driving.
To gain insights into the physical and dynamical origin of the anomalous Hall effect in the TI-FM coupling system, we examine the dependence of the Hall conductance, $\sigma_{xy}$, on the channel conductance $\sigma_{xx}$, defined as

$$\sigma_{xx} = \frac{j_x}{V/L} = -k_F L \frac{e^2}{2\pi \hbar} \int_{\frac{\pi}{2}}^{\frac{\pi}{2}} d\theta |t|^2 \cos \theta,$$

$$\sigma_{xy} = \frac{j_y}{V/L} = -k_F L \frac{e^2}{2\pi \hbar} \int_{\frac{\pi}{2}}^{\frac{\pi}{2}} d\theta |t|^2 \sin \theta. \tag{7.7}$$

Some representative results are shown in Fig. 38 for $V_{dc}/V_{ac} = 0.5179$ (in the transition regime) for the red attractor, where the initial condition is $n = (1, 0, 0)$. Similar results have been found for the blue attractor. In previous systems where an anomalous Hall effect arises, the Hall conductance is typically positively correlated with the channel conductance [307], e.g., $\sigma_{xy} \sim \sigma_{xx}^{1.6}$. However, in our TI-FM coupled system, the correlation is negative. From Eq. (7.7), we see that the total current is divided into the $x$ and $y$ components through the functions $\cos \theta$ and $\sin \theta$, where the quantity $k_F L$ has a physical meaning of the number of available carriers within the ferromagnetic region, the integrals characterize the probabilities of transporting to the $x$ or $y$ directions for a single carrier, and $\frac{e^2}{2\pi \hbar}$ is the fundamental conductance unit. Because of the small probability of backscattering, if more electrons transport along the $x$ direction, there will be fewer electrons transporting in the $y$ direction, and vice versa. This behavior can be seen from Fig. 38, where we have $\sigma_{xy} = 0$ when $|\sigma_{xx}|$ is maximal. Without FM, i.e., for a bare TI, the quantum transmission $|t|^2$ is an even function of $\theta$, leading to zero Hall current. When FM is present, the dynamical coupling between its magnetization and channel current in the TI induces a transverse, Hall current, making time-dependent the relative distribution of electrons in both directions.

Figure 38 indicates that, the Hall versus the channel conductance is a multi-function: for one channel conductance value there are two values of the Hall conductance. The function is symmetrical with respect to the line $\sigma_{xy} = 0$. To understand these features, we examine the relation between
magnetization in the FM and the surface currents in the TI. Figure 39 shows the detailed dynamical behaviors of system for two parameter values: $V_{dc}/V_{ac} = 0.5179$ (during the transition) and $V_{dc}/V_{ac} = 0.525$ (after the transition). In particular, Fig. 39a shows the evolution of the magnetization in the FM for one driving period and Fig. 39b shows the currents during the same time period. Each section in Fig. 39a, marked by different color, corresponds to a section from a local maximum (minimum) to a local minimum (maximum) of the channel conductance in Fig. 39b, as marked by the symbols $A - F$. The attractor in Fig. 39a has its magnetization oscillating close to the $x - z$ plane (the red attractor in Fig. 37). A careful examination of the detail of the dynamical evolution indicates that, when $\sigma_{xx}$ reaches its maximum (marked as $A, C, F$), the Hall conductance $\sigma_{xy}$ is close to zero, and the $x$ component of the magnetization is nearly zero as well. This is consequence of the interaction in the TI-FM coupled system. In particular, Eq. (7.1) stipulates that the $y$ component of the electron momentum is coupled to the $x$ component of the spin. Due to the exchange interaction between the magnetization and the current spin, the electron spin tends to align with the magnetization to minimize the total energy. For $n_x \approx 0$, the electrons tend to polarize their spin along other directions, making $\sigma_x$ close to zero so that the $y$ component of the current becomes vanishingly small. For $n_x \approx 1$ (marked with $B, D, E$ in Fig. 39a), we anticipate that the spin of electrons tend to polarize along the $x$ direction, resulting in a very large $y$ component of the current, as shown in Fig. 39b. There is thus a strong correlation between the direction of the magnetization in the FM and the current direction in the TI.

To explain the symmetry of $\sigma_{xy}$ in Fig. 38, we examine the dynamics of the system around the points $A$ and $C$ in Fig. 39b, where $\sigma_{xy}$ and $\sigma_{xx}$ are approximately an odd and an even functions of time, respectively. As a result, for a particular value of $\sigma_{xx}$, there exists two values of $\sigma_{xy}$ with opposite signs and equal magnitude, which correspond to the two different color sections around
$A$ and $C$, as shown in Fig. 39a. We also note that, Fig. 39b exhibits a plateau region of the Hall conductance, i.e., during the time interval between $D$ to $E$. This is due to a reverse behavior of the magnetization about the $-x$ direction, as marked by the red section in Fig. 39a.

The above analysis can be readily extended to the coexisting state (the blue attractor in Fig. 37), as shown in Figs. 39c and 39d. The reason for a relatively small Hall current in this case is that the magnetization is confined along the $-y$ direction so that the value of $n_x$ is relatively small. The plateau behavior of the Hall conductance is opposite to that in Fig. 39b because the reversed motion lies in the opposite arc of the magnetization sphere.

**7.4. Conclusion**

The exchange coupling between magnetization (e.g., in a FM) and the polarized spin current (e.g., in a TI) can lead to surprising physical phenomena. The dynamics of such coupled quantum systems can be treated semiclassically through the LLG equation [324], which are generically nonlinear. As a result, rich nonlinear dynamical behaviors can arise in the system, including multistability, chaos, and phase synchronization.

The main accomplishments of this paper are twofold: from the perspectives of nonlinear dynamics and physics. Dynamically, we focus on the issue of multistability through a detailed investigation of bifurcation and system’s behaviors in the transition regimes. In particular, we demonstrate that characteristic changes in the system’s final state (or attractor) is associated with emergence of multistability in the transition regime. Prior to the regime, the system exhibits one attractor. As the system enters into the transition regime, a new attractor is born, with its own basin of attraction. Further into the transition regime, the basin of the new attractor expands, while that of the original attractor is suppressed at the same time. At the end of the regime, the basin of the original attrac-
tor disappears, and that of the “new” attractor dominates the entire phase space, completing the transition process and leading to a characteristically different attractor.

Physically, we uncover a novel type of Hall effect: due purely to nonlinear dynamical interactions a current transverse to the channel current on the surface of the TI can arise. As no external magnetic field is necessary, the Hall effect is anomalous. The Hall current exhibits a nontrivial dependence on the channel current. The phase of the Hall current relative to that of the electrical voltage depends on the final state of the system and can exhibit a change of $\pi$ as the system parameter changes through the transition regime. For example, before the transition the system falls into an attractor, associated with which the Hall current is in phase with the electrical driving. The new attractor created in the transition regime has the property that the phase of the associated Hall current is opposite to that of the driving. As a result, after the transition regime is passed, the phase difference between the Hall current and the electrical driving is $\pi$. Another feature is that, the anomalous Hall current has a negative correlation with the channel current, which can again be understood through the nonlinear dynamics of the magnetization in FM.

To our knowledge, the dynamics induced anomalous Hall effect through the spin-transfer torque uncovered in this paper is a novel phenomenon. The underlying coupled system between FM and TI can be realized in experiments. A set of experimentally feasible parameter values can be, e.g., $E = 100\text{meV}$ and $k_F = 1\text{nm}^{-1}$, leading to $L = 100\text{nm}$ and $\xi = 10\text{meV}$, where we assume $\hbar \omega_F = 0.1\text{meV}$ and $eV_0 = 0.1\text{meV}$. An appealing feature of this Hall effect is that the dynamical properties of the Hall current can be controlled readily through the channel voltage, e.g., by modulating the ration between its ac and dc components. The fact that the whole system can exhibit a rich variety of nonlinear dynamical behaviors means equally many possibilities to realize the Hall current. This has potential applications in spintronics.

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Fig. 34. Schematic illustration of configuration and basic interaction of the TI-FM coupled system. (a) A thin layer of insulating ferromagnet sits on a 3D TI. The voltage is applied along the $x$ direction. The effective magnetization, $\vec{m}$, oscillates within the ferromagnet and is coupled to the spin-polarized currents, $j_x$ and $j_y$, in an exchangeable manner. (b) A typical evolution of the normalized magnetization $\vec{n}$. (c) The change in the position of the Fermi surface in the wave vector space corresponding to the adiabatic evolution shown in (b). The central dashed circle corresponds to the case without the magnetization.
Fig. 35. Typical dynamical behaviors of the TI-FM coupled system. (a) Bifurcation diagram of the magnetization with respect to ratio of applied dc and ac voltages. The blue, red and green dots represent \( n_x \), \( n_y \), and \( n_z \), respectively. One chaotic regime is marked by a purple stripe and one phase-synchronization regime is marked by a yellow stripe. (b) The zoom in bifurcation of the transition region which is marked by the cyan strip in (a). (c) A representative time series of the magnetization from the purple chaotic regime. (d) Anomalous Hall current corresponding to (b). (e) A representative time series of the magnetization from the yellow phase-synchronization regime, and (f) the corresponding anomalous Hall current. For better visualization, the \( x \) axis in (a) is rescaled.
Fig. 36. Final states (attractor) before and after transition. (a) Change of the ratio of red states and blue states with system parameter $V_{dc}/V_{ac}$ in the transition region. (b-e) Basins for $V_{dc}/V_{ac}$ = 0.5, 0.5179, 0.5228 and 0.525, respectively. The color is calculated from the mean value of $n_y$ after a considerable time.
Fig. 37. Multistability. (a) For $V_{dc}/V_{ac} = 0.5179$ in the transition regime, two coexisting final states (red and blue attractors) in the $n_x - n_z$ phase space. (b) The corresponding initial conditions that lead to the attractors in (a). (c) A two-dimensional view of (b), where the upper panel is an aerial view and the lower panel is a ground view. (d) Typical time series of magnetization for the red state. (e) Typical time series of the anomalous Hall and channel current densities for the red state. (f) Typical time series of magnetization for the blue state. (g) Typical time series of the anomalous Hall and channel current densities for the blue state. Note that the right $y$ axis limits for (d) and (f) are different.
Fig. 38. Dependence of anomalous Hall conductance on channel conductance. The dependence is plotted for $V_{dc}/V_{ac} = 0.5179$ (in the transition regime) and the red attractor, where the brown dots are results from about 100 oscillating periods and the red dots are results from one period.
Fig. 39. Dynamics of magnetization in the multistability regime and its relation with the surface currents. (a) For $V_{dc}/V_{ac} = 0.5179$ in the transition regime, evolution of magnetization of the red attractor (continuation of the attractor preceding the transition) within one driving period, where the initial condition is $n = (1, 0, 0)$. (b) Corresponding time series of the Hall and channel conductances within the same time period. (c) For $V_{dc}/V_{ac} = 0.525$ (after transition), evolution of magnetization for the blue attractor. (d) Corresponding Hall and channel conductances within the same time period. The symbols $A - F$ mark the local maxima and minima of the channel conductance.
The recently discovered phenomenon of chiral-symmetry protected thermalization gap in Hermitian photonic systems [Nat. Phys. 11, 930-935 (2015)] is striking and counterintuitive as it indicates that the photon coherence can be continuously improved by disorders towards an asymptotic limit. We show that the phenomenon disappears completely in time-independent, non-Hermitian photonic systems even when the chiral symmetry is well preserved. In fact, the degree of thermalization generally increases with the disorder strength as one might intuitively expect. As non-Hermitian characteristics (e.g., weak gain and loss) can be expected in realistic physical situations, the phenomenon of thermalization gap may be observed but only in well controlled and high quality experiments.

8.1. Introduction

Recent years have witnessed a rapid growth of interest in Non-Hermitian systems [342, 343]. In open Hamiltonian systems with a symmetry breaking so that the Hermitian properties can no longer be maintained, surprising physical phenomena can arise [344–349]. For example, in condensed matter physics, the conventional principle of bulk-boundary correspondence stipulates that the bulk of the lattice can be characterized by a topological invariant whose value determines the existence of possible gapless edge states. However, a recent work [299] demonstrated that the violation of the Hermitian properties can induce a fractional topological invariant number and lead to a change in the stability of the edge states, thereby defying the bulk-boundary correspondence. Another example occurs in wave propagation/transport, where the conventional wisdom is that phenomena such as diffusion and localization are caused by random disorders. However, it was demonstrated theoretically and experimentally [350, 351] that a sudden transition from ballistic to diffusive motions can
occur even in ordered, time-independent, non-Hermitian systems maintaining a parity-time reversal (\(PT\)) symmetry. Another remarkable physical phenomenon in non-Hermitian systems is the appearance of exception points in the eigenvalue spectrum about which crossing/anti-crossing transitions can occur and the emergence of a new topological Berry phase associated with paths encircling the exceptional points [352, 353]. Similar to problems associated with resonances and discrete-continuous energy transitions where the eigenvalues of the Hamiltonian are necessarily complex to account for, e.g., the finite lifetime of the state, in non-Hermitian systems the eigenvalues are complex. Experimentally, non-Hermitian physics can be implemented and observed in waveguides, photonic crystals, dielectric microresonators, and even in biological neutral networks [354].

Quite recently, the phenomenon of a chiral symmetry protected photonic thermalization gap has been uncovered in a one-dimensional Hermitian system, theoretically [355–357] and experimentally [357, 357, 358]. A system is said to possess a chiral symmetry if (1) there are eigenvalues (labeled by integers \(m\) and \(-m\)) that appear in pairs whose real and imaginary parts have opposite signs, and (2) the associated eigenstates satisfy the relation: \(\phi_n^m = (-1)^n \phi_n^{-m}\), where \(n\) is the space coordinate. Of interest is how random disorders affect the statistical properties of photon thermal fluctuations. In the absence of any disorder, there is a high degree of coherence among the photons. In this case, a properly defined decoherence measure characterizing the fluctuations, i.e., the normalized intensity correlation, assumes the value corresponding to coherent photon states (e.g., a unity value). When there are arbitrarily weak disorders, there is an abrupt transition in the decoherence measure from unity to a value corresponding to incoherence (e.g., 3) at which the photon statistics can be approximately described by the modified Bose-Einstein distribution. As the strength of the disorders is increased from a near zero value, the decoherence measure decreases from, e.g., 3, but can never reach the unity value, in the systems with chiral symmetry. In fact, the lower bound of the
measure has the value of 2 at which the Bose-Einstein distribution holds. A “thermalization gap” thus arises in the plot of the decoherence measure versus the disorder strength [355–357].

The emergence of photon thermalization gap [355–357,357,357,358] is striking and counterintuitive, as it indicates that the degree of photon coherence in the underlying system can be continuously improved by increasing the disorder strength. This result was obtained for purely Hermitian systems with a chiral symmetry, where no emission and/or absorption was assumed to be present (i.e., the refractive index was assumed to be purely real). In physical reality the refractive index can be expected to be generically complex with an inevitable nonzero imaginary part. This consideration motivated us to investigate thermalization in non-Hermitian photonic systems. While we can impose certain symmetries on the non-Hermitian system, special arrangement of the configuration is required. For example, if we demand that the system to be time independent and possess a $\mathcal{PT}$ symmetry, the real and imaginary parts of the refractive index must then be an even and odd function in space, respectively [267, 268]. While $\mathcal{PT}$ symmetry without such a special arrangement can be realized, a time modulation or spatial engineering of the material along the propagation direction is required [269].

We are thus led to consider the more general situation where we assume that the non-Hermitian system is time independent and does not possess a $\mathcal{PT}$ symmetry. Specifically, we study the photon thermalization statistics for a general class of photonic systems of waveguide array in which the refractive index of an individual element can be complex with either sign (i.e., gain or loss). To be more general, we consider disorders that can either retain or break the chiral symmetry. Our main finding is that the degree of photon coherence continues to deteriorate as the disorder strength is increased, a result in sharp contrast to that in Refs. [355–357]. The implication is that, unless in a well controlled experiment with nearly perfect materials in the intermediate time (propagation distance)
Fig. 40. Symmetry considerations of Hermitian and non-Hermitian photonic systems. For a system described by Hamiltonian $H$, Hermiticity symmetry requires $H = H^\dagger$ and chiral symmetry requires $CHC = H$, with $C = \text{diag}(1, 1, \ldots, 1, -1, \ldots, -1)$. Top row: Hermitian systems; bottom row: non-Hermitian systems; left column: systems for which there is a chiral symmetry breaking; right column: systems with chiral symmetry.

regime, the counterintuitive phenomenon that disorder can continue to improve the coherence of photon fluctuations cannot occur. In fact, in non-Hermitian systems no thermalization gap can be expected.

In Sec. 8.2, we explain how non-Hermitian photonic systems can be realized in realistic situations and describe ways to implement disorders with or without preserving the chiral symmetry. In Sec. 8.3, we present and substantiate our main result that in non-Hermitian systems disorders typically deteriorate photon coherence and, as a result, no thermalization gap can ever arise. We provide a discussion in Sec. 8.4 and a detailed analytic derivation of the system equations in Appendix.
8.2. Non-Hermitian Photonic Systems

The Hamiltonian ($H$) matrix structures of Hermitian/non-Hermitian photonic systems with/without the chiral symmetry are illustrated in Fig. 40, where the Hermitian symmetry requires $H = H^\dagger$ and the system is of chiral symmetry if $CHC = -H$, with $C = \text{diag}(1,1,\ldots,1,-1,\ldots,-1)$ being the chiral symmetry operator. For any of the four combinations, the Hamiltonian matrix can be expressed in a $2 \times 2$ block form, where the diagonal blocks are zero for chiral symmetry systems and non-zero for non-chiral systems. Note that the recent series of works on photon thermalization gap [355–357, 357, 357, 358] focused on the class of systems in panel (a) and (b), while our present work deals with systems in panels (c) and (d).

As a concrete setting to investigate the photon statistics in non-Hermitian systems, we consider an array of one-dimensional, single-mode optical waveguides arranged in the $x$ direction with gain and loss, as shown in Fig. 41. Each waveguide has a complex relative permittivity $\epsilon_n + i\epsilon'_n$, and the waveguides are placed in a surrounding medium with a complex relative permittivity $\epsilon_0 + i\epsilon'_0$.

In the idealized situation where the waveguides are identical and equally spaced, the system can be described by a set of complex, coupled mode equations [351]. In a realistic situation random factors are present, introducing disorders that can be modeled through proper perturbations to the coupled mode equations.

We start from the Helmholtz equation governing wave propagation in the system:

$$[\nabla^2 + k_0^2 \tilde{\epsilon}(x)]\Psi(x, z) = 0,$$

where $z$ is the propagation direction, $\Psi(x, z)$ is the electric field amplitude, $k_0$ is the free space wave vector, and $\tilde{\epsilon}(x)$ is the profile of the relative electric permittivity of the system which can be expressed as

$$\tilde{\epsilon}(x) = \epsilon_0 + i\epsilon'_0 + \sum_{n=1}^{N} [\epsilon_n - \epsilon_0 + i(\epsilon'_n - \epsilon'_0)]\zeta_n(x),$$

where

$$\zeta_n(x) = 1, \quad n = 1, 2, \ldots, N.$$
where $2w$ is the width of the each waveguide and $\zeta_n(x) = \Theta(x - x_n + w) - \Theta(x - x_n - w)$ with $\Theta(x)$ being the Heaviside step function. The effective coupled mode equations can be obtained under the approximation that the eigenmode of the individual waveguide is well confined so that the full width half maximum (FWHM) $\ell$ is much smaller than $d$, the spacing between two adjacent waveguides. The equations are [351]

$$-i\frac{d\phi_n}{dz} = i\kappa_n + (C + iC')(\phi_{n+1} + \phi_{n-1}),$$

(8.3)

where

$$\kappa = \frac{k_0^2}{2\beta} \left[ \epsilon_0' + (\epsilon' - \epsilon_0') \tanh \left( \frac{w}{\ell} \right) \right],$$

$$C = \frac{(\epsilon - \epsilon_0)k_0^2 w}{2\beta \ell} \exp \left( -\frac{d}{\ell} \right),$$

$$C' = \frac{(\epsilon_0' - \epsilon') k_0^2 d}{\beta \ell} \exp \left( -\frac{d}{\ell} \right).$$

(8.4)

The quantity $\phi_n$ in Eq. (8.4) is the field amplitude in the $n$th waveguide and $k_0\sqrt{\epsilon_0} < \beta < k_0\sqrt{\epsilon}$ is the propagation constant along the $z$ direction.

To incorporate disorder-immune chiral symmetry in our non-Hermitian waveguide system, we consider two types of disorders. For the first type, the distance between a pair of adjacent waveguides is randomly modified, as shown in Fig. 41(a). Mathematically, insofar as the approximation $\ell \ll |x_n - x_{n-1}|$ holds, the general form of the coupled mode equations remains the same, except that the coupling constant now assumes a spatial dependence:

$$C \rightarrow C_{n,n\pm1} = \frac{(\epsilon - \epsilon_0)k_0^2 w}{2\beta \ell} \exp \left( -\frac{|x_n - x_{n\pm1}|}{\ell} \right),$$

$$C' \rightarrow C'_{n,n\pm1} = \frac{(\epsilon_0' - \epsilon')k_0^2 d}{\beta \ell} \exp \left( -\frac{|x_n - x_{n\pm1}|}{\ell} \right),$$

where $|x_n - x_{n\pm1}| = d(1 + \xi_1)$ and $\xi_1$ is a random variable uniformly distributed in $[-\Delta C, \Delta C]$. It is apparent that the random modulation in the waveguide spacing will lead to disorders in both the...
Fig. 41. Realizations of two kinds of disorders in non-Hermitian photonic systems of a waveguide array. Both the waveguides and the surrounding medium have a complex reflection index. (a) Spacing disorder in which the distances between nearest waveguides are randomly modified. The disorders will result in randomness in both the real and imaginary parts of the coupling constant. (b) Relative permittivity disorder in which the complex refractive index of each waveguide is randomly modified while keeping the distances between the nearest waveguides constant. As a result, there will be random perturbations upon both the diagonal and off-diagonal elements of the Hamiltonian.
real and imaginary parts of the coupling constant. In a matrix representation of the coupled mode
equation, this type of disorders will be present in the off-diagonal elements only, hence the term
“off-diagonal disorders.” In spite of the presence of waveguide spacing disorders, the system is still
chiral-symmetric.

While the off-diagonal disorders described above preserve the chiral symmetry of the non-
Hermitian system, the second type of disorders we study break the chiral symmetry. Conventionally,
this can be done by introducing disorders into the diagonal elements of the coupling matrix. However,
as can be seen from Eq. (8.4), it is not feasible to introduce diagonal disorders while keeping
the off-diagonal elements unperturbed. Our strategy is then to randomly modify the real part of the
relative permittivities of the individual waveguides while keeping the imaginary part identical. This
way both diagonal and off-diagonal disorders are present to break the chiral symmetry, as shown in
Fig. 41(b). Mathematically, including this kind of disorders entails altering the quantities \( \kappa \) and \( C \)
in the following manner (see Appendix for a detailed derivation):

\[
\begin{align*}
\kappa & \rightarrow \kappa + \left( \epsilon_n - \bar{\epsilon} \right) k_0^2 \frac{w}{\ell} \tanh \left( \frac{w}{\ell} \right), \\
C & \rightarrow C_{n,n+1} = \left( \epsilon_n + \epsilon_{n+1} - \bar{\epsilon} - \epsilon_0 \right) k_0^2 \frac{w}{\ell} \exp \left( -\frac{d}{\ell} \right),
\end{align*}
\]

where \( \epsilon_n \) is the real relative permittivity of the \( n \)th waveguide and \( \bar{\epsilon} \) is the corresponding average
value of all the waveguides. We set \( \epsilon_n = \epsilon (1 + \xi_2) \), where \( \xi_2 \) is a random variable uniformly
distributed in \([-\Delta\beta, \Delta\beta]\).

To characterize the photon statistics in the non-Hermitian system, we use the following three
quantities [355]: the normalized intensity correlation \( g^{(2)}(z) \), the intensity probability distribution
\( P(\mu) \), and the photon-number distribution \( P(n_{ph}) \). In particular, \( g^{(2)}(z) \) characterizes the degree of
randomness of the light in the probability space of disorder realizations, which is defined as [355]

\[
g^{(2)}(z) = \frac{\langle I_x^2(z) \rangle}{165 \langle I_x(z) \rangle^2},
\]
where \( I_x(z) = |\phi_x(z)|^2 \) is the intensity of the electric field at the \( x \)th waveguide and \( \langle \cdot \rangle \) denotes ensemble averaging. For coherent light, we have \( g^{(2)} = 1 \). For thermalized (random or chaotic) light, we have \( g^{(2)} = 2 \), where the intensity correlation can be evaluated at the middle of the waveguide array [355, 356]. One may also consider the normalized intensity correlation between a pair of waveguides, from which non-Gaussian statistics corresponding to photon antibunching have recently been found [359].

The intensity probability distribution \( P(\bar{\mu}) \) and the full photon-number distribution \( P(n_{ph}) \) can exhibit different scaling behaviors for different degrees of the photon thermalization, e.g., coherent, thermalized/chaotic and super-chaotic. In our study, we set the initial excitation at the center of the waveguide array and generate a large number of realizations of the input intensity that obeys the coherent Poisson distribution. After the excitation propagates in the waveguides for certain distance (which is effectively time), we examine the intensity at the central waveguide, which is proportional to the photon numbers. The photon-number distribution can be obtained through the ensemble statistics.

For a Hermitian system, the conventional solution approach is to expand the initial wavefunction in terms of the eigenfunctions and then to calculate the time evolution of each eigenfunction. However, this approach is not suitable for non-Hermitian systems, as the eigenfunctions of a non-Hermitian matrix are generally not orthogonal. We thus resort to a direct numerical solution of the coupled mode equations. For convenience, we use the same parameters as the experiment work [351], i.e., \( C_0 = 0.1 \text{mm}^{-1} \) to rescale all the parameters and set

\[
\alpha = 2 \left( \epsilon_0' - \epsilon' \right) \frac{d}{(\epsilon - \epsilon_0) w} = -0.15
\]

to relate \( C' \) to \( C_0 \) and \( \kappa/C_0 = 0.3 \). For adjacent distance disorders, since the unaffected diagonal elements can be removed by incorporating the quantity \( e^{-\kappa z} \) to all the wave amplitude, i.e., \( \phi(z) = \)
\( E(z) e^{-\kappa t} \). This extra time evolution term contributes to an overall gain or loss, depending on the sign of \( \kappa \), but it is identical for all disorder realizations, which can be canceled out when calculating \( g_0^{(2)} \). For disorders in the real relative permittivity, since the imaginary part is constant, the diagonal \( i\kappa \) term can still be removed. Other parameters are set to be \( d = 17 \mu m, w = 5 \mu m, \epsilon_0/\epsilon = 0.2, \) and \( d/\ell \sim 2 \).

### 8.3. Results

To verify the chiral symmetry in our non-Hermitian system, we examine the eigenvalue spectrum and the associated eigenfunctions for a typical realization of the off-diagonal disorder, as shown in Fig. 42. Mathematically, the chiral symmetry requirement \( CHC = -H \) leads to 
\[ \xi_m = -\xi_{-m} \quad \text{and} \quad \phi_{m}^n = (-1)^m \phi_{-m}^n, \]
where \( \xi_m \) stands for the real or imaginary part of the \( m \)th eigenvalue and \( \phi_{m}^n \) is the corresponding eigenfunction at the \( n \)th waveguide. Figure 42 reveals the continuous existence of the chiral symmetry even in the presence of off-diagonal complex disorders.

An alternative way to test the chiral symmetry is to calculate the commutation between the Hamiltonian and the chiral symmetry operator. We note that, if the disorders occur in the real relative permittivity, the chiral symmetry will be broken.

Figure 43 summarizes our main finding that in non-Hermitian systems, the previously reported chiral symmetry protected photonic thermalization gap disappears. In particular, Figs. 43(a,b) show the dependence of the normalized intensity correlation \( g_0^{(2)} \) on the propagation distance and the disorder strength for the two types of disorders. In both cases, a long propagation distance and a high disorder strength can lead to a relatively high value \( g_0^{(2)} \). This can be understood by noting that the main source of the randomness in the intensity is the gain/loss that behaves as \( \sim \exp(\Delta[\text{Im}(E_n)] \cdot t) \). A higher level of disorder thus leads to a larger value of \( \Delta[\text{Im}(E_n)] \), while a longer propagation distance corresponds to a longer time. For the second type of disorders
Fig. 42. Properties of a non-Hermitian system with off-diagonal disorder. (a) Complex eigenvalue spectrum exhibiting an odd symmetry for both the real and imaginary parts: $\xi_m = -\xi_{-m}$, where $\xi$ stands for the real or imaginary part of the eigenvalue. (b) A representative pair of eigenfunctions with the property $\phi_n^m = (-1)^n \phi_{-n}^m$. 

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Fig. 43. Behavior of photon thermalization in non-Hermitian systems subject to random disorders.

(a,b) Normalized intensity correlation $g_0^{(2)}(z)$ at the center of the waveguide array as a function of the disorder strength and propagation distance $z$ for a system with adjacent distance disorder (off-diagonal disorder) and real relative permittivity disorder, respectively. The number of waveguides in one array is 51. (c) The correlation measure $g_0^{(2)}(zC_0 = 10)$ as a function of the disorder strength for off-diagonal (blue) and permittivity (red) disorders. (d-f) Intensity probability distribution $P(\bar{\mu})$ and photon number distribution $P(n_{ph})$ for a coherent input with a fixed mean photon number $\bar{\mu} = 680$ at the input for different values of the off-diagonal disorder strength. The intensity $I = |\phi|^2$ is represented by the mean photon number $\bar{\mu}$ while the initial photon number is set to be $I = 1$. The left axis indicates $P(\bar{\mu})$ on a linear scale (the blue bar) while the right axis is a semi-logarithmic representation of $P(n_{ph})$ (red). The dashed-dot and the dashed lines represent the fitted exponential and Gaussian-square distributions, respectively, in which the disorder strengths and the corresponding $g^{(2)}$ values are inserted. Due to the system’s being non-Hermitian, eigenvalues are complex. Numerically it is necessary to set a finite (albeit relatively large) distance to prevent energy from diverging.
(i.e., real relative permittivity disorders), the values of \( g_0^{(2)} \) are generally larger as compared to those with the first type of disorders (i.e., adjacent distance or off-diagonal disorders), due to the fact that a nonzero value of \( \Delta \beta \) induces both diagonal and off-diagonal disorders. We observe that, in the small time regime, the main signature of the Hermitian characteristics of the system as reported in Ref. [355] are retained, i.e., \( g_0^{(2)} \) tends to decrease with the disorder strength. However, in the long time (or equivalently, large distance) regime, \( g_0^{(2)} \) increases with the disorder strength. In this regime, the non-Hermitian characteristics dominate, as the main contributions of the imaginary parts of the eigenvalues are from the exponential term. As a result, an increase in the disorder strength will be amplified by the propagation distance, leading to a continuous increase in the value of \( g_0^{(2)} \).

Figure 43(c) shows the behavior of \( g_0^{(2)} \) versus the disorder strength for \( zC_0 = 10 \). We observe a non-decreasing behavior, where the value of \( g_0^{(2)} \) changes continuously from unity to about 3. For longer propagation length, the value of \( g_0^{(2)} \) can exceed 3, due to the non-Hermitian nature of the system. Say we consider \( R \) realizations of the off-diagonal order. Except for the overall gain/loss factor \( \kappa \), the imaginary parts that govern the evolution of the eigenmodes are random. After a long time, the difference in the intensities of the eigenmodes grows exponentially, resulting in significant differences in the intensities of the central waveguide among different realizations. In such a case, we have

\[
g_0^{(2)}(z) = \frac{\langle I_0^2(z) \rangle}{(\langle I_0(z) \rangle)^2} \approx \frac{I_{0,\text{max}}^2(z)/R}{(I_{0,\text{max}}(z)/R)^2} = R, \tag{8.7}
\]

indicating that \( g_0^{(2)} \) can approach the upper bound \( R \).

Figures 43(d-f) show the full photon number statistics for the case of off-diagonal disorders for \( zC_0 = 10.0 \). From the initial condition, we generate an ensemble of input intensity, with the distribution which can approximately be described by the Poisson form: 

\[
P(n) = \frac{\mu^n e^{-\mu}}{n!}
\]

with the mean photon number \( \bar{\mu} \approx 680 \). Due to gain, the effective electric field \( E(z) \) can reach a large value.
Since \( \phi(z) = E(z)e^{-\kappa t} \), the real electric field amplitude can still be moderate for an appropriate value of \( \kappa \). Note that the expression of \( \kappa \) does not depend on the nature of the disorders. We can thus adjust the value of \( \kappa \) to ensure that the energy of the system assumes some reasonable value within a finite distance. Experimentally, the range of the accessible imaginary relative permittivity can be large, where gain can be realized e.g., through photon pumping while loss can be introduced by metal.

Figure 43(d) shows a case where \( g_0^{(2)} = 1.6451 \) and there is a transition from the coherent Poisson distribution to the thermalized Gaussian distribution. About the normal thermal state for which \( g_0^{(2)} \approx 2 \), the intensity distribution is exponential: \( P(I) = (1/\mu)e^{-I/\mu} \), where \( \mu = \langle n_{ph} \rangle \) is the ensemble averaged photon number and the photon number statistics follow the Bose-Einstein distribution [355]. For the superthermal state \( g_0^{(2)} \approx 3 \), the intensity should follow a Gaussian-square type of distribution: \( P(I) = (1/\sqrt{\pi \mu I})e^{-I/\mu} \), which is associated with a modified Bose-Einstein photon number statistics [355]. These behaviors have indeed been observed. In particular, in Figs. 43(e,f), the left side axis is for the blue bar and is on the linear scale of \( P(\bar{\mu}) \) and the right axis is for the red curve \( P(n_{ph}) \) on a semi-logarithmic scale, where the mean photon number \( \bar{\mu} \) is used to mark the strength of the intensity \( I \). From Fig. 43(e), we have \( g_0^{(2)} \approx 1.97 \) and there is an approximately linear dependences of \( P(n_{ph}) \) on \( n_{ph} \) on the semi-logarithmic scale, indicating a Bose-Einstein photon number distribution. The dashed-dot green fitting line for the exponential intensity distribution agrees with the blue bar. In Fig. 43(f), we have \( g_0^{(2)} \approx 2.68 \), the dependence of \( P(n_{ph}) \) on \( n_{ph} \) on the semilogarithmic scale indicates a superthermal distribution, where the dashed magenta fitting curve obeys the Gaussian-square distribution.
8.4. Conclusion

To summarize, we have studied the photon number statistics in non-Hermitian waveguide systems subject to two types of random disorders: one preserving and another breaking the chiral symmetry. We find that, regardless of whether there is a chiral symmetry, the system’s being Hermitian is key to the recently uncovered phenomenon of the photonic thermalization gap. Non-Hermitian photonic systems with gain and loss are typical in realistic situations. For such systems the underlying photon statistics will become progressively random with the disorder level, eliminating the possibility of the emergence of any photonic thermalization gap.

8.5. Derivation of the Coupled Mode Equation

We derive Eq. (8.5) for non-Hermitian systems with non-identical waveguides. Following Ref. [351], we start with a single mode, lossless waveguide of width $2w$ and denote the eigenmode as $\psi_s(x, z) = u(x)e^{i\beta z}$. The relative permittivity of the medium is $\tilde{\epsilon}_s(x) = \epsilon_0 + (\bar{\epsilon} - \epsilon_0)\zeta(x)$. We have

$$\left( \frac{d^2}{dx^2} + k_0^2\tilde{\epsilon}_s(x) - \beta^2 \right)u(x) = 0. \quad (8.8)$$

The electric field $\psi$ can be expanded as

$$\psi(x, z) = \sum_{n=1}^{N} \phi_n(z)u(x-x_n)e^{i\beta z}, \quad (8.9)$$

where $u(x-x_n)$ is the normalized transverse profile of the eigenmode centered at $x_n$ and $\phi_n(z)$ is the amplitude of the electric field of the $n$th waveguide. Substituting the expansion into the
Helmholtz equation, we obtain

\[
\sum_{n=1}^{N} \left[ -2i\beta \frac{d\phi_n(z)}{dz} - i k_0^2 \epsilon_n \phi_n(z) \right] u(x-x_n)
\] (8.10)

\[
= \sum_{n=1}^{N} k_0^2 \left( (\epsilon_n - \bar{\epsilon}) \zeta_n(x) \right)
\]

\[
+ \sum_{k=1, k\neq n}^{N} \left( \epsilon_n - \epsilon_0 \right) \zeta_k(x) + i(\epsilon_0' - \epsilon') \pi(x) \phi_n(z) u(x-x_n),
\]

where \( \pi(x) = 1 - \sum_{k=1}^{N} \zeta_k(x) \). Multiplying this equation by \( u(x-x_m) \) and integrating over the whole space, we obtain

\[
-i \sum_{n=1}^{N} V_{mn} \left( \frac{d\phi_n(z)}{dz} + \frac{k_0^2 \epsilon'_n}{2\beta} \phi_n(z) \right) = \sum_{n=1}^{N} t_{mn} \phi_n(z),
\] (8.11)

where

\[
V_{mn} = \int_{-\infty}^{\infty} u(x-x_m) u(x-x_n) dx,
\]

\[
t_{mn} = C_{mn} + iC'_{mn},
\]

\[
C_{mn} = \frac{k_0^2}{2\beta} \int_{-\infty}^{\infty} \left( \epsilon_n - \bar{\epsilon} \right) \zeta_n(x)
\]

\[
+ \sum_{k=1, k\neq n}^{N} \left( \epsilon_k - \epsilon_0 \right) \zeta_k(x) u(x-x_m) u(x-x_n) dx,
\]

\[
C'_{mn} = \left( \epsilon_0' - \epsilon' \right) k_0^2 \int_{-\infty}^{\infty} u(x-x_m) u(x-x_n) \pi(x) dx.
\]

Note that setting \( \epsilon_n = \epsilon = \bar{\epsilon} \) reduces this set of equations to one with identical waveguides. We see that a change in the real relative permittivity affects the value of \( C_{mn} \) only. To carry out the integration requires the form of \( u(x) \). We approximate the normalization function by

\[
u(x) = \frac{1}{\sqrt{2\ell}} \text{sech}(\frac{x}{\ell}).
\] (8.12)

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From the expression of $C_{mn}$, we see that it will contribute an extra diagonal term $\epsilon_n - \bar{\epsilon}$, which is in general not zero. For $m = n$, $C_{mn}$ can be evaluated:

$$C_{m,m} = \frac{(\epsilon_n - \bar{\epsilon})k^2_0}{2\beta} \int_{-\infty}^{\infty} \zeta_n(x)u(x-x_m)u(x-x_n)dx$$

$$= \frac{(\epsilon_n - \bar{\epsilon})k^2_0}{2\beta} \int_{x_n-w}^{x_n+w} u(x-x_n)u(x-x_m)dx$$

$$\simeq \frac{(\epsilon_n - \bar{\epsilon})k^2_0}{2\beta} \tanh\left(\frac{w}{\ell}\right) \cdot \delta_{m,n}.$$  

For $n = m \pm 1$, we get $C_{mn}$ as

$$C_{m,m\pm 1} = \frac{k^2_0}{2\beta} \int_{-\infty}^{\infty} [(\epsilon_{m\pm 1} - \bar{\epsilon})\zeta_{m\pm 1}(x) + \sum_{k=1,k\neq m\pm 1}^{N} (\epsilon_k - \epsilon_0)\zeta_k(x)]u(x-x_m)u(x-x_{m\pm 1})dx$$

$$= \frac{(\epsilon_{m\pm 1} - \bar{\epsilon})k^2_0}{2\beta} \int_{x_{m\pm 1}-w}^{x_{m\pm 1}+w} u(x-x_m)u(x-x_{m\pm 1}) + \sum_{k=1,k\neq m\pm 1}^{N} \frac{(\epsilon_k - \epsilon_0)k^2_0}{2\beta} \int_{x_k-w}^{x_k+w} u(x-x_m)u(x-x_{m\pm 1})dx$$

$$\simeq \frac{(\epsilon_m + \epsilon_{m\pm 1} - \bar{\epsilon} - \epsilon_0)k^2_0 w}{\beta} \exp\left(-\frac{d}{\ell}\right)(\delta_{m,m+1} + \delta_{m,m-1}).$$

From the expressions of $C_{m,m}$ and $C_{m,m\pm 1}$, we see that the disorders associated with the real part of the relative permittivity contribute to both the diagonal and off-diagonal terms. It is also apparent that, due to the restriction $H = H^T$, $C_{m,m\pm 1}$ exhibits a symmetry between $m$ and $m \pm 1$. 

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REFERENCES


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APPENDIX A

ACHIEVEMENTS DURING PHD STUDIES
Following are the relevant publications on the topics presented in this dissertation


