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Abstract	<p>Pseudospin-1 systems are characterized by the feature that their band structure consists of a pair of Dirac cones and a topologically flat band. Such systems can be realized in a variety of physical systems ranging from dielectric photonic crystals to electronic materials. Theoretically, massless pseudospin-1 systems are described by the generalized Dirac-Weyl equation governing the evolution of a three-component spinor. Recent works have demonstrated that such systems can exhibit unconventional physical phenomena such as revival resonant scattering, superpersistent scattering, super-Klein tunneling, perfect caustics, vanishing Berry phase, and isotropic low energy scattering. We argue that investigating the interplay between pseudospin-1 physics and classical chaos may constitute a new frontier area of research in relativistic quantum chaos with significant applications.</p>
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Chapter 13

Pseudospin-1 Systems as a New Frontier for Research on Relativistic Quantum Chaos

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Abstract. Pseudospin-1 systems are characterized by the feature that their band structure consists of a pair of Dirac cones and a topologically flat band. Such systems can be realized in a variety of physical systems ranging from dielectric photonic crystals to electronic materials. Theoretically, massless pseudospin-1 systems are described by the generalized Dirac-Weyl equation governing the evolution of a three-component spinor. Recent works have demonstrated that such systems can exhibit unconventional physical phenomena such as revival resonant scattering, superpersistent scattering, super-Klein tunneling, perfect caustics, vanishing Berry phase, and isotropic low energy scattering. We argue that investigating the interplay between pseudospin-1 physics and classical chaos may constitute a new frontier area of research in relativistic quantum chaos with significant applications.

13.1 Introduction: What Are Pseudospin-1 Systems and Where Do They Arise?

Solid state materials whose energy bands contain a Dirac cone structure have been an active area of research since the experimental realization of graphene [1, 2]. From the standpoint of quantum transport, the Dirac cone structure and the resulting pseudospin characteristic of the underlying quasiparticles can lead to unconventional physical properties/phenomena such as high carrier mobility, anti-localization, chiral tunneling, and negative refractive index, which are not usually seen in traditional semiconductor materials. Moreover, due to the underlying physics being effectively governed by the Dirac equation, relativistic quantum phenomena such as Klein tunneling, Zitterbewegung, and pair creations can potentially occur in solid state devices and be exploited for significantly improving or even revolutionizing conventional electronics. Uncovers/developing alternative materials with a Dirac cone structure has also been

extremely active [3,4]. In this regard, the discovery of topological insulators [5,6] indicates that Dirac cones with a topological origin can be created, leading to the possibility of engineering materials to generate remarkable physical phenomena such as zero-field half-integer quantum Hall effect [7], topological magnetoelectric effect [8], and topologically protected wave transport [9,10].

A parallel line of research has concentrated on developing photonic materials with a Dirac cone structure, due to the natural analogy between electromagnetic and matter waves. For example, photonic graphene [11,12] and photonic topological insulators [13–18] have been realized, where novel phenomena of controlled light propagation have been demonstrated. Due to the much larger wavelength in optical materials as compared with the electronic wavelength, synthetic photonic devices with a Dirac cone structure can be fabricated at larger scales with a greater tunability through modulations. The efforts have led to systems with additional features in the energy band together with the Dirac cones, opening possibilities for uncovering new and “exotic” physics with potential applications that cannot even be conceived at the present.

The materials to be discussed in this article are those whose energy bands consist of a pair of Dirac cones and a topologically flat band, electronic or optical. For example, in a dielectric photonic crystal, Dirac cones can be induced through accidental degeneracy that occurs at the center of the Brillouin zone. This effectively makes the crystal a zero-refractive-index metamaterial at the Dirac point where the Dirac cones intersect with another flat band [19–23]. Alternatively, configuring an array of evanescently coupled optical waveguides into a Lieb lattice [24–27] can lead to a gapless spectrum consisting of a pair of common Dirac cones and a perfectly flat middle band at the corner of the Brillouin zone. As demonstrated more recently, loading cold atoms into an optical Lieb lattice provides another experimental realization of the gapless three-band spectrum at a smaller scale with greater dynamical controllability of the system parameters [28]. With respect to creating materials whose energy bands consist of a pair of Dirac cones and a topologically flat band, there have also been theoretical proposals on Dice or \mathcal{T}_3 optical lattices [29–34] and electronic materials such as transition-metal oxide SrTiO₃/SrIrO₃/SrTiO₃ trilayer heterostructures [35], 2D carbon or MoS₂ allotropes with a square symmetry [36,37], SrCu₂(BO₃)₂ [38] and graphene-In₂Te₂ bilayer [39]. Dirac cones with a flat band can also arise in a class of mechanical lattices [40].

In spite of the diversity and the broad scales to realize the band structure that consists of two conical bands and a characteristic flat band intersecting at a single point in different physical systems, there is a unified underlying theoretical framework: generalized Dirac-Weyl equation for massless spin-1 particles [31]. Comparing with the conventional Dirac cone systems with massless pseudospin/spin-1/2 quasiparticles (i.e., systems without a flat band), pseudospin-1 systems can exhibit quite unusual physics such as super-Klein tunneling for the two conical (linear dispersive) bands [23,32,41,42], diffraction-free wave propagation and novel conical diffraction [24–27], flat band rendering divergent dc conductivity with a tunable short-range disorder [43], unconventional

Anderson localization [44,45], flat band ferromagnetism [28,46,47], and peculiar topological phases under external gauge fields or spin-orbit coupling [35,48–50]. Especially, the topological phases arise due to the flat band that permits a number of degenerate localized states with a topological origin (i.e., “caging” of carriers) [51]. Most existing works, however, focused on the physics induced by the additional flat band, and the scattering/transport dynamics in pseudospin-1 systems have begun to be studied [52–54].

13.2 Generalized Dirac-Weyl Equation

The effective low-energy Hamiltonian associated with pseudospin-1 Dirac cones can be written, in the unit $\hbar = 1$, as [23,24,41]

$$H_0 = v_g \mathbf{S} \cdot \mathbf{k}, \quad (13.1)$$

where v_g is the magnitude of the group velocity associated with the Dirac cone, $\mathbf{k} = (k_x, k_y)$ denotes the wavevector, and $\mathbf{S} = (S_x, S_y)$ is a vector of matrices with components

$$S_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \quad \text{and} \quad S_y = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}. \quad (13.2)$$

Along with another matrix

$$S_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix},$$

the three matrices form a complete representation of spin-1, which satisfies the angular momentum commutation relations $[S_l, S_m] = i\epsilon_{lmn}S_n$ with three eigenvalues: $s = \pm 1, 0$, where ϵ_{lmn} is the Levi-Civita symbol. It follows from Eq. (13.1) that the energy spectrum consists of three bands that intersect at the Dirac point: a dispersionless flat band $E_0(\mathbf{k}) = 0$ and two linearly dispersive bands $E_\tau(\mathbf{k}) = \tau v_g |\mathbf{k}|$ with $\tau = \pm 1$ being the band index. The corresponding eigenfunctions in the position representation $\mathbf{r} = (x, y)$ are

$$\psi_{\mathbf{k},\tau}(\mathbf{r}) = \langle \mathbf{r} | \mathbf{k}, \tau \rangle = \frac{1}{2} \left[e^{-i\theta}, \sqrt{2}\tau, e^{i\theta} \right]^T e^{i\mathbf{k} \cdot \mathbf{r}}, \quad (13.3)$$

for the dispersive bands and

$$\psi_{\mathbf{k},0}(\mathbf{r}) = \langle \mathbf{r} | \mathbf{k}, 0 \rangle = \frac{1}{\sqrt{2}} \left[-e^{-i\theta}, 0, e^{i\theta} \right]^T e^{i\mathbf{k} \cdot \mathbf{r}}, \quad (13.4)$$

for the flat band, where $\theta = \tan^{-1}(k_y/k_x)$. The current operator is defined from Eq. (13.1) as

$$\hat{\mathbf{j}} = \nabla_{\mathbf{k}} H_0 = v_g \mathbf{S}. \quad (13.5)$$

The local current in a given state $\psi(\mathbf{r}) = [\psi_1, \psi_2, \psi_3]^T$ can thus be expressed as

$$\begin{aligned} \mathbf{j}(\mathbf{r}) &= v_g \psi^\dagger \mathbf{S} \psi \equiv (j_x, j_y) \\ &= \sqrt{2} v_g (\Re[\psi_2^*(\psi_1 + \psi_3)], -\Im[\psi_2^*(\psi_1 - \psi_3)]), \end{aligned} \quad (13.6)$$

which satisfies the common continuity equation

$$\frac{\partial}{\partial t} \rho + \nabla \cdot \mathbf{j} = 0, \quad (13.7)$$

where $\rho = \psi^\dagger \psi$ is the probability density associated with state ψ . From Eqs. (13.3) and (13.4), it can be seen that the associated local current density satisfies $\mathbf{j}_0 = \mathbf{0}$ for the flat band plane-wave, and

$$\mathbf{j}_\tau = v_g (\cos \theta, \sin \theta) = \tau v_g \frac{\mathbf{k}}{|\mathbf{k}|}, \quad (13.8)$$

for the dispersive band plane-wave. In terms of the Berry phase associated with the band structure, one obtains from Eqs. (13.3) and (13.4) the corresponding Berry connections

$$\begin{aligned} \mathcal{A}_\mathbf{k}^\tau &= \langle \mathbf{k}, \tau | i \nabla_{\mathbf{k}} | \mathbf{k}, \tau \rangle = 0, \\ \mathcal{A}_\mathbf{k}^0 &= \langle \mathbf{k}, 0 | i \nabla_{\mathbf{k}} | \mathbf{k}, 0 \rangle = -2 \mathcal{A}_\mathbf{k}^\tau = 0 \end{aligned}$$

for all three bands. The Berry phase is thus given by

$$\Phi_B^{\tau,0} = \oint_{\mathcal{C}_{\mathbf{k}_d}^{\tau,0}} d\mathbf{k} \cdot \mathcal{A}_\mathbf{k}^{\tau,0} = 0, \quad (13.9)$$

for any closed path $\mathcal{C}_{\mathbf{k}_d}^{\tau,0}$ encircling the degeneracy point \mathbf{k}_d of the momentum space defined in each band. It should be noted that the vanishing or 2π quantized Berry phase is consistent with the fundamental properties of spin-1 particles.

A remarkable phenomenon for pseudospin-1 Dirac cone systems, which is not usually seen in conventional Dirac cone systems such as graphene and topological insulators, is super-Klein tunneling [23]. Specifically, following the standard treatment of Klein tunneling for graphene systems [55], one can consider the basic problem of wave scattering from a rectangular scalar (electrostatic) potential barrier defined as $V(x, y) = V_0 \Theta(x) \Theta(D - x)$ with barrier width D and height V_0 . The transmission probability based on the effective Hamiltonian Eq. (13.1) for incident energy $E \neq 0, V_0$ is given by

$$T = \frac{(1 - \gamma^2)(1 - \gamma'^2)}{(1 - \gamma^2)(1 - \gamma'^2) + \frac{1}{4}(\gamma + \gamma')^2 \sin^2(q_x D)}, \quad (13.10)$$

where $\gamma = \tau \sin \theta$, $\gamma' = \tau' \sin \theta'$ with $\tau = \text{sgn}(E), \tau' = \text{sgn}(E - V_0)$, $\theta = \tan^{-1}(k_y/k_x)$ is the incident angle, and $\theta' = \arctan(k_y/q_x)$ with $q_x = \sqrt{(E - V_0)^2 - k_y^2}$. A striking feature of Eq. (13.10) is that, when the incident wave energy is one half of the potential barrier height, i.e., $E = V_0/2$, one has $\tau = -\tau', \theta = \theta'$ and, consequently, perfect transmission with $T \equiv 1$ for *any* incident angle θ - hence the term “super-Klein tunneling.”

13.3 Transport Properties of Pseudospin-1 Systems

A recent work [52] addressed the following question: what types of transport properties can arise from pseudospin-1 systems whose band structure is characterized by coexistence of a pair of Dirac cones and a flat band? To address this question in the simplest possible setting while retaining the essential physics, ballistic wave scattering from a circularly symmetric potential barrier was studied. For conventional Dirac cone systems with pseudospin or spin-1/2 quasiparticles, there has been extensive work on scattering [56–58] with phenomena such as caustics [59], Mie scattering resonance [60], birefringent lens [61], cloaking [62], spin-orbit interaction induced isotropic transport and skew scattering [63, 64], and electron whispering gallery modes [65]. However, there had been no corresponding studies for pseudospin-1 Dirac cone systems prior to the work in Ref. [52].

More specifically, scattering was studied [52] of pseudospin-1 particle from a circularly symmetric scalar potential barrier of height V_0 defined by $V(r) = V_0\Theta(R-r)$, where R is the scatterer radius and Θ denotes the Heaviside function. To characterize the scattering dynamics quantitatively, the scattering efficiency can be used, which is defined as the ratio of the scattering to the geometric cross sections [60]:

$$Q = \sigma/(2R), \quad (13.11)$$

where the scattering cross section σ can be calculated through the far field radial reflected current [52].

There were three main results [52]: revival resonant scattering, super-Klein tunneling induced perfect caustics, and universal low-energy isotropic transport without broken symmetries for massless quasiparticles. First, for small scatterer size, the effective three-component spinor wave exhibits revival resonant scattering as the incident wave energy is varied continuously - a phenomenon that has not been reported in any known wave systems. Strikingly, the underlying revival resonant modes show a peculiar type of boundary trapping profile in their intensity distribution. While the profile resembles that of a whispering gallery mode, the underlying mechanism is quite different: these modes occur in the wave dominant regime through the formation of fusiform vortices around the boundary in the corresponding local current patterns, rather than being supported by the gallery type of orbits through total internal reflections. Second, for larger scatterer size where the scattering dynamics are semiclassical, a perfect caustic phenomenon arises when the incident wave energy is about half of the barrier height, as a result of the super-Klein tunneling effect. A consequence is that the scatterer behaves as a lossless Veselago lens with effective negative refractive index resulting from the Dirac cone band structure. Compared with conventional Dirac cone systems for pseudospin-1/2 particles, the new caustics possess remarkable features such as significantly enhanced focusing, vanishing of the second and higher order caustics, and a well-defined static cusp. Third, in the far scattering field, an isotropic behavior arises at low energies. Considering that there is no broken symmetry so the quasiparticles remain massless,

the phenomenon is quite surprising as conventional wisdom would suggest that the scattering be anisotropic. An analysis of the characteristic ratio of the transport to the elastic time as a function of the scatterer size revealed that the phenomenon of scattering isotropy can be attributed to vanishing of the Berry phase for massless pseudospin-1 particles that results in constructive interference between the time-reversed backscattering paths. Because of the isotropic structure, the emergence of a Fano-type resonance structure in the function of the ratio versus the scatterer size can be exploited to realize effective switch of wave propagation from a forward dominant state to a backward dominant one, and vice versa. In Ref. [52], an analytic theory with physical reasoning was developed to understand the three novel phenomena.

It is possible to conduct experimental test of the phenomena. For example, in a recent work [23], it was demonstrated for a class of two-dimensional dielectric photonic crystals with Dirac cones induced accidentally [19–22] that the Maxwell’s equations can lead to an effective Hamiltonian description sharing the same mathematical structure as that of massless pseudospin-1 particles. Especially, the photonic analogy of the gate potential in the corresponding electronic system can be realized by manipulating the scaling properties of Maxwell’s equations. Recent experimental realizations of photonic Lieb lattices consisting of evanescently coupled optical waveguides implemented through the femtosecond laser-writing technique [24–27] make them prototypical for studying the physics of pseudospin-1 Dirac systems. With a particular design of the refractive index profile across the lattice to realize the scattering configuration, the phenomena can be experimentally tested. Loading ultracold atoms into an optical Lieb lattice fabricated by interfering counter-propagating laser beams [28] provides another versatile platform to test the phenomena, where appropriate holographic masks can be used to implement the desired scattering potential barrier [32, 66]. In electronic systems, the historically studied but only recently realized 2D magnetoplasmon system [67] is described by three-component linear equations with the same mathematical structure of massless pseudospin-1 particles, which can serve as a 2D electron gas system to test the phenomena.

From an applied perspective, the phenomenon of revival resonant scattering can be a base for articulating a new class of microcavity lasers based on the principles of relativistic quantum mechanics. It may also lead to new discoveries in condensed matter physics through exploiting the phenomenon in electronic systems. The phenomenon of perfect caustics can have potential applications in optical imaging defying the diffraction limit as well as in optical cloaking.

13.4 Superscattering of Pseudospin-1 Wave in Photonic Lattice

Another phenomenon is superscattering of pseudospin-1 wave from weak scatterers in the subwavelength regime where the scatterer size is much smaller than wavelength [53]. The phenomenon manifests itself as unusually strong scattering

characterized by extraordinarily large values of the cross section even for arbitrarily weak scatterer strength. The physical origin of superscattering is revival resonances [53], for which the conventional Born theory breaks down. The phenomenon can be experimentally tested using synthetic photonic systems.

In wave scattering, a conventional and well accepted notion is that weak scatterers lead to weak scattering. This can be understood by resorting to the Born approximation. In particular, consider a simple 2D setting where particles are scattered from a circular potential of height V_0 and radius R . In the low energy (long wavelength) regime $kR < 1$ (with k being the wavevector), the Born approximation holds for weak potential: $(m/\hbar^2)|V_0|R^2 \ll 1$. Likewise, in the high energy (short wavelength) regime characterized by $kR > 1$, the Born approximation still holds in the weak scattering regime: $(m/\hbar^2)|V_0|R^2 \ll (kR)^2$. In general, whether scattering is weak or strong can be quantified by the scattering cross section. For scalar waves governed by the Schrödinger equation, in the Born regime the scattering cross section can be expressed as polynomial functions of the effective potential strength and size [68]. For spinor waves described by the Dirac equation (e.g., graphene systems), the 2D transport cross section is given by [58] $\Sigma_{tr}/R \simeq (\pi^2/4)(V_0R)^2(kR)$ (under $\hbar v_F = 1$). In light scattering from spherically dielectric, “optically soft” scatterers with relative refractive index n near unity, i.e., $kR|n - 1| \ll 1$, the Born approximation manifests itself as an exact analog of the Rayleigh-Gans approximation [69], which predicts that the scattering cross section behaves as $\Sigma/(\pi R^2) \sim |n - 1|^2(kR)^4$ in the small scatterer size limit $kR \ll 1$. In wave scattering, the conventional wisdom is then that a weak scatterer leads to a small cross section and, consequently, to weak scattering, and this holds regardless of nature of the scattering particle/wave, i.e., vector, scalar or spinor.

Superscattering of pseudospin-1 wave defies exactly the conventional wisdom [53]. The striking and counterintuitive phenomenon is that extraordinarily strong scattering can emerge from arbitrarily weak scatterers at sufficiently low energies (i.e., in the deep subwavelength regime). Accompanying this phenomenon is a novel type of resonances that can persist at low energies for weak scatterers. An analytic understanding of the resonance was obtained [53] and the resulting cross section was derived, with excellent agreement with results from direct numerical simulations.

13.5 Non-equilibrium Transport in the Pseudospin-1 Dirac-Weyl System

Quantum transport beyond the linear response and equilibrium regime is of great practical importance, especially in device research and development. There have been studies of nonlinear and non-equilibrium transport of relativistic pseudospin-1/2 particles in Dirac and Weyl materials. For example, when graphene is subject to a constant electric field, the dynamical evolution of the current after the field is turned on exhibits a remarkable minimal conductivity behavior [70]. The scaling behavior of nonlinear electric transport in graphene

due to the dynamical Landau–Zener tunneling or the Schwinger pair creation mechanism has also been investigated [71,72]. Under a strong electrical field, due to the Landau–Zener transition, a topological insulator or graphene can exhibit a quantization breakdown phenomenon in the spin Hall conductivity [73]. In addition, non-equilibrium electric transport beyond the linear response regime in 3D Weyl semimetals has been studied [74]. In these works, the quasiparticles are relativistic pseudospin-1/2 fermions arising from the Dirac or Weyl system with a conical type of dispersion in their energy momentum spectrum.

Recently, the transport dynamics of pseudospin-1 quasiparticles were studied [75]. Under the equilibrium condition and in the absence of disorders, the flat band acts as a perfect “caging” of carriers with zero group velocity and hence it contributes little to the conductivity [43,76,77]. However, the flat band can have a significant effect on the non-equilibrium transport dynamics. Through numerical and analytic calculation of the current evolution for both weak and strong electric fields, it was found [75] that the general phenomenon can arise of current enhancement as compared with that associated with non-equilibrium transport of pseudospin-1/2 particles. In particular, for a weak field, the interband current is twice as large as that for pseudospin-1/2 system due to the interference between particles from the flat band and from the negative band, the scaling behavior of which agrees with that determined by the Kubo formula. For a strong field, the intraband current is $\sqrt{2}$ times larger than that in the pseudospin-1/2 system, as a result of the additional contribution from the particles residing in the flat band. In this case, the physical origin of the scaling behavior of the current-field relation can be attributed to Landau–Zener tunneling. These findings suggested that, in general, the conductivity of pseudospin-1 materials can be higher than that of pseudospin-1/2 materials in the nonequilibrium transport regime. Indeed, the interplay between the flat band and the Dirac cones can lead to interesting physics that has just begun to be understood and exploited.

13.6 Discussion: Relativistic Quantum Chaos in Pseudospin-1 Systems

The field of quantum chaos aims to uncover the quantum manifestations or fingerprints of classical chaotic behaviors in the semiclassical limit [78,79]. A vast majority of the works were for nonrelativistic quantum systems described by the Schrödinger equation. Recent years have witnessed a rapid development of Dirac materials [80,81] such as graphene and topological insulators, which are described by the Dirac equation in relativistic quantum mechanics. A new field has thus emerged: relativistic quantum chaos [82,83]. To study the unique physics of classical chaos in relativistic quantum systems is fundamental with potentially significant applications.

Existing works on relativistic quantum chaos [82,83] focused on pseudospin-1/2 systems such as graphene, which are described by the conventional Dirac equation for two-component spinors. Pseudospin-1 systems, due to their unusual

physics, can present a new platform to study relativistic quantum chaos. A technical difficulty that must be overcome is to solve the generalized Dirac-Weyl equation for three-component spinors in arbitrary geometrical domains that generate classical chaos. For example, while scattering of pseudospin-1 particles from a circular potential can be analytically solved [52], at the present there exists no method to solve the scattering problem for a chaotic geometry, e.g., a stadium shaped potential. At the time of writing, author's group is developing a multiple multipole technique to solve the generalized Dirac-Weyl equation for pseudospin-1 system with any given piecewise homogeneous potential, where the multipoles (or "fictitious" sources) are defined in terms of the analytic three-component spinor cylindrical wave basis of eigen-solutions in each sub-region separated by the potential boundaries. In addition, a wave-function matching based scattering matrix approach is being developed to deal with potential of the eccentric annular shape. Both methods are semi-analytic, while the former is more powerful for near-field calculations and is in principle applicable to arbitrary shape of the scattering potential. Preliminary studies have revealed that the methods are highly efficient and accurate, enabling unexpected phenomena to be uncovered such as the existence of an energy range in which pseudospin-1 chaotic cavities defy well known phenomena in quantum chaos such as Q-spoiling [84–86]. It is likely that uncovering, understanding, and exploiting the interplay between pseudospin-1 physics and classical chaos can represent a new frontier in relativistic quantum chaos.

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