Chiral Transport in Anisotropic Materials

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Chiral Transport in Anisotropic Materials

A thesis submitted in partial fulfillment of the requirement for the degree of Bachelor of Science with Honors in Physics from the College of William and Mary in Virginia,

by

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Abstract

Chiral materials are a class of systems in which the momentum of quasiparticles is coupled to a pseudospin degree of freedom, thus affecting their transport properties. In particular, such materials can exhibit Klein tunneling, in which chiral particles tunnel through a potential barrier with probability one due to a suppression of backscattering. In chiral materials with an anisotropic band structure, this tunneling depends nontrivially on the interplay between chirality and the direction of dispersion.

We discuss the consequences of transport in a minimal chiral anisotropic model, highlighting the role of the pseudospin in scattering through a Klein barrier. We implement this model in bilayer phosphorene, a two-dimensional material in which low-energy quasiparticles exhibit both anisotropy and chirality. We find an effective two-band model for the system and investigate the dependence of Klein tunneling on the incident angle of incoming particles. Finally, we propose a scheme to experimentally detect anisotropy of chiral materials through scattering.
Chapter 1

Introduction

The Klein paradox, originally arising in the context of Quantum Electrodynamics and the Dirac equation, is a phenomenon in which relativistic particles are perfectly transmitted through an arbitrarily high potential barrier [3]. The seemingly paradoxical nature of the tunneling is explained by spin conservation and charge-conjugation symmetry, as a particle can only scatter into its antiparticle of the same spin inside the barrier. The energies required for experimental tests in vacuum are elevated, making Klein tunneling difficult to observe.

While high-energy experiments involving Klein tunneling are inherently difficult to realize, another avenue for exploring this phenomenon lies in condensed matter. In a solid, complicated interactions between electrons and the lattice give rise to emergent excitations called quasiparticles [4]. The effective low energy behavior of such quasiparticles can mimic a variety of high-energy particle physics systems. In particular, if a crystal lattice possesses a degree of freedom that acts as spin, it can host spin-mediated phenomena like Klein tunneling.

Recently, Katsnelson, Novoselov, and Geim proposed an experimental test of the Klein paradox in graphene, a two-dimensional honeycomb lattice of carbon atoms in which low-energy particles behave like massless electrons endowed with a “pseudospin” degree of freedom [3]. When electrons are localized in a solid, they are
bound by a potential well originating from atomic Coulomb forces. As a result, Klein tunneling counteracts the effects of localization, increasing conductivity [3]. Unlike its particle physics manifestation, the effect can then be observed at experimentally accessible energy scales in graphene by measuring this conductivity.

Graphene is part of a larger class of chiral materials [5], in which electronic effects depend on the interplay between pseudospin and momentum of charge carriers. Chirality is the projection of momentum onto pseudospin, and quasiparticles that arise in such materials have nonzero chirality. Chiral quasiparticles can also be observed in other two-dimensional materials like bilayer graphene [6] and transition metal dichalcogenides [7], or in three dimensions in Weyl semimetals [8]. In each of these examples, spin conservation constrains physical processes like scattering through a potential barrier.

Not all chiral effects are the same. In ordinary (monolayer) graphene, electron-like quasiparticles are perfectly transmitted through potential barriers because all possible backward-propagating states have opposite spin. This is a consequence of the linear coupling between pseudospin and crystal momentum, which gives rise to opposite spins for left-moving and right-moving particles. In bilayer graphene, however, the coupling between spin and momentum is quadratic, meaning that the counter-propagating states have the same spin as incoming electrons. As a result, incident electrons are perfectly reflected by a potential barrier. Such behavior can be seen as another manifestation of Klein tunneling. Furthermore, the pattern of transmission with linear coupling and reflection with quadratic coupling extends to general odd and even powers of the pseudospin-momentum interaction.

The example of monolayer and bilayer graphene illustrates both the role pseudospin plays in electron transport and the utility of Klein tunneling as a probe for chiral nature in materials. The presence of Klein tunneling indicates whether a ma-
material possesses a pseudospin degree of freedom. Experimental techniques can detect resonances in the resistance of a $p-n-p$ junction in graphene to signal the presence of Klein tunneling [9]. Additionally, the reflective or transmissive nature of the tunneling can further indicate the parity of the chiral coupling.

Because graphene has an isotropic dispersion relation, the tunneling depends only on the chirality of its particles. Klein tunneling at a fixed angle of incidence will yield the same results independent of the angle at which a sample of graphene is rotated. However, there exist chiral materials in which the dispersion relation is fundamentally different along different directions [10, 2]. In such materials, the coupling between pseudospin and momentum is also anisotropic, yielding a Klein tunneling effect that is modulated by the direction of scattering as well as spin-conservation. A natural question arises: what features of the tunneling are solely chiral in nature and what features are due to the anisotropy?

In the following thesis, we describe Klein tunneling in anisotropic chiral materials and present experimentally realizable systems in which this phenomenon occurs. We begin by introducing the Klein paradox as a consequence of spin-conservation. After providing background on the class of chiral materials and the specific case of graphene, we discuss the condensed matter analog of the Klein paradox in such systems. We then develop a model for an anisotropic chiral material that interpolates between two different chiral behaviors. We compare transport in the anisotropic case to that in the isotropic case by varying the angle of incidence, the potential barrier height and length, and the chemical potential in Klein tunneling.

The phosphorus-based analog of graphene, phosphorene, provides a realistic system that exhibits chiral anisotropy [2]. We study the effect of an external electric field on the band gap of phosphorene using a tight-binding model [6]. We develop an effective two-band model of bilayer phosphorene when tuned to a gapless state and
compare it to our general chiral anisotropic model. Through scattering calculations, we show that Klein tunneling smoothly interpolates between even and odd chirality as the direction of charge-carriers is rotated. We conclude by discussing the utility of Klein tunneling in measuring anisotropy in materials and propose experimental configurations to observe such effects.
Chapter 2

Chiral Materials and Klein Tunneling

2.1 Klein Paradox

Although its mechanism is identical to that in condensed matter, the Klein paradox is most naturally explained in a particle physics context. In Klein’s original gedanken-experiment [3], a spin-1/2 particle, like an electron, moves towards a potential bump and, instead of being reflected, is transmitted with probability approaching 1 as the barrier height approaches infinity. In a nonrelativistic system, the Schroedinger equation predicts that a propagating state of energy $E$ incident on a barrier with energy $V > E$ will have an exponentially decaying probability amplitude beyond the barrier. The decay constant is proportional to $\sqrt{V - E}$, indicating that when the barrier height is very large, incoming particles have zero probability of transmission.

Klein tunneling, in which exactly the opposite happens, must therefore be a relativistic effect. Relativistic electrons are no longer described by the Schroedinger equation, but instead obey the Dirac equation[11], which predicts the existence of negative energy states. At the potential barrier, we can no longer treat the scattering as a single-particle problem in quantum field theory due to the creation and annihilation of particle-antiparticle pairs, spoiling the nonrelativistic quantum description.
Instead, when the potential is large enough compared to the incoming particle mass \( (V > 2m) \) [11], the chirality inherent in the Dirac equation allows the particle to scatter into a negative-energy state inside the barrier, called an antiparticle [12]. The higher the potential barrier, the easier it is for particle and antiparticle states to match up. The fundamental feature of this process is spin conservation: as incoming particles have a certain chirality, they can only be transmitted into antiparticles.

If the potential barrier is made into a potential bump, the same phenomenon will occur at the other end of the potential region. The antiparticles created inside the step by the scattering continue to propagate until they in turn scatter back into electrons at the other end. The same mechanism of spin conservation is at work here to produce the net effect of a particle scattering through a (finite) region of high potential.

In the language of condensed matter, when a chiral particle enters a negatively doped region, the only accessible state into which it can scatter while conserving spin is a hole, which then scatters back into a particle on the other end of region. The energy of the electron in this paradigm is the chemical potential \( E_F \) that arises from positive doping. This mechanism is sketched in Fig. 2.1 for free electrons in vacuum and in Fig. 2.2 in a condensed matter system using the framework of chiral dispersion relations.

### 2.2 Chiral Materials

Klein tunneling is a phenomenon that is unique to particles that carry spin, and hence can be realized in chiral materials [3]. In such materials, the Hamiltonian is a linear combination of representations of a spin group, like the Pauli matrices in two dimensions, giving rise to spinor particle states that have a definite spin. Because these Hamiltonians often arise from an effective low-energy description of a condensed
Figure 2.1: Klein Tunneling: An electron incident on a potential barrier with energy much higher the electron energy scatters to an antiparticle/hole with the same spin, which in turn is transmitted back to an electron with probability one. Backscattering is prohibited by spin conservation.

Figure 2.2: Klein Tunneling is displayed in terms of energy bands of a condensed matter system. The incoming chiral particle is scattered to a hole from the same branch of the dispersion, preserving pseudospin ($\sigma$).
matter system, the spin isn’t necessarily the same as particle spin, but as it behaves effectively the same way, it is called pseudospin. In chiral systems, the motion of charge carriers is coupled to this degree of freedom, leading to transport properties distinct from non-chiral materials in which spin is irrelevant. Before discussing general features of Klein tunneling in chiral materials, we turn our attention to perhaps the most well-known physical example of such a system: graphene.

2.2.1 Graphene

It is instructive to consider graphene as a first model of two-dimensional chiral materials. Graphene is a hexagonal layer of \( sp^2 \) hybridized carbon atoms that has strong structural properties due to the strength of the in-plane \( \sigma \)-bonds connecting each carbon atom to its three nearest neighbors and an interesting band structure due to the half-filled \( \pi \)-bond joining \( p_z \) orbitals orthogonal to the plane [5]. Graphene can be seen as a triangular Bravais lattice when we identify two carbon atoms \( A \) and \( B \) as our unit cell, with lattice vectors and reciprocal lattice vectors:

\[
\mathbf{a}_1 = a \sqrt{3}(1, 0), \quad \mathbf{a}_2 = a \sqrt{3} \left( \frac{1}{2}, \frac{\sqrt{3}}{2} \right); \quad \mathbf{b}_1 = \frac{2\pi}{3a}(\sqrt{3}, -1), \quad \mathbf{b}_2 = \frac{4\pi}{3a}(0, 1), \quad (2.1)
\]

where \( a \) is the spacing between neighboring carbon atoms. The Brillouin Zone (BZ) is also hexagonal with a center \( \Gamma \) and two sets of three equivalent points on the corners labeled by \( K \) and \( K' \). The honeycomb crystal lattice of graphene is shown in Fig. 2.3.

Ignoring electron spin, the tight-binding Hamiltonian of the system can be written using second-quantization formalism and setting \( \hbar = 1 \):

\[
H = -t \sum_{\langle i,j \rangle} (a_i^\dagger b_j + \text{h.c.}) - t' \sum_{\langle(i,j)\rangle} (a_i^\dagger a_j + b_i^\dagger b_j + \text{h.c.}), \quad (2.2)
\]

where \( t \) and \( t' \) are positive nearest-neighbor and next nearest-neighbor hopping parameters, and \( a_i \) annihilates an electron and \( a_i^\dagger \) creates an electron at lattice vector

1
**Figure 2.3:** Honeycomb lattice of graphene with its two sublattices highlighted in red and blue.

\( \mathbf{R}_i \) on the \( A \) sublattice (\( b_i \) acts the same way on sublattice \( B \)). The choice of positive \( t \) and \( t' \) is justified because we expect hopping to be energetically favorable. We can diagonalize (2.2) in reciprocal space to find a dispersion relation for graphene, and we expect two bands because of the sublattice degree of freedom.

For simplicity we omit next-nearest neighbor hopping, which breaks particle-hole symmetry [13], and consider the Discrete Fourier Transform of the creation and annihilation operators: 

\[
a_i^\dagger = \frac{1}{\sqrt{N}} \sum_{\mathbf{k} \in \text{B.Z.}} e^{i\mathbf{k} \cdot \mathbf{R}_i} a_{\mathbf{k}},
\]

where \( N \) is the number unit cells in the system. We show the substitution below for one term, where the positions of the three nearest (\( B \)) neighbors to an \( A \) carbon atom are given by \( \delta_1 = a(0,1), \delta_2 = \frac{a}{2}(\sqrt{3},-1), \delta_3 = \frac{a}{2}(-\sqrt{3},-1). \)

\[
\sum_{i,j} a_i^\dagger b_j = \sum_i \sum_{j=1}^3 \frac{1}{N} \sum_{\mathbf{k},\mathbf{k}'} a_i^\dagger e^{-i\mathbf{k} \cdot \mathbf{R}_i} e^{i\mathbf{k}' \cdot (\mathbf{R}_i + \delta_j)} b_{\mathbf{k}'} = \sum_{j=1}^3 \frac{1}{N} \sum_{\mathbf{k},\mathbf{k}'} \sum_i a_i^\dagger e^{i(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{R}_i} e^{i\mathbf{k}' \cdot \delta_j} b_{\mathbf{k}'} =
\]

\[
\sum_{j=1}^3 \frac{1}{N} \sum_{\mathbf{k},\mathbf{k}'} a_i^\dagger e^{i\mathbf{k} \cdot \delta_j} b_{\mathbf{k}'} = \sum_{\mathbf{k} \in \text{B.Z.}} a_i^\dagger \left( \sum_{j=1}^3 e^{i\mathbf{k} \cdot \delta_j} \right) b_{\mathbf{k}}.
\]

(2.3)
This form suggests that we can write out our Hamiltonian in the basis of creation and annihilation operators in reciprocal space as a 2 by 2 matrix:

\[ H = \sum_{k \in \text{B.Z.}} \Psi_k^\dagger H_k \Psi_k \quad H_k = -t \begin{pmatrix} 0 & \gamma(k) \\ \gamma(k)^* & 0 \end{pmatrix}, \quad \gamma(k) = \sum_{j=1}^{3} e^{i k \cdot \delta_j}, \quad \Psi_k = \begin{pmatrix} a_k \\ b_k \end{pmatrix}. \tag{2.4} \]

It is clear that the energy spectrum will be given by \( E_{\pm}(k) = \pm t |\gamma(k)| \), which can be expanded and simplified to arrive at the standard expression for the dispersion relation:

\[ E_{\pm}(k) = \pm t \sqrt{3 + 2 \cos(\sqrt{3} k_y a) + 4 \cos \left( \frac{\sqrt{3}}{2} k_y a \right) \cos \left( \frac{3}{2} k_x a \right)}. \tag{2.5} \]

**Dirac Points**

If we consider the Brillouin Zone of this system we find that the two energy bands are zero, and therefore degenerate, at the six corners of the hexagonal B.Z. The six corners are only two distinct points in reciprocal space because sets of three are separated by reciprocal lattice vectors. The coordinates of the two points can be taken as:

\[ K = \frac{4\pi}{3\sqrt{3}a}(-1,0), \quad K' = \frac{4\pi}{3\sqrt{3}a}(1,0). \tag{2.6} \]

These are known as Dirac points, and at each point \( \gamma(k) \) vanishes and the two bands touch at the Fermi Level of zero.

Because the dynamics of electrons are mainly governed by low energy excitations, we are interested in the behavior of (2.4) near the Dirac points. We can linearize the Hamiltonian around \( K \) by writing the momentum as \( k = K + q \) and then expanding to first order around \( q = 0 \).

\[ \gamma(K + q) \approx \gamma(K) + q \cdot \nabla_q \gamma(K + q) \big|_{q=0} = -\frac{3a}{4}(-i + \sqrt{3})(q_x - iq_y) = -\frac{3a}{2}(q_x - iq_y), \tag{2.7} \]
where at the end we have removed an unphysical phase in the term. This leads to an effective Hamiltonian around $K$ of:

$$H_{K+q} \approx \frac{3ta}{2} \begin{pmatrix} 0 & q_x - iq_y \\ q_x + iq_y & 0 \end{pmatrix} = v_F (q_x \sigma_x + q_y \sigma_y) = v_F \mathbf{\sigma} \cdot \mathbf{q},$$

where $\sigma_i$ are the Pauli Matrices. Here the Hamiltonian acts only on the sublattice degree of freedom of its spinorial eigenstates, in other words its eigenstates are two-component spinors where each component is attached to sublattice $A$ or sublattice $B$. At the other Dirac point we can write out Hamiltonian in a similar way but with a phase shift of $\pi$ in the $x$-components. In both of these cases, the effective crystal momentum $\mathbf{q}$ is linearly coupled with the pseudospin through the Pauli matrices.

We can write out the entire effective low-energy Hamiltonian (around points $K$ and $K'$) as a four by four matrix acting on a four dimensional spinor, where the first two components describe the valley around $K$ and the last two describe the valley around $K'$:

$$H_{\mathbf{q}} = v_F (\tau_z \otimes \sigma_x q_x + 1 \otimes \sigma_y q_y),$$

where $\tau_i, \sigma_i$ are the Pauli Matrices acting on the subvalley (1 or 2) and sublattice ($A$ or $B$) degrees of freedom, respectively. The full effective Hamiltonian in position space is given in second-quantization formalism as:

$$H = -iv_F \int d^2r \bar{\Psi}(r)(\tau_z \otimes \sigma_x \partial_x + 1 \otimes \sigma_y \partial_y)\Psi(r), \quad \Psi^\dagger = (a_1^\dagger \ b_1^\dagger \ a_2^\dagger \ b_2^\dagger).$$

If we again only consider an expansion around $K$, we see that the two component electron spinor $\chi(r) = \begin{pmatrix} \chi_A(r) \\ \chi_B(r) \end{pmatrix}$ is governed by:

$$-iv_F \mathbf{\sigma} \cdot \nabla \chi(r) = i\partial_t \chi(r),$$

which is the Weyl equation [11]: the massless two-dimensional analogue of the Dirac equation, given by $(i\gamma^\mu \partial_\mu - m)\psi = 0$ in natural units. Without the presence of
mass, the Dirac equation decouples into two versions of the Weyl equation for two
spinors of opposite chirality (here corresponding to the subvalley “pseudospin” degree
of freedom). The electrons of long wavelength compared to the lattice spacing thus
behave like massless Dirac fermions in graphene. This is manifested in the dispersion
relation at the Dirac points, which up to linear order in $\mathbf{q}$ is given by:

$$E_{\pm}(\mathbf{q}) = \pm v_F |\mathbf{q}|.$$  \hfill (2.12)

This is the characteristic low-energy dispersion of graphene which lends it its unique
properties. Because the energy bands are gapless and linear, chiral fermions in
graphene behave as if massless and pseudo-relativistic, with the Fermi velocity $v_F$
taking the place of the speed of light $c$.

We can calculate the density of states using number of states below a certain
energy per unit volume, $N(E) = \frac{1}{(2\pi)^2} \int d^2k \theta(E - E(k))$, and differentiating with re-
spect to energy: $\rho(E) = \frac{dN}{dE}$. We find that our linear dispersion relation is manifested
as a linear density of states: $\rho \propto |E|$. As a result, the density of states at the Dirac
points is zero, and graphene is a zero-gap semiconductor [5].

2.2.2 General Chiral Model

We can rewrite the effective Hamiltonian around one Dirac point (2.9) in matrix form
as

$$H = v_F \begin{pmatrix} 0 & q_x - iq_y \\ q_x + iq_y & 0 \end{pmatrix}. \hfill (2.13)$$

Here we notice the characteristic linear coupling to the Pauli spin matrices. In bi-
layer graphene [14], low energy quasiparticles are described by a quadratic effective
Hamiltonian near the $K$-points:

$$H = -\frac{1}{2m} \begin{pmatrix} 0 & (q_x - iq_y)^2 \\ (q_x + iq_y)^2 & 0 \end{pmatrix}, \hfill (2.14)$$
Figure 2.4: Radial slices of the dispersion relation for (a) monolayer and (b) bilayer graphene in the vicinity of a $K$-point. Both materials exhibit zero band gap, yet monolayer graphene is linear while bilayer graphene is quadratic.

where $m$ is the effective mass of the chiral quasiparticles. The dispersion relations between energy and momentum are shown in Fig. 2.4, with a redefined $k = \sqrt{q_x^2 + q_y^2}$ as the magnitude of the crystal momentum. Because we are dealing with two dimensional materials, a true plot of a dispersion relation would show the energy compared to $q_x$ and $q_y$, yet due to the isotropic Hamiltonians (2.13) and (2.14) the radial slice is enough to show the full dispersion.

Different spin couplings give rise to different transport properties. In scattering events, conservation of energy dictates that incoming states must be scattered into reflected, transmitted, or evanescent states of the same energy. The dispersion relation of a two-dimensional material, as previously indicated, is a set of two-dimensional surfaces labeled by three coordinates $(k_x, k_y, E)$ that detail how the energy bands relate to crystal momentum [4]. At fixed energy $E_F$, the allowed momenta values form a slice of one such surface. These slices are called Fermi surfaces (because for ordinary 3D-materials they become surfaces), and indicate the allowable states for a given scattering energy. By looking at the chirality of the states on a Fermi surface, we can understand what processes are allowed and forbidden by spin conservation.
The pseudospin of the allowed states at a positive Fermi energy $E_F$ is plotted in Fig. 2.5 for monolayer and bilayer graphene. These are the incoming states for Klein tunneling depicted in Fig. 2.2. For a given direction of scattering labeled by wavevector $\mathbf{k}$, there is one corresponding state on the Fermi surface. Normal incidence restricts the right-moving states to incoming crystal momentum $\mathbf{k}$, and the left-moving states to $-\mathbf{k}$. Inside the potential barrier, the scattering matches particles to holes. By particle-hole symmetry [3], the pseudospins of the hole states on Fermi surfaces with negative energy are inverted compared to Fig. 2.5. Spin conservation then determines which hole states can be scattered into by the incoming particles.

In the plots, spin projections onto the $x$-axis and $y$-axis are combined to draw each spin vector. As such, vectors pointing in opposite direction are in fact orthogonal, as they represent the states $|s_x = +\frac{1}{2}\rangle$ and $|s_x = -\frac{1}{2}\rangle$. Isotropy does not predicate a preferred direction, so let us restrict our attention to incoming waves in the $x$-direction. In both monolayer and bilayer graphene, such states carry pseudospin $+\frac{1}{2}$. 

Figure 2.5: Pseudospin of states on Fermi surface of positive energy $E_F$ for (a) monolayer and (b) bilayer graphene.
For monolayer graphene, the pseudospin on the opposite side of the Fermi surface in Fig. 2.5 is \(-\frac{1}{2}\). An incident wave with momentum \(k_x\) cannot then scatter into a reflected wave with \(-k_x\) because spin is not conserved, prohibiting backscattering.

On the other hand, the inversion of the Fermi surface for holes means that a hole of momentum \(-k_x\) will have the same pseudospin as the incident particle. This explains the Klein paradox in graphene: incident particles cannot scatter to reflected states by spin conservation, but instead scatter to holes with the same spin inside the potential barrier. A hole moving left is akin to a particle moving right, so such scattering gives rise to perfect transmission through the barrier.

While monolayer graphene exhibits perfect transmission of incident particles on a potential barrier, bilayer graphene exhibits perfect reflection. This is because the states on the Fermi surface of opposite momentum have the same pseudospin. As a result, incident waves can scatter into reflected waves by spin conservation and cannot scatter into holes inside the barrier for the same reason. This phenomenon holds for normally incident scattering across all directions of the Fermi surface: monolayer graphene has opposite spin for opposite momentum states, while bilayer graphene has the same spin.

These qualitative predictions can be confirmed quantitatively by calculating the transmission coefficient of a particle with incident energy \(E_F\) tunneling through a potential barrier of width \(D\) and height \(V\). This is done by finding the scattering wavefunctions at incident energy \(E_F\) inside and outside the barrier. Bloch’s theorem dictates that they will composed of a plane wave, which details the direction of propagation, and the (chiral) eigenstate of the periodic Bloch Hamiltonian (2.13) or (2.14). By matching the wavefunctions and their derivatives at the two boundaries of the potential barrier, we can find the transmission \((T)\) and reflection \((R)\) coefficients for Klein tunneling.
Figure 2.6: Transmission probability across potential barrier of width $D$ for monolayer (red) and bilayer graphene (black). The difference in behaviors is explained by the different chiral couplings to momentum.

The transmission coefficient for monolayer and bilayer graphene is shown in Fig. 2.6. For widths much smaller than the Fermi wavelength ($\lambda = 2\pi/k_F$), even incident particles in bilayer graphene are transmitted, as the long wavelength of the incoming states does not “detect” the small inhomogeneity in potential. As we increase the width of the potential barrier, the transmission falls exponentially for bilayer graphene yet remains at 1 for the monolayer. This is a consequence of spin conservation and the lack of available backscattering states in monolayer graphene.

Using graphene as the base model, we can create a more general Hamiltonian to model a larger class of chiral couplings. Using $q_x$ and $q_y$ to label momentum displacements around some high-energy point in the Brillouin zone, we consider the Hamiltonian

$$H_J = \begin{pmatrix} 0 & q_x e^{iJ\theta} \\ q_x e^{-iJ\theta} & 0 \end{pmatrix},$$

(2.15)

where $q = \sqrt{q_x^2 + q_y^2}$ and $\theta = \tan^{-1}(q_y/q_x)$. The case of $J = 1$ reduces to monolayer graphene, while $J = 2$ reduces to bilayer. Once again, the chirality of the Fermi
Figure 2.7: Pseudospin of states on Fermi surface of positive energy $E_F$ for (a) chiral model with $J = 3$ and (b) bilayer graphene $J = 4$. For even powers of $J$, states of opposite momentum have the same spin, while for odd powers they have opposite spin.

The parameter $J$ in (2.15) labels the winding number of the spin vector around a Fermi surface. When this winding number is odd, states of opposite momenta have opposite spin, spin conservation prohibits reflection, and Klein tunneling gives rise to perfect transmission. When the winding number is even, states of opposite momenta have the same spin, and Klein tunneling becomes reflective in nature.

Using these chiral systems as a “basis”, one can construct a general chiral Hamiltonian: $H = \sum J H_J$. In this case both transmission and reflection are present at normal incidence, yet the highest power of $J$ in the linear combination will dominate. For example, $H = H_3 + H_4$ exhibits mostly Klein reflection like that of bilayer graphene or any evenly-coupled chiral Hamiltonian, with some transmission due to the $H_3$. Nevertheless, any such linear combination will be isotropic, as each $H_J$ is
Figure 2.8: Chirality of Fermi surface at $E_F = 0.2$ eV in anisotropic model. $x$-direction resembles monolayer graphene while $y$-direction resembles bilayer.

individually isotropic.

2.3 Anisotropy in Chiral Materials

To build an anisotropic model that maintains a chirality, we couple momentum linearly in one direction and quadratically in the other. We describe such a system with a Hamiltonian

$$H = tk_x^2\sigma_x + (1 - t)k_y\sigma_y, \quad (2.16)$$

where the parameter $t \in [0, 1]$ determines the relative strength of the couplings. The inherent anisotropy makes (2.16) impossible to write in the chiral basis of $H_J$, yet the presence of the Pauli spin matrices means we can still define a pseudospin for each state on a Fermi surface. The direction of such spins is displayed in Fig. 2.8.
Unlike the isotropic $J$-cases, the spin vector does not wind around the Fermi surface. Instead, along slices in the $k_x$ direction spins at opposite momenta are the same, while along $k_y$ spins at opposite momenta are opposite. The chirality of the Fermi surface suggests that this system is a combination of $H_1$ and $H_2$, yet altered to produce the different chiral behaviors along different directions.

In particular, we expect Klein tunneling to occur along all directions, with its reflective or transmissive nature determined by the power of the chiral coupling. To calculate transmission coefficients, we begin by rescaling the Hamiltonian to treat the linear and quadratic terms on the same footing: $q_x = \sqrt{t} k_x$ and $q_y = (1 - t) k_y$. We consider a plane wave incident on a potential barrier in the $x$-direction, as depicted in Fig. 2.2. If an incoming particle has energy $E_F$ and angle of incidence $\phi$, we solve the dispersion relation of (2.16) for the allowed values of Fermi wavevector: $k_F$, and set $k_x = k_F \cos \phi$ and $k_y = k_F \sin \phi$.

In our rescaled system, $k_F \rightarrow q_F$, changing the angle of incidence. To this end, we consider a rescaled angle of incidence $\varphi = \tan^{-1} \left( \frac{q_y}{q_x} \right)$ that we use in studying the rescaled scattering. To return to the physical angle of incidence, we use the relation

$$\phi = \tan^{-1} \left( \frac{\sqrt{t}}{1 - t \tan \varphi} \right) .$$

As $t$ grows larger, the quadratic term in (2.16) dominates, and the physical angle of incidence for small rescaled angles $\varphi$ is large, indicating that the quadratic region around $q_y = k_y = 0$ dilates. Similarly, when $t$ is small, the effect of (2.17) is to turn large rescaled angles into small physical angles, shrinking the quadratic region and dilating the linear one along $q_x = k_x = 0$. We sketch this dilation in Fig. 2.9, where it is clear that $t$ parametrizes the angular range of linear and quadratic behavior in the material.
Figure 2.9: Dilation from rescaled angular profile to physical profile of anisotropic material in (2.16) (a) Rescaled angle $\varphi$ describes material with equal regions of linear and quadratic coupling, (b) at small $t$, physical system is dominated by linear behavior around $k_x = 0$, (c) at large $t$, physical system is dominated by quadratic behavior near $k_y = 0$.

Keeping track of these dilations from the rescaled system to the physical system, we can calculate the transmission coefficient by matching boundary conditions of the wavefunction at the two interfaces with the potential step. The dispersion relation due to (2.16) gives rise to a quartic equation for $q_F$, where two of the possible solutions are propagating waves and two are evanescent. Bloch’s theorem predicates that the electron wavefunctions in a periodic solid are the product of a plane wave and an eigenstate of the periodic Hamiltonian (2.16) [4].

Starting from a value of $k_F$, we can then write the wavefunction in the different scattering regions. Boundary conditions at infinity restrict our expressions, as the exponentially growing evanescent waves cannot exist outside the finite potential bump, and we stipulate that the incoming particles only hit the potential from one direc-
Figure 2.10: Polar distribution of transmission probability for Klein tunneling in anisotropic model across a potential barrier in the $x$ (quadratic) direction for (a) $V = 2E_F = 0.02$ eV and $D = 2$ nm and (b) $V = 2E_F = 0.04$ eV and $D = 6.5$ nm.

Matching the wavefunctions and their derivatives across the two boundaries, we obtain an expression for the transmission coefficient. In Fig. 2.10 we plot the transmission probability along different (rescaled) angles of incidence.

Our toy model of an anisotropic chiral material displays the expected Klein tunneling behavior, as full transmission is observed along the linear direction $k_x = 0$ and full reflection along the quadratic direction $k_y = 0$. As the Fermi energy and width of the barrier are increased, we see that resonances in the probability begin to develop. Nevertheless, scattering at normal incidence along $k_x$ always like bilayer graphene ($J = 2$), while along $\varphi = \phi = \pi/2$ the transmission remains zero as for monolayer graphene. This simple model thus highlights the anisotropic behavior of Klein tunneling, which smoothly interpolated between perfect transmission and perfect reflection as the direction of transport is rotated.
Chapter 3

Phosphorene

In an effort to find a real material exhibiting the chiral anisotropy of our toy model, we consider the case of phosphorene. phosphorene is a single crystalline layer of black phosphorus with a similar structure to the honeycomb lattice of graphene [2]. Unlike graphene, however, the atoms are staggered in height, giving the lattice a zigzag appearance when looked at from the side and a squished honeycomb appearance from the top. In our tight-binding approximation, we consider two types of hoppings: $t_1$, between adjacent atoms of the same height, and $t_2$, between adjacent atoms of different heights. Each lattice point has two nearest neighbors in-plane and one out of plane. The structure of phosphorene is illustrated in Fig. 3.1, along with the boxed unit cell containing four species of atoms.

Figure 3.1: Phosphorene structure [1] from (a) diagonal view, (b) cross-sectional view, and (c) top view with x as the horizontal axis and y as the vertical.
The unit cell is illustrated in more detail in Fig. 3.3, and the values for our hopping parameters and atom separations are given by \([2]\) \(t_1 = -1.486\ \text{eV}, d_1 = 2.22\ \text{Å}\) and \(t_2 = 3.729\ \text{eV}, d_2 = 2.24\ \text{Å}\), where the vector \(d_2\) is assumed to be only in the \(x\)-direction for simplicity and the bond angle is 98°. Further values of hopping parameters are provided in Fig. 3.2

![Figure 3.2: Table [2] displaying tight-binding parameters for phosphorene.](image)

### 3.1 Tight Binding Model

Neglecting chemical potential for now, which can be added later as “self-hopping”, we can write a tight-binding Hamiltonian for the system in second quantization notation:

\[
H = \sum_{k \in \text{BZ}} \begin{pmatrix} a_k^\dagger & a_k^\dagger & b_k^\dagger & b_k^\dagger \end{pmatrix} \begin{pmatrix} 0 & H_{AA'} & H_{AB} & H_{AB'} \\ H_{AA'}^* & 0 & H_{A'B} & H_{A'B'} \\ H_{AB}^* & H_{A'B}^* & 0 & H_{BB'} \\ H_{AB'}^* & H_{A'B'}^* & H_{BB'}^* & 0 \end{pmatrix} \begin{pmatrix} a_k \\ a_k' \\ b_k \\ b_k' \end{pmatrix},
\]

where the creation and annihilation operators in create and annihilate atoms on the corresponding lattice sites shown in Fig. 3. Using the standard tight-binding procedure in reciprocal space \([4]\), we find the nonzero components of the Hamiltonian by summing over nearest neighbors. For example, \(H_{AB} = \sum_{j=1}^{2} t_j e^{i k \cdot d_{AB}}\), where \(d_{AB}^1\) and \(d_{AB}^2\) are the displacements between \(A\) and its two \(B\) nearest neighbors.
Figure 3.3: Unit cell of phosphorene with four species of atoms and two different hoppings labeled. Atoms in red are higher in the z-direction (out of page) than atoms in blue.

We can add a chemical potential $\mu_0$ by shifting the diagonal of our Hamiltonian by a constant, and introduce an electric field in the $z$-direction by setting a potential difference $\Delta V$ between our higher atoms ($A$ and $B$) and our lower atoms ($A'$ and $B'$). Our new diagonal terms are thus given by $H_{AA} = H_{BB} = -\mu_0 + \Delta V/2$ and $H_{A'A'} = H_{B'B'} = -\mu_0 - \Delta V/2$. For the moment we set $\mu_0 = \Delta V = 0$. Our tight-binding Hamiltonian then takes the following form:

$$H(k_x, k_y) = \begin{pmatrix} 0 & \alpha & \beta & 0 \\ \alpha^* & 0 & 0 & \beta^* \\ \beta^* & 0 & 0 & \alpha^* \\ 0 & \beta & \alpha & 0 \end{pmatrix}, \quad \alpha = 3.73e^{-2.24ik_x}, \beta = -2.97e^{1.46ik_x} \cos(1.68k_y)$$

(3.2)

In particular, we are interested in low-energy behavior of this model near the $\Gamma$-point ($k_x, k_y = 0$), so we must linearize the Hamiltonian and then project out the highest and lowest energy bands. phosphorene is unusual in that the dispersion about $\Gamma$ is linear along the $k_x$ axis in the Brillouin Zone and quadratic along $k_y$. This behavior is shown in Fig. 3.4, along with the band gap of about 1.5 eV.

To linearize the Hamiltonian, we expand about $k_x, k_y = 0$ and keep terms of
linear order. This procedure is an oversimplification, however, because it removes any dependence on \( k_y \). To maintain this, we must expand to quadratic order instead. In this approximation, we arrive at matrix elements \( \alpha \approx 3.73 - 8.36i k_x - 9.36k_x^2 \) and \( \beta \approx -2.97 - 4.33i k_x + 3.17k_x^2 + 4.19k_y^2 \) in (3.2).

![Graphs of \( k_x \) and \( k_y \) slices of the band structure in the vicinity of the \( \Gamma \)-point](image)

Figure 3.4: The \( k_x \) (a) and \( k_y \) (b) slices of the band structure in the vicinity of the \( \Gamma \)-point exhibit linear and quadratic behavior, respectively.

### 3.2 Projected Two-Band Hamiltonian

To study the pseudospin that forms the basis of the unusual Klein paradox transport properties \([3]\), we are interested in the eigenstates of the Hamiltonian and preserving their structure in the projection process. Furthermore, once we have a simplified two-band model, we must introduce an electric field in a manner consistent with the full four-band description of the lattice. It is thus instructive to analyze the eigenvalues of (3.1) at the \( \Gamma \)-point before any sort of linearization or projection is made. In the basis we have chosen for the full Hamiltonian, \( \{ |\psi_A\rangle, |\psi_{A'}\rangle, |\psi_B\rangle, |\psi_{B'}\rangle \} \), the four eigenvalues at \( k_x = k_y = 0 \) take the form

\[
|\psi_{\text{top}}\rangle = \frac{1}{2} \begin{pmatrix} 1 \\ 1 \\ -1 \\ -1 \end{pmatrix}, \quad |\psi_{\text{+}}\rangle = \frac{1}{2} \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}, \quad |\psi_{\text{-}}\rangle = \frac{1}{2} \begin{pmatrix} 1 \\ -1 \\ -1 \\ 1 \end{pmatrix}, \quad |\psi_{\text{bottom}}\rangle = \frac{1}{2} \begin{pmatrix} -1 \\ 1 \\ -1 \\ 1 \end{pmatrix},
\]

(3.3)
where they are associated with the highest, middle two, and lowest bands, respectively. It is interesting to note that $|\psi_+\rangle$ and $|\psi_-\rangle$, which are associated with the low energy bands that exhibit a 1.514 eV band gap at $\Gamma$, are mixed states of all four lattice sites, indicating possible difficulty in choosing a basis that will project out the higher states without loss of information.

To construct a 2 by 2 Hamiltonian out of (3.1), we draw inspiration from [1, 15] and note that we have effectively ignored the difference in height of the unprimed lattice sites and the primed lattice sites in creating our 2D Brillouin Zone. As a result of the symmetry of the lattice under the point group $C_{2h}$ [16], we see that the hoppings between primed and unprimed atoms on the left have the same energies and directions. We can thus ignore height difference altogether, and defining new lattice sites by the atoms right and left of the $t_2$ hopping, we can construct the projected Hamiltonian.

Because we have identified lattice sites $A$ and $B'$ (and $A'$ and $B$) with each other, there are only two of them and the Hamiltonian must necessarily be a two-by-two matrix. Each new lattice site has three hoppings and we can write down the Hamiltonian in the following form:

$$H_1 = \begin{pmatrix} 0 & \alpha + \beta \\ \alpha^* + \beta^* & 0 \end{pmatrix}.$$  (3.4)

Here the electric field is still zero, and we are working in a transformed basis of spinors

$$\Psi = \begin{pmatrix} c_1 |\psi_1\rangle \\ c_2 |\psi_2\rangle \end{pmatrix} \text{ with }$$

$$|\psi_1\rangle = \frac{1}{\sqrt{2}} (|\psi_A\rangle + |\psi_{B'}\rangle), \quad |\psi_2\rangle = \frac{1}{\sqrt{2}} (|\psi_{A'}\rangle + |\psi_B\rangle).$$  (3.5)

We notice that this is the basis of atoms on the right of an $AB$ “pair” ($A$ and $B'$) and atoms on the left ($A'$ and $B$). To return to a four-by-four Hamiltonian, we write these new basis vectors in the old basis as above in (3.5) and choose two more orthogonal vectors to form a basis. A suitable choice of such orthogonal vectors is
\( |\psi_3\rangle \propto (1, 0, 0, -1)^T \) and \( |\psi_4\rangle \propto (0, 1, -1, 0)^T \). In this new basis the Hamiltonian is block diagonal, with the low energy block given by (3.4), and the higher energy block given by

\[
\mathcal{H}_2 = \begin{pmatrix}
0 & \alpha - \beta \\
\alpha^{\ast} - \beta^{\ast} & 0
\end{pmatrix}.
\] (3.6)

Now we can introduce an electric field through a staggered potential of \(-\Delta V/2\) for higher (unprimed) lattice sites and \(\Delta V/2\) for lower (primed) lattice sites. This is best done in the original basis of unmixed lattice sites, where the potential appears on the diagonal of (3.2). We can then transform to the new basis in (3.5) to see how the field affects the lower bands. In this basis, the previously diagonal electric perturbation introduces a tunneling term (an off-diagonal block matrix in the Hamiltonian) between the lower energy bands and the higher energy bands of the form

\[
T = \begin{pmatrix}
-\Delta V/2 & 0 \\
0 & \Delta V/2
\end{pmatrix}.
\] (3.7)

Combining these 2-by-2 blocks we can write our symmetry-basis Hamiltonian compactly as follows:

\[
H = \begin{pmatrix}
\mathcal{H}_1 & T \\
T & \mathcal{H}_2
\end{pmatrix}.
\] (3.8)

Finally, we can include the perturbation in \(\mathcal{H}_1\) due to the mixing with \(\mathcal{H}_2\) mediated by \(T\) through a field theory-like formalism of Green’s functions. Taking \(G_i = (\omega \mathbb{1} - \mathcal{H}_i)^{-1}\) as our unperturbed Green’s functions, we can write the “dressed” Green’s function of the lower bands as a series:

\[
\tilde{G}_1 = G_1 + G_1 TG_2 T G_1 + G_1 TG_2 T G_1 TG_2 T G_1 + \cdots = G_1 + G_1 TG_2 T (G_1 + G_1 TG_2 T G_1 + \cdots),
\] (3.9)

The second equality suggests that we may re-sum the series to get a recursive relation for \(\tilde{G}_1\):

\[
\tilde{G}_1^{-1} = \omega - \tilde{\mathcal{H}}_1 = G_1^{-1}(\mathbb{1} - G_1 TG_2 T).
\] (3.10)
The poles of the dressed Green’s function are the eigenvalues of the matrix, which are solutions to the equation \( \det [\omega - \tilde{H}_1] = 0 \). This yields not only the two lowest eigenvalues, but all of them because we end up with a quadratic equation in \( \omega \).

We can also see this straight from \( H \), whose eigenvalues are the solutions to \( \det [\omega - H] = 0 \). Because \( (\omega - H) \) is a block matrix, and \( (\omega - \mathcal{H}_2) \) is nonsingular for any of the eigenvalues \( \omega \) of \( H \) (simply a consequence of the fact that for nonzero \( T \), the higher eigenvalues of \( H \) will be slightly perturbed from those of its lower block \( \mathcal{H}_2 \)), we can apply the formula for block matrix determinants and arrive at:

\[
\det [\omega - H_1] - T(\omega - H_2)^{-1}T = 0,
\]

which is the same condition as (3.10). We would like to find a \( \tilde{H}_1 \) that is independent of \( \omega \) to represent the perturbed lower-energy Hamiltonian, but unfortunately there is no way to find a solution for all \( \omega \) because the right-hand side of (3.10) depends nontrivially on \( \omega \). The best we can do is perform a low-energy expansion about \( \omega = 0 \) and then keep only the constant term, which yields \( \tilde{H}_1 = H_1 - T\mathcal{H}_2^{-1}T \), a result in agreement with the procedure used in [6] to find a 2-by-2 Hamiltonian for bilayer graphene. In component form, this projected Hamiltonian would be

\[
\tilde{H}_1 = \begin{pmatrix}
0 & \gamma \\
\gamma^* & 0
\end{pmatrix}, \quad \gamma = \frac{|\alpha|^2 + |\beta|^2 + 2i \text{Im}(\alpha^*\beta) + (\Delta V)^2/4}{\alpha^* - \beta^*}
\]

(3.12)

However, for the phosphorene system in a relatively elevated electric field, this projected Hamiltonian has a different band gap than that of the true Hamiltonian \( H \).

To this end, we can follow the more explicit procedure used in [14], and manipulate the above expressions a bit more carefully. We recognize that we have an eigenvalue equation inherent in (3.11), and because we would like to eventually study how the states of the Hamiltonian evolve in the Brillouin Zone, we should be careful about which 2-by-2 matrix acts on the low dimensional eigenvectors. In this way, we can
keep track of the states that correspond to the low-energy bands, which will be the states whose chirality drives the Klein tunneling.

The eigenvalue equation in (3.11) is formulated by identifying $\omega$ as an energy eigenvalue $E$ of the original Hamiltonian, and choosing a vector $\theta$ from the nontrivial null space of $\tilde{H}_1$:

$$[\mathcal{H}_1 + T(E - \mathcal{H}_2)^{-1}T] \theta = E\theta$$  \hfill (3.13)

We recognize that this is simply the first row of the full eigenvalue equation

$$
\begin{pmatrix}
\mathcal{H}_1 & T \\
T & \mathcal{H}_2
\end{pmatrix}
\begin{pmatrix}
\theta \\
\chi
\end{pmatrix}
= E
\begin{pmatrix}
\theta \\
\chi
\end{pmatrix},
$$  \hfill (3.14)

where we have used the second row to arrive at the relation $\chi = (E - \mathcal{H}_2)^{-1}T\theta$, then used to simplify the first row to get (3.13). From (3.14) we recognize that $\theta$ is the state corresponding to the low energy portion of $H$ without the full effects of the perturbation accounted for ($T$ induces mixing of the matrix blocks so that $\theta$ does not correspond exactly to an eigenstate of the perturbed low energy Hamiltonian). Now we can use (3.13) as our starting point and expand around low energies $E$ to find the correct 2-by-2 projection.

We can take advantage of the geometric series expansion for matrices $((1 - A)^{-1} = \sum A^k)$ to write $(E - \mathcal{H}_2)^{-1} = -[\mathcal{H}_2(1 - E\mathcal{H}_2^{-1})]^{-1} = -(1 + E\mathcal{H}_2^{-1} + E^2\mathcal{H}_2^{-2} + \cdots)\mathcal{H}_2^{-1} \approx -\mathcal{H}_2^{-1} - E\mathcal{H}_2^{-2}$. Keeping the linear terms in $E$ allows for a good linear approximation to the eigenvalue equation for the perturbed $\mathcal{H}_1$:

$$(\mathcal{H}_1 - TH_2^{-1}T)\theta = E S \theta, \quad S = (1 + TH_2^{-2}T).$$  \hfill (3.15)

This is not yet an eigenvalue equation because of the matrix $S$, but writing $S = S^{1/2}S^{1/2}$ and changing states to $\Theta = S^{1/2}\theta$ we finally arrive at a proper eigenvalue equation with energy $E$, and we can simply read off the effective 2-by-2 Hamiltonian of our system, which can then be expanded to desired order in $k$:

$$H_{\text{eff}} = S^{1/2}(\mathcal{H}_1 - TH_2^{-1}T)S^{1/2}$$  \hfill (3.16)
3.3 Bilayer phosphorene

In monolayer phosphorene, the band gap increases with applied electric field, and because it starts out at the relatively high value of 1.5 eV, it is more difficult to use for semiconductor applications. It is convenient to instead work with bilayer phosphorene, where we the band gap is smaller ($\sim 0.5$ eV), and can be closed by applying an external electric field. We can simply extend the single layer model to the bilayer case by adding an interlayer hopping $t_{1}^{\perp} = 0.524$ eV [2] between an $A/B'$ atom on the lower layer and two $A'/B$ atoms on the upper layer (and vice versa). Our tight binding model then leads to an 8-by-8 Hamiltonian.

As before, we can add a staggered potential between the two layers to model the electric field. Similarly, applying the same symmetry argument we used for the monolayer (essentially changing the basis) we can reduce the Hamiltonian to two 4-by-4 block matrices and an off-diagonal transfer term which depends on the interlayer hopping [15]. This transfer term can be neglected because the interlayer hopping is small compared to the other terms, and taking one of the two diagonal blocks we end up with an effective Hamiltonian for the four lowest energy bands. From this point, we can again apply the same Green's function formalism to project out the highest and lowest bands, but it is simpler to instead use a $k \cdot p$ approach.

3.3.1 $k \cdot p$ - Hamiltonian

In a $k \cdot p$ expansion, the end result is a Hamiltonian in reciprocal space expanded to low order in $k$ around a point of high symmetry [4]. We thus begin by expanding the 4-by-4 Hamiltonian around the point of interest: in our case the $\Gamma$-point ($k = 0$).
This gives us a matrix of the following form:

\[
H_b(k_x, k_y) = \begin{pmatrix}
0 & \alpha + \beta + \frac{\gamma}{2} & i\frac{\Delta V}{2} & 0 \\
\alpha^* + \beta^* - \frac{\gamma^*}{2} & 0 & 0 & i\frac{\Delta V}{2} \\
-i\frac{\Delta V}{2} & 0 & 0 & \alpha + \beta + \frac{\gamma}{2} \\
0 & -i\frac{\Delta V}{2} & \alpha^* + \beta^* + \frac{\gamma^*}{2} & 0
\end{pmatrix},
\]

(3.17)

where \(\gamma = 1.05 - 4.38ik_x - 8.76k_x^2 - 1.43k_y^2\) is an additional term due to the interlayer hopping and \(\alpha\) and \(\beta\) are the same as before. We can then take the eigenvectors associated with the two lowest (in absolute value) eigenvalues at \(k_x, k_y = 0\), which we will call \(|v_1\rangle\) and \(|v_2\rangle\), and use them to construct a 2-by-2 approximate Hamiltonian that describes just the lowest two energy states:

\[
\mathcal{H}_b(k_x, k_y) = \begin{pmatrix}
\langle v_1|H_b(k_x, k_y)|v_1\rangle & \langle v_1|H_b(k_x, k_y)|v_2\rangle \\
\langle v_2|H_b(k_x, k_y)|v_1\rangle & \langle v_2|H_b(k_x, k_y)|v_2\rangle
\end{pmatrix}.
\]

(3.18)

This approach allows us to focus on just the low-energy dynamics of the system. Looking at the band structure of (3.17), we can see that the band gap is closed by an electric field strength giving rise to potential energy difference of \(\Delta V_0 = 1.094\) eV between the higher and lower atoms in the lattice, which are separated by approximately 2 Å. This is a fairly strong electric field, and so we can start with the expanded Hamiltonian for a lower field like \(\Delta V = 0.5\) eV:

\[
\mathcal{H}_b(k_x, k_y) = \begin{pmatrix}
0.18 - 2.25k_x^2 + 4.81k_y^2 \\
-9.22ik_x & -0.18 + 2.25k_x^2 - 4.81k_y^2
\end{pmatrix} \approx C_1(k_y^2 - C_2k_x^2)\sigma_z - C_3k_x\sigma_y.
\]

(3.19)

where \(C_1 = 4.81\) eV \(\cdot\) Å\(^2\), \(C_2 = 0.47\), and \(C_3 = 9.22\) eV \(\cdot\) Å.

This is a chiral Hamiltonian, as the presence of the Pauli spin matrices in (3.19) gives rise to a pseudospin degree of freedom. The eigenstates of this Hamiltonian are spin-1/2 spinors, and the conservation of this spin engenders a Klein tunneling effect in the material. We can gain intuition about the chirality of the states of (3.18)
by fixing a Fermi energy and plotting the Fermi surface with vectors at each point indicating the spin-components of the states.

This is done by plotting the points \((k_x, k_y)\) that satisfy \(\mathcal{H}_b(k_x, k_y) |\psi\rangle = E_F |\psi\rangle\) for fixed Fermi energy \(E_F\) that is in the range of accessible electronic states (in other words, since the upper and lower bands are symmetric, we must choose a Fermi level above half the band gap). For each point, there is an associated eigenstate \(|\psi\rangle\) that has nonzero spin in the \(y\) and \(z\) directions, so we can graphically visualize its projection onto the spin directions by plotting the vector \((\langle \psi | \sigma_z | \psi \rangle, \langle \psi | \sigma_y | \psi \rangle)\) on the Fermi surface. This generates a vector plot whose form depends on both the Fermi energy and the external electric field. Below we show a few plots characterizing the behavior.

### 3.3.2 Fermi Surfaces

In the following section, the plots on the left are the Fermi surface and spin projections of the states of the Hamiltonian with parameters described in the caption below. To the right, the \(k_x\) and \(k_y\) slices of the band structure of the Hamiltonian is plotted: the red is the dispersion of (3.17), the blue is the dispersion of the 2-by-2 projected bilayer Hamiltonian using the methods of Section 2, and the green is our \(k \cdot p\) effective Hamiltonian above. In the dispersion relations, a horizontal black line indicates the Fermi level, and in the plot of the Fermi surface, the \(k_x\) direction is horizontal while the \(k_y\) is vertical.
Figure 3.5: Electric field: \( \Delta V = 0 \), Band Gap: 0.466 eV, Fermi level: 0.250 eV. Fermi surface is plotted in green on the left with the red arrows indicating the spin projection of the eigenstates. \( k_x \) and \( k_y \) slices of the dispersion is plotted on the right, with red indicating the true dispersion, blue the Green’s function projection, and green the \( k \cdot p \)-expansion.

Figure 3.6: Electric field: \( \Delta V = \Delta V_0 \), Band Gap: 0 eV, Fermi level: 0.200 eV. Fermi surface is plotted in green on the left with the red arrows indicating the spin projection of the eigenstates. \( k_x \) and \( k_y \) slices of the dispersion is plotted on the right, with red indicating the true dispersion, blue the Green’s function projection, and green the \( k \cdot p \)-expansion.
Figure 3.7: Electric field: $\Delta V = 1.4V_0$, Band Gap: 0.341 eV, Fermi level: 0.1 eV. Fermi surface is plotted in green on the left with the red arrows indicating the spin projection of the eigenstates. $k_x$ and $k_y$ slices of the dispersion is plotted on the right, with red indicating the true dispersion, blue the Green’s function projection, and green the $k \cdot p$-expansion.

These plots indicate that the most anisotropic behavior occurs as the electric field is tuned to band gap closing, as in Fig. 3.6. In this regime, the linear dispersion relation along $k_x$ suggests that Klein tunneling along this direction should mimic that of Graphene, with full transmission through an arbitrarily high potential barrier. On the other hand, the dispersion along the $k_y$-direction is quadratic, implying that the transport properties could more closely resemble those of bilayer graphene, in which full transmission becomes zero transmission due to the fact that backscattering now is the process that obeys spin-conservation [3].

Evidence for these observations comes from the plot of the Fermi surface, in which we see that along the $k_x$ direction, the spins for positive and negative momentum
states are opposite, preventing backscattering. By charge-conjugation symmetry, the chirality of the Fermi surface in the valence band is opposite to that displayed in the plots (which display the conduction band), so when the traveling particle enters the potential barrier (effectively placing the Fermi level in the valence band), it can then scatter to a hole inside the barrier because spin is conserved. On the other hand, the spins at $\pm k_y$ are in the same direction in Fig. 3.6, indicating that backscattering is a spin-conserving process in this case. In Fig. 3.7 we see the process of splitting the Fermi surface due to high electric field, which suggests an availability of more scattering states. However

Now that we have found a low-energy model for bilayer phosphorene, a strongly anisotropic example of a chiral two-dimensional material, it is worth revisiting the Hamiltonian to glean the dependence on the external electric field strength. In this way, we will be able to move towards a general description of the chirality of phosphorene at different band gap sizes. First, in order to simplify expressions, we will take the value of the first interlayer hopping parameter to be 0.5 eV instead of the 0.524 eV value given by the tight-binding model we have been using [2] (It is worth noting that a previous tight-binding model from the same authors yielded a value of 0.295 eV for the same hopping [10]).

This does not change the general behavior of the bands, but shifts the critical potential (to close the band gap) to 1.137 eV. Additionally, there is no need to create a dimensionless potential to expand about because our characteristic value for the potential is of order 1. For simplicity, we simply denote the staggered sublattice potential as $V$ in the following.

Including the dependence on the external field, we can write (3.19) as

$$\mathcal{H}(k_x, k_y) = \left[ C_0(V) + C_1(V)k_y^2 - C_2(V)k_x^2 \right] \sigma_z - [C_3(V)k_x]\sigma_y,$$  \hspace{1cm} (3.20)
where the values of the coefficients are given by:

\[
C_0(V) = 0.76 - \frac{\sqrt{1 + V^2}}{2}, \quad C_1(V) = 4.17 + \frac{0.71}{\sqrt{1 + V^2}}, \\
C_2(V) = 6.20 - \frac{4.38}{\sqrt{1 + V^2}}, \quad C_3(V) = -2.19i + \frac{12.64i}{\sqrt{1 + V^2}},
\]

(3.21)

and they have units eV, eV \(\cdot\) \(\hat{A}^2\), eV \(\cdot\) \(\hat{A}^2\), and eV \(\cdot\) \(\hat{A}\), respectively.

Ignoring their units, we can plot the four coefficients together just to understand their general behavior as the external potential changes.

![Figure 3.8](image-url)

Figure 3.8: Magnitude of coefficients describing low-energy effective Hamiltonian plotted against external field value. The y-axis is in units of either eV, eV \(\cdot\) \(\hat{A}^2\), or eV \(\cdot\) \(\hat{A}\) depending on the coefficients.

We can ignore \(C_0\) because of its very small contribution proportional to the other coefficients (effectively it adds a minuscule positive mass term before the critical field and a small negative mass term beyond it). An interesting question is: along which direction should one slice the dispersion in order to get entirely quadratic or entirely linear behavior? In other words, if we slice along \(k_y = \Xi k_x\), what is the coefficient \(\Xi\) that will result in either a quadratic energy-momentum relation or a linear one? It is clear from (3.20) that we get completely quadratic behavior if and only if we slice along \(k_x = 0\). The direction of the completely linear slice varies depending on \(V\), but our dispersion relations in Fig. 3.4 tell us that when we are at \(V = V_0\) there is a very
nearly linear dispersion along \( k_y = 0 \).

More precisely, we can compute the condition for the vanishing of the quadratic coefficients, yielding a “linear slice” along \( k_y = \pm \frac{0.92}{\sqrt{1 + V^2}} k_x \), where we have used the average value of \( C_1(V) \) for \( V \in [0 \text{ eV}, 1.5 \text{ eV}] \) because of its slow variation in the region of interest. This varies from \( k_y = \pm 0.38 k_x \) when there is no external field to \( k_y = \pm 0.70 k_x \) when \( V = V_0 \), yet the dispersion is very nearly linear in almost all directions of slicing except for \( k_x = 0 \).

### 3.4 A More Accurate Model

While the model above captures much of the physics of an anisotropic, chiral 2D material, several simplifications in dropping hoppings and utilizing different values for them in [2] and [10] lead to a dispersion relation that does not match the actual one for phosphorene in energy scale. It is worth returning to the full 8 band model and reduce the amount of simplification to arrive at a two-band model that fully captures the low energy physics of phosphorene, leading to a real example of a chiral anisotropic material.

Using the symmetry argument of (3.4), expanding the hoppings in [15] to second order in \( k_x \) and \( k_y \), and dropping an unimportant constant on the diagonal, we arrive at an accurate four-band effective Hamiltonian for bilayer phosphorene:

\[
H = \begin{pmatrix} H_1 & T \\ T^\dagger & H_2 \end{pmatrix}; \quad H_i = \begin{pmatrix} \alpha k_x^2 + \beta_1 k_y^2 & \gamma_i + \delta_1 k_x^2 + \zeta_i k_y^2 + i\eta_i k_x \\ \gamma_i + \delta_1 k_x^2 + \zeta_i k_y^2 - i\eta_i k_x & \alpha k_x^2 + \beta_1 k_y^2 \end{pmatrix}, \quad T = \frac{-iV}{2} \mathbf{1}.
\]

In the Hamiltonian above, \( V \) is the potential giving rise to the constant electric field, and the coefficients take on values \( \alpha = 1.01 \text{ eV} \cdot \text{Å}^2 \), \( \beta_1 = 2.24 \text{ eV} \cdot \text{Å}^2 \), \( \beta_2 = -1.08 \text{ eV} \cdot \text{Å}^2 \), \( \gamma_1 = 0.97 \text{ eV} \), \( \gamma_2 = 0.56 \text{ eV} \), \( \delta_1 = 4.37 \text{ eV} \cdot \text{Å}^2 \), \( \delta_2 = 3.29 \text{ eV} \cdot \text{Å}^2 \), \( \zeta_1 = 3.63 \text{ eV} \cdot \text{Å}^2 \), \( \zeta_2 = 4.19 \text{ eV} \cdot \text{Å}^2 \), \( \eta_1 = 5.80 \text{ eV} \cdot \text{Å} \), \( \eta_2 = 4.71 \text{ eV} \cdot \text{Å} \).

To perform a \( k \cdot p \)-expansion we diagonalize the Hamiltonian at the \( \Gamma \) point and
use the eigenvectors associated with the two lowest energies (in magnitude) to write a 2-by-2 matrix in the form of (3.18). Defining $\gamma_1 - \gamma_2 = \gamma$, we can express these energies and (unnormalized) states as

$$
\epsilon_{\pm} = \pm \frac{1}{2} \left( \gamma_1 + \gamma_2 - \sqrt{\gamma^2 + V^2} \right), \quad |\pm\rangle = \begin{pmatrix}
i \left( -\gamma + \sqrt{\gamma^2 + V^2} \right) \\
\pm V \\
V
\end{pmatrix}
$$

(3.23)

Defining an electric field-dependent normalization factor $N(V) = (0.67 + 4V^2 - 1.64\sqrt{0.17 + V^2})^{-1}$, we can write the correct two band effective Hamiltonian:

$$
\mathcal{H} = \frac{1}{N} \left[ (C_0 + C_1 k_y^2 + C_2 k_x^2) \sigma_z + (C_3 k_x) \sigma_y + (C_4 k_y^2 + C_5 k_x^2) \right],
$$

(3.24)

where the coefficients are given by

$$
C_0(V) = 0.65 + 3.88V^2 - (1.59 + 2V^2)\sqrt{0.17 + V^2}, \quad C_1(V) = 2.4 + 15.64V^2 - 5.95\sqrt{0.17 + V^2},
$$

$$
C_2(V) = 2.94 + 15.32V^2 - 7.17\sqrt{0.17 + V^2}, \quad C_3(V) = 3.9 + 2.18V^2 - 9.51\sqrt{0.17 + V^2},
$$

$$
C_4(V) = 1.51 + 2.32V^2 - 3.67\sqrt{0.17 + V^2}, \quad C_5(V) = 0.68 + 4.04V^2 - 1.66\sqrt{0.17 + V^2}.
$$

(3.25)

Figure 3.9: Magnitude of corrected coefficients describing correct low-energy effective Hamiltonian plotted against external field value. $C_0$ is not plotted as it is simply an overall shift in energy and will not affect the chirality of the states. The y-axis is in units of either eV, eV \( \cdot \) Å$^2$, or eV \( \cdot \) Å depending on the coefficients.

In Fig. 3.9 we have plotted five of the coefficients in our corrected Hamiltonian for various values of the electric field (ignoring dimension) to get a sense for their
fluctuation near the critical value. One can see that the coefficients of the identity matrix, \( C_4 \) and \( C_5 \), are nearly constant in the region of interest. Given that their only contribution to the system is very small energy shift in the bands away from \( \Gamma \) without affecting the chiral nature of phosphorene, it is justified to work in an approximation where \( C_4 = C_5 = 0 \). Similarly, near our region of interest the constant term \( C_0 \approx 0 \).

Following the developments of the previous sections, we will summarize some results for this adjusted Hamiltonian despite the fact that the general behavior will match that of the previous one (3.20). To begin, the band gap at the \( \Gamma \) point is closed when the field takes on a critical value \( V_0 = 1.47 \) eV. The new Hamiltonian (3.24) is completely quadratic in its dispersion along the \( k_x = 0 \) direction. Because both \( C_1 \) and \( C_2 \) have the same sign, it is impossible to find a “slice” in the dispersion relation such that the quadratic term vanishes, yet near \( \Gamma \) the dispersion is linear along \( k_y = 0 \). Lastly, the chirality of the states on the Fermi surface is very similar to that shown in Figs. 3.5-3.7, with the only difference being the energy scale of chemical potentials decreasing from that of the plots to better fit phosphorene.

### 3.5 Klein Tunneling in Bilayer phosphorene

The anisotropy of bilayer phosphorene is most prominent when there is no band gap, so we restrict our attention to the case in which the electric field attains its critical value. This also ignores the potential effects of the split Fermi surface that occurs when the electric field is greater than the critical value. However, this situation is difficult to realize experimentally due to the strength of the critical field. Furthermore, Fig. 3.7 shows that the splitting of the Fermi surface only affects scattering in the quadratic direction, where now there are additional states to scatter into. The net result of such a process will likely be increased transmission, as each positive \( k_y \)
particle state now has both a particle and a hole state with $-k_y$ to scatter into.

In order to determine the behavior of bilayer phosphorene in Klein tunneling, we find the wavefunction inside and outside a potential bump and match boundary conditions to find the transmission coefficient. Ignoring the coefficients that are not relevant to the chirality of the Hamiltonian, we can rewrite (3.24) as

$$\mathcal{H} = (c_1 k_y^2 + c_2 k_x^2) \sigma_z - c_3 k_x \sigma_y,$$

(3.26)

where $c_1 = C_1(V_0)/N(V_0)$, $c_2 = C_2(V_0)/N(V_0)$, and $c_3 = -C_3(V_0)/N(V_0)$. We can further simplify by rescaling the momenta by defining $q_x = \sqrt{c_2} k_x$, $q_y = \sqrt{c_1} k_y$, and $c = c_3/\sqrt{c_2}$:

$$\mathcal{H} = (q_x^2 + q_y^2) \sigma_z - cq_x \sigma_y.$$  

(3.27)

We now consider our system in polar coordinates, where $q_x = q \cos \varphi$ and $q_y = q \sin \varphi$. Here $\varphi$ will eventually act as an angle of incidence in our scattering, as it determines the momentum direction the incoming particle. We consider scattering in the $x$-direction as shown in Fig. 2.2, with a potential barrier of width $D$ in the $x$-direction and height $V$.

Working in real space, we use the substitution $k_i \rightarrow -i \partial_i$ and a plane wave ansatz of $\psi(x, y) = e^{iq_xx + iq_yy} \begin{pmatrix} a \\ b \end{pmatrix}$ to solve the eigenvalue equation $\mathcal{H}(x, y) \psi(x, y) = E \psi(x, y)$. We find that the energies take on the values

$$E = \pm \sqrt{q^4 + c^2 q^2 \cos^2 \varphi}.$$  

(3.28)

For a given energy of incoming particles, this is a quartic equation for $q$, giving four possible values of crystal momentum. The two solutions correspond to incoming and outgoing waves, while the two evanescent solutions are exponentially localized waves at the interfaces [3]. In our scattering system, the energy of particles is $E_F$, the Fermi energy, when outside the potential barrier and $E_F - V$ inside.
Figure 3.10: Transmission probability across potential barrier of width $D$ and height $2E_F = 0.02$ eV in bilayer phosphorene for normally-incident scattering. The transmission in the quadratic $k_y$ direction (black) exponentially decays, while that in the linear $k_x$ direction remains at probability one.

Consequently, given an angle of incidence $\phi$ and Fermi energy $E_F$, we can find the four solutions for the Fermi wavevector $k_F = k$, which give values $q_x = q_F \cos \varphi$ and $q_y = q_F \sin \varphi$ in our ansatz. We can then plug the ansatz back in to find expressions for the $a$ and $b$, which determine the chirality of the wavefunction $\psi$. Matching boundary conditions at the two interfaces of the potential bump will then give a system of equations that can be solved to find the transmission coefficient, $t$, and the transmission probability, $T = |t|^2$.

Based on the chirality of the Fermi surface, we expect normally-incident tunneling in the $k_x$ direction to mimic monolayer graphene, and tunneling in the $k_y$ direction to mimic bilayer graphene. We compare the transmission coefficients for normal tunneling in these two directions in Fig. 3.10 as we did for graphene mono and bilayers in Fig. 2.6. We notice that along the linear direction, Klein tunneling appears very similar to that of an odd-$J$ chiral material, while along the quadratic direction the
exponential decay of transmission probability to zero matches that of even chirality.

Much like our toy model, we can also study the dependence of Klein tunneling on angle of incidence. The angle of incidence of particles on our potential barrier, which extends in the $x$-direction, is given by $\phi = \tan^{-1}(k_y/k_x)$. However, in our rescaled calculation, we are using a rescaled angle parameter $\varphi = \tan^{-1}(k_y/k_x)$. As outlined by Fig. 2.9 in our toy model, the physical angular axes are dictated by $\varphi$, which in this case is given by $\phi = \tan^{-1}\left(\sqrt{\frac{c_2}{c_1}} \tan(\varphi)\right)$. However, the rescaled angles are very similar to the physical ones, given that $\sqrt{c_2/c_1} \approx 1.08$, and the difference between the two can be ignored.

In Fig. 3.11 we plot the transmission probability of Klein tunneling in phosphorene across a potential barrier in the $y$-direction. The length of the barrier along the $y$-axis is $D = 6$ nm, the Fermi energy is $E_F = 0.02$ eV, and the potential is $V = 0.04$ eV. Because the scattering is in the $y$-direction here, $\phi = \pi/2$ is the direction of normal incidence on this potential barrier. We see that the results agree with those from Fig. 3.10, as Klein tunneling in the linear, transmissive direction smoothly becomes Klein tunneling in the quadratic, reflective direction.

With increased Fermi energy and barrier length, we notice that resonances in the transmission probability begin to develop at different angles. These are a general feature of scattering through a potential barrier, and do not indicate the chirality of the material like the Klein tunneling behavior. It is thus simpler to focus our attention on scattering at normal incidence along differently oriented potential steps.
Figure 3.11: Polar distribution of transmission probability for Klein tunneling across a potential barrier in the $y$ (quadratic) direction for (a) $V = 2E_F = 0.02$ eV and $D = 6$ nm and (b) $V = 2E_F = 0.06$ eV and $D = 10$ nm.

Bilayer phosphorene, at least at low energies, behaves like different chiral materials depending on the direction of propagation of incident particles. Any direction, however, exhibits some form of chiral behavior through Klein tunneling. In a sample of bilayer phosphorene, these altered transport properties can be detected as changes in conductance. In particular, oscillations in the resistance of a $p$-$n$-$p$ gate within a sample are a signature of Klein tunneling [9].

Up until now, we have always taken the potential to be twice the Fermi energy, in order to scatter symmetrically from states with energy $+E_F$ to those with $-E_F$. However, such oscillations in conductance occur when the potential height is varied. To this end, we plot the conductance at different Fermi energies and potentials in Fig. 3.12. In practice, these are controlled by doping the material at different ion concentrations. In the first plot, only transmission through one channel (normal incidence in the linear direction) is considered, while in the second plot we used
Kwant [17] to numerically calculate the conductance of a discretized tight-binding model of (3.26) through all scattering channels.

Figure 3.12: Oscillations in conductance for different barrier heights. In (a) we show transmission probability (proportional to conductance) at normal incidence in the linear direction with $E_F = 0.01$ eV fixed. In (b) we show scattering across all possible channels without $E_F$ fixed.

Fig. 3.12 suggests that we can use experimental techniques to detect the presence of Klein tunneling in phosphorene, which in turn indicates chirality of the material. If instead transport experiments are conducted with sensitivity to the direction of scattering, we can observe the anisotropy of the chiral effects. Bilayer phosphorene has been shown to exemplify the Klein tunneling behavior characteristic of a system that has a linear coupling in one direction, and quadratic in another. For a simple incarnation of a chiral anisotropic material, phosphorene can exhibit complex, detectable transport properties due to the Klein paradox.
Chapter 4

Conclusions and Outlook

In this report, we have outlined the progress in developing a realistic model of an anisotropic chiral material, that of bilayer phosphorene, equipped to host Klein tunneling effects. The Klein paradox, in which chiral particles experience perfect transmission through a potential barrier, can be observed at low energies in condensed matter systems. Materials hosting this phenomenon are called chiral because their low energy quasiparticles have a coupling between momentum and a spin-like degree of freedom. Depending on the parity of this coupling, the Klein paradox can manifest itself in different ways.

For the specific case of monolayer graphene and the general case of materials with an odd chiral coupling, spin conservation prohibits backscattering, and particles are perfectly transmitted through a potential barrier by scattering into hole states of the same chirality. For bilayer graphene and even coupling in general, the reflected state has the same spin as that of the incident particle, giving rise to perfect reflection. Both of these behaviors are incarnations of the Klein paradox, as the transport properties of chiral materials critically depend on the interplay between pseudospin and momentum.

Graphene, in both monolayer and bilayer form, is isotropic in its dispersion relation. We have proposed instead a model of another two-dimensional material that,
while maintaining a chiral coupling, is anisotropic. As a result, the chiral coupling depends on the direction that particles are moving through the material. In one direction, Klein tunneling effects like those of monolayer graphene are observed, while in the orthogonal direction effects arising from a quadratic coupling like bilayer graphene are observed. Klein tunneling smoothly interpolates between the two regimes as the angle of incidence in scattering is changed.

Phosphorene, a single crystalline layer of black phosphorus, provides a physical realization of chiral anisotropy. We have developed low-energy models for monolayer and bilayer phosphorene, discussing the role that an external electric field can play in closing the band gap. The chiral structure of low-energy quasiparticles in gapless, bilayer phosphorene is anisotropic and similar to the proposed toy model. This anisotropy gives rise to the predicted Klein tunneling behavior, with perfect reflection in one direction and perfect transmission in the other.

In real materials impurities give rise to potential barriers that tend to localize electrons. Klein tunneling allows for increased transmission through such barriers, changing the conductivity of the material. As a result, measuring the conductivity (or equivalently resistivity) of a sample can be used to detect its chiral character. In particular, oscillations in the conductance of a $p-n-p$ junction when the doping is altered are an experimental signature of Klein tunneling. Numerical calculations show that bilayer phosphorene exhibits these oscillations, providing an experimentally testable prediction.

The presence or absence of Klein tunneling can be used to detect chirality in a material, because without a pseudospin degree of freedom, effects like perfect transmission for infinitely high potential barriers do not occur. On the other hand, the specific form of Klein tunneling, which requires experiments that distinguish between directions of particle transport, can act as a marker for anisotropy, as we have shown.
for phosphorene. While we have restricted our attention to the simplest cases of chiral anisotropic materials, many more variations can be modeled which act as environments for different manifestations of the Klein paradox.
Bibliography


