Valley separation via trigonal warping

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Monolayer graphene contains two inequivalent local minimum, valleys, located at $K$ and $K'$ in the Brillouin zone. There has been considerable interest in the use of these two valleys as a doublet for information processing. Herein I propose a method to resolve valley currents spatially, using only a weak magnetic field. Due to the trigonal warping of the valleys, a spatial offset appears in the guiding centre co-ordinate, and is strongly enhanced due to collimation. This can be exploited to spatially separate valley states. Based on current experimental devices, spatial separation is possible for densities well within current experimental limits. Using numerical simulations, I demonstrate the spatial separation of the valley states.

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Introduction: Due to the particular symmetry of the honeycomb lattice of monolayer graphene, the valence and conduction bands meet at 6 points. In the immediate vicinity of these points, the dispersion is linear and the Fermi surface consists of two inequivalent cones at points $K$ and $K'$ in the Brillouin zone. These valleys are independent and degenerate, and several works have proposed using these valleys as a doublet for information processing; referred to as valleytronics, in analogy with spintronics\textsuperscript{1, 2}. Since the first proposal over a decade ago, considerable progress has been made with regards to the generation of both static valley polarisations, and valley polarised currents\textsuperscript{3, 4}. Detecting valley polarisation on the other hand has proved to be difficult. An early proposal suggested using superconducting superconducting contacts\textsuperscript{5}. More recently it has been shown that static valley polarisations can be induced and detected via second harmonic generation\textsuperscript{8, 9}. Nonetheless, the detection of valley polarised currents remains an ongoing challenge, with implications for a wide variety of phenomena beyond valleytronics.

In this letter, motivated by recent developments in electron optics in graphene I propose an approach for the detection of valley polarised currents in graphene. Over the past decade, a variety of improvements in material processing have allowed for high mobilities, with free paths of tens of microns\textsuperscript{10}. Very recently, several groups have considered how to form highly collimated electron beams in graphene; Barnard \textit{et al} using absorptive metal contacts to form a pinhole aperture, and Liu \textit{et al} using a parabolic $p-n$ junction as a refinement of the Veselago lens\textsuperscript{11, 12}. Herein I show that collimation, combined with the trigonal warping of the Dirac cone, results in a significant enhancement in the spatial separation between ballistic valley polarised currents. Combined with an appropriate device layout, this spatial separation can be exploited to individually address distinct valley states. Due to the significant enhancement, I find that the required trigonal warping is small, and the required density is well within current experimental limits. It thereby provides a novel method of detecting ballistic valley polarised currents.

Valley separation: The effective Hamiltonian for graphene near the charge neutrality point is Dirac-like, $\mathcal{H} \sim \mathbf{k} \cdot \boldsymbol{\sigma}$, where $\boldsymbol{\sigma}$ are the usual Pauli matrices and reflect the two constituent sub-lattices. At low densities, there is a four-fold degeneracy, due to spin and valley degrees of freedom. The two inequivalent valleys are located at $K$ and $K'$ respectively in the Brillouin zone, and close to the charge neutrality point are cylindrically symmetric. For higher densities, the Fermi surface in each valley $K$ and $K'$ exhibits trigonal warping, the emergence of which is shown in Fig. 1.

With an applied transverse magnetic field, $\mathbf{p} \rightarrow \pi = p + e\mathbf{A}$, where $\mathbf{A}$ is the vector potential. If the applied field is weak, and the electron or hole density is high, the charge carrier dynamics can be described semi-classically, starting from the Heisenberg equation of motion for the operators,

$$\dot{\hat{\pi}} = \{\mathcal{H}, \hat{\pi}\} = eB\dot{\mathbf{v}} \times \mathbf{n} \tag{1}$$

where $\mathbf{n}$ is the unit vector normal to the graphene plane, and $B$ is the magnitude of the applied magnetic field. Note that $\hat{\pi}$ and $\dot{\mathbf{v}}$ are operators. Eq. (1) is general, and holds for a variety of dispersion relations\textsuperscript{13}. In the semiclassical limit, the operator equation, Eq. (1), is converted to a classical equation of the expectation values, which can then be trivially integrated to yield the real space motion of a electron under an applied transverse magnetic field,

$$\mathbf{r}(t) = \frac{\pi \times \mathbf{n}}{eB} \tag{2}$$

where $\mathbf{r} = \langle \mathbf{r} \rangle$ and $\pi = \langle \hat{\pi} \rangle$. This is the equation of motion for cyclotron motion, with the electron following the equienergetic contours of the Fermi surface. Thus at high densities, the semi-classical cyclotron orbits of graphene are trigonally warped.

In Eq. (2), guiding centres of the two valleys are identically located at $(x, y) = (0, 0)$. For an electron optics device, for example, the pin-hole collimator designed in Ref. 11, the initial position of the wave packet is at...
(0, 0), the location of the injector. In addition, for a perfectly collimated beam of electrons, the initial velocity is fully aligned along the x axis, parallel to the channel of the injector. For a cylindrically symmetric Fermi surface, the location of the guiding centre co-ordinate is unchanged. When the Fermi contour becomes trigonally warped, the guiding centre co-ordinate becomes offset, proportional to the magnitude of the trigonal warping. This offset effect is presented in Fig. 2. Since the two valleys exhibit triangular warping with opposite signs, the guiding centre co-ordinate becomes offset, proportional to the magnitude of the trigonal warping; as trigonal warping increases, so does guiding centre co-ordinate offset.

To illustrate the effect analytically, I consider the following approximation for the Fermi momentum, \( p_F \),

\[
p_F \approx \hbar k(1 + su \sin 3\theta)
\]

where \( \theta \) is the polar angle, \( \theta = \tan^{-1} k_y/k_x \), and \( k_0 = \sqrt{\pi n} \). Here \( k_x \) and \( k_y \) are chosen according to Fig. ??.

The valley index, \( s = \pm 1 \), with \( u = ka/4 \), where \( a \) is the lattice constant of graphene. It is important to note that this analytic approach is only valid while \( 3u \ll 1 \), that is, \( u \approx 0.1 \). The transverse velocity must vanish for collimated injection. From Eq. (3), the condition is \( \partial p_y/\partial \theta = 0 \), where \( p_y = p_F \cos \theta \). The guiding centre co-ordinate is

\[
(x_{gc}, y_{gc}) \approx \frac{\hbar k_0}{eB} (-3su, 1 - u)
\]

where \( s \) is once again the valley index. This offset of the two valley states can be clearly seen in Fig. 2b.

Focusing in the half plane, that is, with source and the detector located on the y axis, does not yield any spatial separation between the valley states. However, if an orthogonal device setup is employed, as shown in Fig. 3b, the states can be spatially separated. The real space separation at the collector is

\[
x_+ - x_- \approx 8u \frac{\hbar k_0}{eB}
\]

where \( x_+ \) and \( x_- \) are the real space positions in the plane of the detector. Thus trigonal warping of the valleys in graphene induces a real space separation when combined with an appropriate device setup, with a significant enhancement. This real space separation from collimated injection is shown in Fig. 3b.

Resolution limits: On its own, Eq. (5) tells us little about whether the spatial splitting can be observed. If the broadening of the beam exceeds the spatial separation, then the valley states will overlap and resolution of the distinct valleys currents will not be possible. There are three specific sources of broadening: (1) broadening due to the medium, (2) the spatial resolution of the detector, and (3), the imperfect collimation of the source. Beam broadening due to the medium limits the scale of the focusing device. The path length of the ballistic measurements used in Ref. [11] were \( l_{\text{path}} \approx 3 - 4\mu \text{m} \). For an orthogonal device with a geometry equivalent to that of Fig. 3a, this corresponds to a maximum focusing length, \( l \approx 2\mu \text{m} \). The device should be made as large possible, as the relative resolution of the detector scales as \( w/l \), where \( w \) is the width of the aperture. The mean free path in h-BN encapsulated graphene can be upwards of 10 \( \mu \text{m} \), implying that significantly larger device scales are possible.

Next, let us determine the collimation limit for a pinhole style collimator setup in the orthogonal geometry of Fig. 3b. This can be understood as the area containing all guiding centre co-ordinates, \( (x_{gc}, y_{gc} \in S) \) satisfying the limits, \( y = L/2, -L/2, l - w/2 < x < l + w/2 \). Here \( L \) and \( w \) represent the width and length of the pinhole collimator respectively, while \( l \) is the focusing length. A schematic showing these is presented in Fig. 3. Specifically, the value of interest is the range of \( y_{gc} \), which must be less than the spatial separation of the valley states. Provided the trigonal warping is relatively small, \( u < 0.1 \), the radius of curvature in the local region about \( v_x = 0 \) is identical for both valleys, and the trajectories within

FIG. 1: The emergence of trigonal warping in the two valleys, with \( K (K') \) indicated in red (blue).

FIG. 2: Real space trajectories with collimated injection. Left panel: at low densities, the Fermi surface is nearly cylindrically symmetric, and the trajectory of states in each valley are offset only slightly. Right panel: at high densities trigonal warping results in a guiding centre co-ordinate offset for a collimated source.
the collimator can be approximated by cyclotron orbits. The resulting approximate limit is \( |y_{ge}| < \sqrt{w_{Fe}} - L/2 \), while the “spread” of the beam is double this. In the absence of any addition collimation, the required density for spatial separation for \( w = r_c/6 \) and \( L = r_c/2 \) is \( n \approx 3 \times 10^{13}\text{cm}^{-2} \). Due to the comparatively high density, narrower apertures can be used without reaching the diffraction limit, which can improve the resolution. Alternatively, the spread can be determined from typical values in the literature. For a pinhole collimator like that of Barnard et al, the angular full width half maximum was \( \Delta \theta \sim \pi/9 \), corresponding to a spread of \( \Delta x = \Delta \theta r_c \). For \( x_+ - x_- > \Delta x, 8u > \pi/9 \), which yields a minimum density of \( n \approx 3 \times 10^{13}\text{cm}^{-2} \). Parabolic \( p-n \) junctions, as proposed by Liu et al have a significantly more collimated beam shape, with \( \Delta \theta \sim 5^\circ \), however the beam has larger spatial dimensions, and this is limited by distance of the source to the \( p-n \) parabola. Combinations of parabolic junctions and pinhole aperture can further improve the angular distribution and spatial extent of the beam[14], which would further lower the density. A halving of the beam spread would reduce the required density by a factor of four, placing individual valley resolution tantalisingly close to densities accessible via back-gated devices.

**Numerical simulations:** This can be grounded more firmly via numerical simulation of the device, to determine the required \( u \) and therefore \( n \) for resolution of the individual valleys. Since Eqs. (5) and (6) are valid only for small values of trigonal warping, I consider the energy bands of the usual tight-binding hamiltonian (see, for example, [15]) to determine the equienergetic contours and then use Eq. (2) to determine the dynamics. As already noted, this approach is valid provided \( kr_c > 100 \), and device feature sizes much large than the Fermi wavelength. Plots are generated by considering randomised initial conditions, summing the number of states that pass through the pinhole collimator, and pinhole aperture of the detector plane.

The results of the numerical procedure are presented in Fig. 4. For a device with a pinhole collimator, and a detector with a simple pinhole aperture, the required density is \( \sim 2 \times 10^{13}\text{cm}^{-2} \), with narrow apertures, and longer pinhole channels lowering the required density.
This is well within current experimentally achievable densities for graphene devices[16]. Further improvements by reducing $w$ are possible, however, there is a fundamental limit due to diffraction at low densities. For $n = 1 \times 10^{13}\text{cm}^{-2}$, $\lambda_F \sim 10\text{nm} \ll w = 250\text{nm}$, and naively, the angular spread due to diffraction is $\theta \approx 1/20$, which is significantly less than the collimation limit of the pinhole collimator[11]. The resolution can be further improved via the use of a second pinhole collimator as a detector allowing for resolution of the distinct valleys at lower densities. The principle complication lies in the differing trajectory shapes of the two valleys.

In conclusion, I have shown that the ballistic trajectories of electrons in different valleys of graphene can be spatial separated using a collimating source, and a weak magnetic field. The magnitude of the separation at $\sim 3 \times 10^{13}\text{cm}^{-2}$ is sufficient to fully resolve the individual peaks, and this carrier density is achievable with current gating methods. Additional improvements in resolution are possible with the addition of a second pinhole collimator, and further adjustments to both the width, $w$ and length, $L$ of the collimator. Alternative designs would offer further improvements in resolution. Finally, the basic principle of valley separation outlined here will work for any two dimensional systems where the valleys exhibit trigonal warping, including bilayer graphene, moire superlattices, and two dimensional transitional metal dicalcogenides. This research was partially supported by the Australian Research Council Centre of Excellence in Future Low-Energy Electronics Technologies (project number CE170100039) and funded by the Australian Government. SSRB would like to thank Oleg Sushkov for his critical reading and suggestions.

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