We consider tunneling transport between two parallel graphene sheets where one is a single-layer sample and the other one a bi-layer. In the presence of an in-plane magnetic field, the interplay between combined energy and momentum conservation in a tunneling event and the distinctive chiral nature of charge carriers in the two systems turns out to favor tunneling of electrons from one of the two valleys in the graphene Brillouin zone. Adjusting the field strength enables manipulation of the valley polarization of the current, which reaches its maximum value of 100% concomitantly with a maximum of the tunneling conductance.

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The concept of spintronics continues to stimulate the detailed study of intertwined dynamics of intrinsic (pseudo-)spin-1/2 degrees of freedom and the orbital motion of charge carriers. Graphene-based nanomaterials are particularly attractive systems for spintronics applications because, in addition to their ordinary spin, electrons in graphene also carry an orbital pseudo-spin and a valley-isospin degree of freedom. While the pseudo-spin-up/down eigenstates correspond to an electron’s position on the two equivalent sublattices of graphene’s honeycomb lattice in real space, the valley-isospin quantum number distinguishes states near the $K$ and $K' \equiv -K$ high-symmetry points in reciprocal space. Schematics of the single-layer and bi-layer graphene lattices as well as their (identical) Brillouin zone(s) are shown in panels (a)–(c) of Fig. 1.

The possibility to realize valley-isospin-based spintronics, called valleytronics, in graphene has attracted a lot of interest. The operation of valleytronic devices generally depends on the ability to generate valley-asymmetric charge currents. Mechanisms to separately address electrons from individual valleys necessarily involve the breaking of inversion and/or time-reversal symmetries, e.g., via nanostructuring, coupling to electromagnetic fields, application of mechanical strain, or presence of defects. In many of these situations, the mobility of charge carriers could be compromised by the required inhomogeneity and/or orbital effects of the applied external fields.

Here we propose a valley-filter device that is based on resonant electron tunneling between parallel single-layer and bi-layer graphene sheets. Vertical heterostructures of two-dimensional (2D) crystals have recently been fabricated, and their electronic properties have become the subject of detailed theoretical study. As discussed below, application of a magnetic field parallel to the graphene sheets enables direct tuning of the valley polarization of the tunneling current, with a possible maximum value of 100%. In contrast to other valley-filter designs, no significant modification of the graphene sheets’ electronic structure is required to enable valley-asymmetric transport. As an additional feature, a valley-polarized current is generated simultaneously in both the single-layer and the bi-layer sheets.

Our proposed valley-filter design utilizes the strong link between linear orbital momentum, pseudo-spin and valley isospin for electrons in graphene materials. Due to peculiarities of the honeycomb-lattice band structure, an electron’s pseudo-spin state is locked to its linear motion on the 2D graphene sheet in a way that is normally exhibited by ultra-relativistic
FIG. 1. Structural and electronic properties of graphene. (a) Single-layer graphene has carbon atoms arranged on a honeycomb lattice. Sites on its two equivalent sublattices are indicated by empty and filled circles and labelled $A$ and $B$, respectively. Electrons localized on the $A$ ($B$) sublattice are in pseudo-spin-up (down) eigenstates. (b) In bi-layer graphene, atoms from the $A$ and $A'$ sublattices of the two layers are bonded vertically, while those on $B$ and $B'$ sites are dangling. Electronic excitations at low energy are from the subspaces spanned by $B$ and $B'$ states, which correspond to the pseudo-spin eigenstates for electrons in bi-layer graphene. (c) The first Brillouin zone of single-layer (and bi-layer) graphene. High-symmetry $K$ ($K'$) points are indicated by empty (filled) hexagons. (d)–(f) Pseudo-spin polarization of conduction-band electrons (indicated by red arrows) for the $K$ valley of single-layer graphene [(d)], the $K'$ valley of single-layer graphene [(e)], and the $K$ valley of bi-layer graphene [(f)].

(massless) Dirac fermions. The exact form of this coupling turns out to be different for electrons from the two valleys and also depends on the type of graphene structure, e.g., whether it is a single-layer or a bi-layer sample. See Fig. 1, panels (d)–(f), for an illustration. Furthermore, states with the same wave-vector shift $\mathbf{k} \equiv (k_x, k_y)$ from the high-symmetry point in the conduction and valence bands have opposite pseudo-spin polarization. The characteristic differences between valley-dependent pseudo-spin-momentum locking in single-layer and bi-layer graphene makes it possible to achieve valley separation in a momentum-resolved tunneling structure proposed here.

Tunneling transport between parallel 2D conductors exhibits strongly resonant behavior as a function of in-plane magnetic field $B_\parallel$ and bias voltage $V$ because of the requirement to simultaneously conserve the canonical in-plane momentum and total energy of every tunneled electron. Theoretical descriptions of 2D-to-2D tunneling have been able to explain the experimental observations with great accuracy.
FIG. 2. Visualization of momentum-resolved tunneling between 2D systems in the presence of an in-plane magnetic field. The requirement of simultaneous energy and momentum conservation restricts tunneling to states at intersection points of the Fermi surfaces for the two layers. The pseudo-spin of these states is fixed by the kinetic momentum for electrons in single-layer and bi-layer graphene, and the tunneling probability depends on the matrix element given in Eq. (2).

Recent progress in fabricating tunnel-coupled unconventional 2D systems where the charge carriers’ intrinsic (pseudo-)spin-1/2 degree of freedom is rigidly locked to their orbital motion has stimulated further interest. In particular, it has been shown that the linear (i.e., small-bias) magneto-tunneling conductance for electrons from valley $\gamma$ ($=K$ or $K'$ in graphene, or $\Gamma$ in an ordinary 2D quantum-well system) is given by

$$G^{(\gamma)}(\gamma) = \frac{g_s e^2}{\hbar} 2\pi A \rho_F^{(1)} \rho_F^{(2)} \left[ \left| \Gamma_{u}^{(\gamma)}(Q) \right|^2 + \left| \Gamma_{l}^{(\gamma)}(Q) \right|^2 \right] \times \Theta \left( |Q| - \left| k_F^{(1)} - k_F^{(2)} \right| \right) \Theta \left( k_F^{(1)} + k_F^{(2)} - |Q| \right) \sqrt{ \left[ \left( k_F^{(1)} + k_F^{(2)} \right)^2 - Q^2 \right] \left[ Q^2 - \left( k_F^{(1)} - k_F^{(2)} \right)^2 \right] } \right].$$

Here $Q = (e/\hbar) d B_\parallel \times \hat{z}$ is the magnetic-field-induced shift in kinetic momentum for an electron that has tunneled between two layers spaced vertically at distance $d$. The factor $g_s = 2$ accounts for the real-spin degeneracy, $\rho_F^{(m)}$ is the density of states at the Fermi energy in system $m$ not including real-spin or valley degrees of freedom, $k_F^{(m)}$ is the Fermi wave vector in system $m$, and

$$\Gamma_{u/l}^{(\gamma)}(Q) = \gamma, k_{u/l} - Q/2, \left| \sigma_F^{(1)} \right| \tau_{k_{u/l}} \left| \sigma_F^{(2)} \right\rangle_{\gamma, k_{u/l} + Q/2}$$

are overlap matrix elements between (pseudo-)spinors associated with the electron states at the two intersection points (labelled $u$ and $l$, respectively) of the shifted Fermi circles. See Fig. 2 for an illustration.
In the following, we neglect the \( \mathbf{k} \) dependence of the tunneling matrix\(^{41} \) \( \tau_\mathbf{k} \equiv \tau \) and use the parameterization
\[
\tau = (\tau_0 \sigma_0 + \tau_x \sigma_x + \tau_y \sigma_y + \tau_z \sigma_z) / \sqrt{2}
\]
with complex numbers \( \tau_j \) that encode all possible tunneling processes, including those that are associated with a (pseudo-)spin flip. To be specific, we limit ourselves to the case where both the layers are \( n \)-doped, i.e., where \( \sigma_\mathbf{F}^{(1)} = \sigma_\mathbf{F}^{(2)} \equiv + \). Because of the rigid locking between the pseudo-spin state and the kinetic momentum of single-electron eigenstates in single-layer and bi-layer graphene [see Figs. 1(d)–(f)], it is possible to express the spinors for positive-energy eigenstates in terms of a rotation matrix \( \mathcal{U}(\theta) = \exp(-i\theta \sigma_\mathbf{z}/2) \) and the eigenstates \( |\rightarrow\rangle, |\leftarrow\rangle \) of pseudo-spin projection parallel to the \( x \) axis as
\[
|\sigma_\mathbf{F}^{(\text{sl})}\rangle_{\mathbf{K},\bar{\mathbf{k}}} = \mathcal{U}(\theta_{\bar{\mathbf{k}}}) |\rightarrow\rangle \tag{4a}
\]
\[
|\sigma_\mathbf{F}^{(\text{sl})}\rangle_{\mathbf{K}',\bar{\mathbf{k}}} = \mathcal{U}(\pi - \theta_{\bar{\mathbf{k}}}) |\rightarrow\rangle \equiv \sigma_y \mathcal{U}(\theta_{\bar{\mathbf{k}}}) |\rightarrow\rangle \tag{4b}
\]
\[
|\sigma_\mathbf{F}^{(\text{bl})}\rangle_{\mathbf{K},\bar{\mathbf{k}}} = \mathcal{U}(-2\theta_{\bar{\mathbf{k}}}) |\leftarrow\rangle \tag{4c}
\]
\[
|\sigma_\mathbf{F}^{(\text{bl})}\rangle_{\mathbf{K}',\bar{\mathbf{k}}} = \mathcal{U}(2\theta_{\bar{\mathbf{k}}}) |\leftarrow\rangle \equiv \sigma_x \mathcal{U}(-2\theta_{\bar{\mathbf{k}}}) |\leftarrow\rangle \tag{4d}
\]
Here we indicated states for electrons in single-layer (bi-layer) graphene by the superscript (sl) [(bl)], and \( \theta_{\bar{\mathbf{k}}} = \arctan(\bar{\mathbf{k}}_y/\bar{\mathbf{k}}_x) \). By virtue of the matrix element (2), the magneto-tunneling conductance between graphene sheets is strongly affected by the spinor structure of electron eigenstates\(^{29,30} \) and also depends on the pseudo-spin structure of the tunnel barrier.\(^{30} \)

The total current for tunneling through the barrier will be the sum of contributions from both valleys. However, as we will see below, these contributions need not have equal weight. To quantify the distribution of tunneling transport between the valleys, we consider the valley polarization of the conductance defined as
\[
\chi = \frac{G^{(\mathbf{K})} - G^{(\mathbf{K}')}}{G^{(\mathbf{K})} + G^{(\mathbf{K}')}} \tag{5}
\]
From Eq. (1), we find that \( \chi \) is only a function of the pseudo-spin matrix elements \( \Gamma_\mathbf{u/l}^{(\gamma)}(\mathbf{Q}) \):
\[
\chi = \frac{|\Gamma_\mathbf{u}^{(\mathbf{K})}|^2 - |\Gamma_\mathbf{u}^{(\mathbf{K}')}|^2 + |\Gamma_\mathbf{l}^{(\mathbf{K})}|^2 - |\Gamma_\mathbf{l}^{(\mathbf{K}')}|^2}{|\Gamma_\mathbf{u}^{(\mathbf{K})}|^2 + |\Gamma_\mathbf{u}^{(\mathbf{K}')}|^2 + |\Gamma_\mathbf{l}^{(\mathbf{K})}|^2 + |\Gamma_\mathbf{l}^{(\mathbf{K}')}|^2} \tag{6}
\]
FIG. 3. Comparison of pseudo-spin alignment of states from the $K$ and $K'$ valleys of single-layer graphene (SLG) and bi-layer graphene (BLG) at intersection points of their Fermi circles. The case with equal densities in both layers ($k_{F}^{(sl)} = k_{F}^{(bl)} \equiv k_{F}$) and $Q = Q \hat{x}$ with $Q \approx 2k_{F}$ ($Q \approx -2k_{F}$) is depicted in the upper (lower) panel. Note the parallel (opposite) alignment of pseudo-spins for states from the $K$ ($K'$) valley as $Q \rightarrow 2k_{F}$, and the reversal of alignments for $Q \rightarrow -2k_{F}$.

Without loss of generality, we now consider the situation where the magnetic field $B_{\parallel}$ is applied in $\hat{y}$ direction, i.e., $Q \equiv Q \hat{x}$. Recognizing the fact that $k_{u}$ and $k_{l}$ are then related by mirror symmetry with respect to the $x$ axis allows us to write the tunnelling matrix elements as

$$\Gamma_{u}^{(K)} = \langle \leftarrow | U(2\theta_{k_{u}-Q/2}) \tau U(\theta_{k_{u}+Q/2}) | \rightarrow \rangle, \quad (7a)$$

$$\Gamma_{l}^{(K)} = \langle \leftarrow | U(2\theta_{k_{u}-Q/2}) \sigma_{x} \tau \sigma_{x} U(\theta_{k_{u}+Q/2}) | \rightarrow \rangle, \quad (7b)$$

$$\Gamma_{u}^{(K')} = \langle \leftarrow | U(2\theta_{k_{u}-Q/2}) \sigma_{x} \tau \sigma_{y} U(\theta_{k_{u}+Q/2}) | \rightarrow \rangle, \quad (7c)$$

$$\Gamma_{l}^{(K')} = \langle \leftarrow | U(2\theta_{k_{u}-Q/2}) \tau (-i\sigma_{z}) U(\theta_{k_{u}+Q/2}) | \rightarrow \rangle. \quad (7d)$$

Analysis of the expressions (7) yields analytical results for the valley-polarization $\chi$ of the conductance. For example, when $Q = \pm (k_{F}^{(sl)} + k_{F}^{(bl)})$, we have $\theta_{k_{u}+Q/2} = 0$ and $\theta_{k_{u}+Q/2} = \pi$, which yields

$$\chi(Q \equiv \pm [k_{F}^{(sl)} + k_{F}^{(bl)}] \hat{x}) = \pm \frac{|\tau_{0} - \tau_{x}|^{2} - |\tau_{y} + i\tau_{z}|^{2}}{|\tau_{0} - \tau_{x}|^{2} + |\tau_{y} + i\tau_{z}|^{2}}. \quad (8)$$

Thus a nonvanishing $\chi$ is possible depending on the pseudo-spin structure of the tunneling matrix $\tau$, especially also for the case when pseudo-spin is conserved in a tunneling event ($\tau \equiv \tau_{0} \sigma_{0}/\sqrt{2}$). That this must be the case can be explained based on the form of pseudo-spin states from the single-layer and the bi-layer-graphene system for which tunneling is allowed by simultaneous energy and momentum conservation. See Fig. 3. For example, as $Q \rightarrow k_{F}^{(sl)} + k_{F}^{(bl)}$, the pseudo-spins of states at the ‘kissing’ point of the two Fermi circles
FIG. 4. Valley polarization $\chi$ of the tunneling conductance (red solid curve) and total tunneling conductance $G$ (blue dashed curve) for pseudo-spin-conserving tunneling between vertically separated sheets of single-layer and bi-layer graphene, having equal electron densities. The conductance unit is $G_0 = e^2 M A |\tau_0|^2 / (2\pi \hbar^4 v_F^3)$.

become (oppositely) aligned in the K (K') valley. Thus if the tunneling matrix is of the form $\tau \propto (\tau_0 \sigma_0 + \tau_x \sigma_x)$, the overlap matrix elements (2) restrict tunneling to occur only for electrons from the K valley. Conversely, if $\tau \propto (\tau_y \sigma_y + \tau_z \sigma_z)$, pseudo-spin must be flipped in a tunneling event, and only electrons from the K' valley are able to accommodate that condition with simultaneous energy and momentum conservation. In both situations, the tunneling current will be fully valley-polarized as a result.

The tunneling current will be non-vanishing in general and can even be large under the same conditions that maximize $\chi$. As an example, we provide the expression of the total tunneling conductance for the case when $\tau = (\tau_0 \sigma_0 + \tau_x \sigma_x) / \sqrt{2}$:

$$ G \equiv G^{(K)} + G^{(K')} = \frac{e^2}{\pi \hbar} \frac{M k_F^{(sl)} A}{\hbar^3} \frac{2|\tau_0 + \tau_x|^2 - \text{Re}\{\tau_0 \tau_x^*\}}{\left[\left(k_F^{(bl)} + k_F^{(sl)}\right)^2 - Q^2\right] \left[Q^2 - \left(k_F^{(bl)} - k_F^{(sl)}\right)^2\right]} , \quad (9) $$

where $M$ is the effective mass of electrons in the graphene bi-layer, $v$ the Fermi velocity in the single layer, and $A$ the area of the tunnel-barrier interface between the vertically separated 2D conductors. Clearly, for the condition $Q = \pm [k_F^{(sl)} + k_F^{(bl)}]$ associated with 100% valley polarization of the tunneling current, there is a divergence in the total magneto-tunneling conductance. Specializing $\tau = \tau_0 \sigma_0 / \sqrt{2}$, we can give the result

$$ \chi(Q) = -\cos \left(\theta_{k_u+Q/2} + 2\theta_{k_u-Q/2}\right) , \quad (10) $$
which further simplifies when $k_F^{(\text{sl})} = k_F^{(\text{bl})} \equiv k_F$ to $\chi(Q) = Q/2k_F$. See Fig. 4 for an illustration of the simultaneous occurrence of 100% valley polarization and maximum of tunneling transport, shown there for the special situation of equal densities in the two layers and a pseudo-spin-conserving tunnel barrier.

The efficiency of the valley-filtering device proposed here will be affected by the pseudo-spin structure of the tunnel barrier, which is determined by the geometric placement of the single and bi-layer sheets with respect to each other. Our previously suggested method to determine the full pseudo-spin structure of the tunnel coupling could be employed to optimize the vertical-heterostructure design in this regard. Furthermore, the valley polarization of the tunneling conductance is limited by the available magnitudes of the in-plane magnetic field. Using the case of equal density in the two layers and pseudo-spin-conserving tunneling as an example, we can estimate

$$\chi \leq \min \left\{ 1, \frac{e B^{\text{(max)}} d}{\hbar 4\pi n} \equiv 0.05 \times \frac{B^{\text{(max)}} [\text{T}]}{\sqrt{n [10^{10} \text{cm}^{-2}]}}, \frac{B^{\text{(max)}} [\text{T}]}{d [\text{nm}]} \right\}. \quad (11)$$

Thus in-plane magnetic fields of the order of 10 T are required to generate significant valley polarization in realistic vertical heterostructures of graphene layers.

In conclusion, we have studied tunneling transport between two parallel graphene sheets, one being a single-layer and the other a bi-layer sample. The requirement of simultaneous energy and momentum conservation, together with the distinctive valley-contrasting pseudo-spin-momentum locking in the two different graphene systems, causes a finite valley polarization of the tunneling current when an in-plane magnetic field is applied. For large-enough field magnitude, 100% valley polarization can be achieved, and a significant magnitude of polarization is generally realized concomitantly with large values of the total tunneling current.

In contrast to many other valley-filter designs, the vertical-tunneling-based proposal works without substantially altering the conducting properties of the graphene sheets. As a valley-polarized current is generated in the bulk, the present set-up is ideal for realizing valley-optoelectronic devices as well as applications related to the valley-Hall effect and its inverse. The fact that a valley polarization simultaneously exists in parallel single and bi-layer graphene sheets opens up possibilities for a three-dimensional valleytronic chip design.

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This is based on the realistic assumption that the tunnel-barrier height is much larger than the bandwidth of relevant electronic excitations. In principle, the $k$-dependence of $\tau_k$ can modify the density dependence of tunneling conductances but will not affect the functionality of our proposed valley-filter device.

In real samples, the finite electronic life time will smoothen this divergence into a Lorentzian peak. See, e.g., Ref. 39.