Quantum spin-Hall effect on the Möbius graphene ribbon

Kyriakos Flouris,1 Miller Mendoza Jimenez,1 and Hans J. Herrmann

1ETH Zürich, Computational Physics for Engineering Materials, Institute for Building Materials, Wolfgang-Pauli-Str. 27, HIT, CH-8093 Zürich (Switzerland)

Topological phases of matter have revolutionized quantum engineering. Implementing a curved space Dirac equation solver based on the quantum Lattice Boltzmann method, we study the topological and geometrical transport properties of a Möbius graphene ribbon. In the absence of a magnetic field, we measure a quantum spin-Hall current on the graphene strip, originating from topology and curvature, whereas a quantum Hall current is not observed. In the torus geometry a Hall current is measured. Additionally, a specific illustration of the equivalence between the Berry and Ricci curvature is presented through a travelling wave-packet around the Möbius band.

I. INTRODUCTION

Topological states of matter have been proposed theoretically and observed experimentally [1–3] triggering a surge of research in the context of quantum engineering and condensed matter. The enthusiasm is motivated by the robustness of the topological properties and their tolerance to disorder [4]. Especially useful in technological applications are topological currents as they are robust even in impure systems. Topological protection is a consequence of topological invariants, the most notable being the Chern number [5].

A large fraction of the research is concerned with topological insulators in 2-D [6], which is gradually extending to higher dimensions [7] through combined systems. Graphene, Weyl semi-metals and fractional statistics particles are just a part of the materials associated to the field [8–10]. Simultaneously in condensed matter, another field of great interest are particles constrained to move on curved surfaces. Curvature has immense potential as a novel and pure control mechanism in quantum devices, examples of this have been proposed in graphene systems [11, 12]. Graphene exhibits fascinating properties as a material but also as the platform for two-dimensional physics [13–15]. Furthermore, the honeycomb bipartite lattice of graphene has been shown to exhibit the quantum Hall and the quantum spin-Hall effects in the presence of a magnetic field [16–18]. Additionally, a graphene Möbius ribbon can exhibit topological insulator properties owning to the zig zag edge states [19].

For the Möbius band, although simple to visualize, the geometry is topologically non-trivial. The Möbius strip is the simplest non-trivial fiber bundle, a bundle of the line segment over the circle with a twist. Here, we raise the question of the energy levels of a confined particle on the Möbius graphene strip and the consequence of the curvature to the transport of these particles. We simulate Dirac particles and more specifically we relate them to graphene through the low energy approximation of the band structure. The non-relativistic quantum mechanics on a the Möbius ring have been studied [20] and also non-trivial effects in the Möbius topology have been proposed for molecular devices [21]. Through symmetry arguments it was proposed that the quantum Hall effect cannot exist on the Möbius but the quantum spin-Hall is possible [22]. This result is also confirmed in this work through a direct simulation.

A recurrent theme in recent condensed matter literature is the existence of the quantum Hall effect in the absence of a magnetic field [23, 24]. By avoiding the use of an external field, it is shown that the effect is purely a geometrical consequence. The symmetry of the system is not, as usual, broken by a magnetic field but by an equivalent gauge field originating from the curvature effects of the manifold. In reality, these curvature effects are translated as forces due to the pseudo-potential in a strained graphene sheet.

To this end the electronic and topological properties of a Möbius graphene ribbon are explored numerically using a solver of the Dirac equation in curved space [25, 26]. The method is based on the conceptual similarities between the Dirac and the Boltzmann equations and is an extension of the quantum lattice Boltzmann method [27] to curved space. Through our simulations we observe a quantum spin-Hall current in the bulk of a Möbius graphene strip.

Firstly we introduce the Dirac equation and its extension to curved space and specifically deformed graphene. In the next section, the simulations and results are presented for the Möbius and the torus geometries. The paper finishes with a summary and outlook section. An appendix can be found at the end including a more detailed description of the numerical model (Appendix A) and a calculation of the Berry phase relevant to a Möbius band (Appendix C).

II. THE DIRAC EQUATION IN CURVED SPACE AND GRAPHENE

The original Dirac equation [28] can be written in compact notation:

\[(i\gamma^\mu \partial_\mu - m)\Psi = 0,\]  \hspace{1cm} (1)

in natural units such that \(\hbar = c = 1\) for \(\hbar\), Planck’s constant and \(c\), the speed of light, where \(m\) is the
particle mass, $\mu = 0, 1, 2$ for 2D space-time. where $\Psi = (\Psi^+, \Psi^-) = (\psi_1^+, \psi_2^+, \psi_3^+, \psi_4^+) \in \mathbb{C}^4$ denotes the spinor, and $\gamma^\mu = \gamma^\alpha e^\mu_\alpha$ are the generalized $\gamma$-matrices, where $\gamma^\alpha \in \mathbb{C}^{4 \times 4}$ are the standard $\gamma$-matrices (in Dirac representation). This can be naturally extended to curved space with the addition of a covariant derivative as

$$(iv^\mu D_\mu - m)\Psi = 0,$$  \hspace{1cm} (2)

where $D_\mu$ is the covariant spinor derivative, $e^\mu_\alpha$ is the tetrad (first index: flat Minkowski, second index: curved space-time). Here the tetrad is defined by

$$e^\mu_\alpha g_{\mu\nu} e^\nu_\beta = \eta_{\alpha\beta},$$

where $g_{\mu\nu}$ denotes the metric tensor and $\eta_{\alpha\beta}$ is the Minkowski metric. In 2D the tetrad can be computed directly from the metric. Now defining the covariant derivative as $D_\mu \Psi = \partial_\mu \Psi + \Gamma_\mu \Psi$, where $\Gamma_\mu$ denotes the spin connection matrices given by

$$\Gamma_\mu = -\frac{i}{4}\omega^\mu_\alpha \sigma_{\alpha\beta},$$

where $\sigma_{\alpha\beta} = \frac{i}{2}[\gamma_\alpha, \gamma_\beta]$ and

$$\omega^\mu_\alpha = e^\mu_\nu \nabla_\nu e^{\nu\beta}.$$

The Dirac equation in curved space describes the relativistic Dirac particles (e.g. electrons) moving on arbitrary manifold trajectories, see Appendix B.

A. Theory of strained graphene

To model the single layer carbon atom honeycomb lattice structure we start from the tight binding Hamiltonian which is constructed assuming superposition of local wavefunctions for isolated atoms on a honeycomb lattice [29]. In the low energy limit it has been shown that the tight binding Hamiltonian converges to the Dirac Hamiltonian in the continuum limit,

$$H_D = -iv_f \int \Psi^\dagger \gamma^\mu \partial_\mu \Psi dx,$$  \hspace{1cm} (3)

in natural units, where $\Psi$ is in the chiral representation, $v_f$ is the Fermi velocity. In the context of graphene, the general Dirac spinor is defined as $\Psi = (\Psi_a^K, \Psi_a^{K'}) = (\psi_a^K, \psi_a^{K'}, \psi_a^{K''}, \psi_a^{K'''})$, for sub-lattices $A, B$ and valleys $K, K'$. The convergence from the tight binding Hamiltonian to Eq. (3) can be seen as the Dirac cones in graphene with linear dispersion relation at the conduction and valence band connecting point $E = p$ for $E$, energy and $p$, momentum.

The equation of motion from this Hamiltonian is simply the Dirac equation. In this work, we consider a static space-time metric with trivial time components

$$g_{\mu\nu} = \begin{pmatrix} 1 & 0 \\ 0 & -g_{ij} \end{pmatrix},$$

where the latin indices run over the spatial dimensions. This simplifies the Dirac equation Eq. (2) to

$$\partial_t \Psi + \sigma^a e_a^i (\partial_i + \Gamma_i) \Psi = 0 - i\gamma^0 m \Psi,$$  \hspace{1cm} (4)

with $\sigma^a = \gamma^0 \gamma^a$. After addition of external vector and scalar potentials $A_i(x)$ and $V(x)$ respectively as explained in Ref. [30], the Dirac equation takes the following form:

$$\partial_t \Psi + \sigma^a e_a^i (\partial_i + \Gamma_i - i A_i) \Psi = -i\gamma^0 (m - V) \Psi.$$  \hspace{1cm} (5)

Defining the Dirac current with $J^\mu = \overline{\Psi} \gamma^\mu \Psi$, the conservation law for can be written as $\partial_\mu \rho + \nabla_\mu J^\mu = 0$, where $\rho = \Psi^\dagger \Psi \in \mathbb{R}$ and the $J^i = \overline{\Psi} \gamma^i \Psi \in \mathbb{R}$.

The standard Dirac Hamiltonian for Eq. (5 equation is

$$H_D = -i \int \Psi^\dagger \sigma^a (\partial_a + \Gamma_a - i A_a) \Psi \sqrt{g} dx^2,$$  \hspace{1cm} (6)

For graphene the effective Hamiltonian looks like[31]:

$$H_D^* = -iv_f \int \Psi^\dagger \sigma^a (v_a^{*i} \partial_i + \Gamma_a^* - i A_a^*) \Psi \sqrt{g} dx^2,$$  \hspace{1cm} (7)

where $v_a^{*i} = \delta_a^i + u_a^i - \beta \varepsilon_a$ is the space depended Fermi velocity, $\Gamma_a^* = \frac{1}{m^2} \partial_j v_a^{*j}$ is a complex gauge vector field which guarantees the hermiticity of the Hamiltonian and $A_a^*$ is a strain-induced pseudo-vector potential given by $A_a^* = (A_a^x, A_a^y) = \frac{\beta}{m^2} (\varepsilon_{xx} - \varepsilon_{yy}, \varepsilon_{xy})$, $\beta$ is the material dependent electron Grueiesen parameter, $a$ the lattice spacing and $\varepsilon_{ij} = u_{ij} + \frac{1}{h} \partial_i h \partial_j h$ the general strain tensor with in-plane, $u_{ij}$ and out of plane, $h$ deformations. The term $u_{ai}$ in $v_a^{*i}$ can be interpreted as the deformation potential term and is purely a geometric consequence due to lattice distortion, it does not depend on the material as long as it has the same topology. Comparing this to the standard Dirac Hamiltonian in curved space Eq. (6) we can match both Hamiltonians $H_D$ and $H_D^*$ by fulfilling the following relations:

$$v_a^{*i} = v_f \sqrt{g} e_a^{i1}, \quad \Gamma_a^* = v_f \sqrt{g} e_a^{i1} \Gamma_i, \quad A_a^* = v_f \sqrt{g} e_a^{i1} A_i.$$  \hspace{1cm} (8)

All three can be simultaneously fulfilled by an effective metric tensor derived from the explicit expression of the tetrad [30]. The effective Dirac model for non-uniform strain should describe the particular case of a uniform strain, where both Dirac points in the Brillouin zone are affected the same way and thus considered equivalent. The numerical solutions are obtained with the Quantum Lattice Boltzmann Method as described in Appendix A and Ref. [30].
III. MÔBIUS GRAPHENE STRIP

The system geometry is initialized to the Möbius ribbon by the discrete mapping (or chart),
\[
h^{\alpha}(\theta, r) = \left( \begin{array}{c} (R + wr \cos(\eta \theta/2)) \cos(\theta) \\ (R + wr \cos(\eta \theta/2)) \sin(\theta) \\ wr \sin(\eta \theta/2) \end{array} \right)
\]
with \( \theta \in \{-\pi, \pi\}, r \in \{-L_r/2, L_r/2\}\), half-width \( w \), mid-circle of radius \( R \), number of turns \( \eta \) and at height \( z = 0 \). \( L_r \) is the domain size across the radial direction, for simplicity we set \( L_r/2 = 1 \). In the simulations, we consider a square sheet with reverse periodic and closed boundary conditions on a grid of size \( L_\theta \times L_r = 512 \times 512 \) or \( 100nm \times 100nm \). \( A_\alpha \) is an external potential set to zero.

The metric tensor can be computed from the \( h^{\alpha}(x, y) \) relating the positions of the atoms from the three dimensional flat space (laboratory frame with Minkowski-metric) to the curved space by:
\[
g_{ij} = \frac{\partial h^{\alpha}(\theta, r)}{\partial x^i} \frac{\partial h^{\beta}(\theta, r)}{\partial x^j} \eta_{\alpha \beta},
\]
With this parametrisation the metric is cast to a diagonal form,
\[
g_{ij} = \left( \begin{array}{cc} A^2 & 0 \\ 0 & B^2 \end{array} \right),
\]
where \( A = \sqrt{R + wr \cos(\eta \theta/2) + w^2r^2/4} \) and \( B = w \). The reversed periodic boundary at \( \theta = \pi \) is implemented as \( \Psi(\theta = -\pi, r) = \Psi(\theta = \pi, -r) \). From Ref. [32] a valid current conserving and time-reversal symmetric boundary condition for the Dirac equation can be written as:
\[
\Psi = (\mathbf{v} \cdot \tau) \otimes (\mathbf{n} \cdot \sigma), \quad \mathbf{n} = \mathbf{n}_B,
\]
where \( \mathbf{n}_B \) is the unit vector in the \( r - \theta \) plane normal to the boundary, \( \mathbf{v} \) and \( \mathbf{n} \) are three dimensional unit vectors and \( \tau, \sigma \) are Pauli matrices. In the case of a mass-less particle inside a one-dimensional box, assuming perpendicular reflection, it is sufficient to set \( \Psi_{1,2}(r = -1) = \Psi_{1,2}(r = 1) = 0 \). This closed boundary condition ensures probability conservation for the decoupled Weyl equations such that \( \rho(r = -1) = \rho(r = 1) \) and \( \gamma^\mu(r = -1) = \gamma^\mu(r = 1) = 0 \). Numerically, for the present simulational timescales, there is some small \( (1\%) \), resolution convergent error related to finite size effect of the wavefunction.

The metric tensor, although diagonal, for the typical choice of \( w \sim 1 \) imposes some large gradients on the spin connection \( \Gamma^\alpha \) which introduce numerical instabilities. From the form of the metric it can be shown that for \( w \ll 1 \), the metric variation is minimized resulting in more stability, physically this results in a long and thin strip. It should be noted that this choice of parameterization results in non-zero curvature across the whole domain, seen from the Ricci scalar, Appendix D. Additionally, the choice of \( \theta \) is intentional such that the spin connection is continuous across the reverse periodic boundary, see Fig. 1. This is not the case for the most common convention \( \theta \in \{0, 2\pi\} \). The spin connection (or the Christoffel symbols) is not a gauge independent quantity but the metric and Ricci tensors are. In fact, the complete continuity of the spin connection is only achieved for \( w \ll 1 \), for \( w \sim 1 \) there is still some discrepancy as \( \omega^{\eta \theta}_{jk} \) is not symmetric in \( r \).

Correspondingly to the real space curvature, the Berry connection is not gauge independent but the Berry phase and the Berry curvature are. The similarities of the Ricci and Berry curvatures are further investigated in Appendix C, where we show that a Gaussian wave-packet completing a circle around a Möbius band will attain a phase \( \pi \) equivalent to a Berry phase. This is a consequence of the topology and it represents a specific illustration of the relation between Berry and real space curvature. Furthermore, in Appendix E we present an example of a periodic, quantized alternating current device where a spacial equivalent of Bloch oscillations are observed. The observed oscillations are validated analytically by a set of semi-classical equations of motion dependent on Berry curvature.

To realize the energy levels of a Dirac particle on a Möbius graphene ribbon we initialize the wavefunction to a plane wave solution,
\[
\psi(k, r) = \left( \begin{array}{c} i \sin(k_r r) \\ 0 \\ 0 \end{array} \right)
\]
with \( h = c = 1 \), \( E = |k| \) and \( k = (k_\theta, k_r) \). The wave-functions at some later time-step are shown in Fig. 2.

To study the topological properties and observe a Hall-type effect it is necessary to realize a forward moving wavefunction that explores the complete domain. An electric field is both experimentally challenging and theoretically inconsistent across a periodic system such as the Möbius graphene strip. Additionally, a magnetic field is difficult to keep tangential to such a manifold and un-
Fig. 3(a); for the zero-momentum and $\bar{k}$ for brevity, $k$ manifold. The difference between dependence of the asymmetry ratio on $2$ dashed lines lie on opposite sides relative to the $0$ scenario, indicating a net anomalous velocity effect (in the $r$-direction) as a consequence of a $\theta$ velocity, i.e. a Hall current. The asymmetry ratio, $A_P/A_H$, is plotted in the inset of Fig. 3(a) for two different half-widths $w$, defined by

$$A_P = \frac{\bar{J}_P - \bar{J}_{P,k=0}}{\bar{J}_H - \bar{J}_{H,k=0}},$$

where $\bar{J}_{P,H}$ denote the particle, hole currents for $k = 2\pi/l_0$ and $\bar{J}_{P,H,k=0}$ denote the particle, hole currents for $k = 0$. In practice $\bar{J}_{P,k=0}$ and $\bar{J}_{H,k=0}$ are equal. The dependence of the asymmetry ratio on $w$ suggests that the difference between $\bar{J}_P$ and $\bar{J}_H$ is a consequence of the manifold.

The time evolution of $\bar{J}_P$ and $\bar{J}_{P,k=0}$ for longer time are plotted in the inset of Fig. 3(b). The oscillations are a result of the geometry and the closed boundary condition as they are also present for $\bar{J}_{P,k=0}$. There is no obvious non-zero average $\bar{J}_P$, or quantum Hall current. Nevertheless, the non-zero asymmetric ratio and its dependence on $w$ imply again a net anomalous velocity effect. In Fig. 3(b) the time evolution of the average particle-hole space-integrated current $\langle J_{PH} \rangle = |\bar{J}_P - \bar{J}_H|$, is plotted for two different non-zero $k$. The result clearly shows a quantum spin-Hall current (or particle-antiparticle current), which is $k_0$ dependent. The effect is a transient result as there is no constant electric field in order to measure a stationary state solution. Since a Möbius band has only one boundary, it is easier to visualize the result when projected to a rectangle (simulational domain), where the current is flowing towards one direction.

The spin-Hall current is a consequence of the curvature and topology of the system. The gauge field breaking the symmetry of the system is the spin connection matrix $\Gamma$, similar to a twisting magnetic field. For graphene, these curvature effects are realized as forces due to the pseudo-potential in a strained sheet [31]. The correspondence between a magnetic field and curvature is also evident from Appendix C, as the Berry phase is directly related to the Aharanov-Bohm effect.
The time-evolution of the azimuthal current $J^\phi$ for a non-zero momentum particle, (dotted line) and hole (dashed line) wavefunctions. The solid line represents a particle wavefunction with $k_\theta = 0$.

The space integrated spin-Hall current is then a result of the topology, i.e. the twist. This can be understood theoretically as a space-averaged current would not be affected by the 'sharpness' of the twist and any 'flat' regions are irrelevant. Moreover, assuming geometrical disorder is not greater than the cumulative effect of the twist, the bulk current will not be affected more than a perturbative correction. Furthermore, it is established that the quantum levels on the Möbius strip are quantized with respect to $k_\theta$, see Ref. [20]. The current measured here is then quantized with respect to $k_\theta$. Therefore, the response is identified as a quantum spin-Hall current, which can be used to define a Hall conductivity.

IV. THE TORUS

To investigate the relevance of topology and curvature, a similar but simpler shape is also simulated. The system is initialized to the torus geometry by the discreet mapping,

$$h = \begin{pmatrix} (R + w \cos(\phi)) \cos(\theta) \\ (R + w \cos(\phi)) \sin(\theta) \\ w \sin(\theta) \end{pmatrix},$$

with $\theta, \phi \in \{-\pi, \pi\}$, width $w$, mid-circle of radius $R$, $R, w \in \mathbb{R}_{>0}$, both boundaries are periodic. In this parametrization the metric is diagonal and $\phi$ dependent $g_{ij} = \text{diag}((R + w \cos(\phi))^2, w^2)$. In Fig. 5 the time-evolution of the azimuthal current $J^\phi$ is plotted for a particle, (dotted line) and hole (dashed line) wavefunctions as in Sec. III. The solid line represents a particle wavefunction with $k_\theta = 0$. Here, it is evident that a Hall current develops in the presence of a $\theta$ velocity. The different topology, i.e. the absence of the twist and closed boundaries, results in a simpler behaviour, where a transverse current develops as a consequence of curvature.

V. CONCLUSIONS AND OUTLOOK

We have presented a study of the topological and geometrical transport properties of a Möbius graphene ribbon. The challenges and resolutions in simulating such a system were outlined. The continuity of the spin connection was achieved by a gauge transformation and limiting the half-width of the ribbon. We provide some possible numerical wavefunction solutions of the Möbius ribbon.

In the absence of a magnetic field, we measure a quantum spin-Hall current on the graphene ribbon originating from topology and curvature, whereas a quantum Hall current is not observed. This result also represents an example of the correspondence between a magnetic field and a curved manifold. The torus geometry is simulated for comparison, where a Hall current is measured. Additionally, a concrete illustration of the equivalence between the Berry and Ricci curvature is presented through a travelling wave-packet around the Möbius band. Finally we propose a periodic quantized alternating current device with a curved graphene sheet.

Building on these results, higher order and different types of topologies can be further investigated in the context of curvature. Without the need of a magnetic or electric field and by further understanding the properties of topological graphene sheets, simple and topologically robust quantum devices could be developed just by exploiting their geometry.

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Appendix A: Curved-space quantum lattice Boltzmann

The quantum lattice Boltzmann (QLB) method used for solving the Dirac equation as minimally coupled to curved space is an extension of the original method developed by Succi et al. [27]. The method exploits the conceptual similarities between the Dirac equation and the Boltzmann equation on the lattice. We present here the QLB method for a three-dimensional manifold, with straightforward usage to lower dimensional systems.

1. The Dirac equation

The classical Boltzmann equation for a particle density distribution function \( f(x_a, v_a, t) \) is given by

\[
\partial_t f + v^i \partial_{v_i} f = C[f] - F^a \partial_{v^a} f, \tag{A1}
\]

the left-hand side describes the advection of the distribution function, velocity \( v^a \), whereas the right-hand side describes the collisions between particles and the effect of external forces \( F^a \). Furthermore, the Dirac equation in curved space in Eq. 2 can be cast into a kinetic theory form,

\[
\partial_t \Psi + \sigma^a \partial_{v^a} \Psi = C[\Psi] + F[\Psi]. \tag{A2}
\]

Therefore, similarly to the Boltzmann equation, the left-hand side represents the ‘free streaming’ step along matrix valued ‘velocities’ \( \sigma^a \) and the right-hand side contains a ‘collision term’ and a ‘Forcing term’.

The collision term of Eq. A2 is represented by

\[
C = -\left( i m \gamma^0 + \sigma^a e^a_i \Gamma_i \right), \tag{A3}
\]

where \( m \) is the fermion mass, and the ‘forcing term’ by

\[
F = -\sigma^a (e^a_i - \delta^a_i) \partial_i. \tag{A4}
\]

The symbols have their usual meaning. The partial derivative of the Dirac equation is distributed between the
streaming part and the forcing term resulting in a lattice compatible streaming operator of the form \( \partial_t + v^a \partial_a \), where \( v^a \in \mathbb{R} \). The forcing term is a consequence of the generalized Dirac matrices \( \gamma^i = e^{t} \gamma^a \) and captures the bulk of the curvature effects. The partial derivative in Eq. A4 is approximated by a local finite difference scheme on the lattice.

2. Diagonal streaming operator

In order to obtain a diagonal streaming operator the complex \( \sigma \)-matrices have to be diagonalized first, which also yields a diagonal velocity matrix with eigenvalues \( \pm 1 \). The digitalization is achieved by:

\[
X^\dagger_a \sigma^a X_a = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \gamma^0 \quad \text{for } a = 0, 1, 2,
\]

with unitary transformation matrices \( X_1, X_2, X_3 \) given by

\[
X_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 \end{pmatrix}, \quad X_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & i & 0 & 1 \\ -i & 0 & i & 0 \\ -1 & 0 & -1 & 0 \\ 0 & -1 & 0 & -i \end{pmatrix}, \quad X_3 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 & -1 \\ 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 \end{pmatrix}.
\]

The streaming and collision operations are performed in successive steps using operator splitting as simultaneous diagonalization of three \( \sigma \)-matrices is not possible:

\[
\Psi(t + \frac{\Delta t}{D}) = \exp(-\Delta t \sigma^1 \partial_1 + \frac{\Delta t}{D} (C + F)) \Psi(t),
\]

\[
\Psi(t + \frac{2\Delta t}{D}) = \exp(-\Delta t \sigma^2 \partial_2 + \frac{\Delta t}{D} (C + F)) \Psi(t + \frac{\Delta t}{D}),
\]

\[
\Psi(t + \Delta t) = \exp(-\Delta t \sigma^3 \partial_3 + \frac{\Delta t}{D} (C + F)) \Psi(t + \frac{2\Delta t}{D}),
\]

where \( D = 3 \) denotes the dimension. Each streaming step can be diagonalized by left multiplying with \( X_a^\dagger \).

\[
X^\dagger_a \Psi(t + \frac{\Delta t}{D}) = \exp(-\Delta t \sigma^a \partial_a + \Delta t (\tilde{C}_a + \tilde{F}_a)) \Psi_a(t),
\]

with the definitions:

\[
\tilde{C}_a := \frac{1}{2} X_a^\dagger C X_a, \quad \tilde{F}_a := \frac{1}{2} X_a^\dagger F X_a,
\]

for \( a = 1, 2, 3 \) (no Einstein summation is used here), and the exponential approximated as

\[
\exp(-\Delta t \sigma^a \partial_a + \Delta t (\tilde{C}_a + \tilde{F}_a)) \approx (\mathbb{1} - \Delta t \sigma^a \partial_a + \Delta t (\tilde{C}_a + \tilde{F}_a)) + (\mathbb{1} - \frac{\Delta t}{2} \tilde{C}_a)^{-1} (\mathbb{1} + \frac{\Delta t}{2} \tilde{C}_a).
\]

The expansion of the collision operator \( e^{\Delta t \tilde{C}_a} \) is unitary and thus conserves exactly the probability of the wavefunction. The streaming \( e^{-\Delta t \sigma^a \partial_a} \) and forcing \( e^{\Delta t \tilde{F}_a} \) operators are not expanded in analogous as this is prohibited by the derivative. A simple \( 2^{nd} \)-order expansion is performed limiting the probability norm to \( \Delta t^2 \) accuracy. The operator splitting contains an error of \( O(\Delta t^3) \), as \( e^{\Delta t X} e^{\Delta t Y} = e^{\Delta t (X + Y) + 1/2 \Delta t^2 [X,Y]} = e^{\Delta t (X + Y) + O(\Delta t^3)} \).

The manifold is described by a chart \( h \) defined in linear space (see Appendix. B) discretized on a regular rectangular lattice. The curved space quantum Lattice Boltzmann method evolves the spinor \( \Psi = (\Psi^+, \Psi^-) = (\Psi_1^+, \Psi_2^+, \Psi_1^-, \Psi_2^-) \) from \( t \) to \( t + \delta t \). Once the operators are split, the following algorithm is performed consecutively for each lattice direction \( n_a \), where \( n_1 = (1, 0) \), \( n_2 = (0, 1) \) and \( a = 1, 2 \).

1. Rotation: The spinor is rotated by \( X_a \)

\[
\tilde{\Psi}_a(x,t) = X_a^\dagger \Psi(x,t).
\]

2. Collisions and curvature: The collision and force operators are applied on the rotated spinor,

\[
\tilde{\Psi}_a(x,t) = (\Delta t \tilde{F}_a + (1 - \frac{\Delta t}{2} \tilde{C}_a)^{-1} (1 + \frac{\Delta t}{2} \tilde{C}_a)) \tilde{\Psi}_a(x,t),
\]

where \( \tilde{\Psi}_a(x,t) \) denotes an auxiliary field,

\[
\tilde{C}_a = \frac{1}{2} X_a^\dagger C X_a = -i \frac{m}{D} (X_a^\dagger \gamma^0 X_a) - \gamma^0 e^a \Gamma_i ,
\]

\[
\tilde{F}_a \tilde{\Psi}_a(x,t) = (e^a - \delta^a) \left( \tilde{\Psi}_a(x + n_a \Delta t, t) - \tilde{\Psi}_a(x, t) \right),
\]

3. Streaming: The spinor components are streamed to the closest grid points along the lattice direction \( \pm n_a \),

\[
\tilde{\Psi}_a(x,t + \frac{\Delta t}{2}) = \tilde{\Psi}_a(x \mp n_a \Delta t, t).
\]

4. Inverse Rotation: The spinor is rotated back by \( X_a \)

\[
\tilde{\Psi}_a(x,t + \frac{\Delta t}{2}) = X_a \tilde{\Psi}_a(x,t + \frac{\Delta t}{2}).
\]

5. Repeat steps 2-4 for the next spatial direction

The external potentials \( V(x) \), scalar, and \( A(x) \), vector are added to the collision operator Eq. A7 such that

\[
\tilde{C}_a = \frac{1}{2} X_a^\dagger C X_a = -i \frac{m}{D} (m - V)(X_a^\dagger \gamma^0 X_a) - \gamma^0 e^a (\Gamma_i - i A_i).
\]
The simulation for strained graphene is carried out with modified Eqs. (A7,A8) such that
\[ \tilde{C}_a \rightarrow \sqrt{g}\tilde{c}_a, \quad e^a \rightarrow \sqrt{g}e^a. \]
The additional factor of \( \sqrt{g} \) originates from the volume element of the Hamiltonian Eq. (7).

Appendix B: Riemannian geometry

The Latin indices run over the spatial dimensions and Einstein summation convention is used for repeated indices.

A \( D \) dimensional curved space is represented by a Riemannian manifold \( M \), which is locally described by a smooth diffeomorphism \( h \), called the chart. The set of tangential vectors attached to each point \( y \) on the manifold is called the tangent space \( T_y M \). In the fluid model, all the vector quantities are represented as elements of \( T_y M \). The derivatives of the chart \( h \) are used to define the standard basis \( (e_1,...,e_D) = \frac{\partial h}{\partial x^1},...\frac{\partial h}{\partial x^D}. \)

The metric tensor \( g \) can be used to measure the length of a vector or the angle between two vectors. In local coordinates, the components of the metric tensor are given by
\[ g_{ij}(x) = e_i(x) \cdot e_j(x) = \frac{\partial h}{\partial x^i} \cdot \frac{\partial h}{\partial x^j}. \] (B1)
where \( \cdot \) is the standard Euclidean scalar product.

For a given metric tensor, the vector \( v = v^i e_i \in T_y M \) has a norm \( ||v||_g = \sqrt{v^i g_{ij} v^j} \) and a corresponding dual vector \( v^* = v^i e_i \in T^*_y M \) in the cotangent space, which is spanned by the differential 1-forms \( dx^i = g(e_i,.) \). The coefficients \( v_i \) of the dual vector are typically denoted by a lower index and are related to the upper-index coefficients \( v^i \) by contraction with the metric tensor \( v_i = g_{ij} v^j \) or equivalently, \( v^i = g^{ij} v_j \), where \( g^{ij} \) denotes the inverse of the metric tensor. The upper-index coefficients \( v^i \) of a vector \( v \) are typically called covariant components, whereas the lower-index coefficients \( v_i \) of the dual vectors \( v^* \) are known as the contravariant components.

A necessary feature for the description of objects moving on the manifold is parallel transport of vectors along the manifold. The tangent space is equipped with a covariant derivative \( \nabla \) (Levi-Civita connection), which connects the tangent spaces at different points on the manifold and thus allows to transport a tangent vector from one tangent space to the other along a given curve \( \gamma(t) \).

The covariant derivative can be viewed as the orthogonal projection of the Euclidean derivative \( \partial \) onto the tangent space, such that the tangency of the vectors is preserved during the transport. In local coordinates, the covariant derivative is fully characterized by its connection coefficients \( \Gamma^i_{jk} \) (Christoffel symbols), which are defined by the action of the covariant derivative on the basis vector, \( \nabla_j e_k = \Gamma^i_{jk} e_i \). In the standard basis, \( e_i = \frac{\partial h}{\partial x^i}, \) the Christoffel symbols are related to the metric by
\[ \Gamma^i_{jk} = \frac{1}{2}g^{il}(\partial_j g_{kl} + \partial_k g_{lj} - \partial_l g_{jk}). \] (B2)

Acting on a general vector \( v = v^i e_i \), the covariant derivative becomes:
\[ \nabla_k v = (\partial_k v^i + \Gamma^i_{jk} v^j) e_i, \] (B3)
where the product rule has been applied, using that the covariant derivative acts as a normal derivative on the scalar functions \( v^i \). Extending to tensors of higher rank, for example the second order tensors \( T = T^{ij} \),
\[ \nabla_k T = (\partial_k T^{ij} + \Gamma^i_{kl} T^{lj} + \Gamma^j_{kl} T^{il}) e_i \otimes e_j \] (B4)
in this work the basis vectors \( e_i \) are generally dropped. Compatibility of the covariant derivative with the metric tensor implies that \( \nabla_k g^{ij} = \nabla_k g_{ij} = 0 \). This property allows us to commute the covariant derivative with the metric tensor for the raising or lowering of tensor indices in derivative expressions.

The motion of the particle can be described by the curve \( \gamma(t) \), which parametrizes the position of the particle at time \( t \). The geodesic equation, \( \nabla_T^\gamma = 0 \), in local coordinates \( \gamma(t) = \gamma^i(t) e_i \) is defined by
\[ \ddot{\gamma}^i + \Gamma^i_{jk} \dot{\gamma}^j \dot{\gamma}^k = 0. \] (B5)
The geodesic equation can be interpreted as the generalization of Newton’s law of inertia to curved space. The solutions of Eq. (B5) represent lines of constant kinetic energy on the manifold, i.e. the geodesics. The Riemann curvature tensor \( R \) can be used to measure curvature, or more precisely, it measures curvature-induced change of a tangent vector \( v \) when transported along a closed loop.
\[ R(e_i, e_j) v = \nabla_i \nabla_j v - \nabla_j \nabla_i v. \] (B6)

In a local coordinate basis \( e_i \), the coefficients of the Riemann curvature tensor are given by
\[ R^i_{ijk} = g(R(e_i, e_j) e_k, e_l) = \partial_j \Gamma^l_{ik} - \partial_k \Gamma^l_{ij} + \Gamma^l_{jm} \Gamma^m_{ik} - \Gamma^l_{km} \Gamma^m_{ij}. \] (B7)

Contraction of \( R^i_{ijk} \) to a rank 2 and 1 tensor yields the Ricci-tensor \( R_{ij} = R^k_{ikj} \) and the Ricci-scalar \( R = g^{ij} R_{ij} \) respectively, which can also be used to quantify curvature.

The gradient is defined as the \( \nabla^i f = g^{ij} \partial_j f \), the divergence as \( \nabla_i v^i = \frac{1}{\sqrt{g}} \partial_i (\sqrt{g} v^i) \), and the integration over curved volume as \( V = \int_V Q dV \), where \( dV = \sqrt{g} dx^1...dx^D = :\sqrt{g} d^D x \) denotes the volume element. \( \sqrt{g} \) denotes the square root of the determinant of the metric tensor.

It should be clarified that in the simulations there is no time curvature and \( g_{ij} \) denotes the curved space metric.
Appendix C: Berry phase on the Möbius ribbon

To solve the Dirac equation, minimally coupled to curvature, Eq. 2, with \( A_i = 0 \) and assuming that the wave-packet has a negligible profile, \( \delta r \rightarrow 0 \), the connection component of the covariant derivative can be absorbed into the wavefunction such that

\[
\Psi \rightarrow \Psi \exp \left( i \int_{r_e}^{r_e+\delta r} \Gamma_i dr \right)
\]

\[\text{(C1)}\]

where \( r_e \) is the center of mass position and \( \Gamma_i \) is the spin connection matrix. For a Gaussian wavepacket with spread \( \sigma \) and momentum \( k \)

\[
\Psi(r, k) = \frac{1}{\sqrt{2\pi\sigma^2}} \left( \begin{array}{c} 1 \\ 0 \\ 0 \\ -1 \end{array} \right) e^{i \frac{\sigma^2}{4\pi} r^2 + ik \cdot r}.
\]

\[\text{(C2)}\]

This wavefunction effectively minimally couples the standard Dirac equation to curved space through the spin connection. Defining the Berry connection as

\[
A_n^i(R) = i \langle \Psi(R) | \partial R | \Psi(R) \rangle
\]

\[\text{(C3)}\]

for some parameter space \( R \) and eigen-function \( n \). The Berry phase can be calculated from the complete loop integral of the connection

\[
\gamma = \oint_0^{2\pi} A(R) g^{ij} dR.
\]

\[\text{(C4)}\]

In a similar manner to the treatment of the Aharonov-Bohm effect from Berry [33], we define the fast and slow coordinates as \( R \) and \( r \) respectively such that \( \Psi(R) \rightarrow \Psi(r-R) \). For the Möbius band, choosing the real space as the parameter of integration and restricting the motion to one-dimension \( r \in 0, 2\pi \), the center of the band, the wavefunction takes the form

\[
\Psi_r(R-r) = \frac{1}{\sqrt{2\pi\sigma^2}} \left( \begin{array}{c} 1 \\ 0 \\ 0 \\ -1 \end{array} \right) e^{i \int R \Gamma_i dr_e e^{-\frac{\sigma^2 r^2}{4\pi} + ik \cdot r}}.
\]

\[\text{(C5)}\]

From Eq. C3 the explicit form of the wavefunction implies that \( \mathcal{A}_n^i = Tr \Gamma_i \). The implication of these results is that the Berry connection and curvatures can be directly related to the real space affine connection and Ricci curvature tensor under some conditions.

As a consequence, the phase change of a wavepacket moving around a Möbius band can be calculated from the Berry phase. Integrating naively around the band

\[
\gamma = \oint_0^{2\pi} \text{Tr} \langle \Psi_r | \partial_r \Psi_r \rangle g^{ij} dr,
\]

\[\text{(C6)}\]

where the Tr denotes the trace of the resulting matrix and it takes into account the spinor nature of the Dirac wavefunction, yields a trivial result: \( \gamma = 0 \). The caveat is that, in this coordinate basis, for both half-width and half-radius equal to unity \( \Gamma_r \) simplifies to a diagonal matrix such that

\[
\left(\begin{array}{cccc}
\frac{1}{2} i \cos \left(\frac{\pi}{2}\right) & 0 & 0 & 0 \\
0 & \frac{1}{2} i \cos \left(\frac{\pi}{2}\right) & 0 & 0 \\
0 & 0 & \frac{1}{2} i \cos \left(\frac{\pi}{2}\right) & 0 \\
0 & 0 & 0 & -\frac{1}{2} i \cos \left(\frac{\pi}{2}\right)
\end{array}\right).
\]

\[\text{(C7)}\]

\( \Gamma_r \) is discontinuous when \( \theta = 2\pi \rightarrow 0 \). To make the function single valued we can perform a gauge transformation such that \( \Psi \rightarrow \Psi' = \Psi e^{i\gamma} \). This implies that \( \gamma' = \gamma - \frac{1}{2} dr/2 = -\pi \). Therefore the wavefunction picks up a phase of \( \pi \) as it moves around the band, a consequence of the specific topology.

Appendix D: Ricci scalar for Möbius band

The Ricci scalar for Möbius band is non-zero across the whole domain for the specific choice of parameters

\[\text{Figure 5. The Ricci scalar of the Möbius band for half-width } w = 0.1 \text{ and mid-circle of radius } R = 1.\]

Appendix E: Quantized alternating current

graphene strip

To further investigate the potential of curvature on curved graphene sheets we propose a periodic system with alternating current (AC) behaviour which is quantized according to its shape. The system geometry is initialized by the discreet mapping (or chart),

\[
h^\alpha(x, y) = \begin{pmatrix} x \\ y \\ y \sin(\eta x/2) \end{pmatrix}
\]

\[\text{(E1)}\]

with \( x \in \{0, 2\pi\} \), \( r \in \{-L_y/2, L_y/2\} \), with \( L_y \) being the domain size in the \( y \) dimension, see Fig. 6. The boundaries are periodic along the \( x \)-direction and closed at \(-L_y/2, L_y/2\).
A Gaussian wave-packet is initialized as
\[
\Psi(\mathbf{r}, \mathbf{k}) = \frac{1}{\sqrt{2\pi\sigma^2}} \left( \frac{1}{\lambda \epsilon^{i\theta}} \right) e^{-\frac{|\mathbf{r}|^2}{8\sigma^2} + i\mathbf{k} \cdot \mathbf{r}},
\]
where \( \lambda = \pm 1 \) is the band index, \( \theta = \arctan(k_y/k_x) \), \( \sigma \) is a measure for the width, \( \mathbf{r} = (x, y) \), \( x, y \) are the two space dimensions, \( \mathbf{k} = (k_x, k_y) \), \( k_x, k_y \) represent the \( x \) and \( y \) momenta respectively. \( k_z \) is initialized to one, \( k_y \) to zero and \( \lambda \) to plus one. In the simulations, we consider a rectangular sheet with periodic boundary conditions on a grid of size \( L_x \times L_y = 256 \times 128 \) or \( 20nm \times 5nm \), \( A_n \), the external potential is set to zero. The norm of the wavefunction, \( ||\Psi||^2 \), i.e. the probability density, \( \rho \) is plotted in Fig. 6 for the initial and a later time-step. The domain is initialized to a close boundary in the \( y \) direction and periodic across \( x \).

The center of charge density
\[
\bar{\rho} = \left[ \int_{area} r \cdot \rho dA - \int_{area} r \cdot \rho(t=0) dA \right] / \int_{area} \rho dA,
\]
where \( dA = dx dy \), is plotted as a time evolution in Fig. 7. The oscillations can be understood as the geometrical equivalent to the Bloch oscillations and they are a consequence of the sinusoidal, periodic domain. The frequency is quantized relative to \( \eta \). For a slowly perturbed Hamiltonian and expanding around the wave-packet center \( c \), \( H = H_0 + \Delta H \), assuming a periodic system that can be described with a Bloch wavefunction, the semiclassical equations of motion are given by [33]
\[
\dot{r}_c = \frac{\partial \varepsilon}{\partial q} - (\Omega_{qr} \cdot \dot{r}_c + \Omega_{qq} \cdot \dot{q}_c) - \Omega_{qt}, \quad \dot{q}_c = \frac{\partial \varepsilon}{\partial r} - (\Omega_{qr} \cdot \dot{q}_c + \Omega_{rr} \cdot \dot{r}_c) - \Omega_{rt},
\]
where \( r_c, q_c \) are the center of mass position and momentum of the wavepacket, \( \varepsilon \) is the band energy and
\[
\Omega_{qr} = (\Omega_{qr})_{\alpha \beta} = \partial q_\alpha A_{\beta} - \partial r_\beta A_{\alpha}, \quad \text{is the Berry curvature and} \ A_{\alpha} \text{ the Berry connection. As seen in Appendix C, the Berry phase, and thus Berry curvature, can be related directly to the spin connection } \Gamma_{\mu} \text{ through } A^\mu_r \left( \mathbf{R} \right) = i \langle \Psi(\mathbf{R}) | \partial_\mu | \Psi(\mathbf{R}) \rangle \Rightarrow A_{R_\mu} = \text{Tr}(\Gamma_{\mu} | \Psi \rangle \langle \Psi |) \text{ for some parameter space } \mathbf{R} \text{ and eigen-function } n. \text{ The non zero terms of Eqs. (E4,E5) for the specific geometry are } \dot{r}_c = \partial \varepsilon / \partial q \approx v_f, \quad \dot{q}_c = \Omega_{rr} \cdot \dot{r}_c, \text{ which imply:}
\]
\[
\frac{\partial q_\alpha}{\partial r_\beta} = (\Omega_{rr})_{\alpha \beta}.
\]

For small local wave-packet \( \delta q_\alpha = \int (\Omega_{rr})_{\alpha \beta} d\beta = \int (\partial r_\alpha A_{\beta} - \partial r_\beta A_{\alpha}) d\beta \) and thus \( \delta q_\eta \propto \sin(\eta x) \) and \( \delta q_\eta \propto \cos(\eta x) \). Therefore, the oscillations can be explained by a real space Berry curvature description of the system as well as the classical geodesic equation of a manifold.

The frequency of these Bloch-like oscillations are quantized according to \( \eta \). Finally, as the center of mass density would be equivalent to a driven oscillating current the system can be implemented as a periodic, quantized AC device.