Brillouin zone doubling causes fermion doubling
for a staggered lattice discretization of the Dirac equation

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When the massless Dirac fermions on the surface of a topological insulator are placed on a 2D lattice, a second species may appear at the Brillouin zone boundary — a lattice artefact known as “fermion doubling”. To avoid this, a staggered space-time lattice discretization has been developed in the literature, with one single Dirac cone in the Brillouin zone of the original square lattice. Here we show that the staggering doubles the size of the Brillouin zone, which actually contains two Dirac cones. We find that this fermion doubling causes a spurious breakdown of Klein tunneling, which can be avoided by an alternative single-cone discretization scheme.

I. INTRODUCTION

A topological insulator is Nature’s way to work around the “no-go” theorem for the impossibility to place a single species of massless Dirac fermions on a two-dimensional (2D) lattice [1]. The work-around consists in spatially separating two Dirac cones, one on the top surface and one on the bottom surface of the 3D material [2–5]. Since working with a 3D lattice is computationally expensive, there is a need for methods to implement a single Dirac cone on a 2D lattice [1].

A method with highly attractive features has been developed by Hammer, Pötz, and Arnold (HPA) [6, 7] and applied to a variety of problems in condensed matter physics [7–10]. They have implemented a space-time lattice discretization of the Dirac equation

\[ i\hbar \frac{\partial}{\partial t} \Psi(r, t) = v_0 \sum_{\alpha = x, y} (p_\alpha + eA_\alpha)\sigma_\alpha \Psi(r, t) + V\Psi(r, t), \]

which in the absence of scalar and vector potentials \(V, A\) produces the bandstructure

\[ \sin^2(\varepsilon \delta t/2) = \gamma^2 \sum_{\alpha = x, y} \sin^2(a_0 k_\alpha/2), \quad \gamma \equiv \frac{v_0 \delta t}{a_0} \leq \frac{1}{\sqrt{2}}. \]

Here \(a_0\) and \(\delta t\) are the lattice constants in space and time, \(\hbar\) and \(\varepsilon\) are crystal momentum and quasi-energy [11]. \(v_0\) is the energy-independent velocity of the massless electrons (Dirac fermions), and the \(\sigma_\alpha\)'s are Pauli spin matrices. Eq. (2) has a single Dirac point at \(k = 0\) in the domain \(|k_\alpha| < \pi/a_0\).

A unique property of the HPA technique is that it is fully gauge invariant [5, 6]. It is also highly efficient, because the time evolution is governed by a direct, rather than implicit, difference equation, which moreover is local in real space. Since these features have all been elusive for single-cone discretization schemes, we were motivated to investigate the technique in some detail.

Our central finding, presented in Sec. II, is that the bandstructure (2) actually has two inequivalent Dirac cones in the first Brillouin zone: The Dirac points at \(k = 0\) and \(k = (2\pi/a_0, 0)\) are not related by a reciprocal lattice vector. The Brillouin zone doubling can be avoided by using a different space-time lattice, which has a bandstructure of the same form as Eq. (2) — but with the sine replaced by a tangent [12]. We simulate Klein tunneling by means of these two methods in Sec. III and conclude in Sec. IV.

II. BRILLOUIN ZONE DOUBLING

The HPA technique modifies a staggered lattice discretization known as Susskind fermions [13, 14] and implemented in 2 + 1 space-time dimensions in Ref. 15. In that approach the two components of the spinor \(\Psi = (u, v)\) are discretized on separate lattices, displaced (staggered) from each other by \(a_0/2\) and evaluated at alternating time slices (see Fig. 1).

The Susskind fermion quasi-energy bandstructure [15],

\[ \cos^2 \varepsilon \delta t = (1 - \gamma^2 + \gamma^2 \cos a_0 k_\alpha \cos a_0 k_\beta)^2, \quad \gamma \leq 1, \]

has two inequivalent Dirac cones in the first Brillouin zone \(B\) shown in Fig. 1, defined by

\[ B = \{k_x, k_y \in \mathbb{R} | -\pi/a_0 < k_x, k_y \leq \pi/a_0\}. \]

This is an improvement over the naive discretization, without staggering, which would have four inequivalent Dirac cones, at \((a_0 k_x, a_0 k_y) = (0, 0), (\pi, \pi), (\pi, 0),\) and \((0, \pi)\). Susskind fermions do not have the last two, but the first two Dirac cones remain.

In Fig. 1, d we show the HPA modification of the staggered lattice discretization. Comparison with Fig. 1, c shows that the HPA unit cell has one half the area of the unit cell of the original square lattice. Accordingly, the first Brillouin zone \(B'\), defined by

\[ B' = \{k_x, k_y \in \mathbb{R} | -2\pi/a_0 < |k_x \pm k_y| \leq 2\pi/a_0\}, \]

has twice the area of \(B\).

Inspection of the HPA dispersion (2) then shows that, indeed, within \(B\) there is only a single Dirac cone, at
FIG. 1. Comparison of two types of staggered grids for the spatial discretization of Dirac fermions, in the Susskind fermion approach (panel a, corresponding Brillouin zone $B$ in panel c) and in the HPA modification (panel b, Brillouin zone $B'$ in panel d). The black and white dots distinguish the $u$ and $v$ amplitudes of the spinor wave function $\Psi = (u,v)$. The blue squares give the unit cell of the lattice in real space, the grey square is the first Brillouin zone in momentum space, the red dots indicate two inequivalent Dirac points.

FIG. 2. Quasi-energy bandstructure of the HPA staggered lattice discretization, for $\gamma = 1/\sqrt{2}$, in the first Brillouin zone $B'$ given by Eq. (5). There are two inequivalent Dirac cones, at center and corner of the Brillouin zone.

FIG. 3. Three snapshots of the time-dependent simulation of Klein tunneling, in two alternative methods of discretization of the Dirac equation. A potential barrier of height $V_0 = 1.41 \hbar/\delta t$ is located between the dotted lines. A wave packet at lower energy ($\bar{E} = 0.35 \hbar/\delta t$) is normally incident on the barrier. The color scale shows $|\Psi|^2$ normalized to unit peak height at each of the three times.

III. KLEIN TUNNELING

The second Dirac cone at the corner of the Brillouin zone $B'$ is at a relatively large momentum, so it will not play a role if the potentials are smooth: only momenta near $k = 0$ then matter. But if the potentials vary on the scale of the lattice constant, then the fermion doubling has noticeable consequences.

We investigate that here for Klein tunneling [16, 17]: Massless Dirac fermions are transmitted with unit probability when they approach a potential barrier at normal incidence, because conservation of chirality does not allow backscattering within a single Dirac cone. Coupling to a second cone will spoil that.

We contrast the numerical results following from the HPA staggered lattice technique [5] with those obtained using a manifestly single-cone discretization method [12] (a split-operator implementation of the Stacey discretization [18–20]). To make this paper self-contained, both methods are summarized in App. A. Our numerical codes are available at a repository [21].

We calculate the time dependence of a state $\Psi(x,y,t)$ incident along the $x$-axis on a rectangular barrier of height $V_0$ and width $50 a_0$. The initial state is a Gaussian wave packet,

$$\Psi(x,y,0) = (2\pi\sigma^2)^{-1/2} e^{i k_0 x} e^{-(x^2+y^2)/2\sigma^2} \begin{pmatrix} 1 \\ 1 \end{pmatrix},$$

with parameters $k_0 = 0.5/a_0$, $\sigma = 30 a_0$. We choose the time step $\delta t$ such that $\gamma = v_0 \delta t/a_0 = 1/\sqrt{2}$. The mean energy is $\bar{E} = \hbar v_0 k_0 = 0.35 \hbar/\delta t$, much less than the barrier height.

As shown in Figs. [3 and 4] when $V_0$ is larger than $\bar{E}$ the wave packet is fully transmitted when the Dirac equation is discretized using the split-operator method,
reaches the bandwidth.

V example, when $V_0$ is close to $E$ the wave packet disperses side ways and backwards in the barrier region, hence the dashed dip in both curves. For the split-operator discretization $T \approx 1$ once $V_0 \gtrsim E$, while for the staggered discretization $T$ drops significantly below 1 well before $V_0 - E$ reaches the bandwidth.

![Fig. 4. Transmission probability $T$ through the potential barrier of Fig. 3 as a function of the barrier height $V_0$. The blue and red curves are for, respectively, the split-operator discretization and the staggered lattice discretization. The mean energy $\bar{E} = 0.35\hbar/\delta t$ of the incident wave packet is indicated, as well as the finite bandwidth $\pi\hbar/\delta t$ of the staggered discretization.](image)

but not in the HPA staggered lattice discretization. For example, when $V_0 = 2E$ we find, respectively, $T = 1.00$ and $T = 0.87$. We attribute the difference to fermion doubling.

To establish this, we have repeated the calculation with a periodic modulation of the barrier height,

$$V(x, y) = \begin{cases} 0 & \text{if } |x/a_0 - 300| > 25, \\ V_0 + \delta V \sin q_0 x & \text{if } |x/a_0 - 300| < 25. \end{cases}$$

\begin{equation}
\sin^2(\varepsilon/\delta t/2) = \frac{(V_0\delta t/2)^2 + \gamma^2 \sin^2(q_0 k_x/2)}{1 + (V_0\delta t/2)^2}. \tag{8}
\end{equation}

The gap at $k = 0$ equals $2V_0$ for $V_0\delta t \ll 1$.

**IV. CONCLUSION**

In conclusion, we have uncovered a difficulty of staggered space-time lattice discretizations of the Dirac equation. In 2D staggered fermions *a la* Susskind have two Dirac cones in the Brillouin zone. To eliminate this lattice artefact known as fermion doubling, Hammer, Pütz, and Arnold introduced a space-time lattice with bandstructure

$$\varepsilon = \pm 2 \arcsin \left( v \sqrt{\sin^2 (k_x/2) + \sin^2 (k_y/2)} \right) \tag{9}$$

(in units where $a_0$ and $\delta t$ are 1). The Susskind fermion Brillouin zone is $-\pi < k_x, k_y < \pi$ and in that Brillouin
zone the bandstructure \[1\] has only a Dirac cone at the origin \(k = 0\).

What we have found is that this bandstructure is accompanied by Brillouin zone doubling: Along the \(k_z\)-axis it extends from \(-2\pi < k_z < 2\pi\), so the Dirac cone at \(k = (2\pi, 0)\) is independent from the one at the origin — they are not related by a reciprocal lattice vector. We have shown that this fermion doubling has physical consequences in the breakdown of Klein tunneling.

To ascertain that fermion doubling is at the origin of these effects, we have compared with an alternative space-time discretization using a split-operator technique \[12\], with bandstructure

\[
\varepsilon = \pm 2 \arctan \left( v \sqrt{\tan^2(k_x/2) + \tan^2(k_y/2)} \right). \tag{10}
\]

The replacement of sine by tangent avoids the Brillouin zone doubling, essentially because \(\sin(k/2)\) is \(4\pi\)-periodic in \(k\), while \(\tan(k/2)\) is \(2\pi\)-periodic. The Dirac cones at \(k = 0\) and \(k = (2\pi, 0)\) are now equivalent, related by a reciprocal lattice vector, and indeed we recover the Klein tunneling with unit probability expected for massless Dirac fermions.

The staggered lattice discretization has one feature that the split-operator discretization lacks: the possibility to include the vector potential in a fully gauge invariant way via the Peierls substitution \[5, 6\]. We are inclined to think that this is an intrinsic limitation of the split-operator discretization lacks: the possibility to include the vector potential in a fully gauge invariant way via the Peierls substitution \[5, 6\]. We are inclined to think that this is an intrinsic limitation of this approach of Ref. 12. We summarize these two methods.

1. Staggered lattice approach

Hammer, Pötz, and Arnold \[3\] discretize the \(2 + 1\) dimensional Dirac equation on the space-time lattice shown in Fig. 7. The two components of the wave function \(\Psi = (u, v)\) are evaluated on two different lattices, staggered in both space and time. The \(v\)-lattice is obtained from the \(u\)-lattice by a translation of \(\delta t/2\) in the time direction and by \(a_0/2\) in the \(x\)-direction. A translation of either \(u\)-lattice or \(v\)-lattice by \(a_0/2\) in the \(x\)-direction without a time translation defines a third lattice of points \(S_{u,v} = (x_n, y_m, t_s)\), the red points in Fig. 7. Each of these three lattices is face-centered square in the \(x-y\) plane, with the unit cell and Brillouin zone \(B'\) of Fig. 7b, d.

The finite-difference equation for the \(u\) component is (abbreviating \(\gamma = v_0\delta t/a_0\))

\[
i[u(x_n, y_m, t_s + \frac{1}{2}\delta t) - u(x_n, y_m, t_s - \frac{1}{2}\delta t)] = -i\gamma[v(x_n + \frac{1}{2}a_0, y_m, t_s) - v(x_n - \frac{1}{2}a_0, y_m, t_s)] + \delta t \frac{2\hbar}{\gamma} V(x_n, y_m, t_s) u(x_n, y_m, t_s + \frac{1}{2}\delta t) + u(x_n, y_m, t_s - \frac{1}{2}\delta t)], \tag{A1a}
\]

for \((x_n, y_m, t_s \pm \frac{1}{2}\delta t)\) on the \(u\)-lattice. The arguments of the \(v\)-component are then located on the \(v\)-lattice. Similarly,
the finite-difference equation for the $v$-component is

$$i[v(x_n, y_m, t_s + \frac{1}{2}\delta t) - v(x_n, y_m, t_s - \frac{1}{2}\delta t)] = -\gamma[u(x_n + \frac{1}{2}a_0, y_m, t_s) - u(x_n - \frac{1}{2}a_0, y_m, t_s)]$$

$$+ \gamma[u(x_n, y_m + \frac{1}{2}a_0, t_s) - u(x_n, y_m - \frac{1}{2}a_0, t_s)] + \frac{\delta t}{2\hbar}V(x_n, y_m, t_s)[v(x_n, y_m, t_s + \frac{1}{2}\delta t) - v(x_n, y_m, t_s - \frac{1}{2}\delta t)],$$

(A1b)

The unitary Fourier transform operator $\mathcal{F}$ performs a change of basis, so that the $r$-dependent operators are evaluated in the real-space basis and the $k$-dependent operators are evaluated in the momentum basis — at minimal computational cost. The cost of a Fast Fourier Transform scales as $N\log N$ on an $N$-site lattice.

The eigenvalues $e^{i\epsilon t}$ of $U$ for $V = 0$ depend on $k$ according to

$$\tan^2(\varepsilon\delta t/2) = \gamma^2[\tan^2(a_0k_x/2) + \tan^2(a_0k_y/2)].$$

(A4)

The quasi-energy $\varepsilon$ is real for any $\gamma > 0$. The bandstructure in the first Brillouin zone is plotted in Fig. 8 for $\gamma = 1/\sqrt{2}$.

Appendix B: Gap opening for the staggered lattice discretization

Because the staggered lattice discretization has two Dirac cones in the Brillouin zone, the gapless Dirac point is not protected by time-reversal symmetry — a gap can open without violating Kramers degeneracy. Here we show this by an explicit calculation.

The gap opening mechanism can be described as “fold and split”: a potential that varies on the scale of the lattice constant $a_0$ folds the Dirac cone at $k = (2\pi/a_0, 0)$ onto the cone at $k = (0, 0)$, and then the upper and lower cone can split apart while preserving the double degeneracy required by Kramers theorem.

We consider the periodic potential $V(x, y) = V(x + a_0, y) = V(x, y + a_0)$ and solve the finite difference equations (A1) for the Bloch state $\Psi(x + a_0, y, t) = e^{ia_0k_x}\Psi(x, y, t)$, $\Psi(x, y + a_0, t) = e^{ia_0k_y}\Psi(x, y, t)$. There are four independent equations, involving the spinor amplitudes

$$u_1(t) = u(0, 0, t - \delta t/2), \quad u_2(t) = u(a_0/2, a_0/2, t - \delta t/2), \quad v_1(t) = v(a_0/2, 0, t), \quad v_2(t) = v(0, a_0/2, t),$$

(B1)

and potential values $V_A = V(0, 0), V_B = V(a_0/2, a_0/2), V_C = V(a_0/2, 0), V_D = V(0, a_0/2)$. The four equations can be written in the matrix form
The eigenvalues $e^{\pm \delta t}$ of the matrix product $\mathcal{P}^{-1} \mathcal{Q}$ give the bandstructure $\varepsilon(k_x, k_y)$. One readily recovers Eq. (2) for $V(x, y) \equiv 0$. For the potential $V(x, y) = V_0 \cos(2\pi x/a_0)$ we set $V_A = V_D = V_0$, $V_B = V_D = -V_0$. Along the line $k_y = 0$ we then find the result (8), with a gap at $k = 0$ of size

$$\Delta \varepsilon = \frac{4}{\delta t} \arcsin \left( \frac{V_0 \delta t / 2}{\sqrt{1 + (V_0 \delta t / 2)^2}} \right).$$

We note that the topological protection of the Dirac cone for the split-operator discretization (A3) was established in Ref. [12].
[22] C. L. Kane, *Topological band theory and the $\mathbb{Z}_2$ invariant*, Contemporary Concepts of Condensed Matter Science 6, 3 (2013) doi:10.1016/B978-0-444-63314-9.00001-9.