Topological aspects of fermions on a honeycomb lattice

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with **Dipankar Chakrabarti** & **Antonio Rago** JHEP**06**(2009)060

Novel Lattice Fermions and their Suitability
for High-Performance Computing and Perturbation Theory, MITP Mainz 6/3/23

Preamble

Two very influential papers related to
graphene emerged from our community around 2007-08

D.T. Son, Phys. Rev. B**75** (2007) 235423

suggested that the presence of electrostatic interactions between charged excitations in graphene may destabilise the semimetallic ground state of the tight-binding model leading to a gapped ground state characterised by $\langle\bar{\psi}\psi\rangle \neq 0$
The semimetal-insulator transition, expected at small flavor number N and large interaction strength g^2 may correspond to a Quantum Critical Point

M. Creutz, JHEP**04**(2008) 017

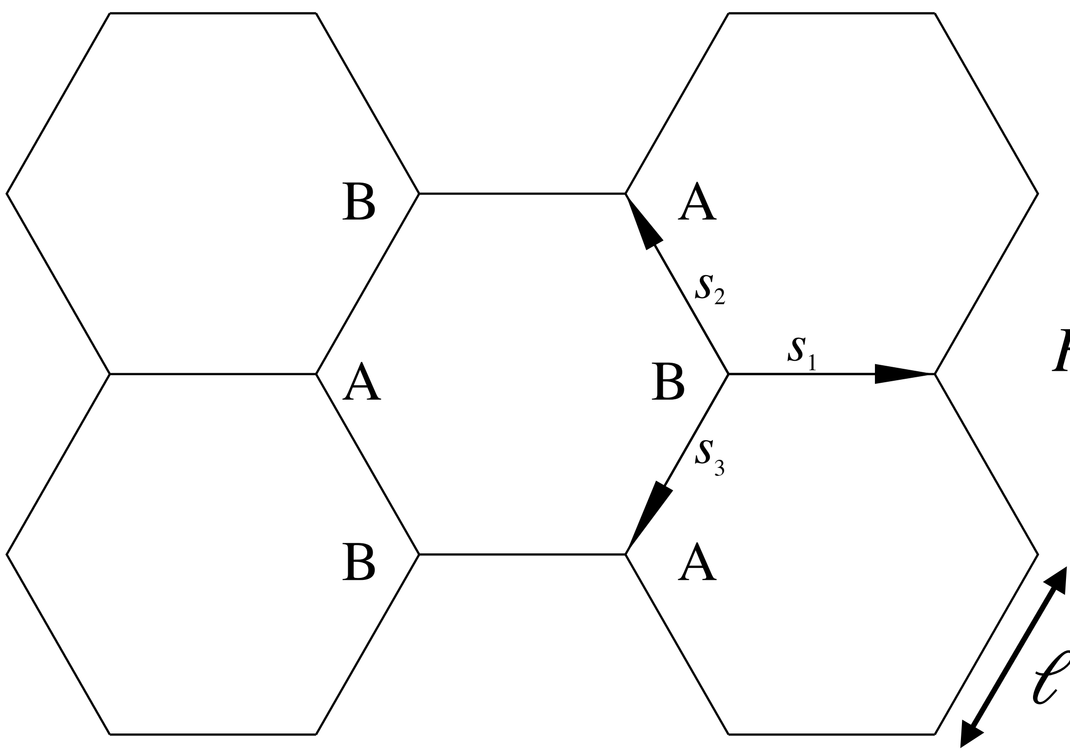
argued that tight-binding graphene is an instance of "minimal doubling" required by the Nielsen-Ninomiya theorem, and proposed related models based on (hyper)-cubic lattices potentially offering simulation advantages.
This kicked off a flurry of activity in proposing and analysing novel fermion actions.

The following work was our attempt to initiate analysis of non-perturbative features of minimally-doubled fermions

Relativity in Graphene

P.R. Wallace, Phys. Rev. **71** (1947) 622

The electronic properties of graphene were first studied theoretically almost 75 years ago



$$\vec{s}_1 = (1,0)\ell; \quad \vec{s}_{2,3} = \left(-\frac{1}{2} \pm \frac{\sqrt{3}}{2}\right)\ell$$

Rules of the Dance

On each carbon atom there can reside 0, 1 or 2 electrons which can hop between sites

$$H = -t \sum_{\vec{r}\in B} \sum_{i=1}^{3} b^\dagger(\vec{r})U(\vec{r},\vec{s}_i)a(\vec{r}+s_i) + a^\dagger(\vec{r}+\vec{s}_i)U^\dagger(r,\vec{s}_i)b(\vec{r})$$

tight-binding Hamiltonian

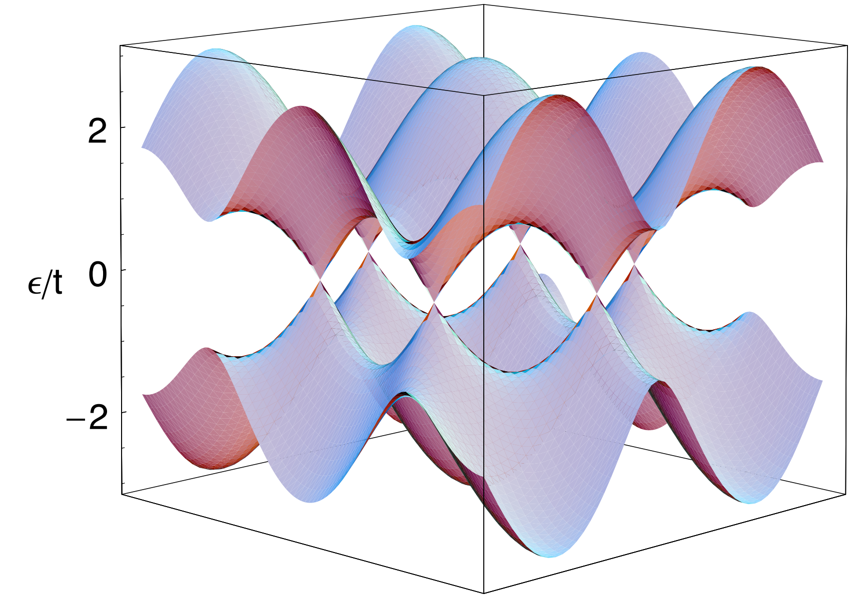
describes hopping of electrons in π-orbitals from A to B sublattices and *vice versa*

In momentum space $$H_0 = H[U=1] = \sum_k \left(\Phi(\vec{k})a^\dagger(\vec{k})b(\vec{k}) + \Phi^*(\vec{k})b^\dagger(\vec{k})a(\vec{k})\right)$$

with $$\Phi(\vec{k}) = -t\left[e^{ik_x\ell} + 2\cos\left(\frac{\sqrt{3}k_y\ell}{2}\right)e^{-i\frac{k_x\ell}{2}}\right]$$

Define states $|\vec{k}_\pm\rangle = (\sqrt{2})^{-1}[a^\dagger(\vec{k}) \pm b^\dagger(\vec{k})]|0\rangle$

$$\Rightarrow \langle \vec{k}_\pm | H | \vec{k}_\pm \rangle = \pm(\Phi(\vec{k}) + \Phi^*(\vec{k})) \equiv \pm E(\vec{k})$$



Energy spectrum is symmetric about $E = 0$

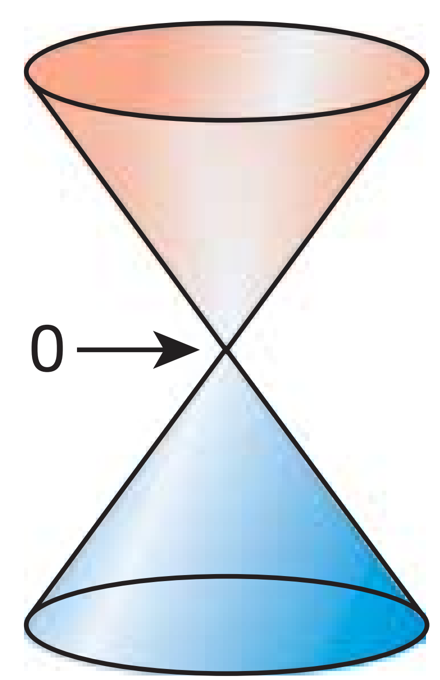
Half-filling (neutral "undoped" graphene) has zero energy at **Dirac points** at corners of first Brillouin Zone:

Two independent Dirac points

$$\Phi(\vec{k}) = 0 \;\Rightarrow\; \vec{k} = \vec{K}_\pm = \left(0, \pm\frac{4\pi}{3\sqrt{3}\ell}\right)$$

Taylor expand @ Dirac point

$$\Phi(\vec{K}_\pm + \vec{p}) = \pm v_F[p_y \mp ip_x] + O(p^2)$$



the pitch of the cone is the Fermi velocity

$$v_F = \frac{3}{2}tl$$

Define modified operators $a_{\pm}(\vec{p}) = a(\vec{K}_{\pm} + \vec{p})$ etc.

Now combine them into a "4-spinor" $\Psi = (\, b_+, a_+, a_-, b_-)^{tr}$

$$\Rightarrow \quad H \simeq v_F \sum_{\vec{p}} \Psi^\dagger(\vec{p}) \begin{pmatrix} & p_y + ip_x & & \\ p_y - ip_x & & & \\ & & & -p_y - ip_x \\ & & -p_y + ip_x & \end{pmatrix} \Psi(\vec{p})$$

$$= v_F \sum_{\vec{p}} \Psi^\dagger(\vec{p}) \vec{\alpha}.\vec{p}\, \Psi(\vec{p})$$

Dirac Hamiltonian

$$\{\alpha_i, \alpha_j\} = 2\delta_{ij}$$

ie. low-energy excitations are massless fermions with **Fermi velocity**

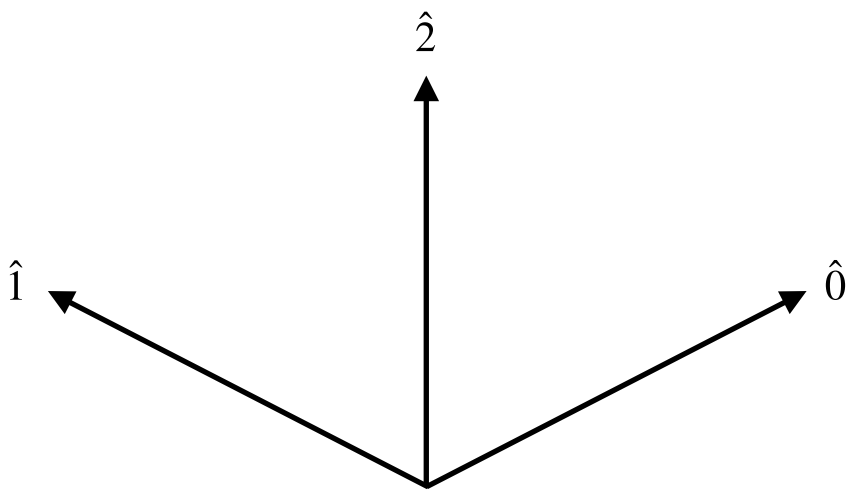
$$v_F = \frac{3}{2} tl \approx \frac{1}{300} c$$

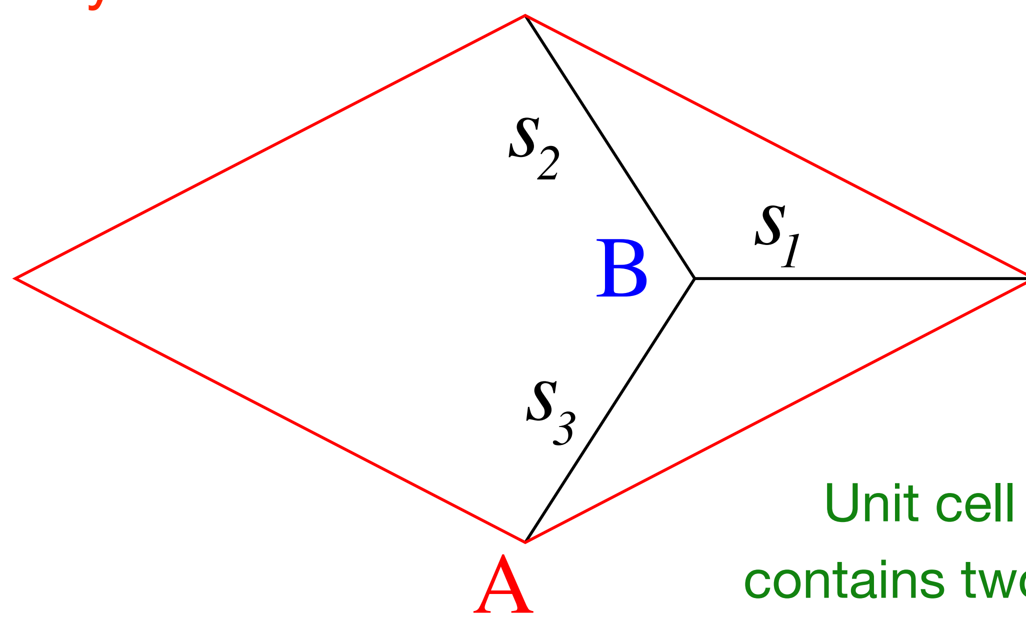
For monolayer graphene the number of flavors $N = 2$

(2 C atoms/cell × 2 Dirac points/zone × 2 spins = 2 flavors × 4 spinor)

We will recast the tight-binding Hamiltonian as the Lagrangian density of a 2d Euclidean quantum field theory

$$\mathscr{L}_{2d} = \bar{\chi} i D \chi = \bar{\chi}_B i D \chi_A + \bar{\chi}_A i D \chi_B$$





$$\chi(x) = \begin{pmatrix} \chi_A(x) \\ \chi_B(x) \end{pmatrix}$$

Unit cell labelled by spatial x contains two inequivalent sites A,B

with $$(D\chi)(x) = D_1(x)\chi(x+\hat{0}) + D_1(x-\hat{0})\chi(x-\hat{0})$$
$$+D_2(x)\chi(x+\hat{2}) + D_2(x-\hat{2})\chi(x-\hat{2}) + D_3(x)\chi(x)$$

$$D_1(x) = \begin{pmatrix} 0 & 0 \\ U(x,\vec{s}_1) & 0 \end{pmatrix} \quad D_1(x-\hat{0}) = \begin{pmatrix} 0 & U^*(x-\hat{0},\vec{s}_1) \\ 0 & 0 \end{pmatrix} \quad D_2(x) = \begin{pmatrix} 0 & 0 \\ U(x,\vec{s}_2) & 0 \end{pmatrix} \quad D_2(x-\hat{2}) = \begin{pmatrix} 0 & U^*(x-\hat{2},\vec{s}_2) \\ 0 & 0 \end{pmatrix}$$

$$D_3(x) = \begin{pmatrix} 0 & U^*(x,\vec{s}_3) \\ U(x,\vec{s}_3) & 0 \end{pmatrix}$$

$$D^\dagger = D$$ D is hermitian

We have introduced a background gauge connection $U(x,\vec{s}_i)$, $i = 1,2,3$ on the 3 links emerging from the B site towards an A site

As before, define continuum two-spinor fields

ψ_α, $\alpha = 1,2$

in the neighbourhood of the Dirac points

$$\psi_1 = (\chi_{B+}, \chi_{A+})^T; \quad \bar{\psi}_1 = (\bar{\chi}_{B+}, \bar{\chi}_{A+})$$

$$\psi_2 = (\chi_{A-}, \chi_{B-})^T; \quad \bar{\psi}_2 = (\bar{\chi}_{A-}, \bar{\chi}_{B-})$$

The same steps lead to a long-wavelength theory describing two independent massless flavors

$$S_0 \simeq \frac{3\ell}{2} \sum_{\vec{p}} \bar{\psi} \begin{pmatrix} i\vec{p}\,.\,\vec{\sigma} & \\ & -i\vec{p}\,.\,\vec{\sigma} \end{pmatrix} \psi$$

Recall staggered fermions in 2d also yield 2x2-component spinors in long-wavelength limit

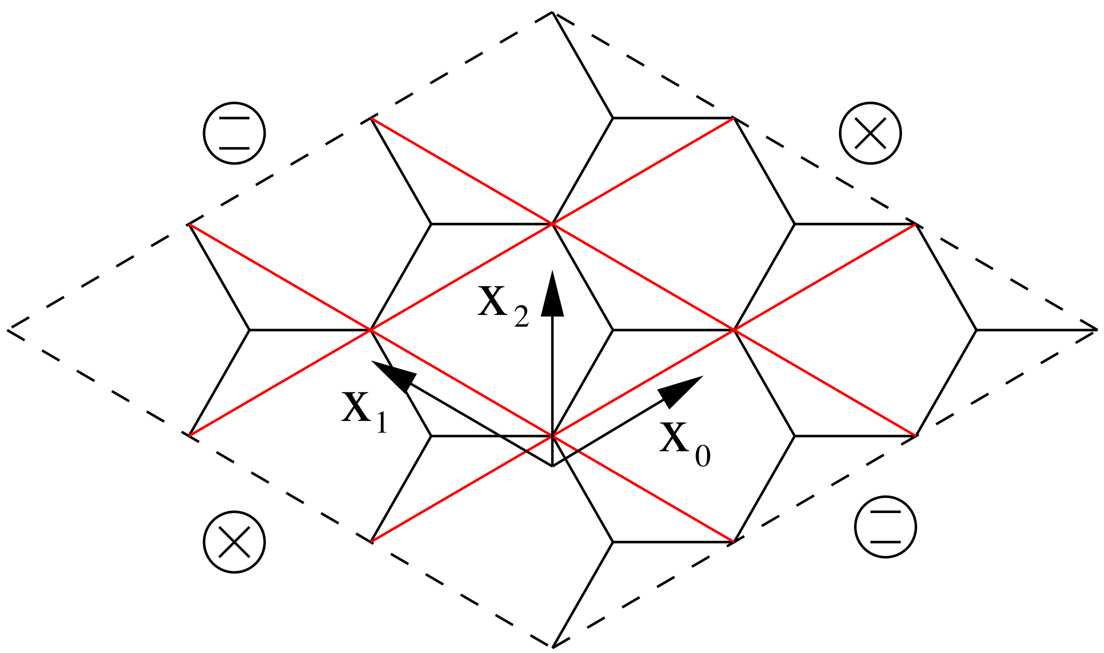
For Euclidean fermions in 2d define **chirality** in terms of a matrix $\gamma_5 \sim i\sigma_1\sigma_2$

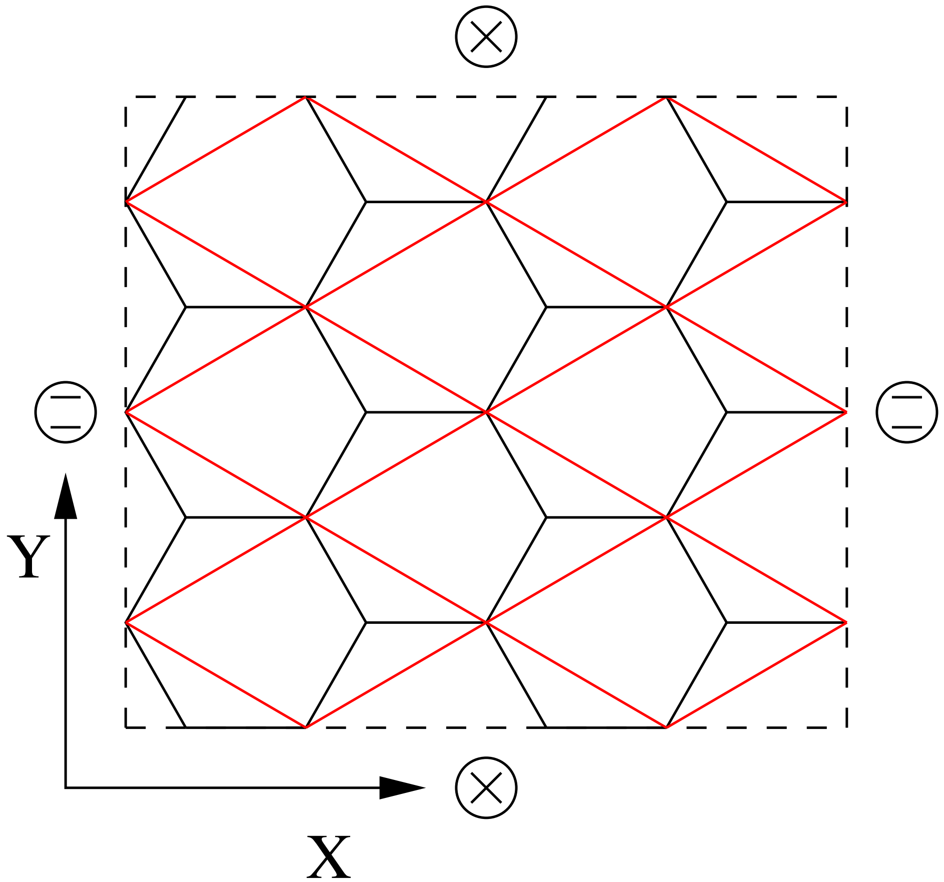
$$\gamma_5 = i \begin{pmatrix} \sigma_1 & \\ & -\sigma_1 \end{pmatrix} \begin{pmatrix} \sigma_2 & \\ & -\sigma_2 \end{pmatrix} = \begin{pmatrix} -\sigma_3 & \\ & -\sigma_3 \end{pmatrix}$$

$$\Rightarrow \; \bar{\psi}\gamma_5\psi = -\bar{\chi}_{B+}\chi_{B+} + \bar{\chi}_{A+}\chi_{A_+} - \bar{\chi}_{A-}\chi_{A-} + \bar{\chi}_{B-}\chi_{B-}$$

in terms of the original lattice fields

In order to define a translationally-invariant finite system suitable for numerical studies, there are two inequivalent compactifications





"primitive"

$$f(x + L_0\hat{0}) = f(x + L_1\hat{1}) = f(x)$$

contains $L_0 L_1$ distinct hexagons

"perpendicular"

contains $L_X L_Y$ distinct hexagons

Index Theorem

For any background abelian gauge configuration we can define a quantised integer-valued topological charge Q

$$Q = \frac{1}{2\pi}\int d^2x F_{12}(x)$$

with $F_{12} = \partial_x A_y - \partial_y A_x$

magnetic flux density

Now consider eigensolutions of the Dirac equation $D[U]\,|\,\psi_i\rangle = E_i\,|\,\psi_i\rangle$

The Atiyah-Singer index theorem asserts that eigenmodes of this equation satisfy

$$Q = \sum_i \langle\psi_i\,|\,\gamma_5\,|\,\psi_i\rangle = n_+ - n_-$$

where $n_\pm$ count positive/negative chirality modes with $E = 0$

The mode chirality $\langle\psi\,|\,\gamma_5\,|\,\psi\rangle \equiv 0$ for any mode with $E \neq 0$ if $\{D, \gamma_5\} = 0$

Lattice fermion formulations in common use don't satisfy this relation in general. Examining the recovery of the index theorem is an important test of non-perturbative properties

eg. J. Smit & J.C. Vink, Nucl. Phys. **B286** (1987) 485

A simple test (following Smit & Vink) uses homogeneous background flux $F_{12} = \omega$

Convenient gauge choice: $A_x(x,y) = -\omega y; \quad A_y(x,y) = 0$

Square lattice:

Demand gauge equivalence of A_x related by y-boundary condition:

$$A_x(y=0) = A_x(y = L_y a) + i\Omega_y \partial_x \Omega_y^{-1} \quad \text{with} \quad \Omega_y(x,y) = e^{i\omega L_y a x}$$

Imposing periodicity in x as well results in quantisation of ω: $\Omega_y(0,y) = \Omega(L_x a, y) \;\Rightarrow\; \omega = \dfrac{2\pi Q}{L_x L_y a^2} = \dfrac{2\pi Q}{\mathscr{A}}$

Honeycomb lattice:

the area of a hexagonal plaquette is $\frac{\sqrt{3}}{2}a^2$, with $a = \sqrt{3}\ell$

Primitive compactification:

$$U(x, \vec{s}_1) = \exp\left(-i\frac{\sqrt{3}}{2}\omega x_0 a^2\right); \quad U(x,\vec{s}_2) = U(x,\vec{s}_3) = 1$$

$$U(x_0 = L_0 - 1, x_1, \vec{s}_3) = \exp\left(-i\frac{\sqrt{3}}{2}\omega L_0 x_1 a^2\right)$$

$$\Rightarrow \quad \omega = \frac{4\pi}{\sqrt{3L_0L_1a^2}}Q$$

The perpendicular case is left as an exercise… 🙂

Analytic continuum result
(single flavor)

$$D|\psi_n\rangle = \sum_{\mu=1}^{2} D_\mu[A]\sigma_\mu|\psi_n\rangle = E_n|\psi_n\rangle$$

$$|\psi_{n\pm}(x,y)\rangle \propto \sum_{l=-\infty}^{\infty} e^{2\pi i \frac{x}{L_x}(j+l|Q|)} e^{-\frac{1}{2}|\omega|(y\pm\frac{L_y}{|Q|}(j+l|Q|))^2} H_n\left(\sqrt{|\omega|}\left(y \pm \frac{L_y}{|Q|}(j+l|Q|)\right)\right)|\phi_\pm\rangle$$

$$j = 0,1,\ldots,|Q|-1 \qquad \phi_+ = \begin{pmatrix}0\\1\end{pmatrix}; \quad \phi_- = \begin{pmatrix}1\\0\end{pmatrix}; \qquad \omega = \frac{2\pi}{\mathscr{A}}Q$$

Spectrum: $E_{n\pm}^2 = (2n+1)|\omega| \mp \omega$ $\quad n=0$ yields zero modes with $\langle\gamma_5\rangle = \mathrm{sgn}\omega$

Re-index: $E_m^2 = 2m|\omega|; \quad m = 0,1,2,\ldots$ $\qquad g_m = \begin{cases} |Q| & m=0 \\ 2|Q| & m>0 \end{cases}$

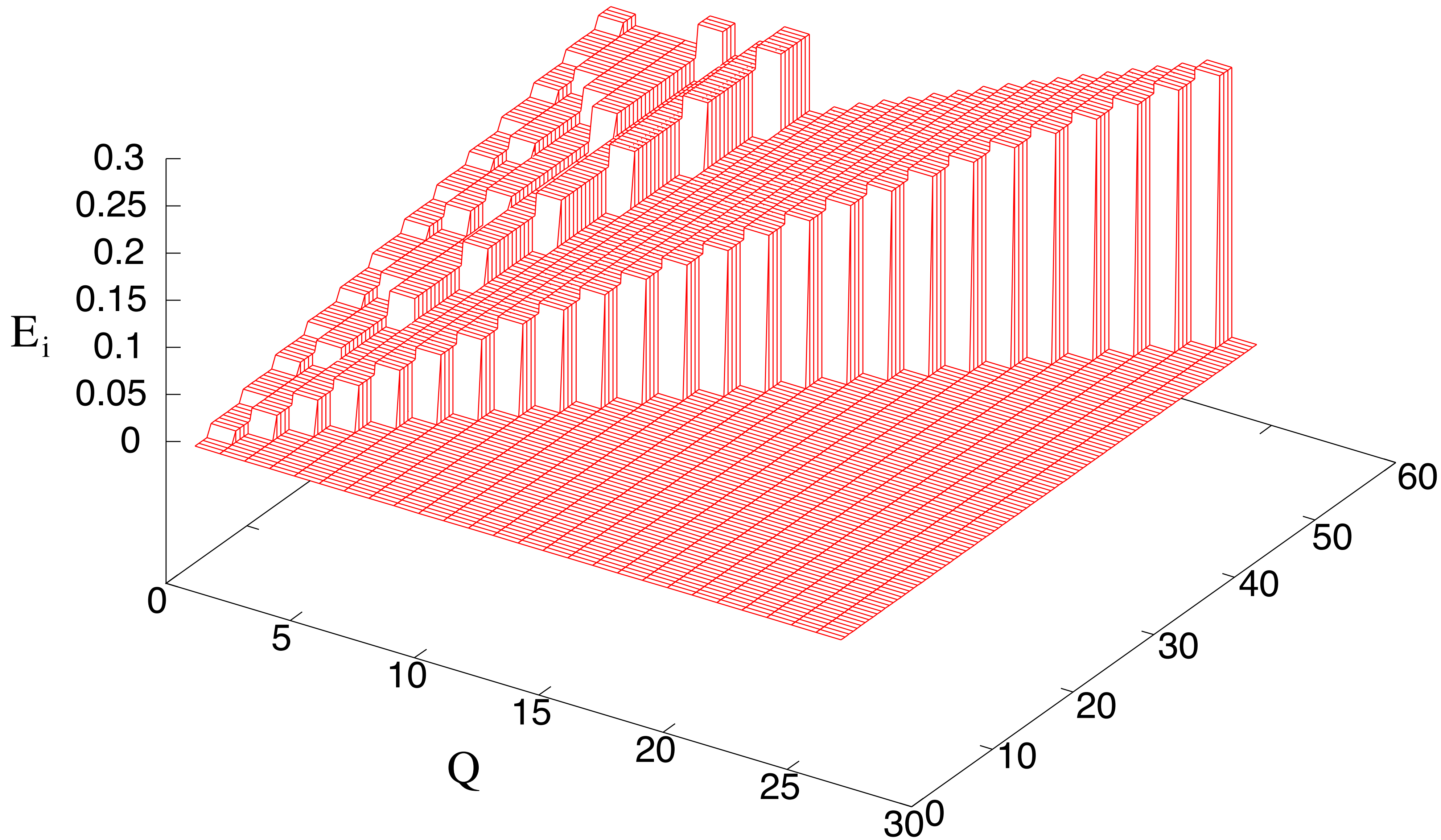
m labels the Landau level

Spectral degeneracy g_m is consistent with the anomalous quantum Hall Effect
- the smoking gun for relativity in graphene

G.W. Semenoff PRL **53** (1984) 2449

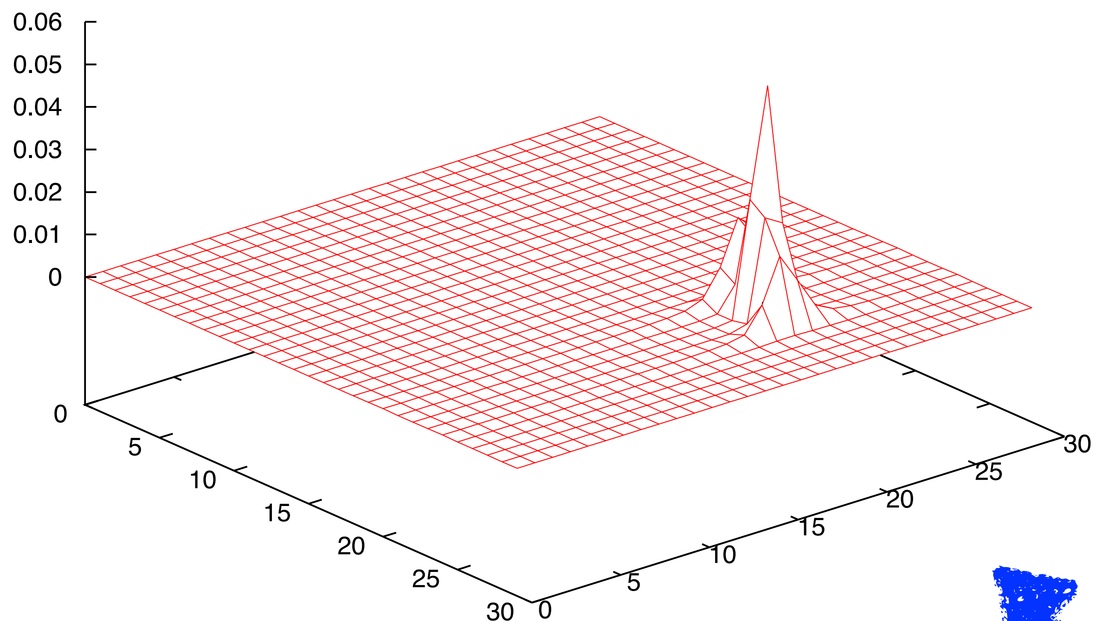
Numerical Solution

E_i^2 on 30×30 primitive lattice, $i = 1,\ldots,60$

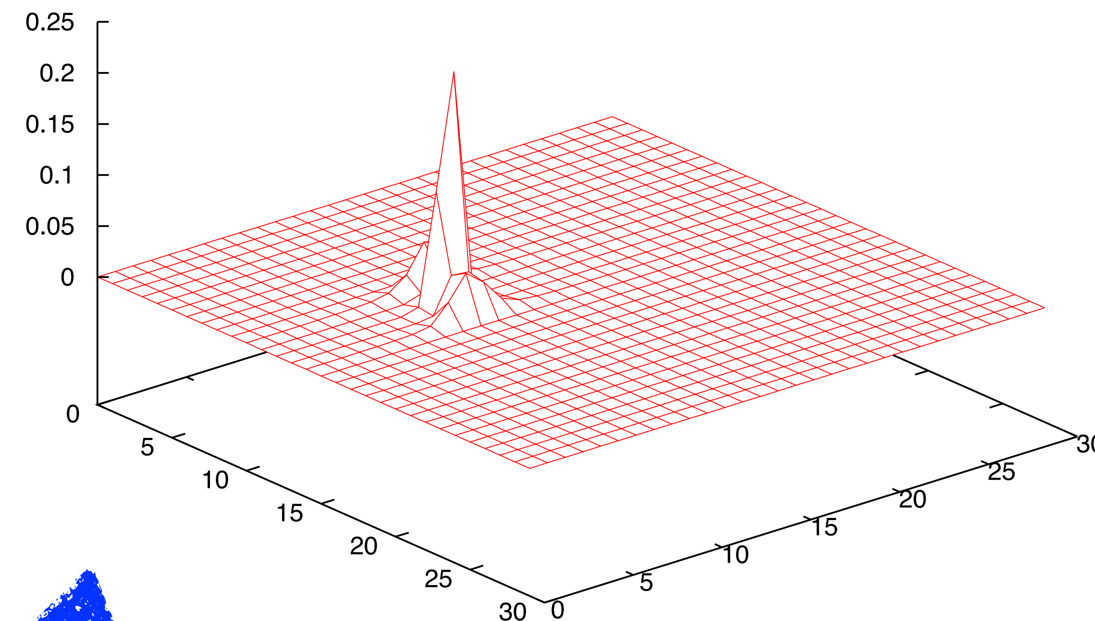


- Recall for 2 flavors degeneracy is $2g_m$
- Zero mode “carpet” has $E_i \simeq 0$ within machine precision
- Perpendicular lattice yields identical spectrum

The low-lying modes are highly-localised around the Dirac points in Fourier space

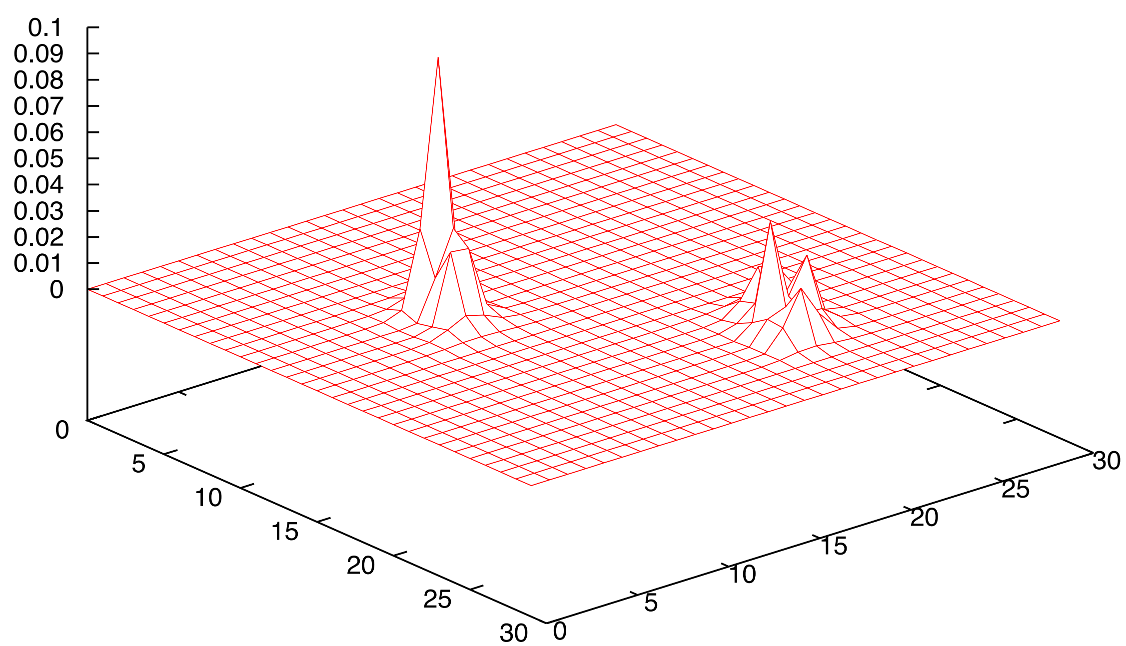


$E = 0$, A sub lattice



$E = 0$, B sub lattice

The zero modes only have support on the $A+$ and $B-$ field components



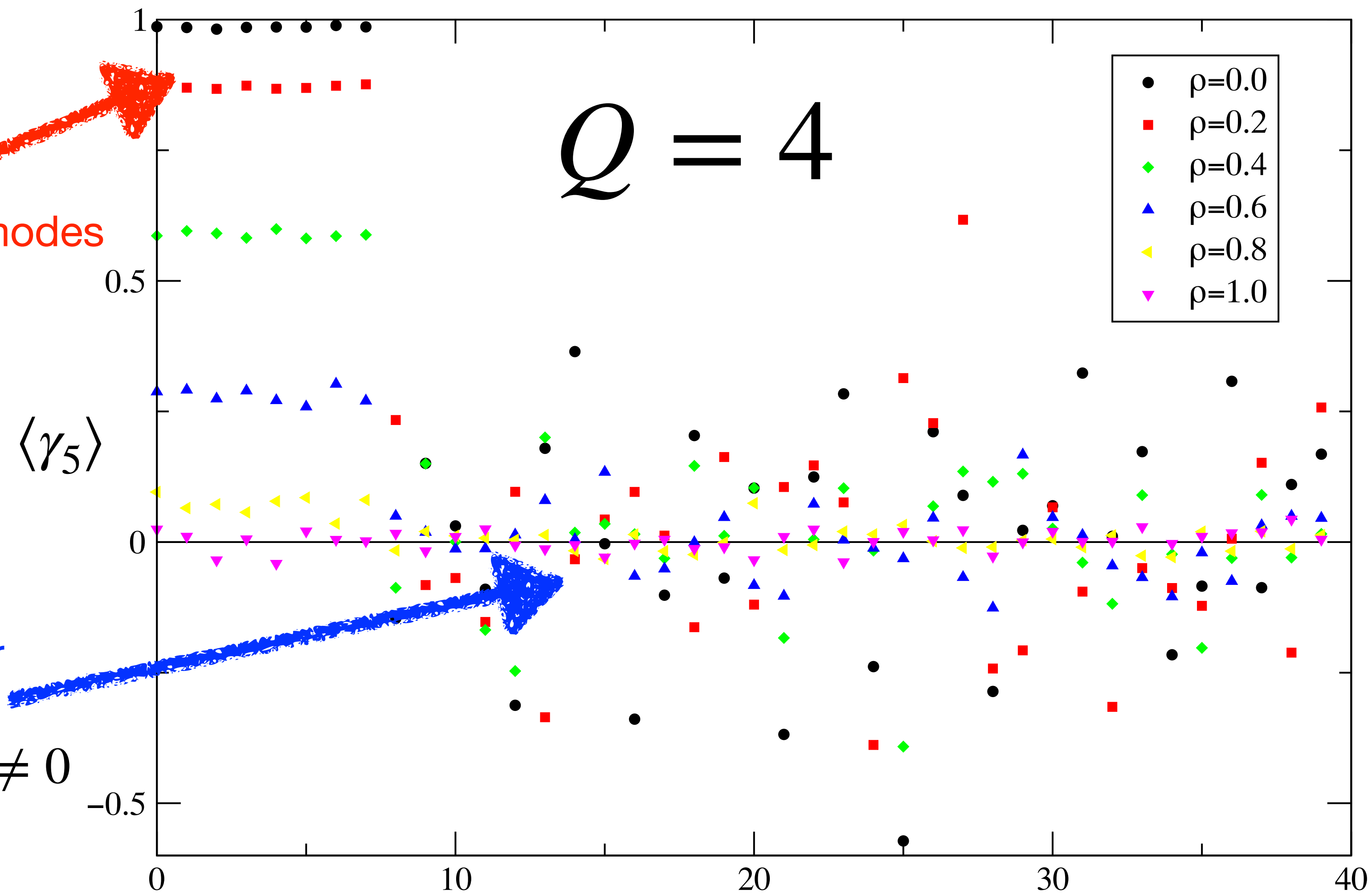
$E \neq 0$, A sub lattice

see Alim & Möller SFU Technical Report 2008-14 for details of the Fourier transform on a honeycomb

Mode Chirality

30×30 lattice, $Q = 4$, $i = 1,\ldots,40$

$2|Q|$ topological zero modes



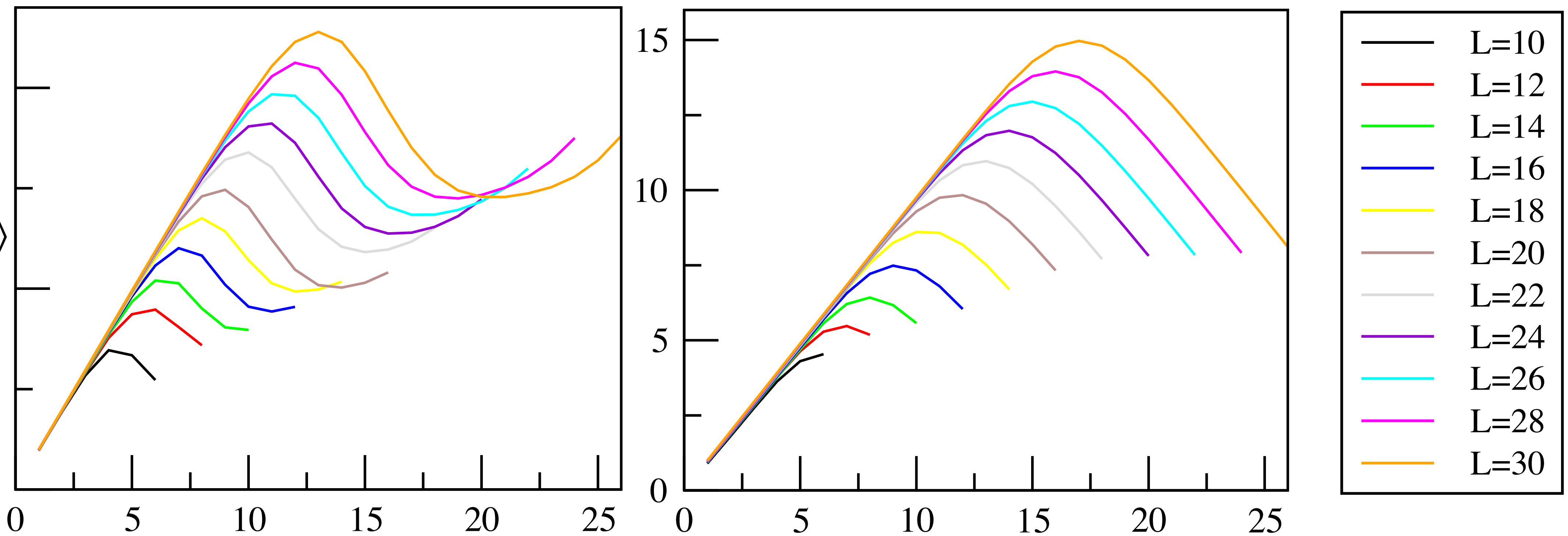
$$\sum_{k=1}^{4|Q|} \langle k | \gamma_5 | k \rangle = 0$$ over degenerate modes with $E \neq 0$

- $\langle \gamma_5 \rangle = -\langle \chi_{B+} | \chi_{B+} \rangle + \langle \chi_{A+} | \chi_{A+} \rangle - \langle \chi_{A-} | \chi_{A-} \rangle + \langle \chi_{B-} | \chi_{B-} \rangle$ is evaluated in Fourier space
- Each Fourier mode $\chi_{A,B}(\vec{k})$ counted as $\pm$ depending on which Dirac point is nearer
- Black points evaluated on smooth gauge background
- Coloured points following $U(\vec{r}, \vec{s}_i) \mapsto \Omega^*(\vec{r}) U(\vec{r}, \vec{s}_i) \Omega(\vec{r} + \vec{s}_i)$ with $\Omega(\vec{r}) = e^{i\rho\hat{\vartheta}(\vec{r})}$
- Random gauge transformation $\hat{\vartheta}(\vec{r})$ leaves spectrum unchanged
- Random gauge transformation degrades chirality signal: chirality is ***not*** gauge-invariant

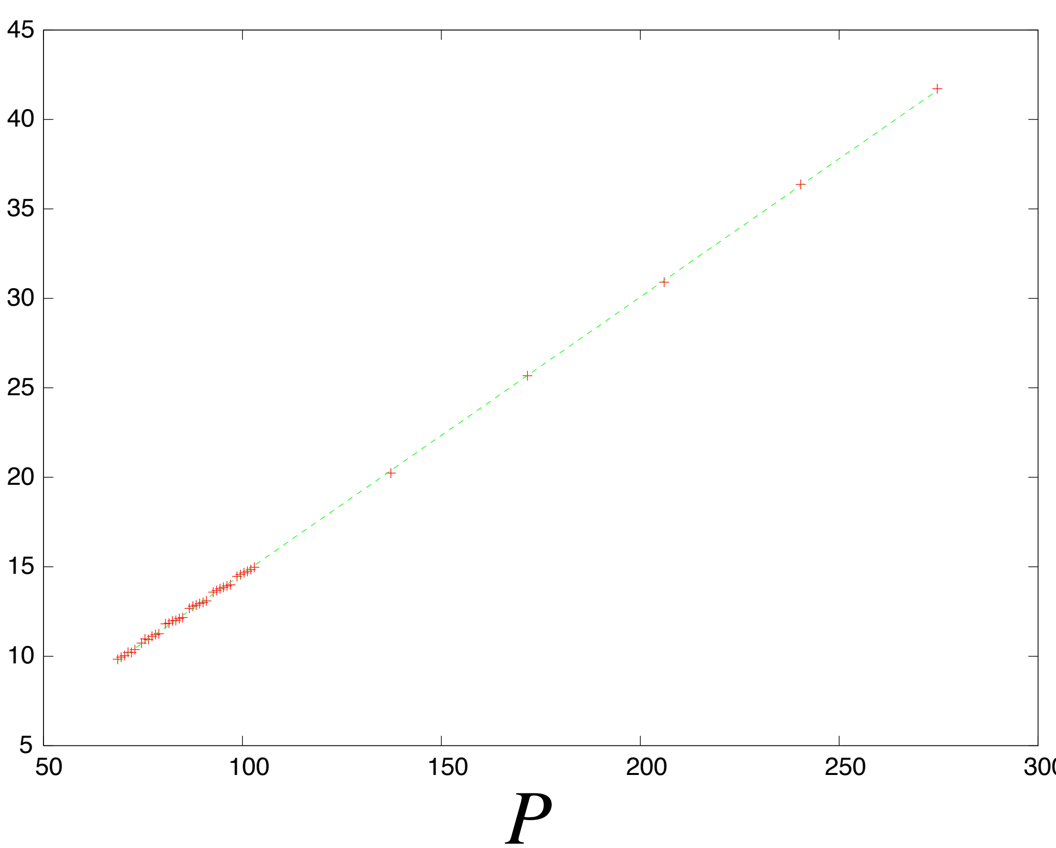
There is a natural upper limit to the topological charge which can be faithfully reproduced by the index theorem, which grows with system size

Primitive **Perpendicular**

$$Q^{\text{index}} = \sum_i \langle i|\gamma_5|i\rangle$$



$$Q^{flux} = \frac{\mathcal{A}\omega}{2\pi}$$



In fact the maximum $Q^{\text{index}}_{\text{max}}$ depends linearly on the perimeter P of the system

eg. for a perpendicular compactification

$$P = 3L_X + \frac{\sqrt{3}}{4} L_Y$$

smooth transition function Ω_y requires $\omega L_y a^2 \ll 2\pi$

$$\Rightarrow \quad Q^{\text{index}}_{\text{max}} \ll \frac{\sqrt{3}}{2} L_x$$

Lessons Learned

Staggered fermions are smarter than you think!

The gauge-invariant interpretation of staggered lattice fields
in terms of explicit spin/flavor components was solved long ago:

either in real space (Kluberg-Stern et al, NP**B220(**1983)447)
here the continuum field $\psi(x)$ is defined within a 2^d hypercube

or momentum space (van den Doel & Smit, NP**B228**(1983)122)
here the continuum field $\psi(k)$ is evenly distributed across all Dirac points

The two recipes coincide in the long-wavelength limit (Daniel & Kieu, PL**B175**(1986)73)
In either case the chirality operator $\bar{\psi}(\gamma_5 \otimes 1)\psi$ has the point-split form $\bar{\chi}(x)\mathcal{U}\chi(x \pm \hat{1} \pm \hat{2})$

whereas here we have assigned each flavor to a distinct Dirac point
The chirality operator $\bar{\psi}(\gamma_5 \otimes 1)\psi$ is a sum of bilinears which is local in momentum space

In hindsight, there's been a missed opportunity to perform a similar analysis for minimally doubled fermions *à la* Creutz-Borici on a square lattice.