Graphene at the Edge

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Quantum Field Theory at the Boundary,
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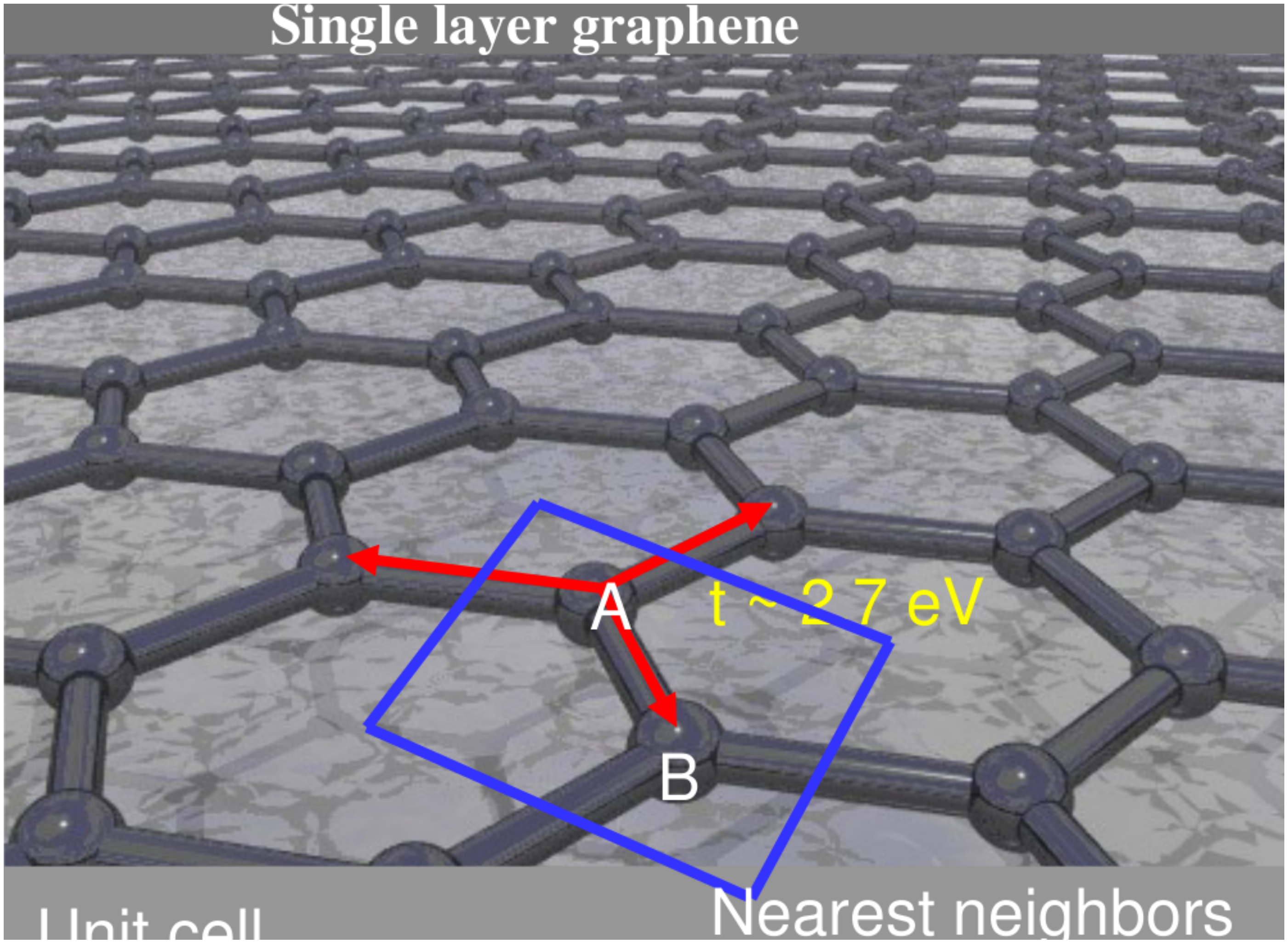
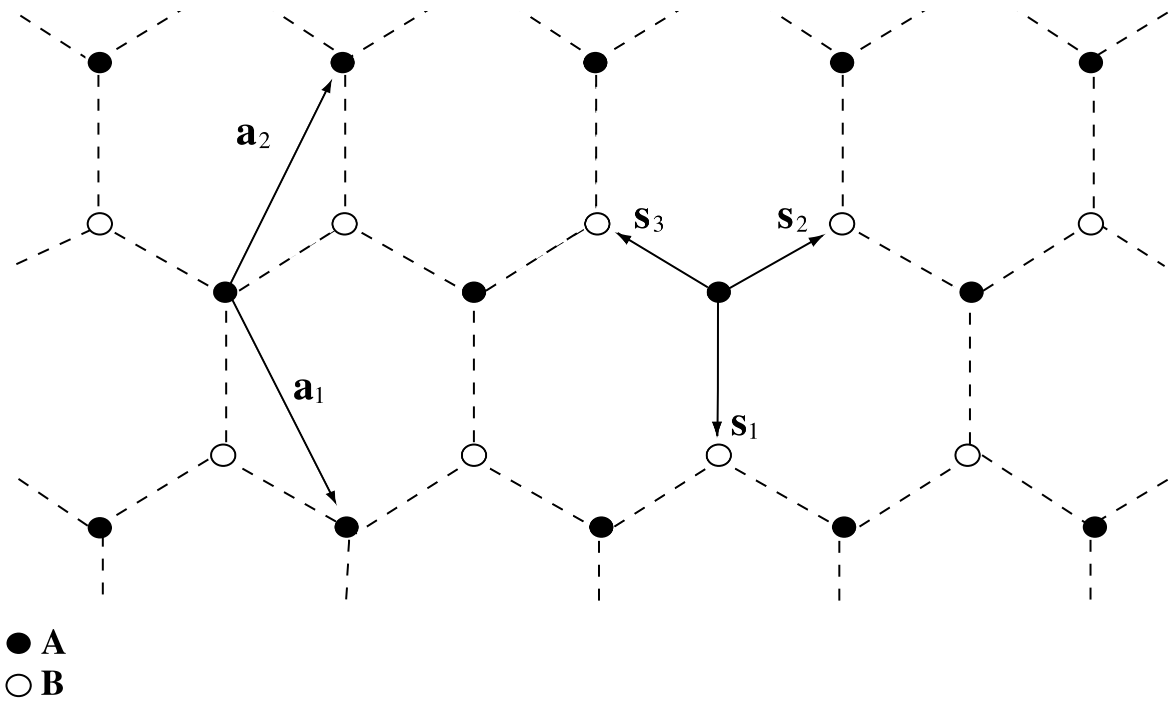
Graphene

A one-atom thick layer of Carbon atoms with a hexagonal lattice



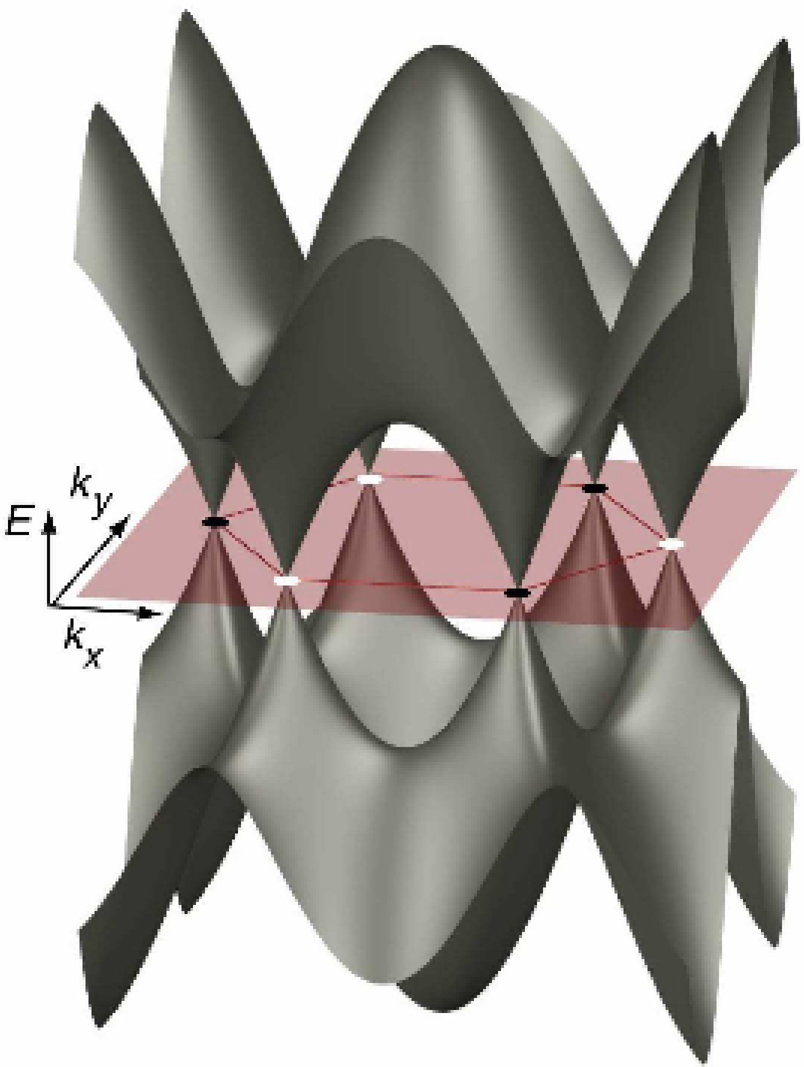
Tight-binding model



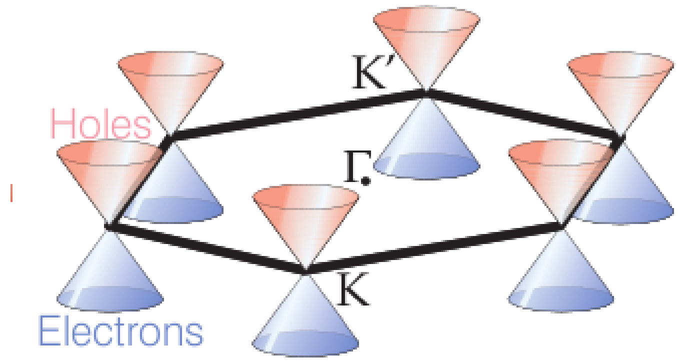
hexagonal lattice = two triangular sub-lattices $\vec{A}$ and $\vec{B}$ connected by vectors $\vec{s}_1, \vec{s}_2, \vec{s}_3$.

$$H = \sum_{\vec{A},i} \left(t\ b^{\dagger}_{\vec{A}+\vec{s}_i}\, a_{\vec{A}} + t^*\ a^{\dagger}_{\vec{A}} b_{\vec{A}+\vec{s}_i} \right)$$

Band structure of graphene



Linearize spectrum near degeneracy points



$$E(k) = \hbar v_F |\vec{k}| \quad v_F \sim c/300,$$

$$\psi(k) \approx \begin{bmatrix} \psi_A^{(1)}(k-K) \\ \psi_B^{(1)}(k-K) \end{bmatrix} \text{ and } \approx \begin{bmatrix} \psi_A^{(2)}(k-K') \\ \psi_B^{(2)}(k-K') \end{bmatrix}$$

$$H_{\text{Dirac}} = \hbar v_F \begin{bmatrix} 0 & k_x - ik_y & 0 & 0 \\ k_x + ik_y & 0 & 0 & \\ 0 & 0 & 0 & k_x + ik_y \\ 0 & 0 & k_x - ik_y & 0 \end{bmatrix}$$

SU(4) symmetry

Notation: interchange valleys $A \leftrightarrow B$ in $\psi^{(2)}$:

$$\psi(k) \approx \begin{bmatrix} \psi_A^{(1)}(k-K) \\ \psi_B^{(1)}(k-K) \end{bmatrix} \quad \text{and} \quad \approx \begin{bmatrix} \psi_B^{(2)}(k-K') \\ \psi_A^{(2)}(k-K') \end{bmatrix}$$

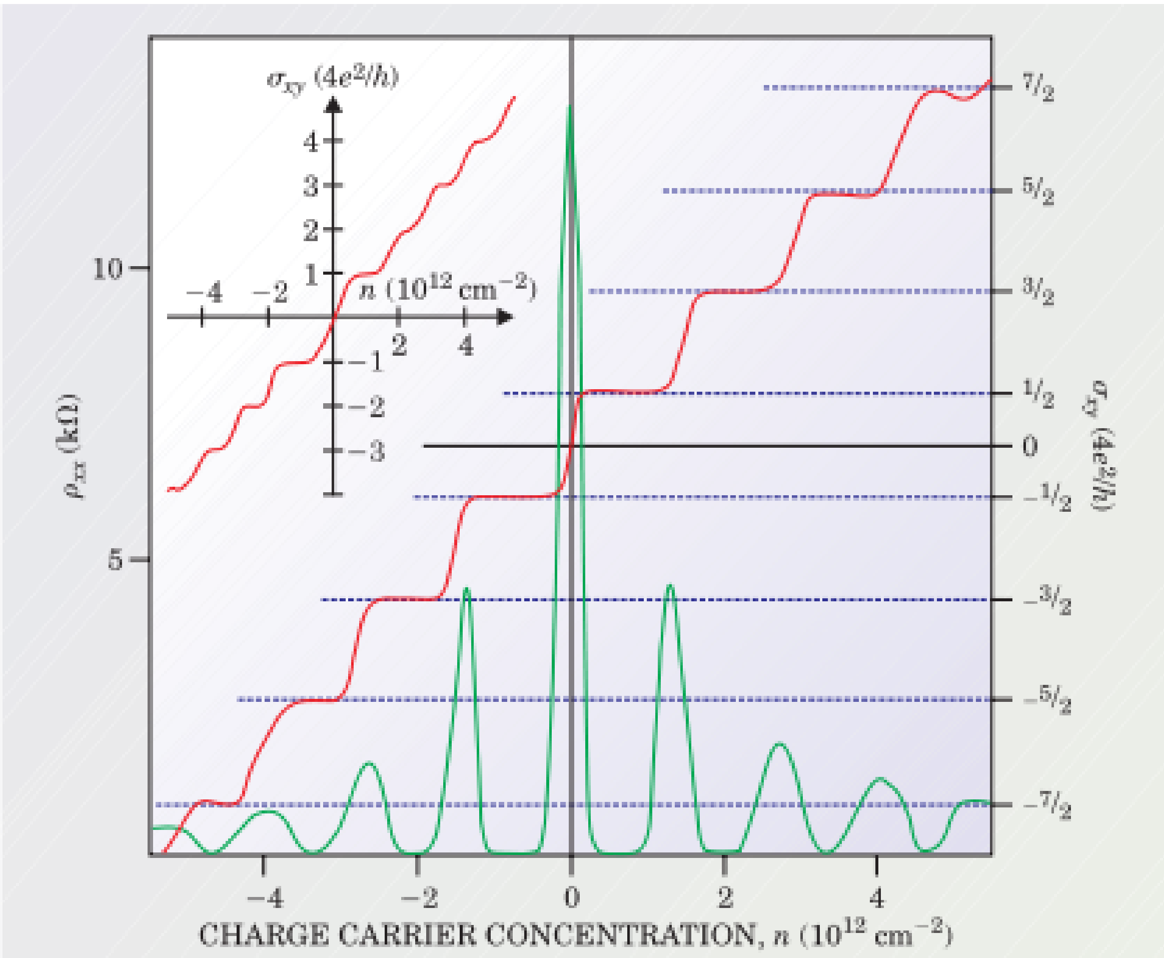
Then, they obey identical Dirac equations

$$H_{\text{Dirac}} = \hbar v_F \begin{bmatrix} 0 & k_x - ik_y \\ k_x + ik_y & 0 \end{bmatrix}$$

two valleys $+$ two spin states $=$ **SU(4) symmetry**

K. Novoselov et. al. *Nature 438, 197 (2005)*

Y. Zhang et. al. *Nature 438, 201 (2005)*



$$\sigma_{xy} = 4\frac{e^2}{h}\left(n + \frac{1}{2}\right)$$

SU(4) symmetry

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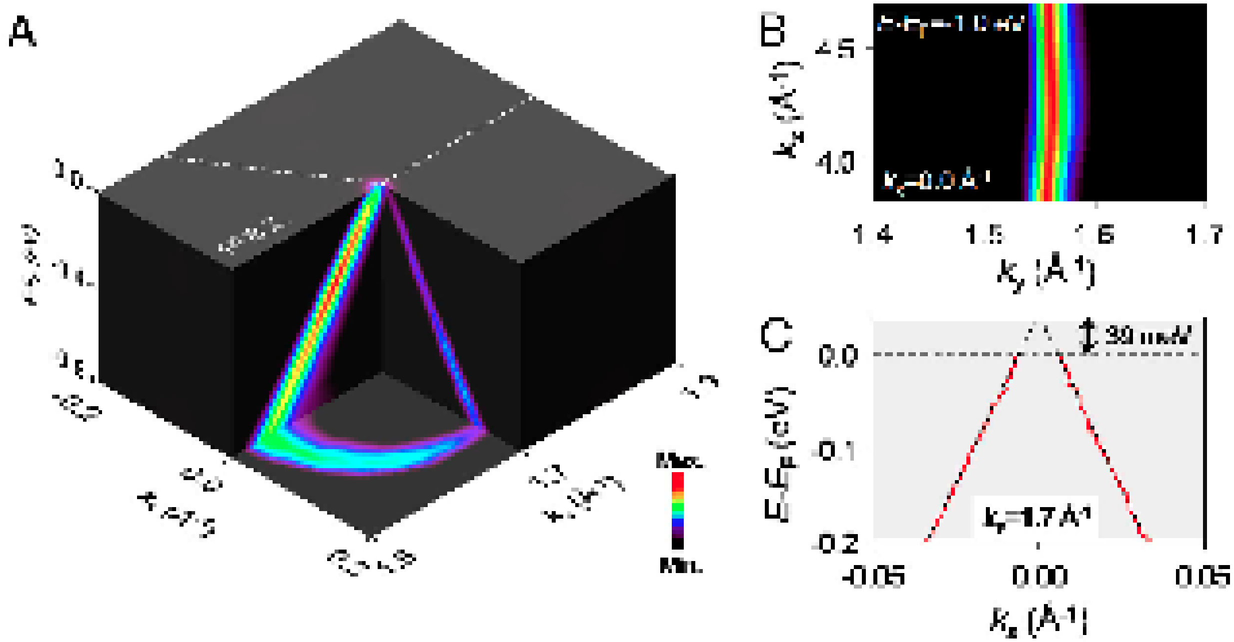
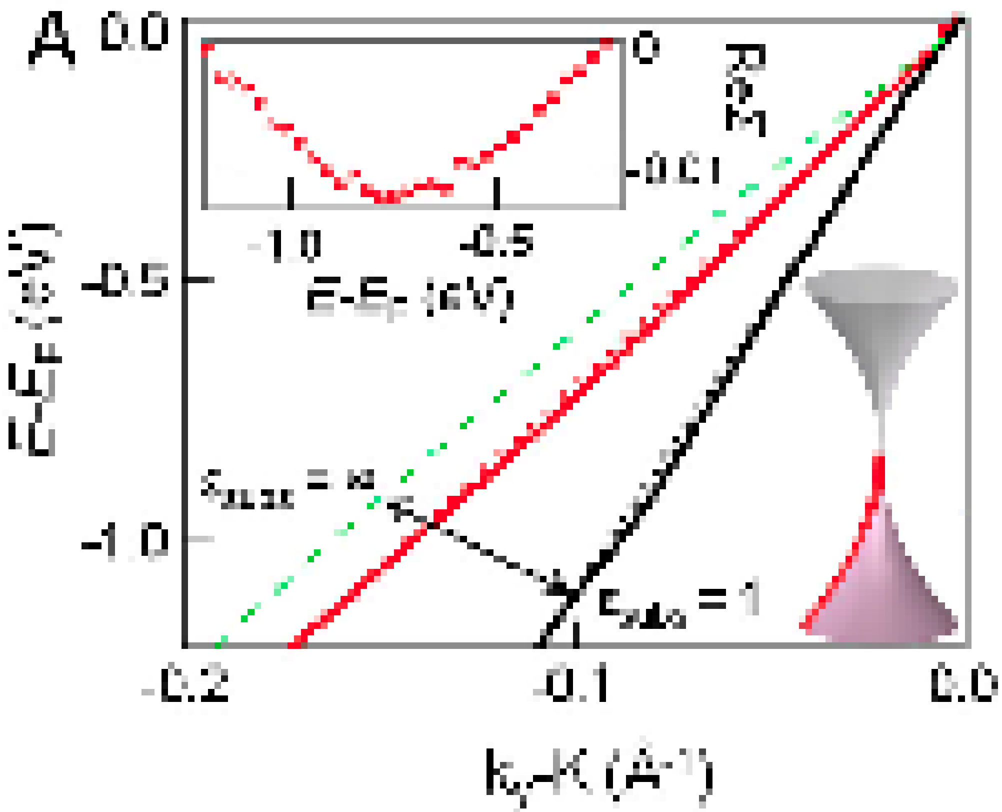
Relativistic QFT $\mathcal{L} = -i\bar{\psi}\gamma^\mu \partial_\mu \psi$

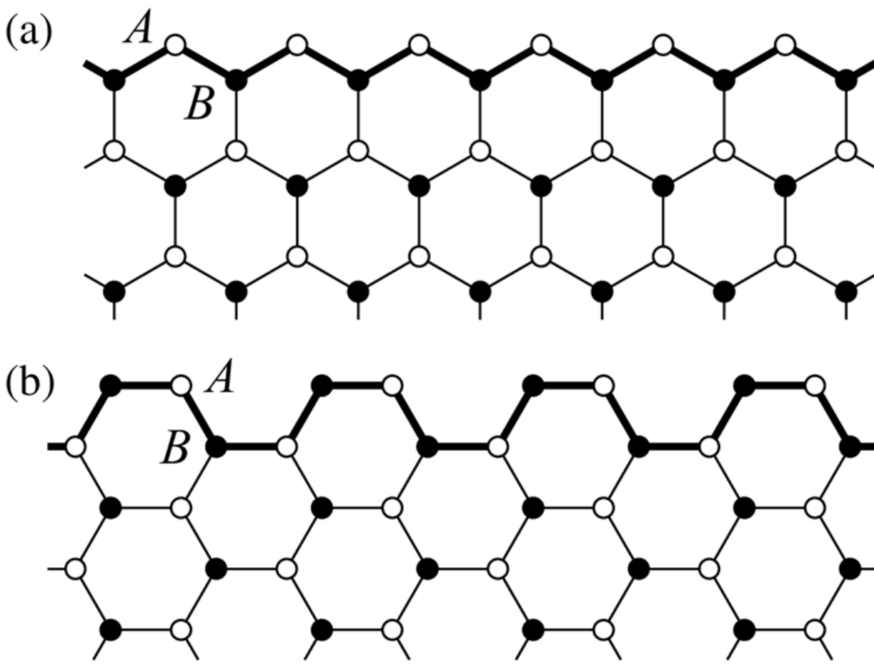
$\psi(x)$ is 2-component spinor of SO(2,1) and 4 rep of SU(4)

SO(3,2) conformal symmetry

interactions are non-relativistic, break scale invariance....but


A
B
C
4.5
4.0
1.4
1.5
1.6
1.7
0.0
-0.1
-0.2
-0.05
0.00
0.05
Max.
Min.


A
0.0
-0.5
-1.0
E-E_F (eV)
-0.2
-0.1
0.0
k_y-K (Å^-1)
0
-0.01
ReΣ
-1.0
-0.5
E-E_F (eV)
ε_subs = 1



ge. The edge is indicated by

Massless Dirac field on a half-space

$x^\mu = (x, y, t)$: $\qquad 0 \leq x < \infty \qquad -\infty < y, t < \infty$

$$\gamma^\mu \partial_\mu \psi(x) = 0$$

Hamiltonian is Hermitian if

$$J^1(0, y, t) \;=\; 0 \quad \rightarrow \quad \bar{\psi}(0, y, t)\gamma^1\psi(0, y, t) = 0$$

$$\{\gamma^\mu, \gamma^\nu\} = 2\eta^{\mu\nu} = 2\mathrm{diag}(-1, 1, 1)$$

guaranteed by the family of linear boundary conditions

$$\lim_{x\to 0} \;\left[1 - \left(i\gamma^0 \cos\varphi + \gamma^1 \sin\varphi\right)\right]\; \psi(x, y, t) \;=\; 0$$

Most interesting for special cases

$\varphi = \frac{\pi}{2} : \left[1 - \gamma^1\right]\; \psi(0, y, t) = 0$ armchair $\rightarrow$ **BCFT** ~~**edge** states~~

$\varphi = 0 : \; \left[1 - i\gamma^0\right] \psi(0, y, t) = 0$ zigzag $\rightarrow$ ~~**BCFT**~~ **edge states**

Conformal transforms which preserve boundary

translations

$$iH\ \psi = \partial_t \psi(t,x,y) \quad , \quad iP_y\ \psi = \partial_y \psi(t,x,y)$$

Lorentz

$$iM_{ty}\ \psi = \left(t\partial_y + y\partial_t + \gamma^1\right)\psi(t,x,y)$$

Scale

$$i\Delta\ \psi = \left(-t\partial_t + x\partial_x + y\partial_y + 1\right)\psi(t,x,y)$$

Conformal

$$iK^t\ \psi = \left[\frac{1}{2}(t^2+x^2+y^2)\partial_t - t(x\partial_x + y\partial_y) + \frac{1}{2}(x\gamma^2 - y\gamma^1)\right]\psi(t,x,y)$$

$$iK^y\ \psi = \left[\frac{1}{2}(t^2-x^2+y^2)\partial_y + y(x\partial_x - t\partial_t) + \frac{1}{2}(t\gamma^1 - x\gamma^0)\right]\psi(t,x,y)$$

Preserve armchair boundary condition $[1-\gamma^1]\psi\big|_{x=0} = 0$

M_{ty}, K^0, K^y not symmetries of zigzag boundary $[1-i\gamma^0]\psi\big|_{x=0} = 0$

Fermionic BCFT

$$\mathcal{L} = -i\bar{\psi}\gamma^\mu\partial_\mu\psi + \text{interactions} \qquad \left[1-\gamma^1\right]\ \psi(0,y,t) = 0$$

$$< \psi(w)\bar{\psi}(w') >= \frac{i}{4\pi}\frac{-\gamma^t(t-t') + \gamma^x(x-x') + \gamma^y(y-y')}{\left[-(t-t')^2 + (x-x')^2 + (y-y')^2 + i\epsilon\right]^{\frac{3}{2}}} - \frac{i}{4\pi}\frac{-\gamma^t(t-t') + \gamma^x(x+x') + \gamma^y(y-y')}{\left[-(t-t')^2 + (x+x')^2 + (y-y')^2 + i\epsilon\right]^{\frac{3}{2}}}\gamma^x$$

Chiral condensate

$$< \bar{\psi}(t,x,y)\psi(t,x,y) >= -\frac{i}{8\pi}\frac{1}{x^2} \qquad < \bar{\psi}(t,x,y)\gamma^\mu\psi(t,x,y) >= 0$$

Zero-field Hall conductivity localized at the edge, $\sigma_{xy} = \frac{e}{4\pi\hbar}\frac{1}{x}$

canceled by fermion doubling in graphene

Zigzag Edge state solutions in graphene

valleys with 2 $[1 - i\gamma^0]\psi\Big|_{x=0} = 0$ and $[1 + i\gamma^0]\psi\Big|_{x=0} = 0$

Edge states also found in the tight binding lattice model:

M. Fujita, K. Wakabayashi, K. Nakada, and K. Kusakabe, Journal of the Physical Society of Japan 65, 1920 (1996).

This early work also conjectured that the edges are spin Ferromagnetic. This was based on mean field theory and density functional arguments. A proof that they are Ferromagnetic for the weakly coupled repulsive Hubbard model and a weak Coulomb interaction was given in

Z.Shi, I.Affleck, Phys. Rev. B 95, 195420 (2017).

S. Biswas and G.W.S. work in progress.

Zigzag Edge state solutions of the Dirac equation

$[1 - i\gamma^0]\psi\big|_{x=0} = 0$ or $[1 + i\gamma^0]\psi\big|_{x=0} = 0$ in the basis where the Dirac equation is

$$\begin{bmatrix} -i\partial_t & -i\partial_x - \partial_y \\ -i\partial_x + \partial_y & -i\partial_t \end{bmatrix} \begin{bmatrix} u(t,x,y) \\ v(t,x,y) \end{bmatrix} = 0$$

with $v(t,0,y) = 0$ which has the edge state solutions

$$\psi(t,x,y) = \sqrt{\frac{|k|}{\pi}} \begin{bmatrix} e^{k(x+iy)} \\ 0 \end{bmatrix} \qquad -\infty < k < 0$$

or with $u(t,0,y) = 0$ which has the edge state solutions

$$\psi(t,x,y) = \sqrt{\frac{|k|}{\pi}} \begin{bmatrix} 0 \\ e^{-k(x-iy)} \end{bmatrix} \qquad 0 < k < \infty$$

C, P, T Anomaly

$[1 - i\gamma^0]\psi\big|_{x=0} = 0 \quad \to \text{C, P, T} \to \quad [1 + i\gamma^0]\psi\big|_{x=0} = 0$

(some) restoration of these symmetries by doubling fermions

$$\psi_0^{(1)}(t,x,y) = \sqrt{\frac{|k|}{\pi}} \begin{bmatrix} e^{k(x+iy)} \\ 0 \end{bmatrix} \qquad -\infty < k < 0$$

$$\psi_0^{(2)}(t,x,y) = \sqrt{\frac{|k|}{\pi}} \begin{bmatrix} 0 \\ e^{-k(x-iy)} \end{bmatrix} \qquad 0 < k < \infty$$

- Charge neutral ground state has $\frac{1}{2}$ of zero modes filled
- P and $P_y = 0$ ground state would have equal numbers of $\psi_0^{(1)}(t,x,y)$ and $\psi_0^{(2)}(t,x,y)$ filled.
- Δ invariant ground state has sets of zero modes either completely filled or completely empty

Doubled Fermions with spin (à la Graphene)

$$\psi^{(1)}_{0\uparrow}(t,x,y) = \sqrt{\frac{|k|}{\pi}}\begin{bmatrix} e^{k(x+iy)} \\ 0 \end{bmatrix} \;,\; \psi^{(1)}_{0\downarrow}(t,x,y) = \sqrt{\frac{|k|}{\pi}}\begin{bmatrix} e^{k(x+iy)} \\ 0 \end{bmatrix}$$

$$\psi^{(2)}_{0\uparrow}(t,x,y) = \sqrt{\frac{|k|}{\pi}}\begin{bmatrix} 0 \\ e^{-k(x-iy)} \end{bmatrix} \;.\; \psi^{(2)}_{0\downarrow}(t,x,y) = \sqrt{\frac{|k|}{\pi}}\begin{bmatrix} 0 \\ e^{-k(x-iy)} \end{bmatrix}$$

C,P,T,Δ invariant states

$$\text{Ferromagnetic}: \qquad \left| \begin{matrix} \text{filled} & \text{empty} \\ \text{filled} & \text{empty} \end{matrix} \right\rangle$$

$$\text{anti} - \text{Ferromagnetic}: \qquad \left| \begin{matrix} \text{filled} & \text{empty} \\ \text{empty} & \text{filled} \end{matrix} \right\rangle$$

Degenerate Perturbation Theory

Find eigenvalues and eigenvectors of

$$< \text{degenerate state}| \ H_I \ |\text{degenerate state}' >$$

$$H_I = \int d^2x d^2x' \frac{1}{2} \psi_s^{(A)\dagger}(x)\psi_s^{(A)}(x)V(\vec{x},\vec{x}')\psi_{s'}^{(A')\dagger}(x')\psi_{s'}^{(A')}(x')$$

$$\text{or} \quad -\int d^2x \frac{1}{2}[\bar{\psi}(x)\psi(x)]^2 \text{or} \ -\int d^2x \frac{1}{2}\bar{\psi}(x)\gamma^\mu\psi(x)\bar{\psi}(x)\gamma_\mu\psi(x)$$

C,P,T,Δ invariant states

$$\text{Ferromagnetic :} \qquad H_I \left| \begin{matrix} \text{filled} & \text{empty} \\ \text{filled} & \text{empty} \end{matrix} \right\rangle = 0$$

$$\text{anti} - \text{Ferromagnetic :} \qquad H_I \left| \begin{matrix} \text{filled} & \text{empty} \\ \text{empty} & \text{filled} \end{matrix} \right\rangle = 0$$

Conclusions

- We have studied some aspects of the Dirac field in 2+1-dimensions on a 1/2-space.
- Boundary conditions violate discrete symmetries which can be restored by doubling (as occurs in graphene).
- Zigzag boundary conditions have edge states. Repulsive interactions lead to spin Ferromagnetism of electrons populating the edges.
- It would be interesting to understand the stability of the Ferromagnetic state, i.e. the nature of spin waves.