Magnetism on the Edges of Graphene Ribbons

Hamed Karimi and Ian Affleck

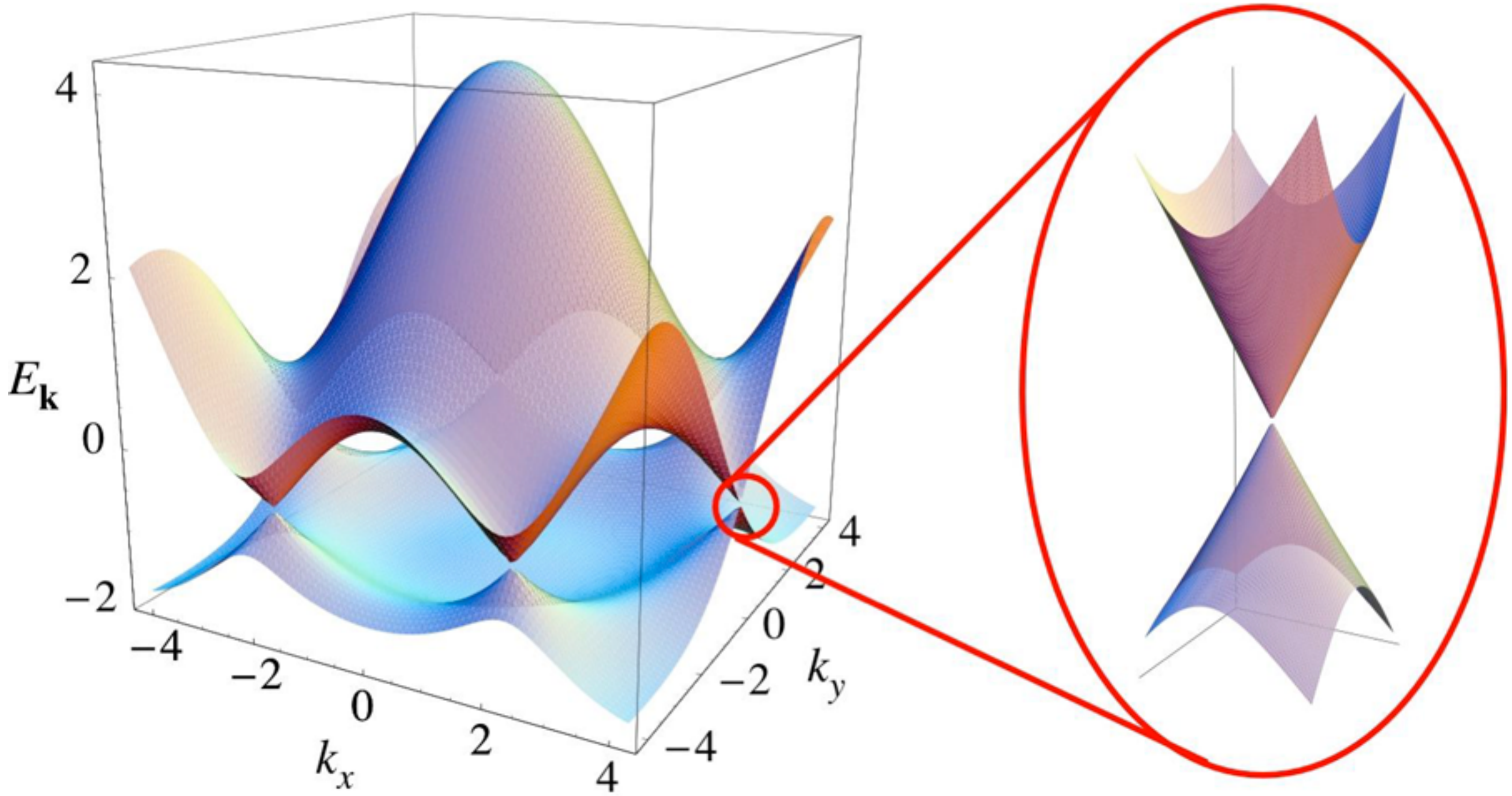
Numerical and Analytic Methods for Strongly Correlated Systems

Outline

- Introduction, edge modes
- Is graphene a strongly correlated material?
- Rigorous proof of ferromagnetism in 1D model
- Excitons
- More realistic models
- (Edge-bulk interactions)
- Conclusions
- Open Questions

Introduction

- Graphene is a single layer of carbon atoms
- Half-filled π-orbitals give simple honeycomb lattice tight-binding band structure



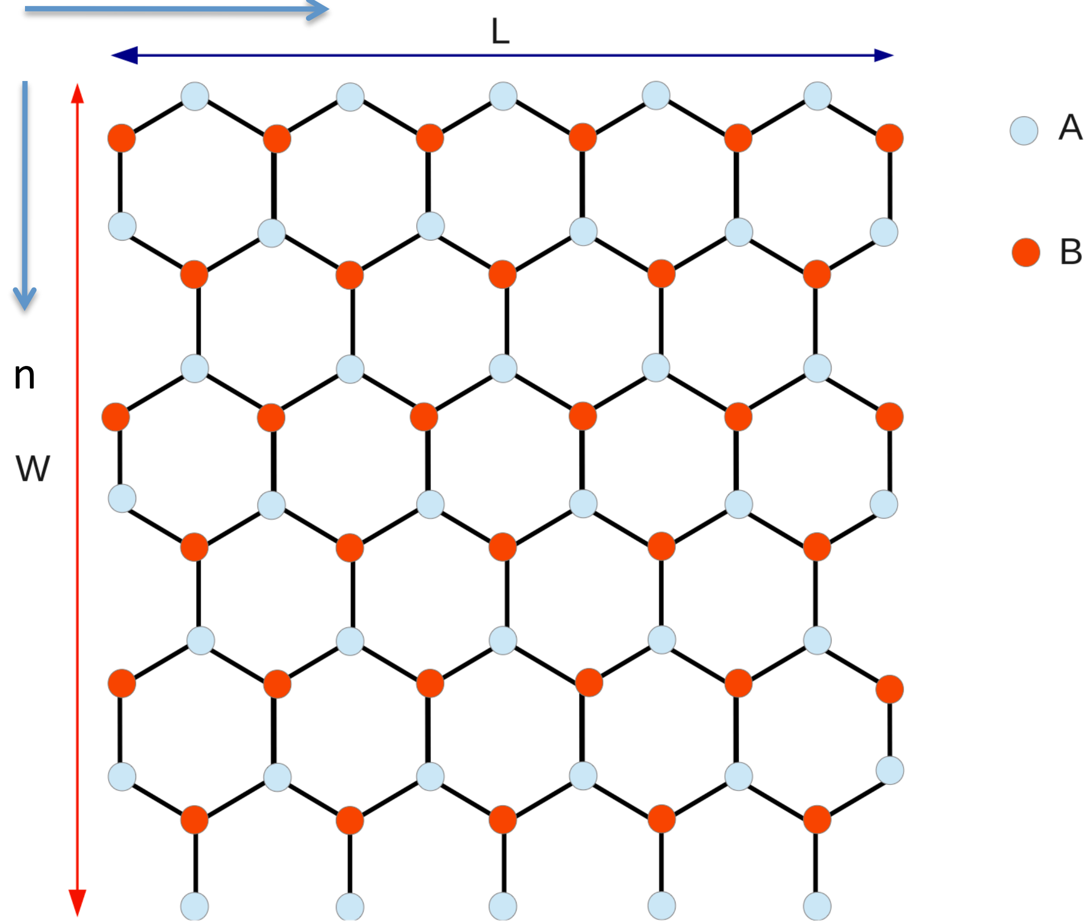
2 inequivalent Dirac points in Brillouin zone, where

$$E(\vec{k}) \approx \pm v_F \left| \vec{k} - \vec{K}_i \right| \qquad \text{(i=1,2)}$$

Simple types of edges of ribbons:

zigzag

armchair



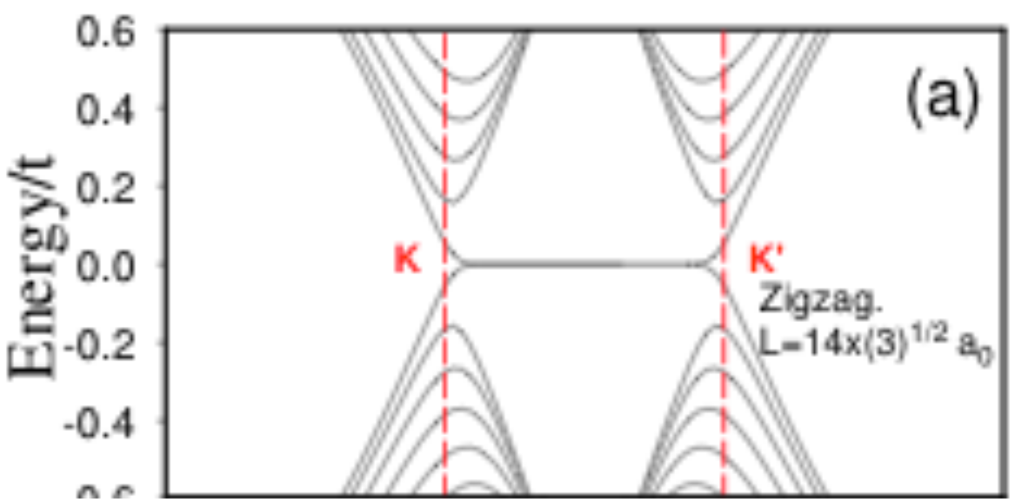
bearded

For non-interacting semi-infinite system with zigzag edge there are exact zero energy states localized near edge:

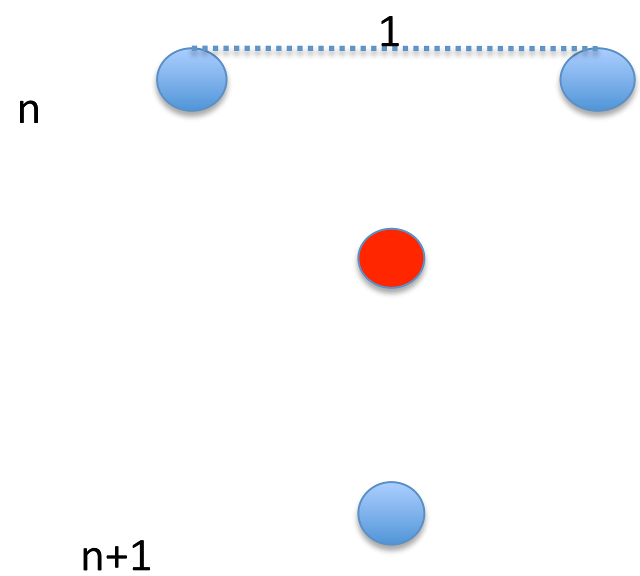
$$\phi(m,n) \prec \exp(ik_x m)[-2\cos(k_x/2)]^{-n}$$

n=0,1,2,… for |k|>2π/3.

N.B. k=±2π/3 are Dirac points



Proof: Wave-function only non-zero on A-sites



$$\left(e^{ik/2} + e^{-ik/2}\right)\phi(n) + \phi(n+1) = 0$$

Including Interactions

•weak Hubbard interactions have little effect, *with no boundaries* even at half-filling, since 4-Fermi interactions are irrelevant in (2+1) dimensional Dirac theory (ψ has d=1)
•Dirac liquid phase stable up to U_c~4t
•But they have a large effect on flat edge bands which have effectively infinite interaction strength
•Mean field theory and numerical methods indicate ferromagnetic ordering on each edge
•Antiferromagnetic order between edges in ZZ case at half-filling

Actually, screening of long range Coulomb interaction is poor in graphene, especially with chemical potential at Dirac points. Should treat actual Coulomb interaction. This is marginal. Dimensionless coupling constant:

$$\alpha_{eff} = \frac{e^2}{\hbar v_F \varepsilon} \approx 1$$

since $c/v_F \approx 1$.

Projected 1D Hamiltonian

$$H = \frac{U}{2}\sum_{k,k',q}\Gamma(k,k',q)[c^{+}_{k+q,\sigma}c_{k,\sigma} - \delta_{q,0}][c^{+}_{k'-q,\sigma'}c_{k',\sigma'} - \delta_{q,0}]$$

$$\Gamma(k,k',q) \equiv \sum_{n=0}^{\infty} g_n(k)g_n(k')g_n(k+q)g_n(k'-q)$$

Schmidt & Loss (repeated spin indices summed)
Here $g_n(k)$ is the wave-function of the edge state of momentum k at distance n from the edge:

$$g_n(k) = \theta(\pi/3 - |k-\pi|)[2\cos(k/2)]^n\sqrt{1-(2\cos(k/2)^2}$$

Due to restricted range of k this geometric series decays exponentially

- We can simply prove exact ground state of H_{1D} is fully polarized ferromagnet
- This follows because we can write it as a sum of non-negative terms:

$$H = \frac{1}{2}\sum_{n,q} O_n^+(q) O_n(q), \quad [O_n^+(q) = O_{-n}(q)]$$

$$O_n(q) \equiv \sum_{k,\sigma} g_n(k) g_n(k+q)[c_{k+q,\sigma}^+ c_{k,\sigma} - \delta_{q,0}]$$

- The fully polarized state is annihilated by all $O_n(q)$ operators
- Can prove this is unique ground state (up to spin rotation)

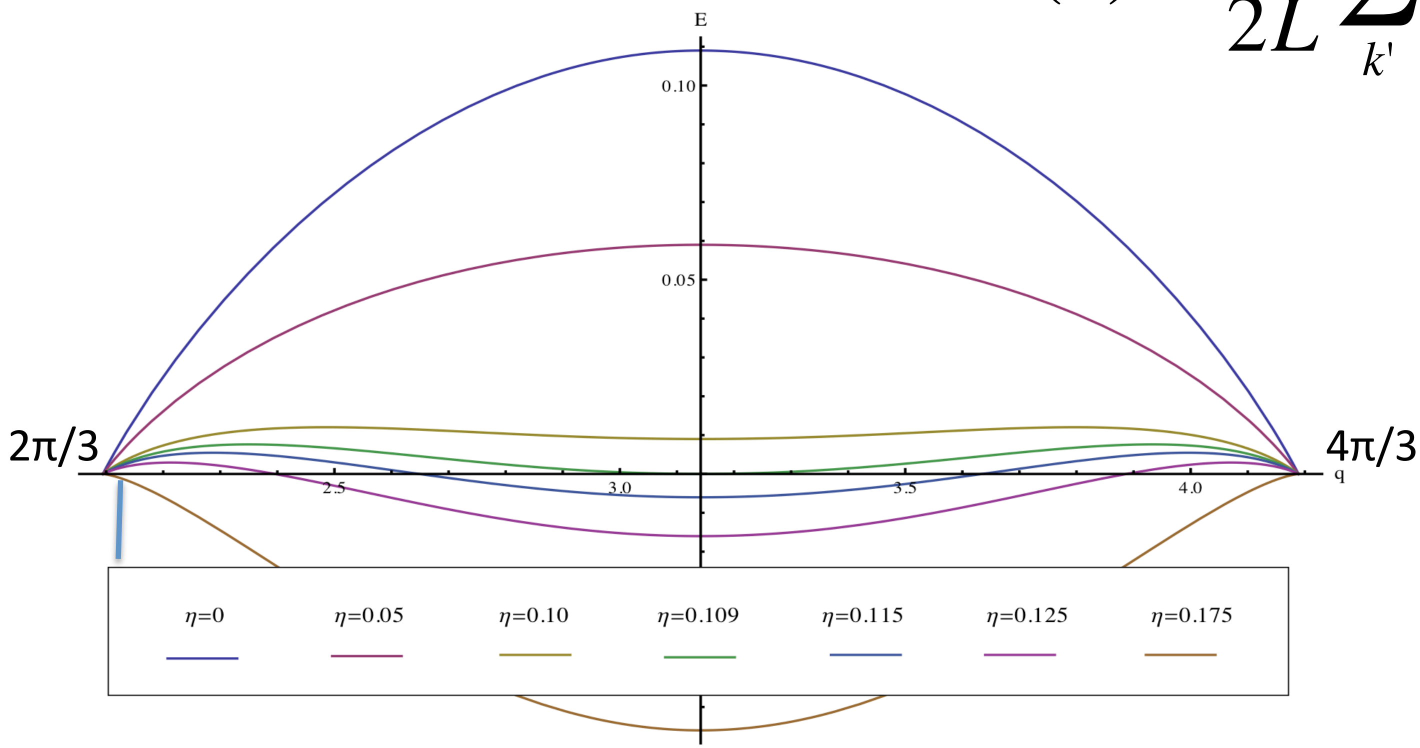
Uniqueness of ground state follows from observing that $O_n(q)|\psi>=0$ for all n implies

$$[c^{+}_{k+q,\sigma}c_{k,\sigma} + c^{+}_{-k,\sigma}c_{-k-q,\sigma} - 2\delta_{q,0}]\,|\Psi>=0,\ \forall k$$

We can then prove ferromagnetic states are only ones to satisfy these conditions for all k,q

- N.B.-unusual particle-hole symmetry: $c_k \leftrightarrow c_k^+$
- Interaction energy and dispersion are both O(U)
- Energy to add ($\downarrow$) or remove ($\uparrow$) particle relative to fully polarized spin $\uparrow$ state:

$$E(k) = \frac{U}{2L}\sum_{k'}\Gamma(k,k',0)$$

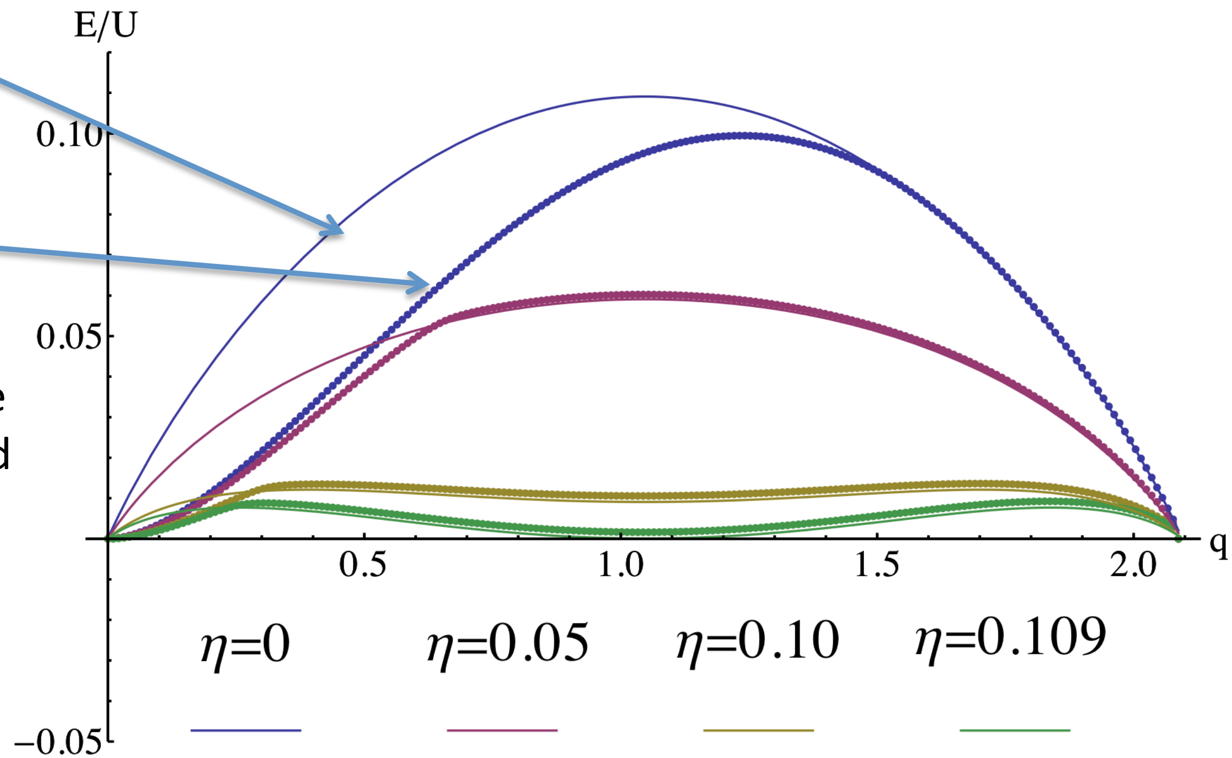


Since it is only a 2-body problem, it is feasible to study ΔM=-1 exciton numerically despite complicated interactions (L<602)

Bottom of 2 particle continuum

Bound exciton

Near q=2π/3 we see free particle hole pair at band edges



•Graphene has 2nd neighbour hopping:t_2/t ~.1 ?
•We might expect a potential acting near edge, V_e
•For U, t_2, V_e<<t, modification to edge Hamiltonian is:

$$\delta(H - \varepsilon_F N) = \frac{\Delta}{L}\sum_{k,\alpha}(2\cos k + 1)e^{+}_{k\alpha}e_{k\alpha} \; , \;\; \Delta = t_2 - V_e$$

•Here we assume ε_F is held at energy of Dirac points, $\varepsilon_F = 3t_2$
•This breaks particle-hole symmetry

For $\Delta>0$, energy to add a spin down electron is decreased near $k=\pi$ or for $\Delta>0$, energy to remove a spin up electron Is decreased near $k=\pi$

•Increasing Δ causes the exciton to become unbound (except close to q=0)

•For $|\Delta|>\Delta_c$~.109 U the edge starts to become doped at k near π (while ε_F is maintained at energy of Dirac points)

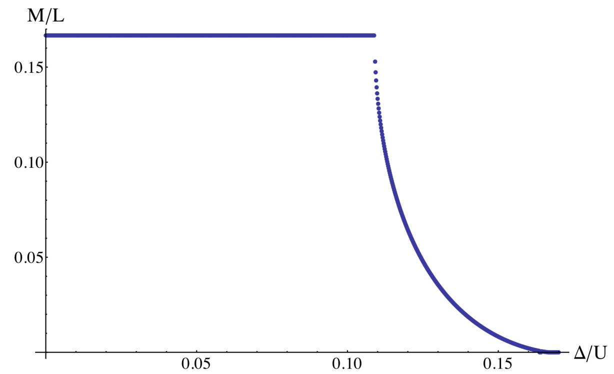
•Since exciton is unbound it is plausible that we get a non-interacting state with no spin down electrons for Δ<0 or filled band of spin up electrons, Δ>0

- We confirmed this by looking at ΔM=-2 states near $\Delta=\Delta_c$ numerically ($L \leq 74$)

– no bi-exiton bound states

- State with no spin down electrons (or no spin up holes) is non-interacting for our projected on-site Hubbard model since particle of same spin don’t interact with each other

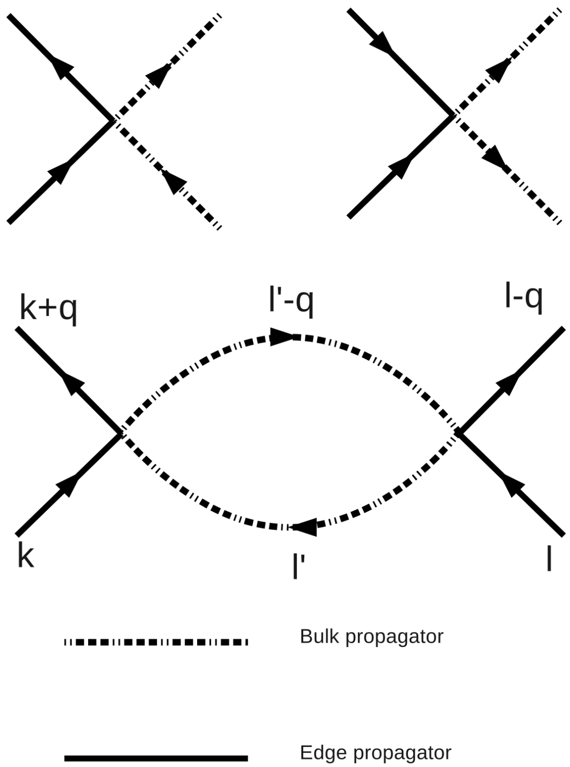
•Gives simple magnetization curve



2nd neighbor extended Hubbard interactions (must couple A to A sites) would turn this into a (one or two component) Luttinger liquid state

Effect of Edge-Bulk Interactions

- Decay of edge states into bulk states is forbidden by energy-momentum conservation
- But integrating out bulk electrons induces interactions between edge modes



We may calculate induced Interactions for small 1/W, q and ω using Dirac propagators with correct boundary conditions

•Most important interactions involve spin operators of edge states $\mathbf{S}_{U/L}(q,\omega)$ on upper and lower edges – like RKKY

•At energy scales $<<v_F/W$, inter-edge interactions is simply

$$H_{\text{inter}} = J_{\text{inter}} \vec{S}_U \cdot \overline{S}_L \ , \quad J_{\text{inter}} = \pm .2 \frac{U^2}{tW^2}$$

•Ferromagnetic for zigzag-bearded ribbon or antiferromagnetic for zigzag-zigzag case

•Consistent with S=(1/2)L or 0 for zigzag-bearded or zigzag-zigzag ribbon, respectively (Lieb's Theorem)

Lieb's Theorem:
Spin of ground state is $|N_A - N_B|/2$ for U>0 Hubbard model at half-filling with hopping between A and B sites only.

Ribbon with zigzag-bearded edges has $N_A - N_B = L$.

Ribbon with zigzag-zigzag edges has $N_A - N_B = 0$.

•Intra-edge interaction induced by exchanging bulk electrons is long range and retarded but this effect is reduced for Dirac liquid compared to Fermi liquid

•Example: exciton dispersion gets a correction:

$$E(q) \approx .36Uq^2 - \sqrt{3}(4-\pi)(U^2/t)q^2 \ln q^2$$

•O(U^2) term *increases* energy of a spin flip, thus further stabilizing ferromagnetic state

•To investigate effects of edge-bulk interactions more systematically, I hope to develop a Renormalization Group method

•A type of boundary critical phenomenon in (2+1) dimensions:

•Gapless (2+1) D Dirac fermions interacting with spin polarized semi-metallic edge states

Like a Kondo or Anderson model in one higher Dimension:Kondo: 0D impurity, interacting with 1D Dirac fermions

Graphene: “impurity” is now 1D edge, interacting with 2D Dirac fermions

Conclusions

•Small U/t limit is a tractable starting point for studying graphene edge magnetism

•Rigorous result on 1D edge Hamiltonian indicate full polarization in simplest model

•t_2 and edge potential lead to edge doping but ground state may remain free for Hubbard model

•Edge-bulk interactions stabilize inter-edge magnetic ground state and introduce long range retarded interactions

(H. Karimi and I.A., Phys Rev B, 2012)

Open Questions

-can higher orders in U/t be controlled?

(Can we develop a renormalization group approach?)

-does ferromagnetism survive with:

- -long range Coulomb interactions
- -bulk doping away from Dirac points
- -chiral (rather than zigzag) edges

[M. Schmidt, M, Golor, T. Lang, S. Wessel, PRB 87, 245431 (2013)]

- -disorder?

-will ferromagnetism be seen experimentally?

-will it be useful for spintronics?