Magnetism on the Edges of Graphene Ribbons

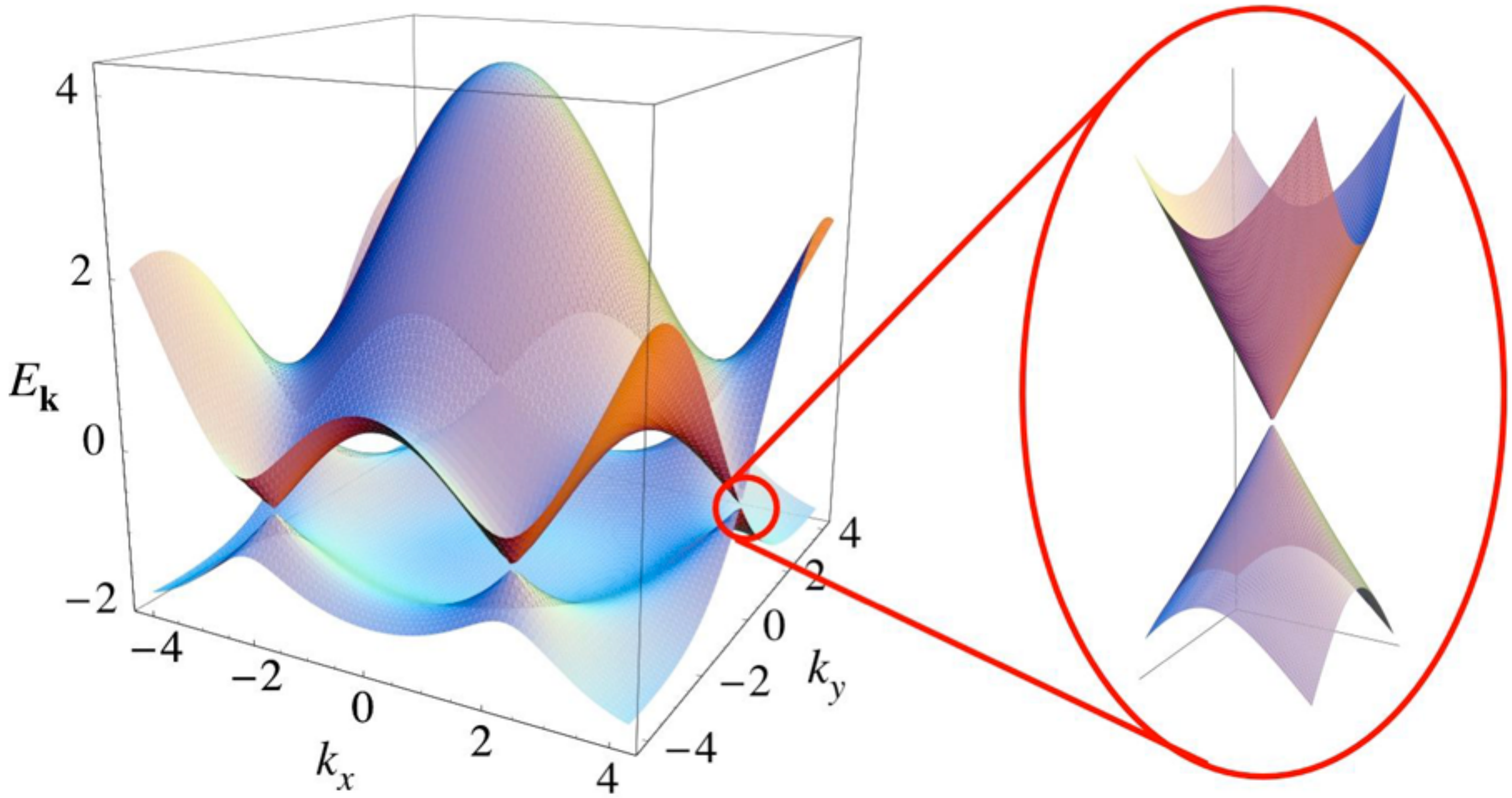
Hamed Karimi and Ian Affleck

Outline

- Introduction
- Edge modes, 1D model
- Lieb's theorem
- Rigorous bound in 1D model
- Excitons
- More realistic models
- Edge-bulk interactions

Introduction

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



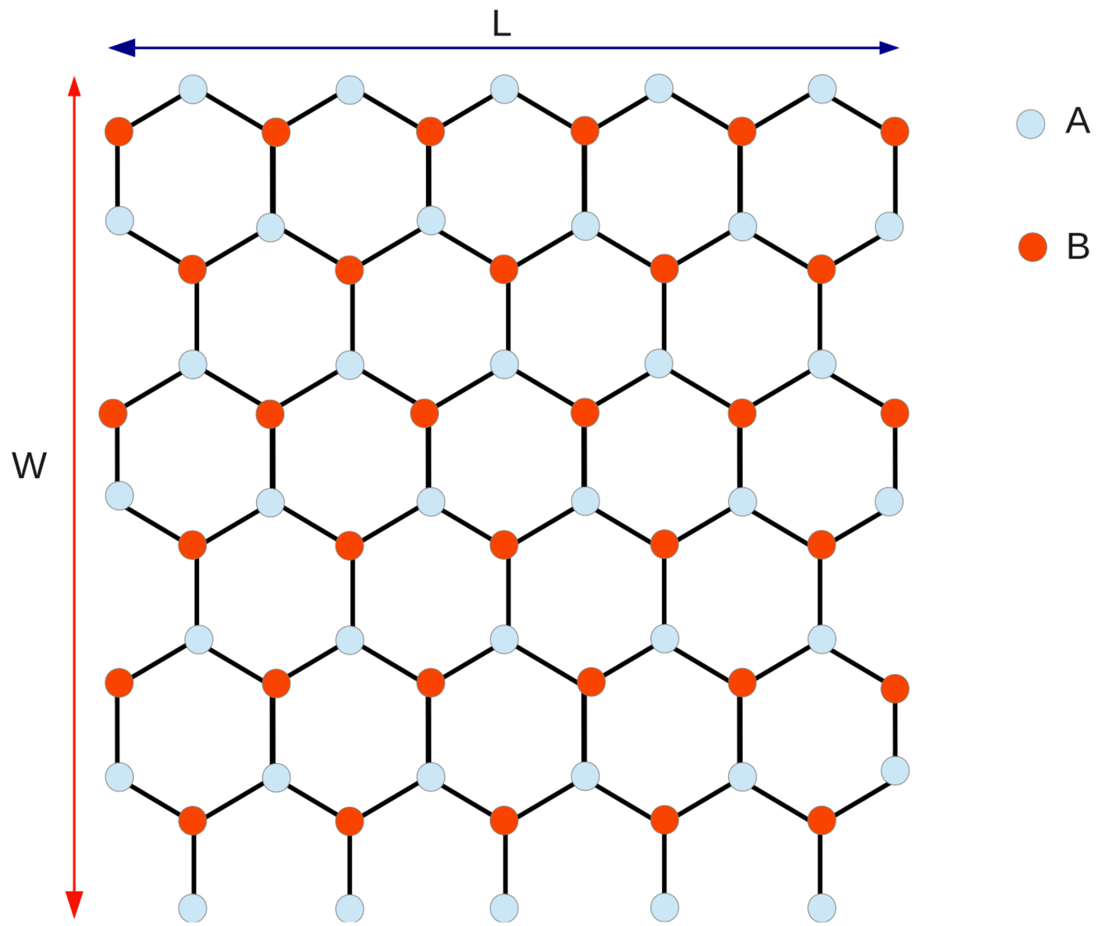
2 inequivalent Dirac points in Brillouin zone, where

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

Simple types of edges of ribbons:

zigzag

armchair



bearded

For zigzag-bearded (ZB) case, with convenient notation, there are exact zero energy states existing only on A-sites with:

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

•Localized near bearded edge (n=0) for $|k_x|<2\pi/3$ and near zigzag edge (n=W) for $|k_x|>2\pi/3$

•N.B. $k_x=\pm 2\pi/3$ are the Dirac points

•For zigzag-zigzag (ZZ) case there are 2 bands with $|k_x|>2\pi/3$ and $|E|\sim\exp[-W]$, which are $\pm$ combinations of upper & lower edge states

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

•Dirac liquid phase stable up to U_c~t

•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

Lieb's Theorem

1988: $U>0$ Hubbard model on bipartite connected lattice at half-filling has unique ground state total spin multiplet with $S=(1/2)|N_A-N_B|$ where N_A, N_B are numbers of sites on A and B sub-lattice

-ZB case: $S=(1/2)L$, ZZ $S=0$

-for $U<<t$ we expect negligible perturbation of unpolarized Dirac liquid ground state

- so in ZB case, spin must come from edge states
- there are L edge states so they must be fully polarized
- for W>>1 upper and lower edges very weakly interact so ~L/3 electrons on (upper) zigzag edge must have spin ~(1/2)L/3 and ~2L/3 electons on (lower) zigzag edge must have spin ~(1/2)2L/3 (fully polarized!)
- Must be ferromagnetic coupling between upper and lower edge (as shown below)
- For ZZ case, spin~ (1/2)L/3 on both edges but must be antiferromagetic inter-edge coupling (as shown below)

Projected 1D Hamiltonian

$$\mathcal{H}_e = \frac{U}{L}\sum_{k,k',q}\Gamma(k,k',q)e_\uparrow^\dagger(k+q)e_\uparrow(k)e_\downarrow^\dagger(k'-q)e_\downarrow(k') - \frac{U}{2L}\sum_{k,k',\alpha}\Gamma(k,k',0)e_\alpha^\dagger(k)e_\alpha(k).$$

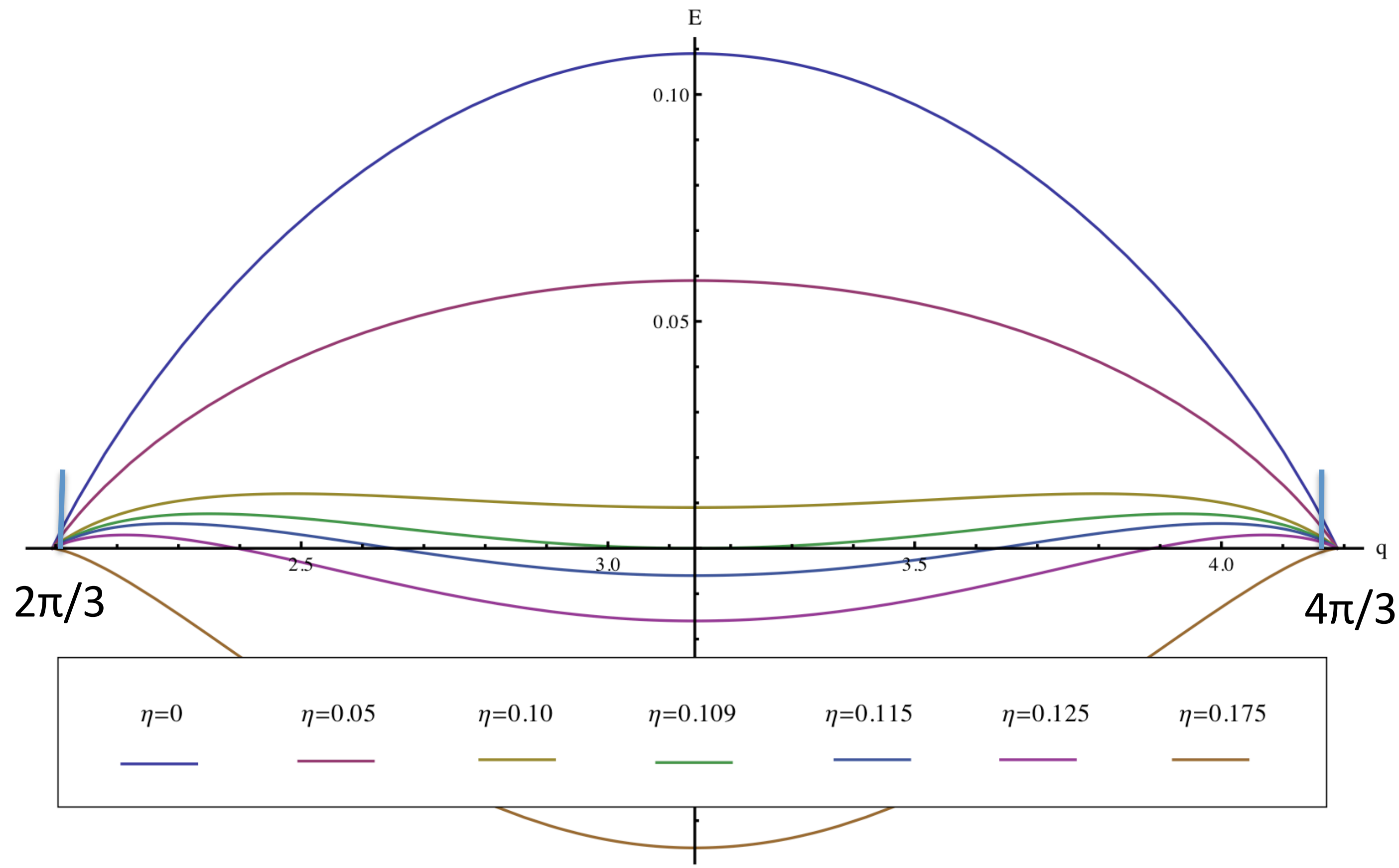
$$\Gamma(k,k',q) = \frac{\left\{\left[1-\left(2\cos\frac{k}{2}\right)^2\right]\left[1-\left(2\cos\frac{k+q}{2}\right)^2\right]\left[1-\left(2\cos\frac{k'}{2}\right)^2\right]\left[1-\left(2\cos\frac{k'-q}{2}\right)^2\right]\right\}^{1/2}}{1-16\cos\frac{k}{2}\cos\frac{k+q}{2}\cos\frac{k'-q}{2}\cos\frac{k'}{2}}.$$

- NB- both terms are O(U)
- Has unusual type of particle-hole symmetry:

$e_k \rightarrow e_k^+$ (same value of k)

Fully polarized state [M~(1/2)L/3] is clearly (at least) a local minimum since energy to add a spin down particle or remove a spin up particle >0

Energy to add (🡇) or remove (🡅) particle



•What if we remove a spin up particle and add a spin down particle- creating a $\Delta M=-1$ exciton?

•This is just a 2-body problem but involves complicated function $\Gamma(k,k',q)$.

Using symmetry: $\Gamma(l,k+q,k-l)=\Gamma(k,-l,q)$, to find 2-body eigenstates of total momentum q we just need to diagonalize LxL matrix

$$M_{kl}^{(q)} = \frac{U}{2L}\left[-2\Gamma(k,-l,q) + \delta_{kl}\sum_{k'}[\Gamma(k,k',0) + \Gamma(k+q,k',0]\right]$$

We can prove $M^{(q)}$ is positive for all q $\neq 0, \underline{+}2\pi/3$:
This follows from $M_{kl} \leq 0$, $k \neq l$, if we can prove

$$M_{ii} > -\sum_{j \neq i} M_{ij}, \quad \forall i$$

$$\sum_{i,j} v_i M_{ij} v_j = \sum_i v_i^2 M_{ii} + \sum_{i \neq j} v_i M_{ij} v_j > -(1/2) \sum_{i \neq j} v_i^2 + v_j^2 - 2 v_i v_j) M_{ij} > 0$$

We can prove $M^{(q)}$ is positive for all q $\neq 0, \pm 2\pi/3$:

This follows from $M_{kl} \leq 0$, $k \neq l$, if we can prove

$$M_{ii} > -\sum_{j \neq i} M_{ij}, \quad \forall i$$

Or equivalently: $$\sum_{k'} \Gamma(l+q,k',0) + \Gamma(l,k',0) - 2\Gamma(l,k',q)] > 0$$

This can be proven using the form for Γ:

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

$$g_n(k) = \sqrt{1-[2\cos(k/2)]^2}\,[2\cos(k/2)]^n$$

Only zero energy states are $S^-|F\rangle$, part of spin multiplet

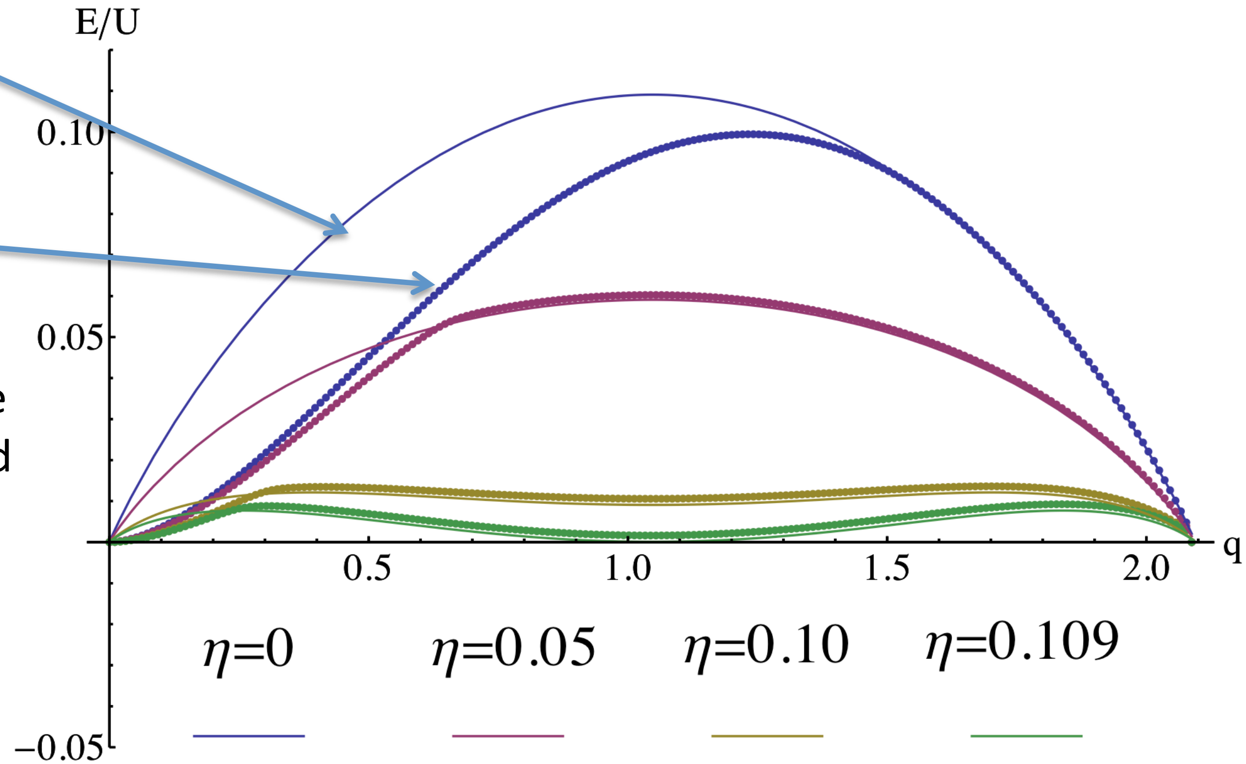
- Fully polarized edge state is consistent with Lieb’s Theorem
- It is a kind of spin-polarized semi-metal with a trivial ground state despite strong interactions

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 $k=\pi$

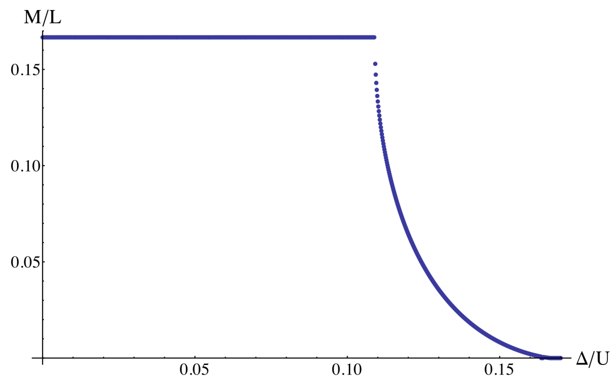
•Increasing Δ causes the exciton to become unbound (except close to q=0)

•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 elecrons For $\Delta<0$ or filled band of spin up electrons, $\Delta>0$

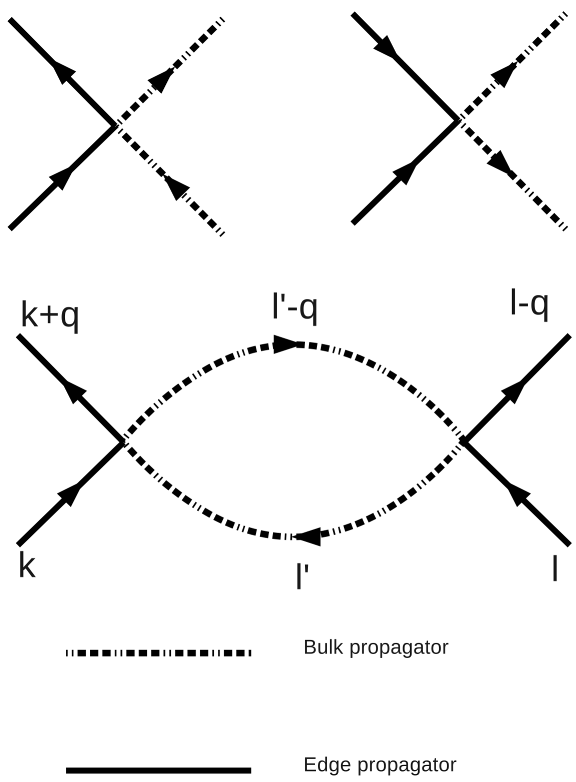
- We confirmed this by looking at $\Delta M=-2$ states near $\Delta=\Delta_c$ – no biexiton bound states
- State with no spin down electrons (or no spin up holes) is non-interacting for our projected on-site Hubbard model since particle of same spin don’t interact with each other

•Gives simple magnetization curve
•2nd neighbour 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

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

•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

•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:

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

•To investigate effects of edge-bulk interactions more systematically, we plan to use Renormalization Group

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

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

Conclusions

- Small U/t limit is a tractible starting point for studying graphene edge magnetism
- Both Lieb's theorem and rigorous result on 1D edge Hamiltonian indicate full polarization in simplest model
- t_2 and edge potential lead to 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