Interactions and magnetism in graphene boundary states

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Outline

1 Model
   - Hamiltonian and symmetries
   - Effective description for boundary states

2 Results
   - Empty band and half filling
   - General fillings

3 Conclusions
Midgap states

- Edges of nano-structured graphene, or vacancies, cracks lead to localized states that increase density of states close to Dirac point.

- Strong effect of interactions due to poor screening.

Nearest neighbor hopping:

\[ H_{TB} = -t \sum_{\langle i,j \rangle, \sigma} \left( c_{\sigma,i}^\dagger c_{\sigma,j} + h.c. \right) \]

Symmetry of energy spectrum
Hamiltonian and symmetries

Interaction term $V$:

$$H = H_{TB} + V$$

$$V_H = U \sum_i \left( n_i^{\uparrow} - \frac{1}{2} \right) \left( n_i^{\downarrow} - \frac{1}{2} \right)$$

$$V_C = \frac{1}{2} \sum_{i \neq j} \frac{e^2}{r_{ij}} (n_i - 1)(n_j - 1) + V_H$$

System has electron-hole symmetry around half filling

Good quantum numbers:

Spin, $S$, $S_z$, momentum along edge (around tube) $M$. 
Effective description for boundary states

- Filled valence band, \( N_e \) electrons in \( N_B \) boundary states.

\[
H = H_{VB} + V_{BB}
\]

\[
H_{VB} = \sum_mE_m n_m
\]

- Potentials \( E_m \) can be expressed by boundary states

\[
\delta_{r,r'} = \sum_i\psi_i(r)^*\psi_i(r') = 2\sum_v\psi_v(r)^*\psi_v(r') + \sum_m\psi_m(r)^*\psi_m(r')
\]

- Effective Hamiltonian expressed only in terms of boundary states.
- Interaction between boundary electrons \( V_{BB} \) treated exactly.
- All symmetries of full Hamiltonian are conserved.
Strong dispersion ($v_F^* = v_F U/3t$)

Hubbard and Coulomb interaction differ for empty band (non-magnetic and charged edge).

Hubbard and Coulomb coincide at half filling (magnetic and charge-neutral edge). Convergence of band.
Magnetic properties of edge as function of filling

- Magnetic edge close to half filling.
- Strong spin alternations of ground state for low occupations.

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Interacting graphene boundary states
April 2008 7 / 10
Spin of lowest energy state depends on total linear momentum

For certain fillings the ground state is a doublet with two possible values of $M \Rightarrow$ Persistent current in presence of magnetic field
Conclusions

- Effective model allows a detailed analysis of interaction effects on localized states in graphene beyond mean field approximations.
- Band dispersion is derived
- Magnetism close to half filling of edge states and an alternation between spin polarized and unpolarized ground states for a nearly empty/filled band.
- Connection between momentum along the edge and spin degree of freedom.

Thanks for your attention
Edge states visible in STM as peaks in local density (T=77K,UHV), two peaks expected for magnetic edge.