Electron interactions and broken symmetry phases in graphene

Jeil Jung and Allan H. MacDonald, Department of Physics, University of Texas at Austin

References: Phys. Rev. B 84, 085446 (2011) and Phys. Rev. B 80, 235417 (2009)

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Abstract

The physics of nonlocal exchange interactions in graphene sheets is treated within a π-orbital tight-binding model using a Hartree-Fock approximation and Coulomb interactions modified at short distances by lattice effects and at large distances by dielectric screening. The strong non-locality of exchange effects in systems with isolated band crossings at energies close to the Fermi level leads to renormalization of Fermi velocity and eventually to broken symmetry states for strong enough interactions.

We show the role played by lattice scale details of the effective Coulomb interaction at neutrality point in determining the character of broken symmetry states at zero field and in the quantum Hall regime.

Hartree-Fock non-local exchange in graphene

Enhancement of non-local exchange near isolated band crossings in graphene
Reference: Phys. Rev. B 84, 085446 (2011)

Band hamiltonian

$$H_0(\mathbf{k}) = \begin{pmatrix} 0 & \gamma_0 t(\mathbf{k}) \\ \gamma_0 t^*(\mathbf{k}) & 0 \end{pmatrix}$$

Exchange potential

$$V_X(\mathbf{k}) = \begin{pmatrix} V_X^{AA}(\mathbf{k}) & V_X^{AB}(\mathbf{k}) \\ V_X^{BA}(\mathbf{k}) & V_X^{BB}(\mathbf{k}) \end{pmatrix}$$

Electrostatic Hatree / Exchange Fock

$$V_{HF} = \sum_{\mathbf{k}\lambda\lambda'} U_H^{\lambda\lambda'} \left[\sum_{\mathbf{k}'} \langle c^\dagger_{\mathbf{k}'\lambda'} c_{\mathbf{k}'\lambda'} \rangle \right] c^\dagger_{\mathbf{k}\lambda} c_{\mathbf{k}\lambda} - \sum_{\mathbf{k}\mathbf{k}'\lambda\lambda'} U_X^{\lambda\lambda'}(\mathbf{k}'-\mathbf{k}) \langle c^\dagger_{\mathbf{k}'\lambda'} c_{\mathbf{k}'\lambda} \rangle c^\dagger_{\mathbf{k}\lambda} c_{\mathbf{k}'\lambda'}$$

Real space

$$U_H^{ll'} \simeq \frac{1}{N_K^2} \sum_{i,j} V_{\rm eff}(|\mathbf{L}_{ij}^{ll'}|),$$

$$U_X^{ll'} \simeq \frac{1}{N_K^2} \sum_{ij}^{N_K} e^{i(\mathbf{k}'-\mathbf{k})\mathbf{L}_{ij}^{ll'}} V_{\rm eff}(|\mathbf{L}_{ij}^{ll'}|).$$

$$V_{\rm eff}(d) = 1/(\epsilon_r \sqrt{a_o^2 + d^2})$$

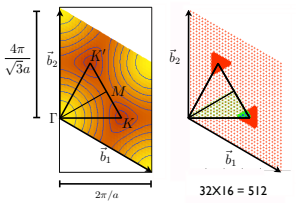
Momentum space

$$U_H^{ll'} = \frac{1}{A} \sum_{\mathbf{G}} e^{i\mathbf{G}\cdot(\tau_l - \tau_{l'})} |f(|\mathbf{G}|)|^2 \widetilde{V}(|\mathbf{G}|),$$

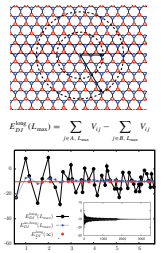
$$U_X^{ll'}(\mathbf{q}) = \frac{1}{A} \sum_{\mathbf{G}} e^{i\mathbf{G}\cdot(\tau_l - \tau_{l'})} |f(|\mathbf{q}-\mathbf{G}|)|^2 \widetilde{V}(|\mathbf{q}-\mathbf{G}|),$$

$$f(q) = [1 - (r_o q)^2]/[(1 + (r_o q)^2]^4]$$

Adaptive k-point sampling in the primitive cell



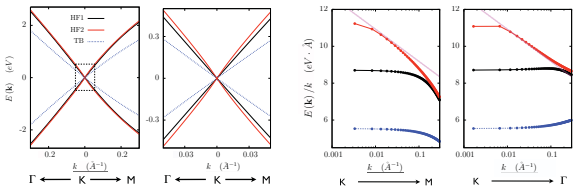
Real space truncation and Ewald sum



Velocity enhancement and logarithmic divergence

The exchange enhanced velocity $v_{HF} = v_F\left[1 + \frac{\alpha_{ee}}{4}\ln\left(\frac{p_c}{ka}\right)\right]$, where $\alpha_{ee} = \frac{e^2}{\varepsilon_r \hbar v_F}$

can be fitted with the parameter value $p_c = 30 \pm 3$.

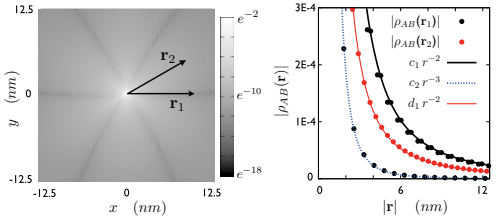


The diagonal AA exchange term in the sublattice basis is proportional to the onsite U and does not contribute in the velocity enhancement.

$$V_X^{AA}(\mathbf{k}) = -\frac{1}{2N_K^2} \sum_{\mathbf{k}',i,j}^{N_K} e^{i(\mathbf{k}'-\mathbf{k})\mathbf{L}_{ij}^{AA}} V_{\rm eff}(|\mathbf{L}_{ij}^{AA}|) = -\frac{1}{2N_K} \sum_{i,j}^{N_K} \delta_{i,j} V_{\rm eff}(|\mathbf{L}_{ij}^{AA}|) = -\frac{U}{2}.$$

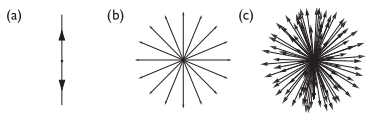
$$V_X^{AB}(\mathbf{k}) = \frac{1}{2N_K^2} \sum_{\mathbf{k}'}^{N_K} \sum_{i,j} e^{i(\mathbf{k}'-\mathbf{k})\mathbf{L}_{ij}^{AB}} V_{\rm eff}(|\mathbf{L}_{ij}^{AB}|) \frac{f(\mathbf{k}')}{|f(\mathbf{k}')|} \equiv \frac{1}{2N_K} \sum_{i,j}^{N_K} e^{-i\,\mathbf{k}\,\mathbf{L}_{ij}^{AB}} \rho_{AB}(\mathbf{L}_{ij}^{AB})\, V_{\rm eff}(|\mathbf{L}_{ij}^{AB}|).$$

The enhancement is due to the off diagonal AB density matrix term which has a slow power law decay in real space, together with the long range Coulomb tail.



$$\rho_{AB}(\mathbf{r}) \simeq e^{i\mathbf{K}\cdot\mathbf{r}} \frac{A_0}{(2\pi)^2} \int_{|\mathbf{k}|<k_c} d\mathbf{k}\; e^{i\mathbf{k}\mathbf{r}}\, \widetilde{\rho}_{AB}(\mathbf{k}) \simeq \frac{C_d}{r^d}$$ for systems with linear isolated band crossing

the slow decay of the density matrix is related with the abrupt change of pseudospin direction when we move across the Fermi point.



1D - Odd parity 2D - Vortex 3D - Hedgehog

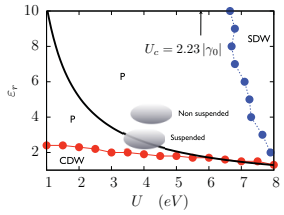
$$\frac{\partial V_X^{AB}(k)}{\partial k} \simeq \frac{1}{2\Omega}\frac{\partial}{\partial k} \int d\mathbf{r}\; e^{-i\mathbf{k}\mathbf{r}} \rho_{AB}(\mathbf{r})\, V_{\rm eff}(|\mathbf{r}|) \simeq C_{\tilde{B},d} \int_a^{k^{-1}} dr\, r^d \frac{1}{r^{d+1}} \propto \ln\left(\frac{1}{ka}\right)$$

Broken symmetry phase diagram as a function of interaction strength.

We have a competition of band energy, electrostatic direct term (DI) and exchange.

$$\delta E_{DI} = \frac{(\delta n)^2}{2}\left[U + \sum_{j\in A} V_{ij} - \sum_{j\in B} V_{ij}\right].$$

We treat as separate parameters the onsite U and the Coulomb tail screened by the dielectric constant.



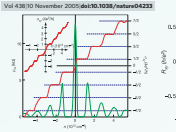
Quantum Hall ferromagnetism in a perpendicular magnetic field

Theory of the magnetic-field-induced insulator in graphene

Reference: Phys. Rev. B 80, 235417 (2009)

Preliminaries

Early measurements of quantum Hall effect in graphene at filling factors $\nu = 4(n+1/2)$



The Landau levels in graphene are 4-fold degenerate, twofold degeneracy in spin and valley

Valley K

$$\Psi(K,n) = e^{ik_x x}\begin{pmatrix} \pm\phi_{n-1}(y - k_x\ell^2) \\ \phi_n(y - k_x\ell^2) \end{pmatrix}$$

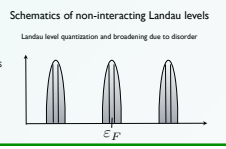
Valley K'

$$\Psi(K',n) = e^{ik_x x}\begin{pmatrix} \pm\phi_n(y - k_x\ell^2) \\ \phi_{n-1}(y - k_x\ell^2) \end{pmatrix}$$

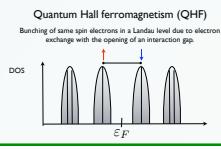
Sublattice selective wave functions for n=0 levels. In the continuum model valley = sublattice

$$\Psi(K,0) = e^{ik_x x}\begin{pmatrix} 0 \\ \phi_0(y - k_x\ell^2) \end{pmatrix} \qquad \Psi(K',0) = e^{ik_x x}\begin{pmatrix} \phi_0(y - k_x\ell^2) \\ 0 \end{pmatrix}$$

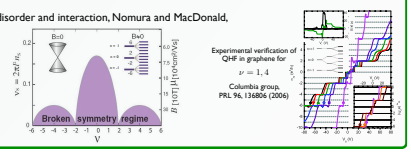
Schematics of non-interacting Landau levels



Quantum Hall ferromagnetism (QHF)

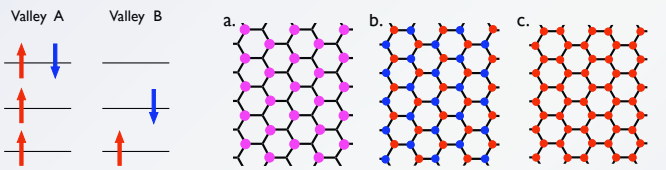


QHF, disorder and interaction, Nomura and MacDonald,

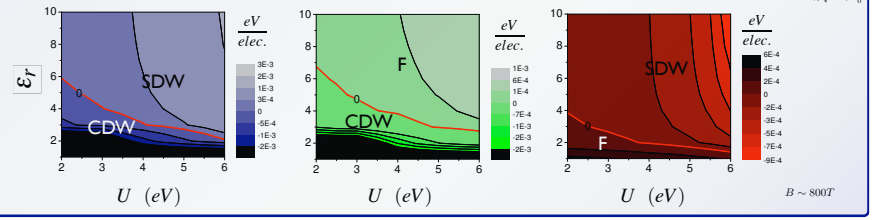


Bulk physics

Different possible filling schemes of n=0 levels at half filling within a collinear spin mean field description, leading to density wave (charge or spin) or spin polarized ferromagnetic solutions in the bulk

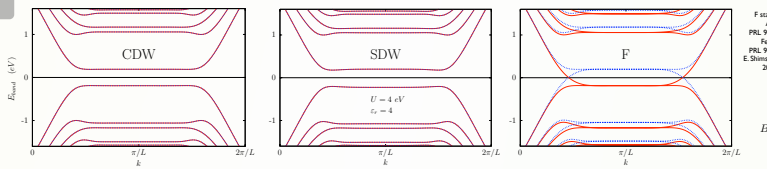


Within a Hartree-Fock theory the density wave states are energetically favored over F solutions. We distinguish the onsite repulsion U from the Coulomb tail using the definition $V_{\rm eff}(r) = \frac{1}{\varepsilon_r\sqrt{r^2 + r_0^2}}$



Ribbons

Using a ribbon geometry (armchair) we can verify that the density wave solutions do not support conducting edge states that cross the Fermi level at half filling



F state discussed by Abanin et al. PRL 98, 196806 (2007); Fertig and Brey, PRL 97, 116805 (2006); E. Shimshoni et al. PRL 102, 206408 (2009)

The density wave solutions show a substantial Landau level mixing (deviation from dotted horizontal line), related with the selective sublattice occupation of n=0 levels.