Excitonic mass generation in Honeycomb lattice

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Outline

1. Introduction

Dirac electrons Coulomb interaction Excitonic order parameters(Previous works)

2. Honeycomb lattice model

Formulation Self-consistent equation Results

3. Summary

Massless Dirac electron system in solid

Graphene



 α –(BEDT–TTF)₂I₃

P. Wallace, Physical Review 71: 622-634. (1947) (Graphite)

A. Geim, K. Novoselov Nature 438 (2005) 197.



$$H_{eff} = \hbar \sum_{\rho=0}^{3} \mathbf{v}_{\rho} \cdot \mathbf{\tilde{k}} \sigma_{\rho}$$

Effective Weyl Hamiltonian



K. Kajita, et al., J. Phys. Soc. Jpn. 61, 23 (1992).N. Tajima, et al., J. Phys.Soc. Jpn. 75, 051010 (2006).

S. Katayama, A. Kobayashi, Y. Suzumura, JPSJ. 75 (2006) 054705

Weyl Hamiltonian





$$H_{0,k}^{R,L} = \pm k_x \hat{\sigma}_x + k_y \hat{\sigma}_y$$
$$V_0(q) = \frac{2\pi e^2}{\varepsilon_0 |q|}$$
$$H' \equiv \int d\mathbf{r} \int d\mathbf{r}' V_0(\mathbf{r} - \mathbf{r}') n(\mathbf{r}) n(\mathbf{r}')$$

 $H = H_0 + H'$

Electron correlation



Excitonic mass generation



Mean field order parameters
which contribute to mass generation
$$\hat{\sigma} : sublattice \\
\hat{\tau} : valley$$

$$4^{2}=16 \text{ degrees} of freedom$$

$$\Psi_{k}^{+}(\hat{\sigma}_{3} \otimes \hat{\tau}_{0})\Psi_{k} = \sum_{\tau=R,L} (A_{k}^{\tau+}A_{k}^{\tau} - B_{k}^{\tau+}B_{k}^{\tau}) \\
\Psi_{k}^{+}(\hat{\sigma}_{3} \otimes \hat{\tau}_{3})\Psi_{k} = \sum_{\tau=R,L} sign(\tau)(A_{k}^{\tau+}A_{k}^{\tau} - B_{k}^{\tau+}B_{k}^{\tau}) \\
\Psi_{k}^{+}(\hat{\sigma}_{1} \otimes \hat{\tau}_{1})\Psi_{k} = A_{k}^{R+}B_{k}^{L} - B_{k}^{R+}A_{k}^{L} + h.c. \\
\Psi_{k}^{+}(\hat{\sigma}_{1} \otimes \hat{\tau}_{2})\Psi_{k} = -iA_{k}^{R+}B_{k}^{L} - iB_{k}^{R+}A_{k}^{L} + h.c.$$

D.V.Khveshchenko, J. Phys.: Condens. Matter **21** (2009) 075303 S. Raghu et al., Phys. Rev. Lett. **100** (2008) 156401

	q	$R \leftrightarrow L$	physical content	$\langle C^{\dagger}C' angle$	matrix
Δ_{0}^{even}	0	even	CDW/SDW	$\langle A^{\dagger}A - B^{\dagger}B \rangle$	$\sigma_3 \otimes \tau_0$
$\Delta_{0}^{\mathrm{odd}}$	0	odd	QAH/ QSH	$\langle A^{\dagger}A - B^{\dagger}B \rangle$	$\sigma_3 \otimes \tau_3$
$\Delta_{Q}^{\mathrm{even}}$	Q	even	BOW (charge/spin)	$\langle A^{\dagger}B + B^{\dagger}A \rangle$	$\sigma_1 \otimes \tau_1$
$\Delta_{oldsymbol{Q}}^{\mathrm{odd}}$	Q	odd	flux	$\langle A^{\dagger}B + B^{\dagger}A \rangle$	$\sigma_1 \otimes \tau_2$

Honeycomb lattice





Formulation

$$H = t \sum_{\langle i,j \rangle} \left(c_i^+ c_j + c_j^+ c_i \right) + \frac{1}{2} \sum_{i,j} V_{ij} n_i n_j - \left(\frac{U}{2} + \mu \right) \sum_i n_i$$

$$V_{ij} = \begin{cases} \frac{e^2}{\varepsilon |R_i - R_j|} & i \neq j \\ U & i = j \end{cases} \qquad H = H_0 + H'$$

$$n_i = c_{i\uparrow}^+ c_{i\uparrow} + c_{i\downarrow}^+ c_{i\downarrow}$$

Mean field theory

$$H'_{MF} = U \sum_{k} \left\{ \left[\sum_{k'} \left\langle A_{k'}^{+} A_{k'} \right\rangle \right] A_{k}^{+} A_{k} + \left[\sum_{k'} \left\langle B_{k'}^{+} B_{k'} \right\rangle \right] B_{k}^{+} B_{k} \right\} - \sum_{k,k',q} V(q) \left\{ \left\langle A_{k+q}^{+} A_{k'+q} \right\rangle A_{k}^{+} A_{k} + \left\langle B_{k+q}^{+} B_{k'+q} \right\rangle B_{k}^{+} B_{k} \right\} - \sum_{k,k',q} \widetilde{V}(q) \left\{ \left\langle A_{k+q}^{+} B_{k'+q} \right\rangle B_{k}^{+} A_{k} + \left\langle B_{k+q}^{+} A_{k'+q} \right\rangle A_{k}^{+} B_{k} \right\}$$



Self-consistent equation

excitonic order parameters

singlet • triplet

$$\Delta_{k}^{\text{singlet}} = \Delta_{k,s,s'} \delta_{s,s'}$$
$$\Delta_{i,k}^{\text{triplet}} = \sum_{s,s'} (\hat{s}_{i})_{s,s'} \Delta_{k,s,s'}$$

$$\Delta_{k,s,s'}^{q=0} = \sum_{k,s,s'}^{11} - \sum_{k,s,s'}^{22} \Delta_{k,s,s'}^{q=Q} = \left(\sum_{k,s,s'}^{41} + \sum_{k,s,s'}^{32} + c.c. \right) / 2$$

$$\Sigma_{k,s,s'}^{ab} = \frac{1}{N} \sum_{q} W(q) \left\langle \Psi_{k+q,s'}^{b+} \Psi_{k+q,s}^{a} \right\rangle$$

linearized self-consistent field equation

$$\varepsilon_{k+q} = \hbar v_F \left| k + q \right|$$

$$\lambda \Delta_k = \sum_q W(q) \frac{\Delta_{k+q}}{2\varepsilon_{k+q}} \tanh \frac{\varepsilon_{k+q}}{2T}$$

q=0,singlet case

$$W(q) = V_l(q) - U + \left[V_l(q) - \widetilde{V}(q)\right]_{q=0}$$

Comes from

neutrality condition.

q=0,triplet case $W(q) = V_{I}(q) + U$ q=Q case $W(q) = \frac{\widetilde{V}(q) + \widetilde{V}(-q)}{2}$

Order parameters in momentum space







Summary

We study about excitonic mass generation in Honeycomb lattice model.

In continuum model, several excitonic orders are degenerated.

We find that in lattice model, the degeneracy of excitonic orders is broken.

For realistic parameter U=1.2t(graphene), BOW state is stable for α >0.8.

band-representation

$$\Psi_{k,s}^{+}\hat{U}^{+}\hat{U}\hat{H}_{k,s,s'}^{MF}\hat{U}^{+}\hat{U}\Psi_{k,s'} = \Phi_{k,s}^{+}\hat{H}_{k,s,s'}^{band}\Phi_{k,s'} \qquad \Phi_{k,s}^{+} = \begin{pmatrix} a_{\tilde{k},s}^{R+} & b_{\tilde{k},s}^{R+} & b_{\tilde{k},s}^{L+} & a_{\tilde{k},s}^{L+} \end{pmatrix}$$

$$\begin{split} U_{R} &= \frac{1}{\sqrt{2}} \begin{pmatrix} e^{\frac{i\theta}{2}} & e^{\frac{-i\theta}{2}} \\ e^{\frac{i\theta}{2}} & -e^{\frac{-i\theta}{2}} \end{pmatrix} \qquad U_{L} = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{\frac{-i\theta}{2}} & e^{\frac{i\theta}{2}} \\ e^{\frac{-i\theta}{2}} & -e^{\frac{i\theta}{2}} \end{pmatrix} \qquad a_{\vec{k},\sigma}^{+} : conduction \\ \\ H_{k}^{band(0)} &= \frac{\sqrt{3}}{2} \begin{pmatrix} \left| \vec{k} \right| & 0 & 0 & 0 \\ 0 & -\left| \vec{k} \right| & 0 & 0 \\ 0 & 0 & -\left| \vec{k} \right| & 0 \\ 0 & 0 & 0 & \left| \vec{k} \right| \end{pmatrix} \qquad b_{\vec{k},\sigma}^{+} : valence \qquad k,a \qquad V(k-k') \qquad k,b \\ \text{sublattice -representation} \qquad \qquad band-representation \\ \Delta_{\vec{k},s,s'}^{q=Q} &= \left[\frac{1}{N} \sum_{q} \left\{ \widetilde{V}(q) \left\langle A_{\vec{k}+q,s'}^{R+} B_{\vec{k}+q,s}^{L} \right\rangle + \widetilde{V}(-q) \left\langle B_{\vec{k}+q,s'}^{R+} A_{\vec{k}+q,s}^{L} \right\rangle + c.c. \right\} \right] / 2 \\ &= \frac{1}{N} \sum_{q} \frac{\widetilde{V}(q) + \widetilde{V}(-q)}{2} \left(\left\langle a_{\vec{k}+q,s'}^{R+} b_{\vec{k}+q,s'}^{L} \right\rangle - \left\langle b_{\vec{k}+q,s'}^{R+} a_{\vec{k}+q,s}^{L} \right\rangle + c.c. \right) \end{split}$$

BOW(Honeycomb)



$$H = -\sum_{\boldsymbol{r} \in \Lambda_A} \sum_{i=1}^{3} (t + \delta t_{\mathbf{r},i}) a_{\boldsymbol{r}}^{\dagger} b_{\boldsymbol{r}+\boldsymbol{s}_i} + \text{H.c.} \qquad (1)$$

$$\delta t_{\boldsymbol{r},i} = \Delta(\boldsymbol{r}) e^{i\boldsymbol{K}_+ \cdot \boldsymbol{s}_i} e^{i\boldsymbol{G}\cdot\boldsymbol{r}}/3 + \text{c.c.,} \qquad \boldsymbol{K}_{\pm} = \pm (\frac{4\pi}{3\sqrt{3}\alpha}, 0).$$

$$\boldsymbol{G} := \boldsymbol{K}_+ - \boldsymbol{K}_-,$$

BOW in Honeycomb lattice correspond to the Kekulé distortion.

C. Y. Hou et al., Phys. Rev. Lett. 98 186809(2007)

Topological aspect of the quantum mechanics

Berry接続
$$\mathbf{A}_n = -\mathbf{i} \langle n | \partial_{\kappa} | n \rangle$$
 n: band index

Berry曲率

$$\mathbf{B}_{n} = \nabla \times \mathbf{A}_{n}$$

$$B_{n}^{z} = -\mathbf{i} \sum_{m(\neq n)} \frac{\langle n | \partial_{k_{x}} H | m \rangle \langle m | \partial_{k_{y}} H | n \rangle}{(E_{n} - E_{m})^{2}} + \mathbf{c.c.}$$
Berry phase $\Phi = \int_{\mathbf{S}} \mathbf{B} \cdot d\mathbf{S} = \int_{\mathbf{S}} \nabla \times \mathbf{A} \cdot d\mathbf{S} = \oint_{\mathbf{C}} \mathbf{A} d\mathbf{X}$
Chern number (2D) $V_{n\sigma} = \frac{1}{2\pi} \int_{\mathbf{BZ}} d^{2}k B_{n\sigma}^{z} = 0, \pm 1, \pm 2, \dots$

ホール伝導率



F. D. M. Haldane, PRL 61, 2015 (1988).
S. Raghu, X. L. Qi, C. Honerkamp, and S. C. Zhang, PRL 100, 156401 (2008).

The simplest Hamiltonian with non-zero Chern number

$$H = \alpha_{x}k_{x}\sigma_{x} + \alpha_{y}k_{y}\sigma_{y} + \alpha_{z}\Delta\sigma_{z} \qquad \left(\alpha_{x}, \alpha_{y}, \alpha_{z} = \pm 1\right)$$
Parameter space $\mathbf{X} = (k_{x}, k_{y}, \Delta)$
Eigen energy $E_{\pm} = \pm X$
Eigen function $\left(\begin{array}{c} \Psi_{+} = \frac{1}{\sqrt{2X(X - \alpha_{z}\Delta)}} \begin{pmatrix} \alpha_{x}k_{x} - i\alpha_{y}k_{y} \\ -\alpha_{z}\Delta + X \end{pmatrix} \\ \Psi_{-} = \frac{1}{\sqrt{2X(X + \alpha_{z}\Delta)}} \begin{pmatrix} \alpha_{x}k_{x} - i\alpha_{y}k_{y} \\ -\alpha_{z}\Delta - X \end{pmatrix} \\ \text{using} \quad \partial_{k_{x}}H = \alpha_{x}\sigma_{x} \quad \partial_{k_{y}}H = \alpha_{y}\sigma_{y}$

$$B_{-}^{\Delta} = -i \frac{\left(\Psi_{-}^{+} \cdot \partial_{k_{x}} H \cdot \Psi_{+} \right) \left(\Psi_{+}^{+} \cdot \partial_{k_{y}} H \cdot \Psi_{-} \right)}{\left(E_{-} - E_{+} \right)^{2}} + c. c. = -\alpha_{x} \alpha_{y} \alpha_{z} \frac{\Delta}{2X^{3}} \Rightarrow Ch_{-} = -\frac{\alpha_{x} \alpha_{y} \alpha_{z}}{2}$$

Lower (filled) band "Magnetic monopole"

"magnetic monopole" and discontinuity of Chern number



Topological insulator with TRS (time-reversal symmetry) = a combined system of two subsystems with opposite sign Chern numbers Kane-Mele model (graphene + spin-orbit interaction) PRL 95, 226801 (2005)

<u>A4</u>

Direct calculation of Berry's phase gauge field using the Hamiltonian for alpha-(BEDT-TTF) $_2I_3$

Fictitious "magnetic field" given by Berry's phase gauge field

$$B_{n\sigma}^{\Delta} = -i \sum_{m(\neq n)} \frac{\langle n\sigma | \partial_{k_x} H | m\sigma \rangle \langle m\sigma | \partial_{k_y} H | n\sigma \rangle}{(E_{n\sigma} - E_{m\sigma})^2} + \text{c.c.}$$

$$=-\mathrm{i}\sum_{m(\neq n),\alpha_{1}\sim\alpha_{4}}\frac{\langle n|\alpha_{1}\rangle\langle\alpha_{1}|\partial_{k_{x}}H|\alpha_{2}\rangle\langle\alpha_{2}|m\rangle\langle m|\alpha_{3}\rangle\langle\alpha_{3}|\partial_{k_{y}}H|\alpha_{4}\rangle\langle\alpha_{4}|n\rangle}{(E_{n\sigma}-E_{m\sigma})^{2}}+\mathrm{c.\,c.}$$

$$=-\mathrm{i}\sum_{\substack{m(\neq n),\alpha_{1}\sim\alpha_{4}}}\frac{d_{n\alpha_{1}\sigma}(\mathbf{k})\partial_{k_{x}}H_{\alpha_{1}\alpha_{2}\sigma}(\mathbf{k})d_{m\alpha_{2}\sigma}^{*}(\mathbf{k})d_{m\alpha_{3}\sigma}(\mathbf{k})\partial_{k_{y}}H_{\alpha_{3}\alpha_{4}\sigma}(\mathbf{k})d_{n\alpha_{4}\sigma}^{*}(\mathbf{k})}{\left(E_{n\sigma}-E_{m\sigma}\right)^{2}}+\mathrm{c.c.}$$

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n = 2, m = 1 $\alpha_1, \alpha_2, \alpha_3, \alpha_4 = 1, 2, 3, 4$ **k** : in BZ

excitonic mass generation in graphene

Static RPA: Khveshchenko, D. V., and H. Leal, 2004, Nucl. Phys. B 687, 323 Strong k-dependence of $\Delta(k)$ $\alpha_c = 1.13$

Effect of renormalized velocity: $\varepsilon_{h}(k) = \hbar v |k|^{1-\eta}$ Khveshchenko, D. V., 2009, J. Phys.: Condens. Matter 21, 075303.

$$T_c \approx \frac{\Delta}{\left|\ln\left(1 - \tilde{\alpha}_c / \alpha_c\right)\right|} \quad \left(\tilde{\alpha} = \frac{\alpha}{1 + \pi N \alpha / 4}\right) \qquad \qquad \frac{\Delta(0)}{\hbar v \Lambda} \approx 0.001 \qquad \Delta \approx k_{\rm B} T_c \approx 4 \,\mathrm{mev}$$

Dynamical RPA on-shell: $\Delta(p, \varepsilon = \hbar v p)$ Gamayun, O. V., E. V. Gorbar, and V. P. Gusynin, 2010, Phys. Rev. B 81, 075429. $\alpha_c = 0.92$ 面直磁場によりα、減少、Δ増大 **Monte Carlo calculations:**

Hands, S., and C. Strouthos, 2008, PRB 78, 165423. Drut et al.,2009, PRB 79, 241405(R); RPL 102, 026802; PRB 79, 165425. $\alpha_c = 1.1$

Polarization function with $\Delta(k)$ and anomalous Green function

J-R. Wang et al., J. Phys.: Condens. Matter 23 (2011) 155602

$$\Pi(\mathbf{q})$$
 ***** = **** + *** 〇 *** + *** 〇 *** + *** 〇 *** + *** 〇 *** GG *** FF GG *** FF GG *** FF

グラフェンにおける電気抵抗



F. Amet, J. R. Williams, K. Watanabe, T. Taniguchi, and D. Goldhaber-Gordon PRL 110, 216601 (2013)

シリコン基板上においたグラフェンの電気抵抗(右図インセット)

