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Kekulé-modulated α-T_3 model

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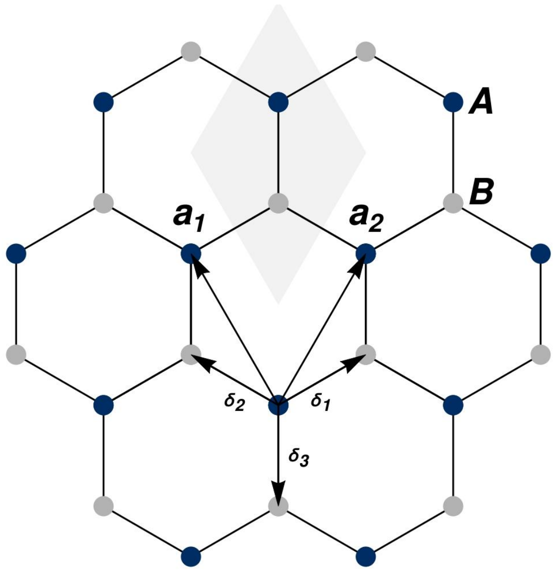
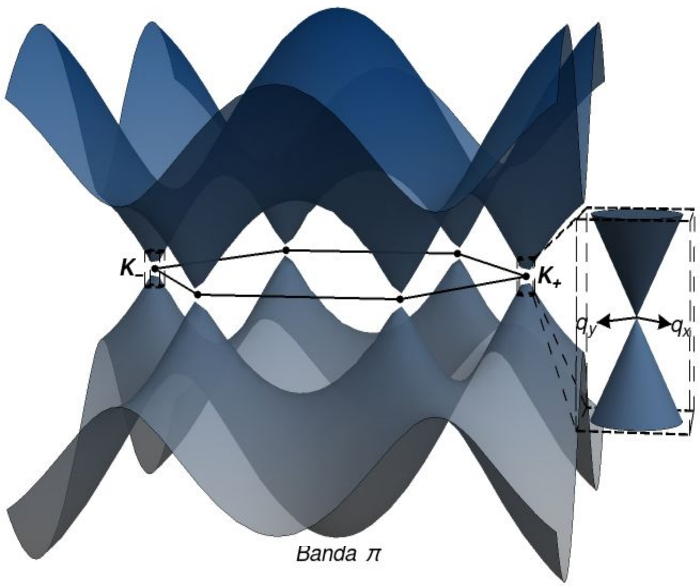
Introduction

Graphene



Honeycomb lattice

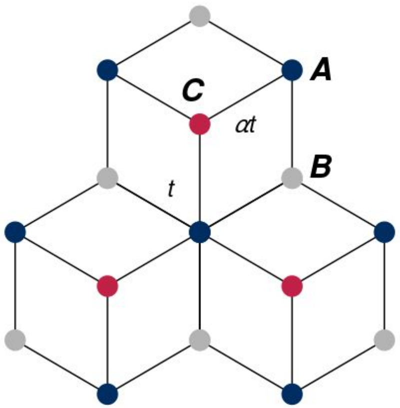


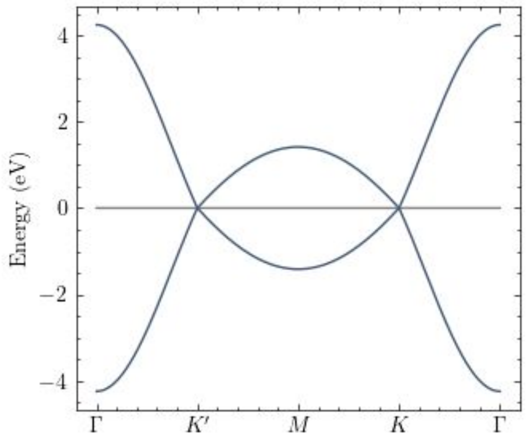
Electronic dispersion

- Dirac Hamiltonian $$\mathcal{H}_\xi(\boldsymbol{q}) = \xi \hbar v_F (\tau_z \otimes \boldsymbol{q} \cdot \boldsymbol{\sigma})$$

- Novoselov, K. S., et al. (2005). *Nature*, *438*(7065), 197-200.
- Neto, A. C., et al. (2009). *Rev. Mod. Phy.*, 81(1), 109.

The α-T_3 model





T_3 lattice

Electronic dispersion

- Hamiltonian $\mathcal{H}(\boldsymbol{k}) = \begin{pmatrix} 0 & f(\boldsymbol{k}) & 0 \\ f^*(\boldsymbol{k}) & 0 & \alpha f(\boldsymbol{k}) \\ 0 & \alpha f^*(\boldsymbol{k}) & 0 \end{pmatrix}$

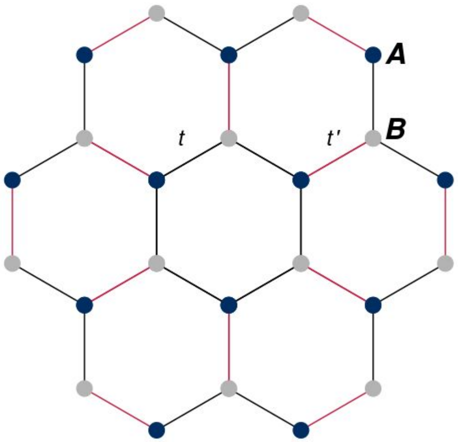
$$0 \leq \alpha \leq 1$$

The parameter α provides a continuous transition between honeycomb and T_3 lattice.

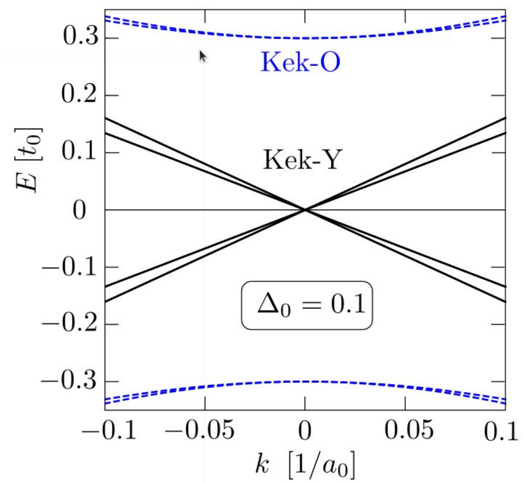
Raoux, A., et al. (2014). *Phy. Rev. Lett.*, *112*(2), 026402.

Kekulé-distorted graphene

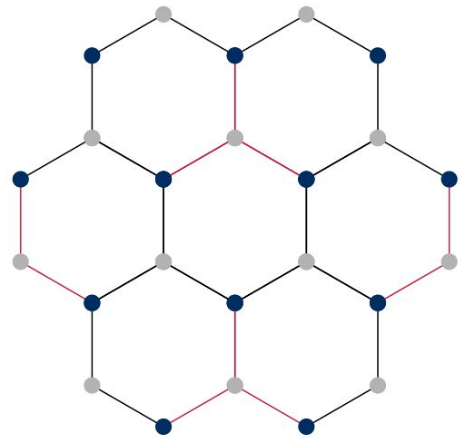
Kek-O (ν=0)



Dispersion relation



Kek-Y (ν=±1)



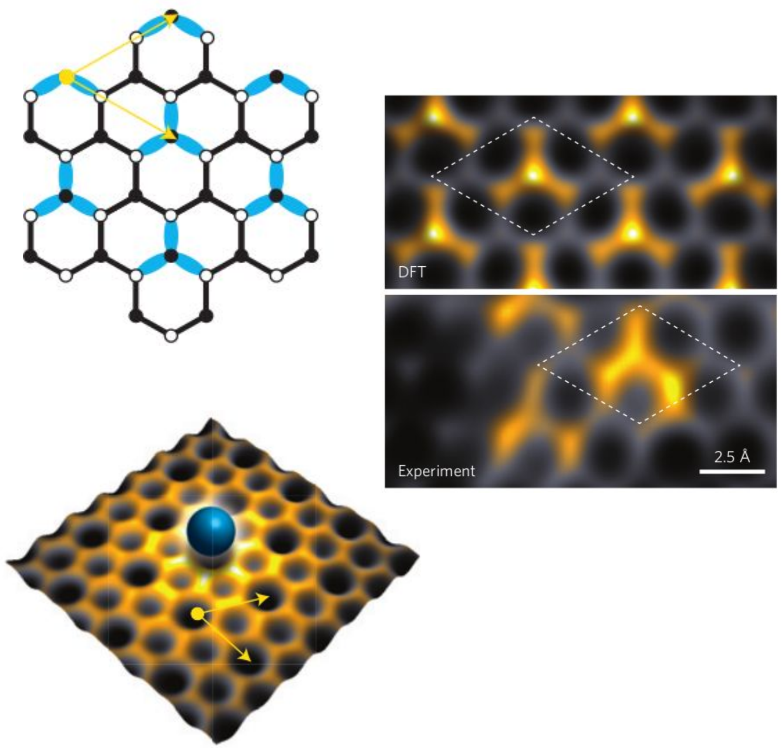
- Bond density-wave: $t_{\boldsymbol{r},n}/t = 1 + \mathbb{R}e\{\tilde{\Delta} e^{i(p\boldsymbol{K}_+ + q\boldsymbol{K}_-)\cdot\boldsymbol{\delta}_n + i\boldsymbol{G}\cdot\boldsymbol{r} - i2(p+q)\pi/3)}\}$
- Low-energy Hamiltonian

$$\mathcal{H}(\boldsymbol{p}) = \begin{pmatrix} v_F \boldsymbol{\sigma}\cdot\boldsymbol{p} & \tilde{\Delta} Q_\nu \\ \tilde{\Delta}^* Q_\nu^\dagger & v_F \boldsymbol{\sigma}\cdot\boldsymbol{p} \end{pmatrix} \qquad Q_\nu = \begin{cases} 3t\sigma_0, & \nu = 0 \\ v_F(\nu p_x - i p_y)\sigma_0, & \nu = \pm 1 \end{cases}$$

- Chamon, C. (2000). *Physical Review B*, *62*(4), 2806.
- Gamayun, O. V., et al. (2018). *New Journal of Physics*, *20*(2), 023016.

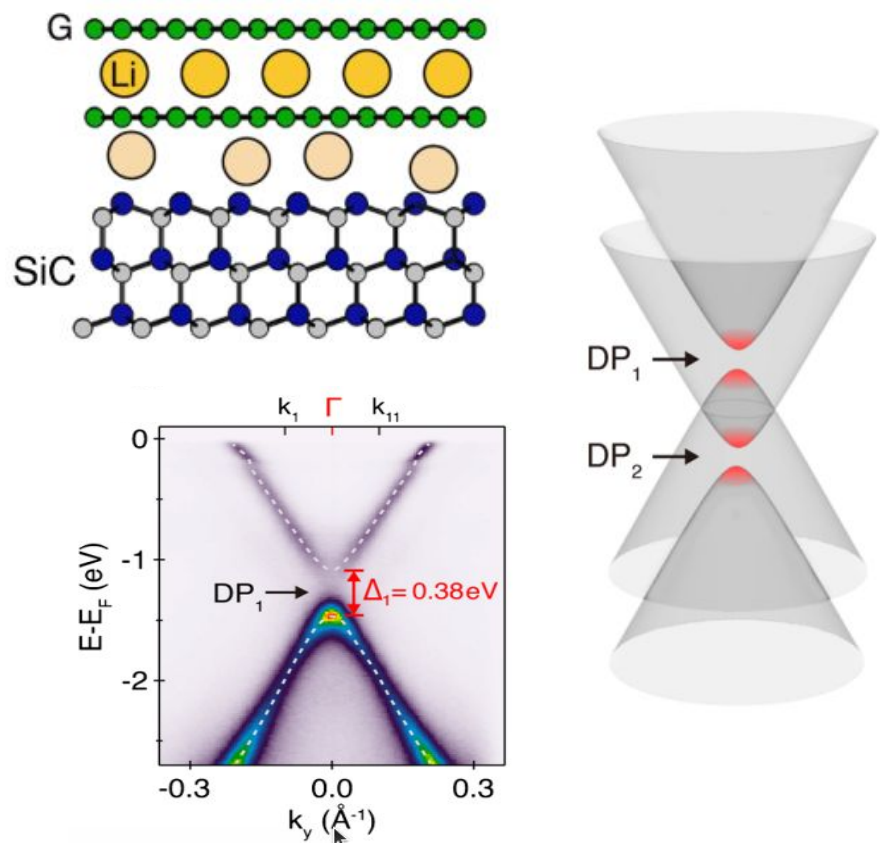
Experimental evidence to KD graphene

Kek-Y



Gutiérrez, C., et al. (2016). *Nat. Phy.*, *12*(10), 950-958.

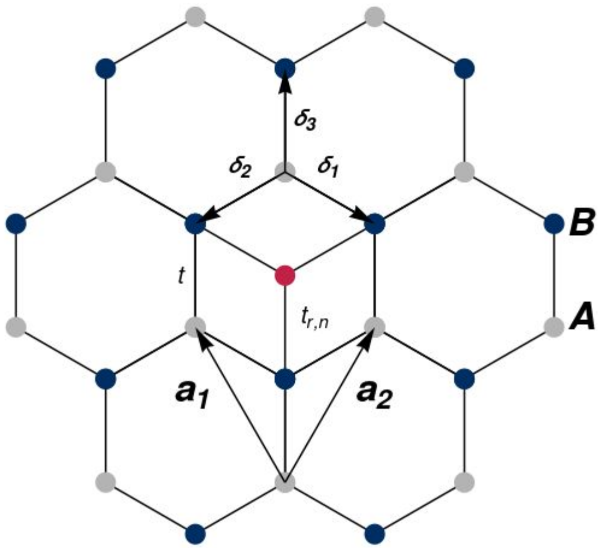
Kek-O



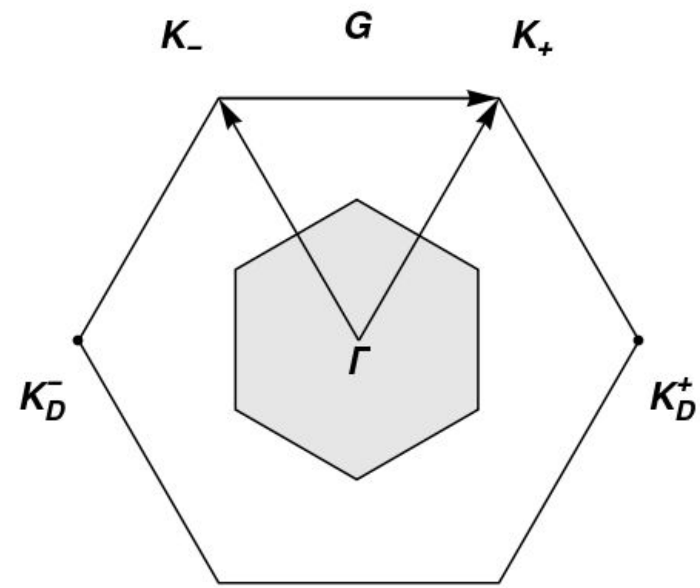
Bao, C., et al. (2021). *Phy. Rev. Lett.*, *126*(20), 206804.

Kekulé-modulated α-T_3 model

Crystal structure



Unit cell



1BZ

$$\boldsymbol{\delta}_1 = \frac{1}{2}(\sqrt{3}, -1), \quad \boldsymbol{\delta}_2 = -\frac{1}{2}(\sqrt{3}, 1), \quad \boldsymbol{\delta}_3 = (0, 1)$$

$$\boldsymbol{a}_1 = \boldsymbol{\delta}_3 - \boldsymbol{\delta}_1, \qquad \boldsymbol{a}_1 = \boldsymbol{\delta}_3 - \boldsymbol{\delta}_2$$

$$\boldsymbol{K}_\pm = \frac{2\pi\sqrt{3}}{9}(\pm 1, \sqrt{3})$$

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

Tight-binding model

Real-space formulation

- Tight-binding Hamiltonian

$$H = -t \sum_{\boldsymbol{r}} \sum_{n=1}^{3} b^\dagger_{\boldsymbol{r}} a_{\boldsymbol{r}-\boldsymbol{\delta}_n} - \alpha \sum_{\boldsymbol{r}} \sum_{n=1}^{3} t_{\boldsymbol{r},n} b^\dagger_{\boldsymbol{r}} c_{\boldsymbol{r}+\boldsymbol{\delta}_n} + H.c$$

- Hopping of B-C bonds

$$t_{\boldsymbol{r},n} = t[1 + 2\mathbb{R}e(e^{i(p\boldsymbol{K}_+ + q\boldsymbol{K}_-)\cdot\boldsymbol{\delta}_n + i\boldsymbol{G}\cdot\boldsymbol{r}})], \qquad p, q \in \mathbb{Z}_3$$

$$q - p \mod 3 = -2$$

Transformation to momentum space

- Hamiltonian in momentum space

$$H = -\Psi_{\boldsymbol{k}}^{\dagger} \begin{pmatrix} \mathbf{0} & \boldsymbol{\mathcal{F}}(\boldsymbol{k}) & \mathbf{0} \\ \boldsymbol{\mathcal{F}}(\boldsymbol{k})^{\dagger} & \mathbf{0} & \alpha\boldsymbol{\mathcal{E}}(\boldsymbol{k}) \\ \mathbf{0} & \alpha\boldsymbol{\mathcal{E}}(\boldsymbol{k})^{\dagger} & \mathbf{0} \end{pmatrix} \Psi_{\boldsymbol{k}}$$

$$\Psi_{\boldsymbol{k}} = (a_{\boldsymbol{k}}, a_{\boldsymbol{k}-\boldsymbol{G}}, a_{\boldsymbol{k}+\boldsymbol{G}}, b_{\boldsymbol{k}}, b_{\boldsymbol{k}-\boldsymbol{G}}, b_{\boldsymbol{k}+\boldsymbol{G}}, c_{\boldsymbol{k}}, c_{\boldsymbol{k}-\boldsymbol{G}}, c_{\boldsymbol{k}+\boldsymbol{G}}),$$

$$\mathcal{F}(\boldsymbol{k}) = \begin{pmatrix} f_0 & 0 & 0 \\ 0 & f_{-1} & 0 \\ 0 & 0 & f_1 \end{pmatrix}, \qquad \mathcal{E}(\boldsymbol{k}) = \begin{pmatrix} f_0 & \Delta f_0 & \Delta^* f_0 \\ \Delta^* f_{-1} & f_{-1} & \Delta f_{-1} \\ \Delta f_1 & \Delta^* f_1 & f_1 \end{pmatrix}$$

$$\Delta = e^{i2\pi(p+q)/3}, \qquad f_n = f(\boldsymbol{k} + n\boldsymbol{G}) \qquad f(\boldsymbol{k}) = t\sum_{n=1}^{3} e^{i\boldsymbol{k}\cdot\boldsymbol{\delta}_n}$$

Low-energy Hamiltonian

- Hamiltonian ($\alpha \ll 1$)

$$H = -\boldsymbol{\Psi}_{\boldsymbol{k}}^{\dagger} \begin{pmatrix} \mathbf{0} & \mathcal{F}(\boldsymbol{k}) & \mathbf{0} \\ \mathcal{F}^{\dagger}(\boldsymbol{k}) & \mathbf{0} & \alpha\mathcal{E}(\boldsymbol{k}) \\ \mathbf{0} & \alpha\mathcal{E}^{\dagger}(\boldsymbol{k}) & \mathbf{0} \end{pmatrix} \boldsymbol{\Psi}_{\boldsymbol{k}}$$

$$\mathcal{F}(\boldsymbol{k}) = \begin{pmatrix} f_{-1} & 0 \\ 0 & f_1 \end{pmatrix}, \qquad \mathcal{E}(\boldsymbol{k}) = \begin{pmatrix} f_{-1} & \Delta f_{-1} \\ \Delta^* f_1 & f_1 \end{pmatrix},$$

$$\boldsymbol{\Psi}_{\boldsymbol{k}} = (a_{\boldsymbol{k}-\boldsymbol{G}}, a_{\boldsymbol{k}+\boldsymbol{G}}, b_{\boldsymbol{k}-\boldsymbol{G}}, b_{\boldsymbol{k}+\boldsymbol{G}}, c_{\boldsymbol{k}-\boldsymbol{G}}, c_{\boldsymbol{k}+\boldsymbol{G}})$$

- Low-energy approach ($\alpha \ll 1$)

$$f_{\pm 1} = \hbar v_F(\mp k_x + k_y i), \qquad v_F = \frac{3t}{2\hbar}$$

Diagonalization of Hamiltonian

- Dispersion relation

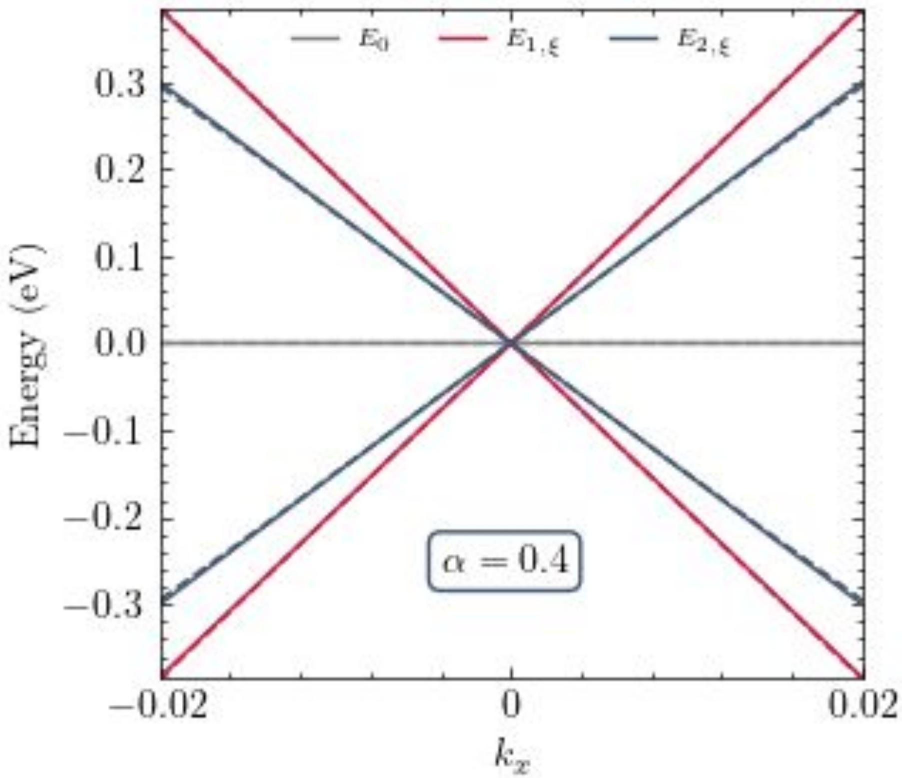
$$E_0 = 0, \qquad E_{1,\pm} = \pm v_F p, \qquad E_{2,\pm} = \pm v_F p\sqrt{1+4\alpha^2}$$

$$p = \hbar|\boldsymbol{k}|$$

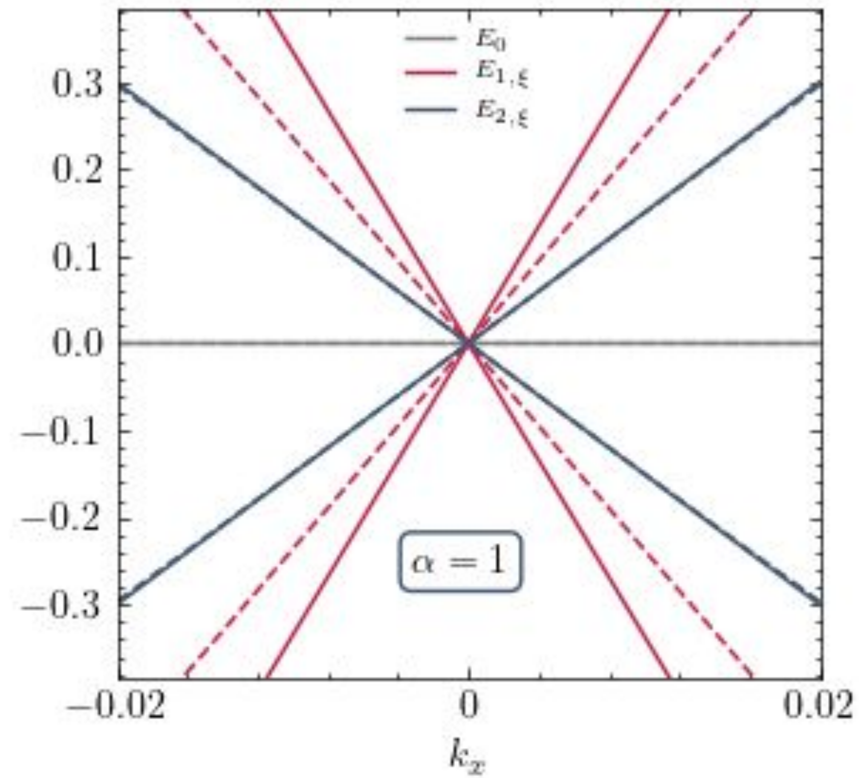
- Eigenfunctions

$$\Psi_0^1 = \frac{1}{\sqrt{2\alpha^2+1}}\begin{pmatrix} -\alpha e^{i2\theta} \\ -\alpha e^{-i2\theta} \\ 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \qquad \Psi_0^2 = \frac{1}{\sqrt{2\alpha^2+1}}\begin{pmatrix} -\alpha e^{i2\theta} \\ -\alpha e^{-i2\theta} \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \quad \Psi_{1,\pm} = \frac{1}{2}\begin{pmatrix} \pm e^{2i\theta} \\ \mp e^{-2i\theta} \\ e^{i\theta} \\ 1 \\ 0 \\ 0 \end{pmatrix}, \qquad \Psi_{2,\pm} = \frac{\alpha}{\sqrt{4\alpha^2+1}}\begin{pmatrix} \frac{e^{2i\theta}}{2\alpha} \\ \frac{e^{-2i\theta}}{2\alpha} \\ \pm\frac{\sqrt{4\alpha^2+1}e^{i\theta}}{2\alpha} \\ \mp\frac{\sqrt{4\alpha^2+1}e^{-i\theta}}{2\alpha} \\ 1 \\ 1 \end{pmatrix}$$

$$\theta = \tan^{-1}(p_x/p_y)$$



Dispersion relation for small α



Dispersion relation for large α

Thank you!

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