Emergence of Dirac Electron Pair in Charge Ordered State of Organic Conductor α-(BEDT-TTF)$_2$I$_3$

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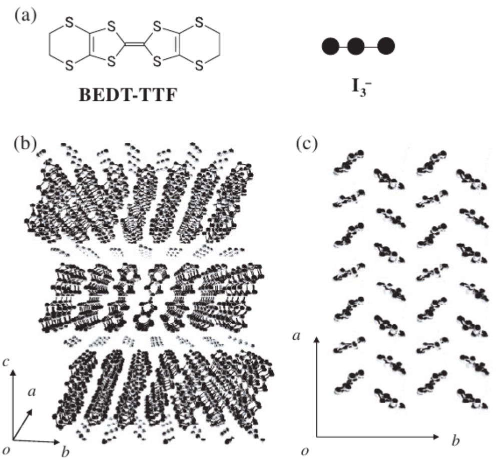
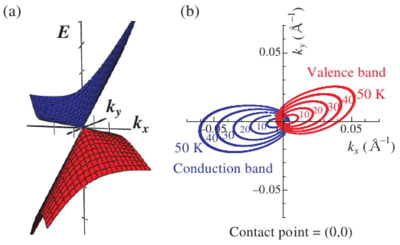
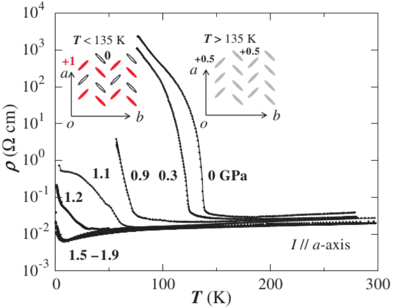
The Organic Conductor α-(BEDT-TTF)$_2$I$_3$







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Outline: study of the (V_a, P_a) phase diagram

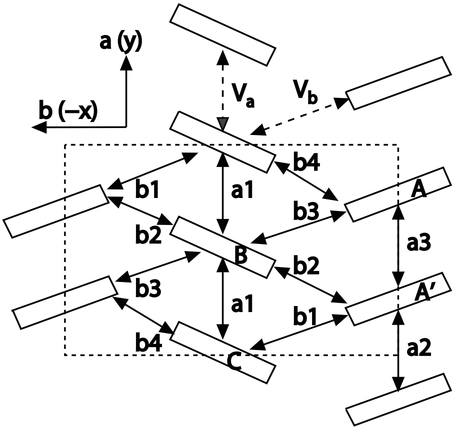
- Tight-binding model for α-(BEDT-TTF)$_2$I$_3$
  with mean field for e-e interaction

- $\mathbf{2 \times 2}$ effective Hamiltonian (Luttinger-Kohn representation)

- Berry curvature and Berry phase

The Organic Conductor α-(BEDT-TTF)$_2$I$_3$

- Insulating stripe Charge Ordered (CO) phase
- Charge Ordered Metallic (COM) phase
- Superconducting state in the presence of charge ordering
- Zero Gap State (ZGS) with a massless Dirac spectrum



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Hartree mean-field theory

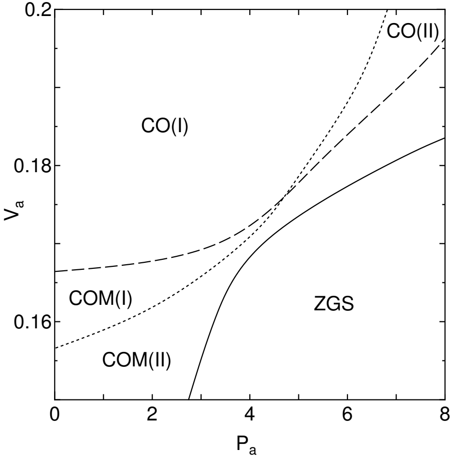
$$H = \sum_{(i\alpha:j\beta),\sigma} (t_{i\alpha;j\beta}\; a^\dagger_{i\alpha\sigma} a_{j\beta\sigma} + \mathrm{h.c.}) + \sum_{i\alpha} U\; a^\dagger_{i\alpha\uparrow}\; a^\dagger_{i\alpha\downarrow} a_{i\alpha\downarrow} a_{i\alpha\uparrow}$$
$$+ \sum_{(i\alpha:j\beta),\sigma,\sigma'} V_{\alpha\beta}\; a^\dagger_{i\alpha\sigma} a^\dagger_{j\beta\sigma'} a_{j\beta\sigma'} a_{i\alpha\sigma},$$

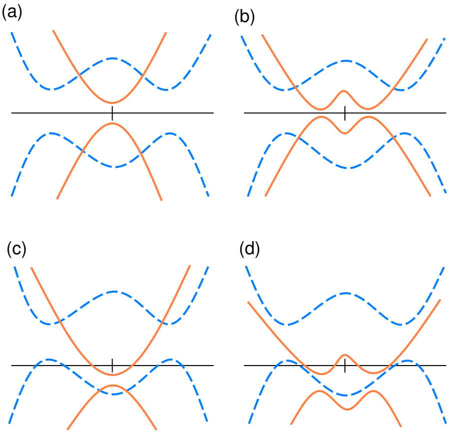
$$\Downarrow$$

$$H_\sigma(\mathrm{k}) = \sum_{\alpha\beta} \tilde{\epsilon}_{\alpha\beta\sigma}(\mathrm{k}) a^\dagger_{\mathrm{k}\alpha\sigma} a_{\mathrm{k}\beta\sigma}$$

$$\tilde{\epsilon}_{\alpha\beta\sigma}(\mathrm{k}) = I_{\alpha\sigma}\delta_{\alpha\beta} + \epsilon_{\alpha\beta}(\mathrm{k})$$
$$I_{\alpha\sigma} = U_\alpha \langle n_{\alpha-\sigma}\rangle + \sum_{\beta'\sigma'} V_{\alpha\beta'} \langle n_{\beta'\sigma'}\rangle$$
$$\epsilon_{\alpha\beta}(\mathrm{k}) = \sum_{\delta} t_{\alpha\beta} e^{\mathrm{ik}\cdot\delta}$$

Phase diagram



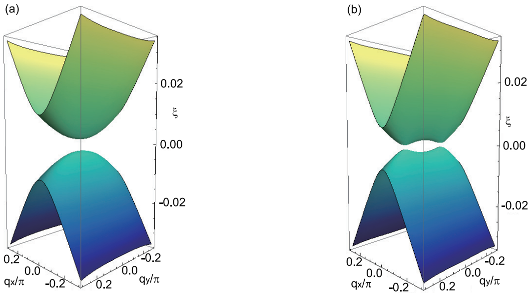


Effective 2-band Hamiltonian

$$H^{LK}(\mathrm{k}_M + \mathrm{q}) = f_0(\mathrm{q})\sigma_0 + f_1(\mathrm{q})\sigma_1 + f_2(\mathrm{q})\sigma_2 + f_3(\mathrm{q})\sigma_3$$

$$\xi_\pm(\mathrm{q}) = f_0(\mathrm{q}) \pm \sqrt{f_1(\mathrm{q})^2 + f_2(\mathrm{q})^2 + f_3(\mathrm{q})^2}$$

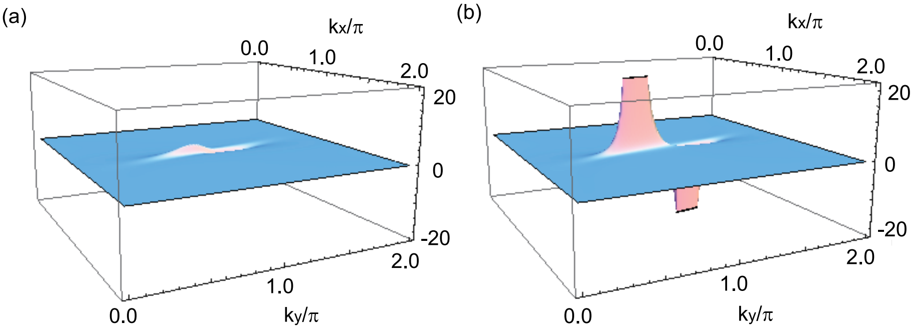
$$\Delta(\mathrm{q}) = \frac{\xi_+(\mathrm{q}) - \xi_-(\mathrm{q})}{2} \simeq \Delta + \frac{1}{2}(q_x\ q_y) S_M \begin{pmatrix} q_x \\ q_y \end{pmatrix} + \cdots$$



Berry curvature associated with the topological transition

$$B_{n\sigma}(\mathbf{k}) = -\mathbf{i}\sum_{m\neq n} \frac{v^x_{nm\sigma}(\mathbf{k})v^y_{mn\sigma}(\mathbf{k})+c.c.}{(\xi_{n\sigma}(\mathbf{k})-\xi_{m\sigma}(\mathbf{k}))^2}$$

$$v^{x,y}_{nm\sigma}(\mathbf{k}) = \langle n\sigma(\mathbf{k})|\partial_{k_{x,y}}H_\sigma(\mathbf{k})|m\sigma(\mathbf{k})\rangle = \sum_{\alpha\beta} d_{n\alpha\sigma}(\mathbf{k})^* d_{m\beta\sigma}(\mathbf{k})\partial_{k_{x,y}}\epsilon_{\alpha\beta}(\mathbf{k})$$



Berry phase and Chern number

$$Ch_{1\uparrow} = \frac{1}{2\pi}\int_{BZ} dS B_{1\uparrow}(\mathbf{k}) = 0$$

$$\Gamma(\mathbf{k}_\pm) = \frac{1}{2\pi}\int_{S(\mathbf{k}_\pm)} dS B_{1\uparrow}(\mathbf{k}) \neq 0$$