Manipulation of band gap upon photoexcitation of an excitonic insulator

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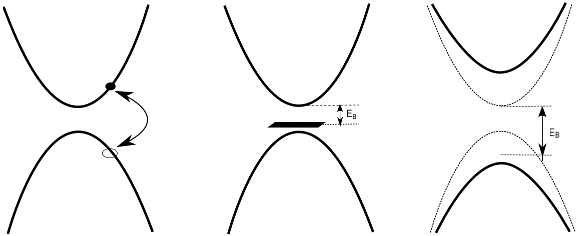
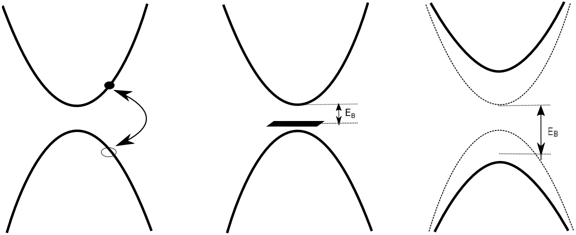
Semiconductor

- Exciton is a bound pair of electron and hole due to Coulomb interaction
- Excitonic insulator: spontaneous symmetry breaking due to Coulomb interaction predicted by Mott in the early 60's



Semiconductor

- Exciton is a bound pair of electron and hole due to Coulomb interaction
- Excitonic insulator: spontaneous symmetry breaking due to Coulomb interaction predicted by Mott in the early 60's
- Semiconductor and semimetal limit
- Experimental candidates: semiconducting(Ta_2NiSe_5) and semimetal($1T - TiSe_2$)

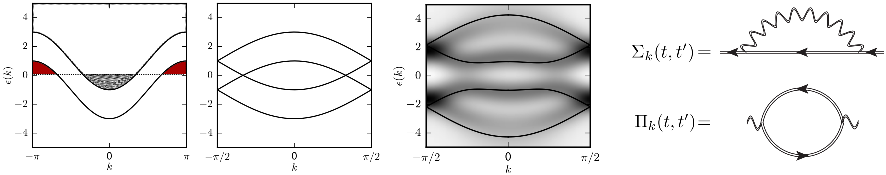


Semi-metal

Two band spin-less fermions with longer range interaction

$$H = \sum_{k\alpha}(\epsilon_{k\alpha} + \Delta_\alpha)c^\dagger_{k,\alpha}c_{k,\alpha} + \frac{1}{2}\sum_{i,j}\sum_{\alpha\alpha'} V^{\alpha\alpha'}_{|i-j|} n_{i\alpha} n_{j,\alpha'}$$
$$H_{dip} = \sum_k A(t) c^\dagger_{k,1} c_{k,0} + H.c.$$

Symmetry breaking: spatial symmetry and charge conservation within the bands $\langle c^\dagger_{k+Q,1} c_{k,2}\rangle \neq 0$
Time dependent Hartree-Fock and GW approximation



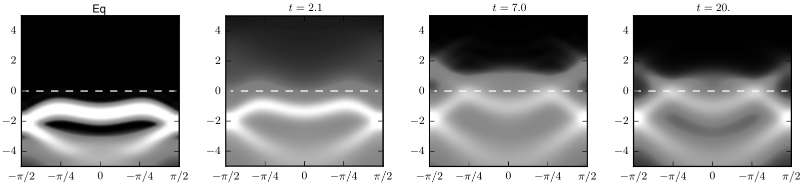
t-ARPES

Time dependent PES

$$I(\omega, t_p) = \mathrm{i} \int dt dt' S(t) S(t') e^{\mathrm{i}\omega(t-t')} G_k^<(t_p + t, t_p + t')$$

$S(t)$ is probe pulse envelope.

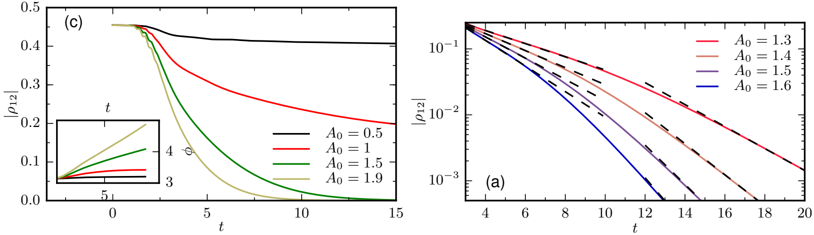
- Photo excitation with strong pulse
- Partial photoinduced population in the upper band
- Strong excitation close the gap, weak only partially



Dynamics of order parameter

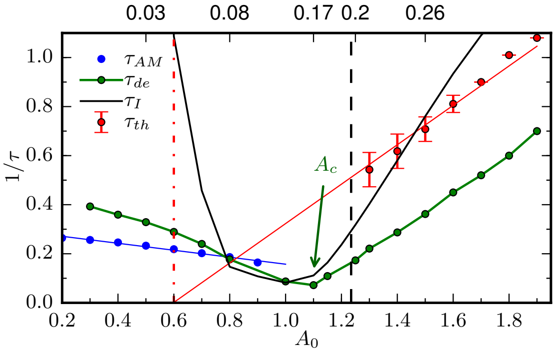
Order parameter $\langle c^\dagger_{k+Q,1} c_{k,2} \rangle$

- Reduction of the order parameter
- Different long time limit for weak(strong) excitations
- For strong excitation two time dynamics



Dynamical phase transition

- Prethermalization scenario: system is in the long lived trapped state
- Critical slowing down at nonthermal critical point
- Long time dynamics and thermal critical point: temperature vs doping
- Connection with PES



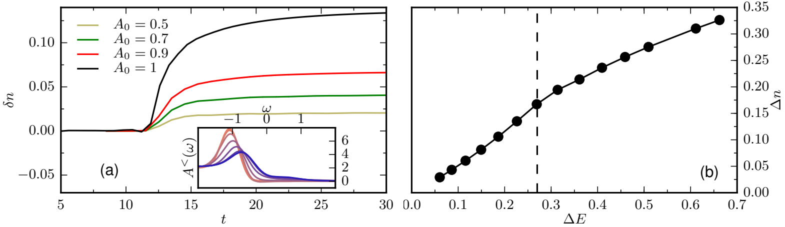
Gap closure

Transfer of kinetic energy to condensate

- Gap prevents fast recombination
- Intraband relaxation due to el.-el. scattering
- Impact ionization

Screening scenario

- Screening decrease the effective interaction



Screening

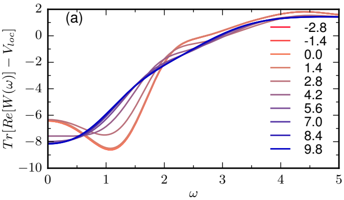
Frequency dependent interaction

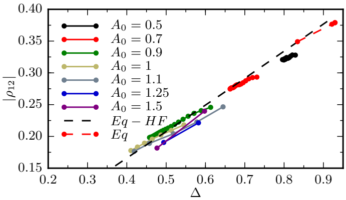
$$W_q(\omega) = \epsilon_q(\omega)^{-1} V_q$$

- How to construct low energy model ?
- Which energy scale is responsible for gap dynamics

"Phenomenological" approach

$$V_{eff} = \Delta / |\rho_{12}|$$

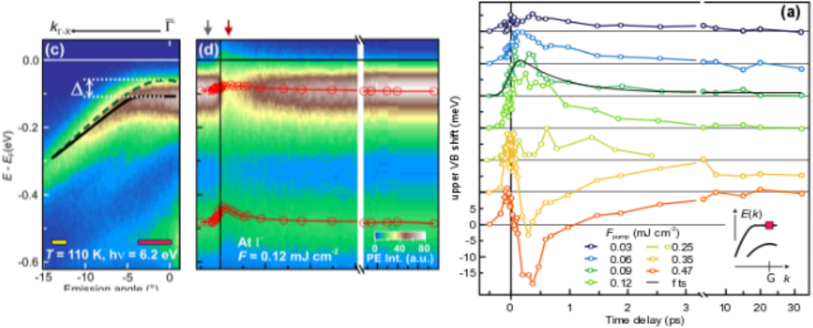




Semiconductor - gap enhancement

t-ARPES on Ta_2NiSe_5:

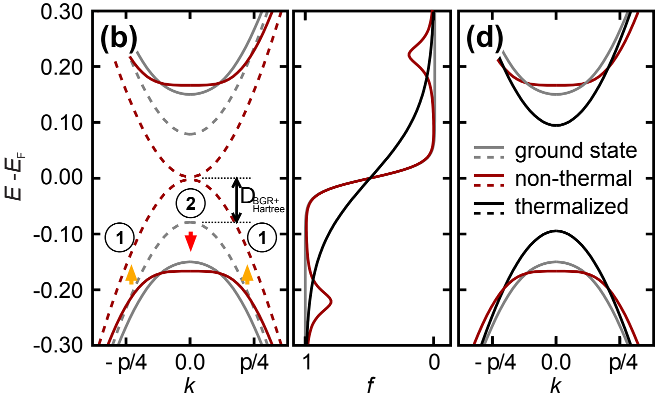
- Gap increase as one lowers temperature - possible excitonic insulator
- After photo-excitation momentum dependent renormalization of gap size
- Weak excitation vs strong excitations



Proposed mechanism

Hartree-Fock with nonthermal distribution function

- Fast intra-band relaxation of electrons
- Bottleneck due to presence of the gap
- Hartree shift leads to more resonating states at $k = 0$



Conclusions

Semimetal limit and gap closure
Semiconductor limit and gap manipulation

- Gap closure for semimetal: DG et.al., Phys. Rev. B 94, 035121 (2016)
- Selene Mor et.al., Band-gap enhancement in semiconductor limit: arXiv:1608.05586