TRANSIENT DYNAMICS IN AN EXCITONIC INSULATOR:

FAST COMPUTATION OF NONEQUILIBRIUM GREEN'S FUNCTIONS

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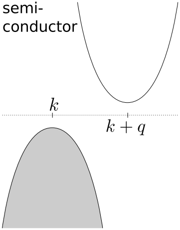
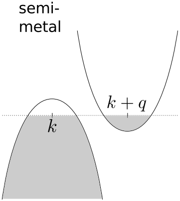
WHAT? EXCITONIC INSULATOR (EI) PHASE[1]

Indirect semiconductor (small gap) or -metal (small overlap)





Reduce the gap below exciton binding energy $\Rightarrow$ EI phase

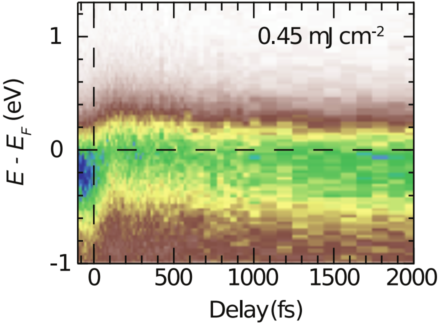
Reduce the overlap $\Rightarrow$ reduce the number of free carriers $\Rightarrow$ less screening $\Rightarrow$ EI phase

$\sim$ BCS superconductivity: electrons form Cooper pairs

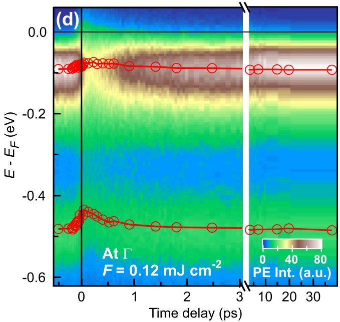
[1] N. F. Mott, Phil. Mag. **6**, 287 (1961); L. V. Keldysh and Yu. V. Kopaev, Sov. Phys. Solid State **6**, 2219 (1965); D. Jérome, T. M. Rice, and W. Kohn, Phys. Rev. **158**, 462 (1967)

WHY? RECENT TIME-DOMAIN EXPERIMENTS

Time-resolved ARPES measurements for materials exhibiting the EI phase [$TiSe_2$ and Ta_2NiSe_5]



S. Hellmann, *et al.*, EPJ Web of Conferences **41**, 03022 (2013)



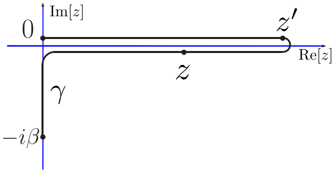
S. Mor, *et al.*, Phys. Rev. Lett. **119**, 086401 (2017)

Critical photoexcitation observed: band gap can be either enhanced (∼ increased exciton condensation) or decreased

HOW? TIME-PROPAGATION OF GREEN FUNCTIONS[2] [3]

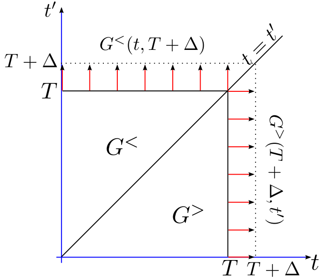
- Two-time Green's functions defined on the Keldysh contour

$$G(z,z') = -\mathrm{i}\langle T_\gamma[\hat{\psi}(z)\hat{\psi}^\dagger(z')]\rangle$$



- Integro–differential equations

$$[\mathrm{i}\partial_z - \underbrace{h}_{\text{System}}]G = \delta + \int_\gamma \underbrace{\Sigma}_{\text{Many-body effects}} G$$



- Expensive for both CPU and RAM

[2] A. Stan, N. E. Dahlen, and R. van Leeuwen, J. Chem. Phys. **130**, 224101 (2009)

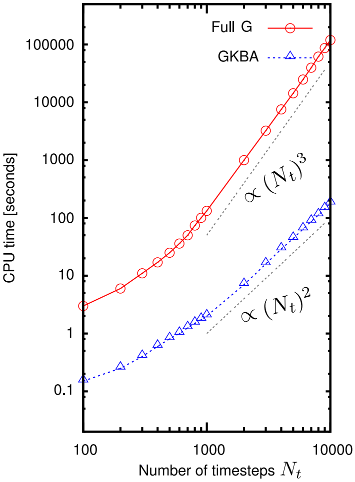
[3] G. Stefanucci and R. van Leeuwen, *Nonequilibrium Many-Body Theory of Quantum Systems: A Modern Introduction*, (Cambridge University Press, Cambridge, 2013)

GENERALIZED KADANOFF–BAYM ANSATZ (GKBA)[4 5]

- Full Green's function reconstructed from time-diagonal
  $G^{\lessgtr}(t,t') \approx$
  $\mathrm{i}\left[G^{\mathrm{R}}(t,t')G^{\lessgtr}(t',t') - G^{\lessgtr}(t,t)G^{\mathrm{A}}(t,t')\right]$

- Approximate propagators
  $G^{\mathrm{R/A}}(t,t') \approx$
  $\mp \mathrm{i}\theta[\pm(t-t')]\exp\left[-\mathrm{i}h(t-t')\right]$

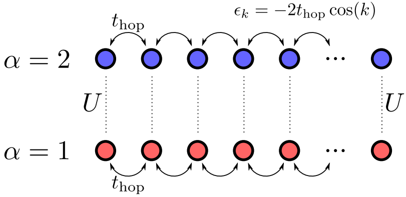
$\Rightarrow$ Evolution of a time-local density matrix $\rho(t) \equiv -\mathrm{i}G^{<}(t,t)$



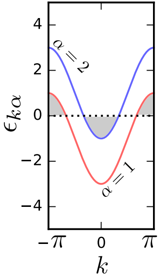
[4]P. Lipavský, V. Špička, and B. Velický, Phys. Rev. B **34**, 6933 (1986)
[5]S. Hermanns, K. Balzer, and M. Bonitz, Phys. Scr. **T151**, 014036 (2012)

MODEL FOR THE EXCITONIC INSULATOR[6]

One-dimensional two-band system with interband Hubbard interaction



$$
\begin{aligned}
\hat{H}(t) &= \hat{H}_{\mathrm{eq}} + \hat{H}_{\mathrm{ext}}(t), \\
\hat{H}_{\mathrm{eq}} &= \sum_{k\alpha} (\epsilon_{k\alpha} + \Delta_\alpha)\hat{c}^\dagger_{k\alpha}\hat{c}_{k\alpha} + \frac{1}{2}\sum_i U \hat{c}^\dagger_{i,1}\hat{c}_{i,1}\hat{c}^\dagger_{i,2}\hat{c}_{i,2}, \\
\hat{H}_{\mathrm{ext}}(t) &= \sum_k (E(t)\hat{c}^\dagger_{k,2}\hat{c}_{k,1} + \mathrm{h.c.})
\end{aligned}
$$



Excitonic order parameter: $\langle \hat{c}^\dagger_{(k+\pi)1}\hat{c}_{k2}\rangle \overset{!}{\neq} 0$

[6] D. Golež, P. Werner, and M. Eckstein, Phys. Rev. B **94**, 035121 (2016)

EQUILIBRIUM BY MATSUBARA GREEN FUNCTION

$$
\begin{aligned}
k^{\mathrm{M}}(\tau-\tau') &\equiv -\mathrm{i}k(-\mathrm{i}\tau,-\mathrm{i}\tau') \qquad (k=G,\Sigma) \\
(-\partial_\tau - h_{\mathrm{eq}})G^{\mathrm{M}}(\tau-\tau') &= \delta(\tau-\tau') + \int_0^\beta \mathrm{d}\bar{\tau}\,\Sigma^{\mathrm{M}}(\tau-\bar{\tau})G^{\mathrm{M}}(\bar{\tau}-\tau')
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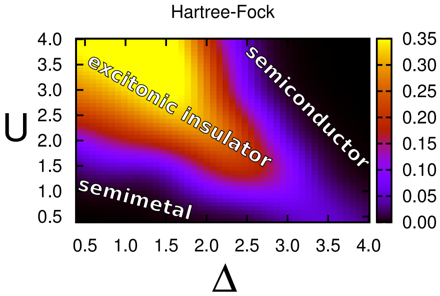
"Phase diagrams" using different self-energy approximations



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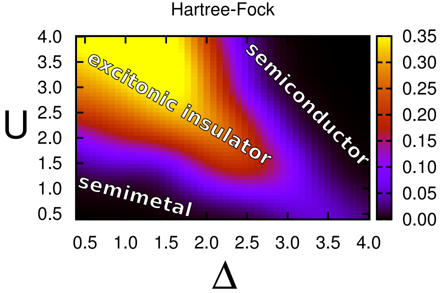

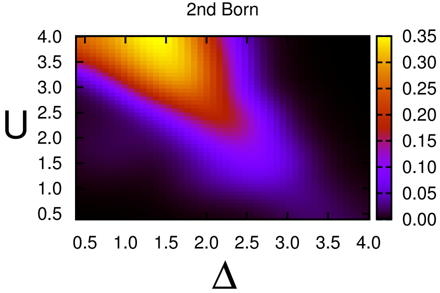

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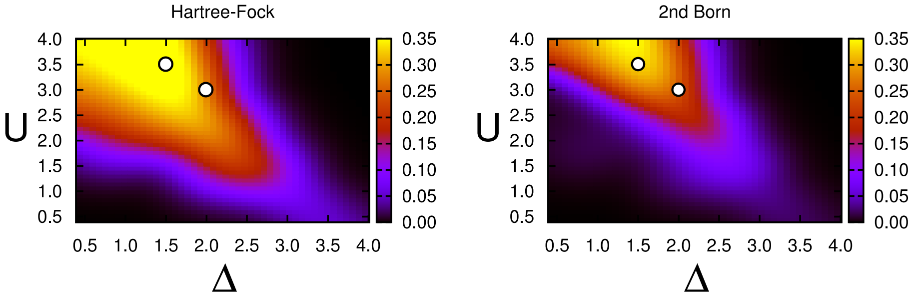
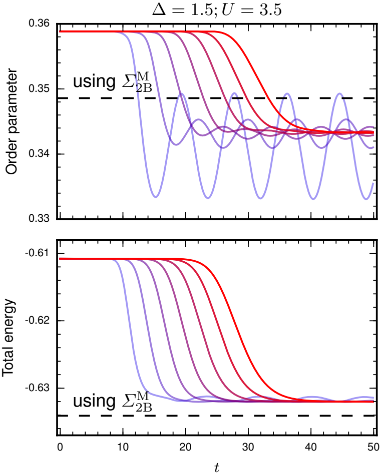


EQUILIBRIUM BY GKBA (ADIABATIC SWITCHING)



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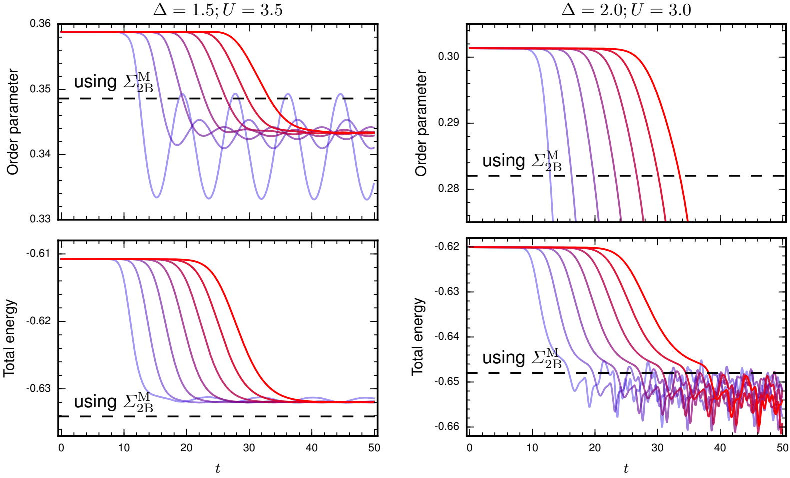

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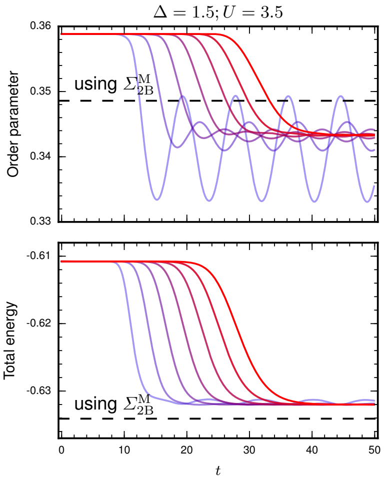
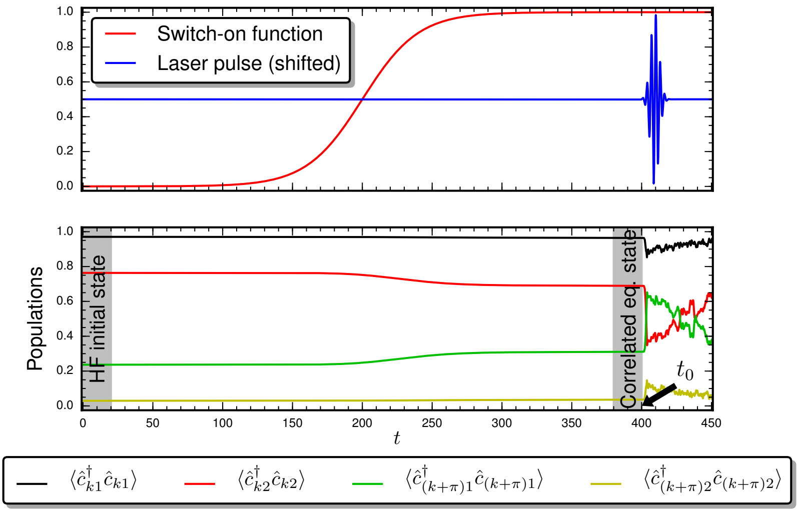


OUT-OF-EQUILIBRIUM: POPULATIONS AND ORDER



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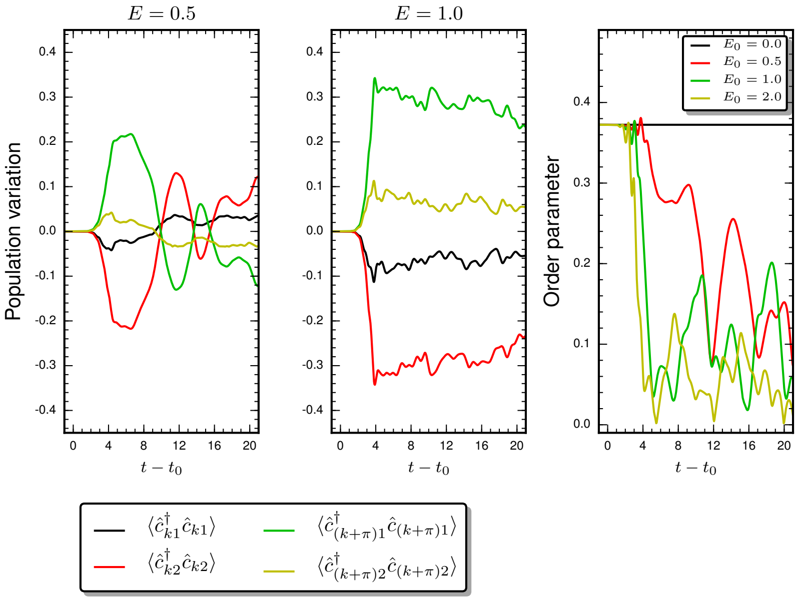

SUMMARY

- Ultrafast experiments available in materials exhibiting the excitonic insulator phase
- Theoretical description is a challenge (electronic correlations, transient regime, ...)
- Generalized Kadanoff–Baym Ansatz computationally more applicable (must be careful though!)
- Preliminary results show light-induced population inversion and melting of the excitonic condensate