ULTRAFAST MANY-BODY CORRELATIONS

IN AN EXCITONIC INSULATOR OUT OF EQUILIBRIUM

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Emmy Noether-Programm DFG Deutsche Forschungsgemeinschaft

FNSNF Swiss National Science Foundation

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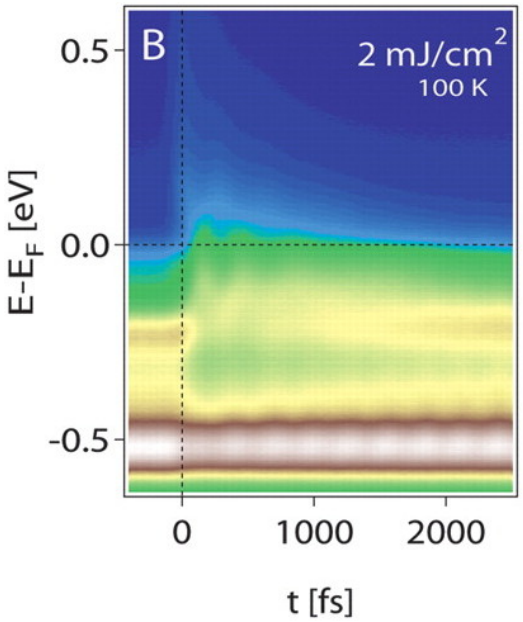
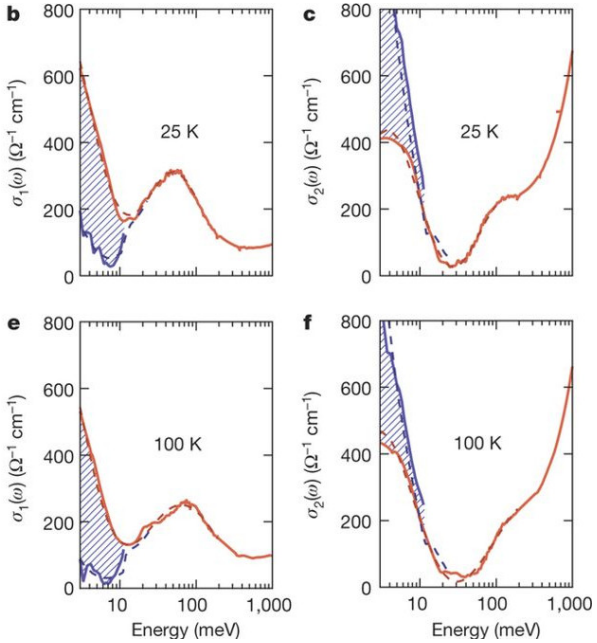
TRANSIENT SPECTROSCOPY OF ORDERED PHASES

Charge-density wave



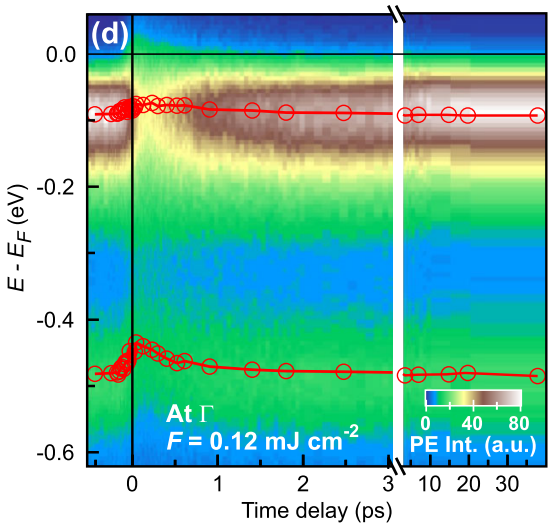
F. Schmitt *et al.*, Science **321**, 1649 (2008)

Superconductivity



M. Mitrano *et al.*, Nature **530**, 461 (2016)

Excitonic insulator



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

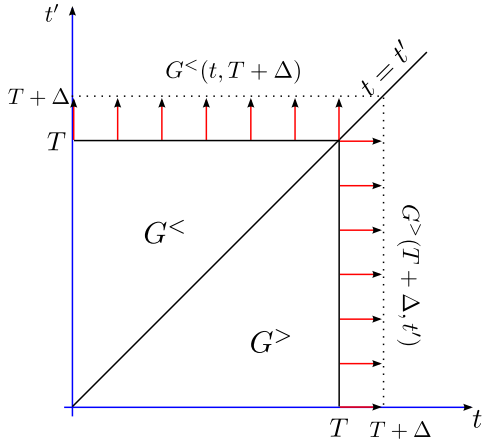
NONEQUILIBRIUM GREEN'S FUNCTION THEORY*†

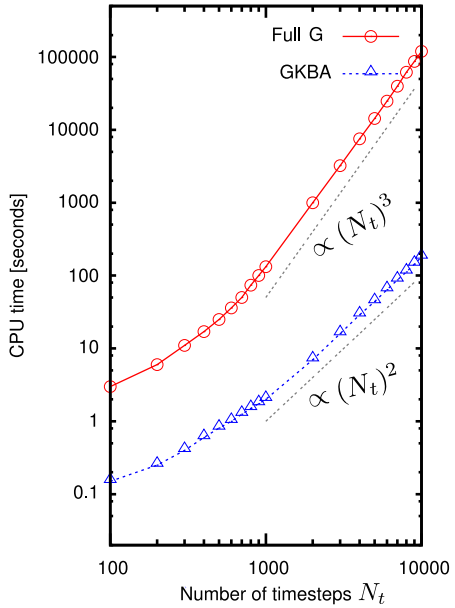
- Two-time Green's functions
  $G(t,t') = -\mathrm{i}\langle T[\hat{\psi}(t)\hat{\psi}^\dagger(t')]\rangle$
  (expensive for both CPU and RAM)

$$[\mathrm{i}\partial_t - h\,]G = \delta + \int \mathrm{d}t\ \Sigma\ G$$

System Many-body effects

- Generalized Kadanoff–Baym Ansatz (GKBA) as cheaper alternative
  $G^{\lessgtr}(t,t') \approx$
  $\mathrm{i}\left[G^{\mathrm{R}}(t,t')G^{\lessgtr}(t',t') - G^{\lessgtr}(t,t)G^{\mathrm{A}}(t,t')\right]$
- This work: GKBA for ordered phases



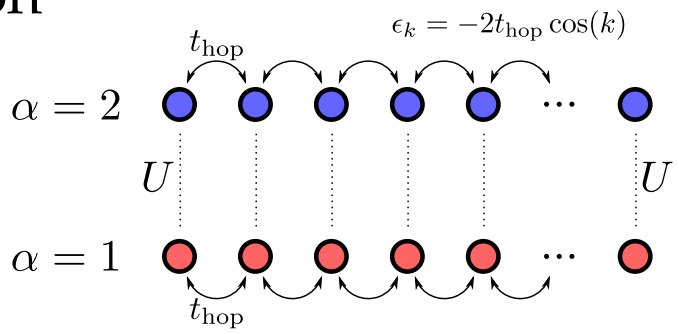


*A. Stan, N. E. Dahlen, and R. van Leeuwen, J. Chem. Phys. **130**, 224101 (2009)

†R. Tuovinen, D. Golež, M. Schüler, P. Werner, M. Eckstein, and M. A. Sentef, Phys. Status Solidi B (2018) (`arXiv:1808.00712`)

MODEL FOR THE EXCITONIC INSULATOR* †

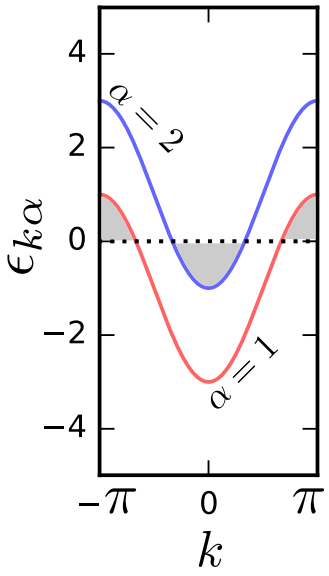
One-dimensional two-band system with interband Hubbard interaction



$$\hat{H}(t) = \hat{H}_{\rm eq} + \hat{H}_{\rm ext}(t),$$

$$\hat{H}_{\rm eq} = \sum_{k\alpha}(\epsilon_{k\alpha} + \Delta_\alpha)\hat{c}^\dagger_{k\alpha}\hat{c}_{k\alpha} + \sum_i U\hat{c}^\dagger_{i,1}\hat{c}_{i,1}\hat{c}^\dagger_{i,2}\hat{c}_{i,2},$$

$$\hat{H}_{\rm ext}(t) = \sum_k (E(t)\hat{c}^\dagger_{k,2}\hat{c}_{k,1} + \text{h.c.})$$



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

($\sim$ BCS superconductivity: electrons form Cooper pairs)

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

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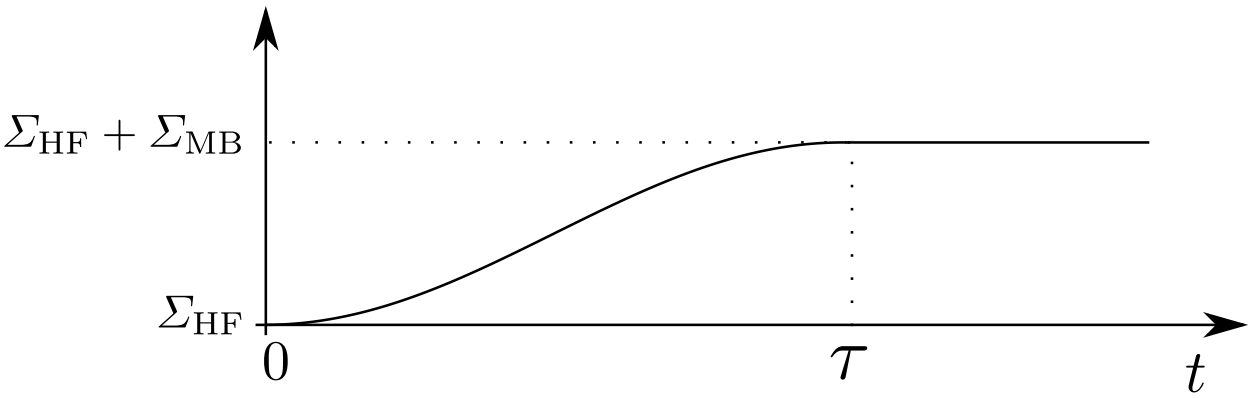
EQUILIBRIUM BY GKBA: ADIABATIC SWITCHING*



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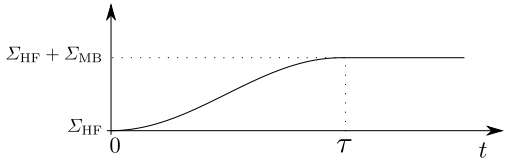

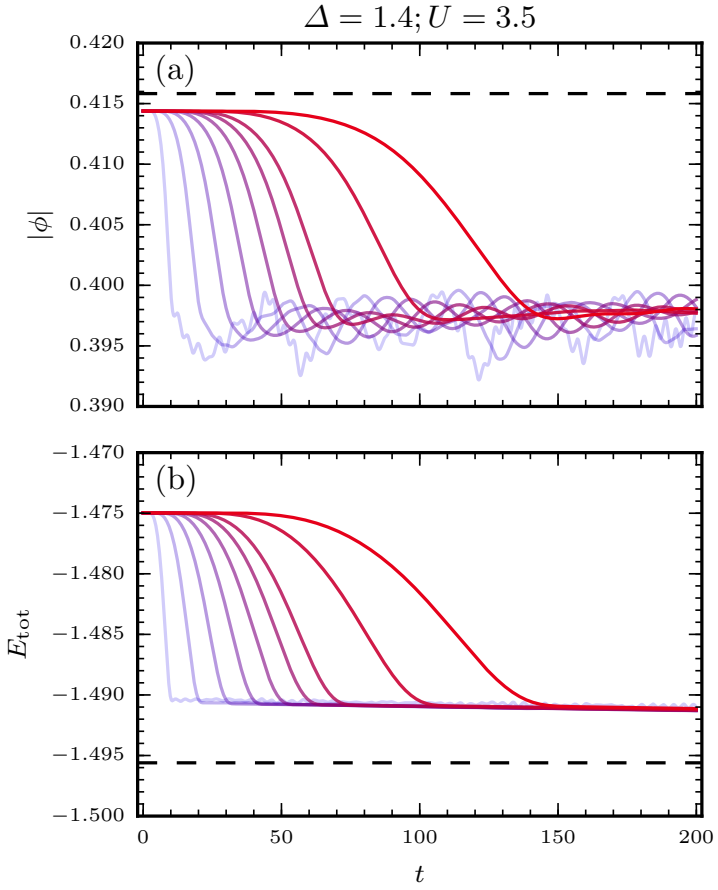

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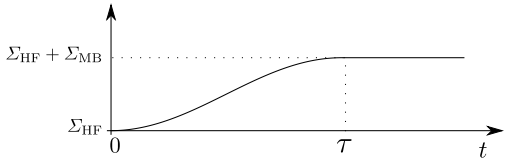

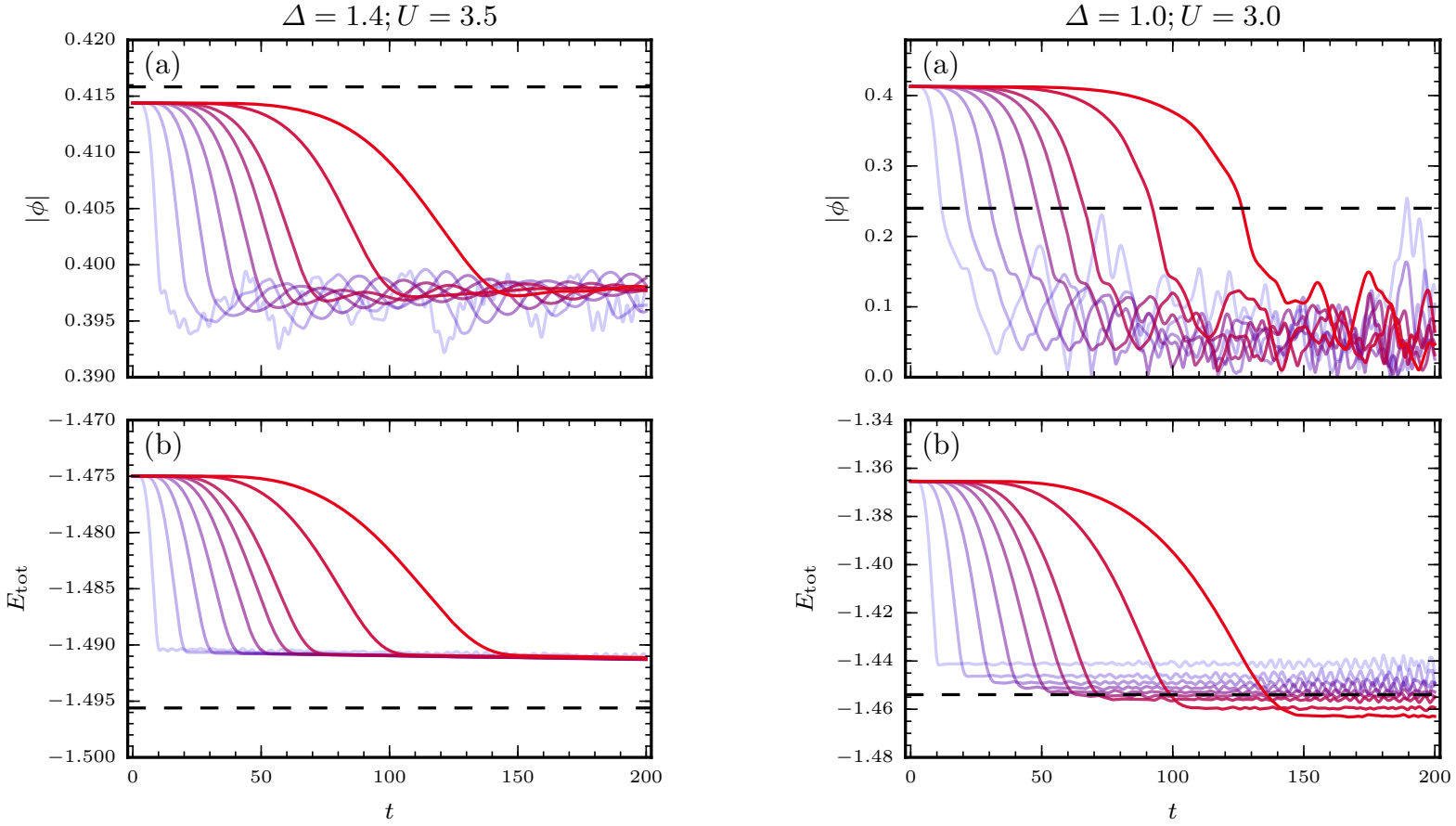

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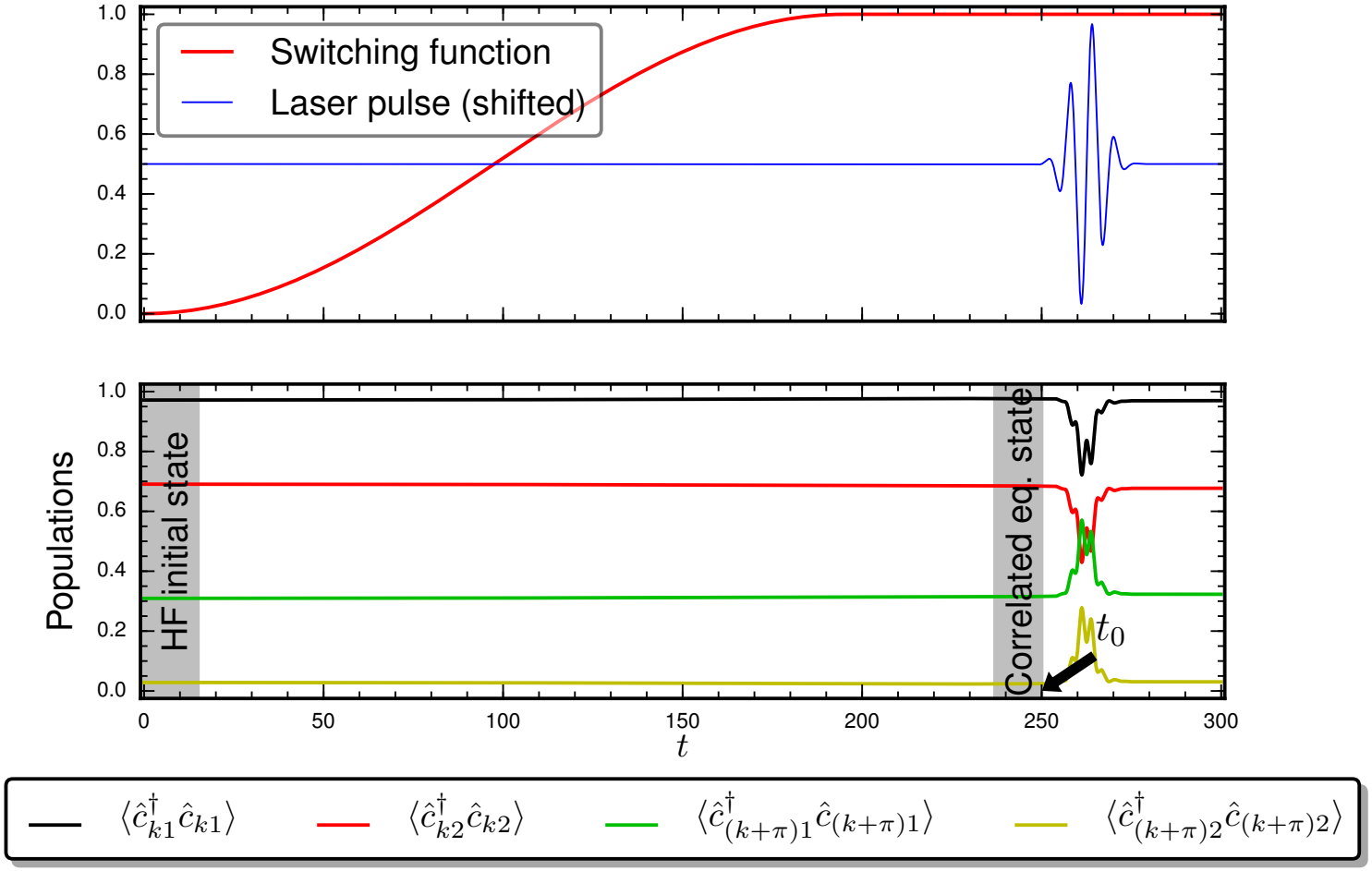
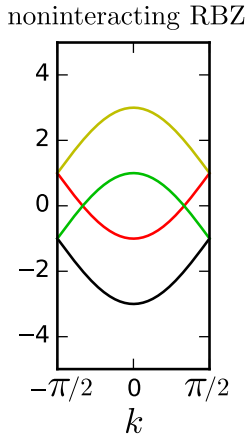
OUT-OF-EQUILIBRIUM: POPULATIONS AND ORDER





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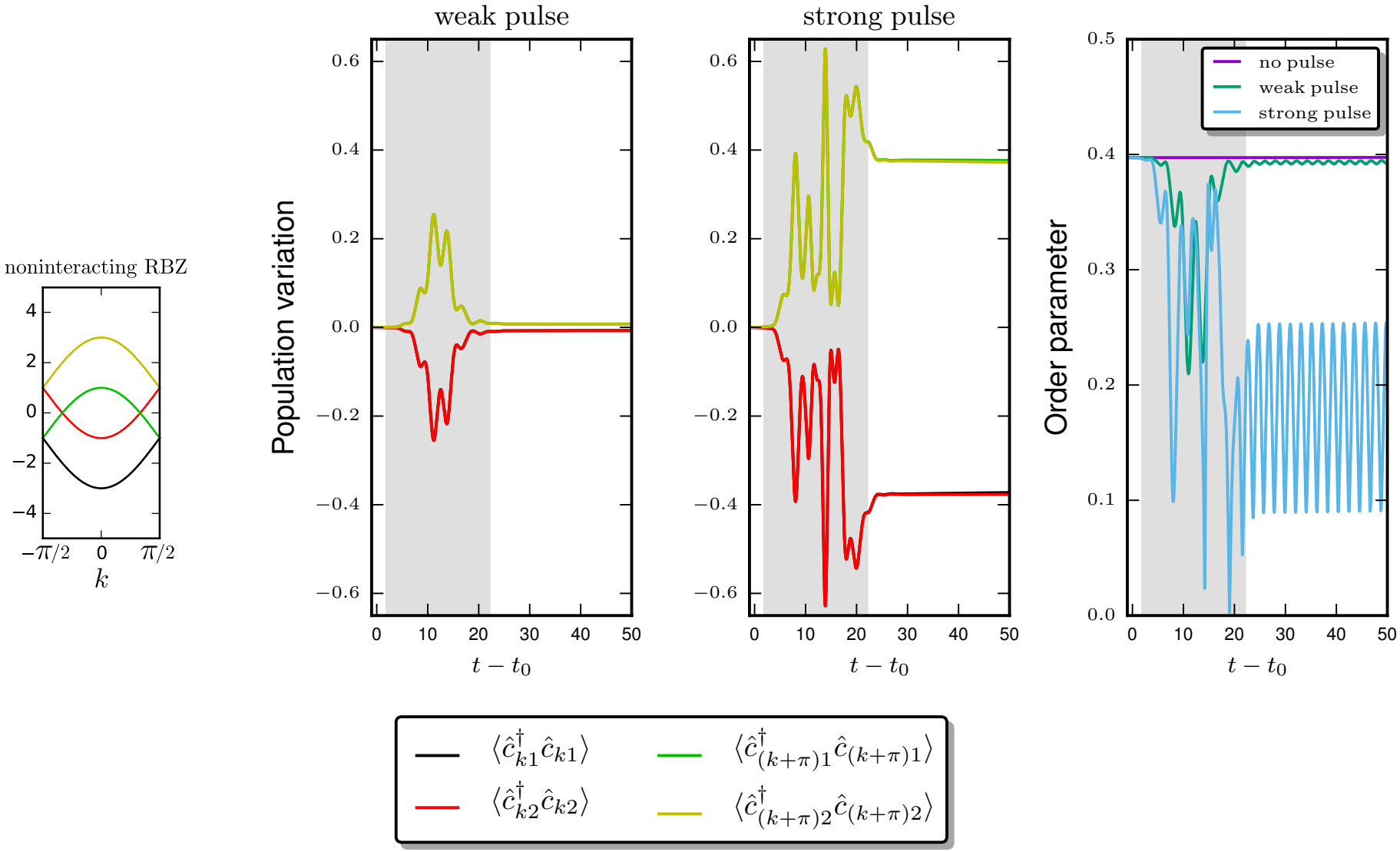

SUMMARY

- Ultrafast experiments available in, e.g., transition-metal dichalcogenide materials exhibiting the EI phase
- Theoretical description is a challenge (electronic correlations, transient regime, . . .)
- Generalized Kadanoff–Baym Ansatz computationally tractable (assess validity vs. full KBE)
- Equilibrium: symmetry-broken correlated initial state with nonzero excitonic order parameter (using the GKBA)
- Out-of-equilibrium: light-induced population inversion and melting of the excitonic condensate

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postdoc position available
starting fall 2019
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FNSNF Swiss National Science Foundation
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