Quadratic *e-ph* coupling

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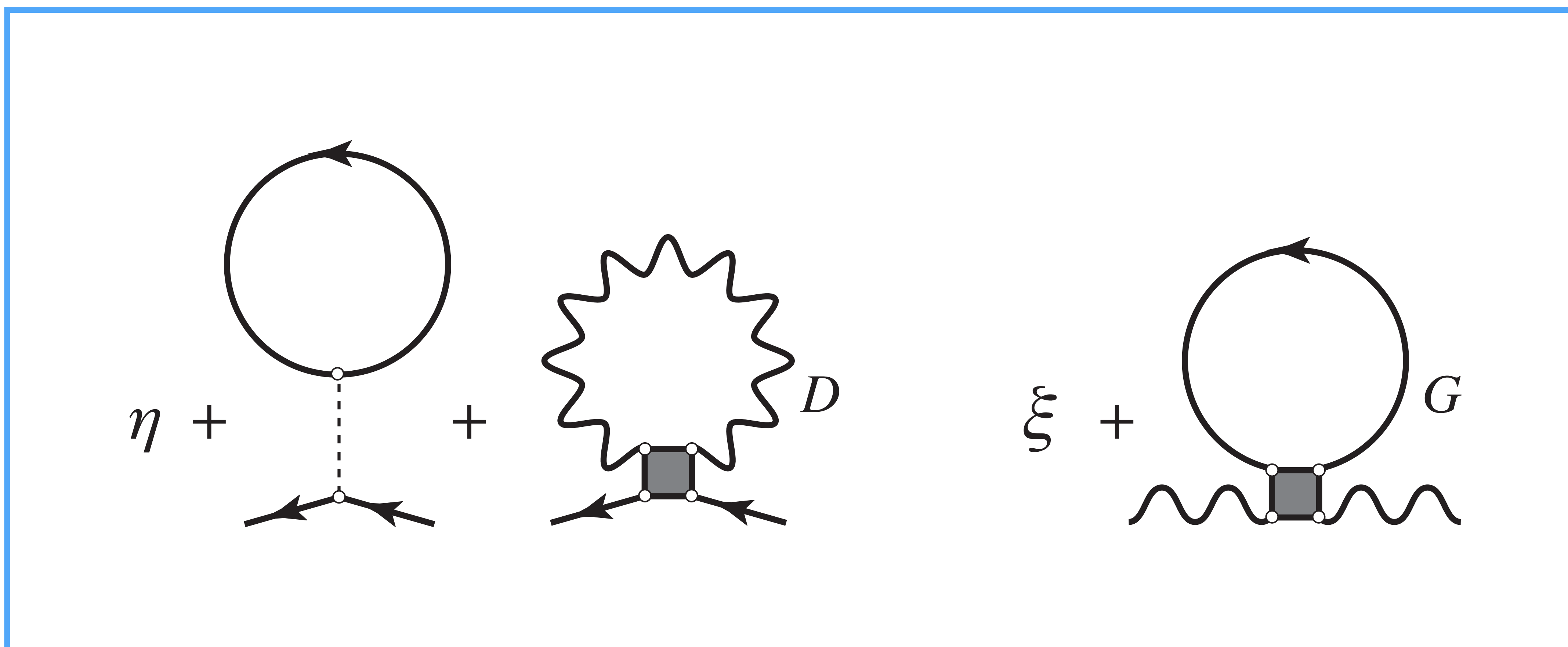


Acknowledgements

- Michael Schüler—NEGF for electron-plasmon coupling
  Phys. Rev. B **93**, 054303 (2016), **NESSY**-code
- Andrea Marini—Functional approach to arbitrary strong *e-ph* interaction
  Phys. Rev. B. **98**, 075105 (2018)
- Gianluca Stefanucci and Robert van Leeuwen—PSD approximations
  Phys. Rev. B. **90**, 115134 (2014)

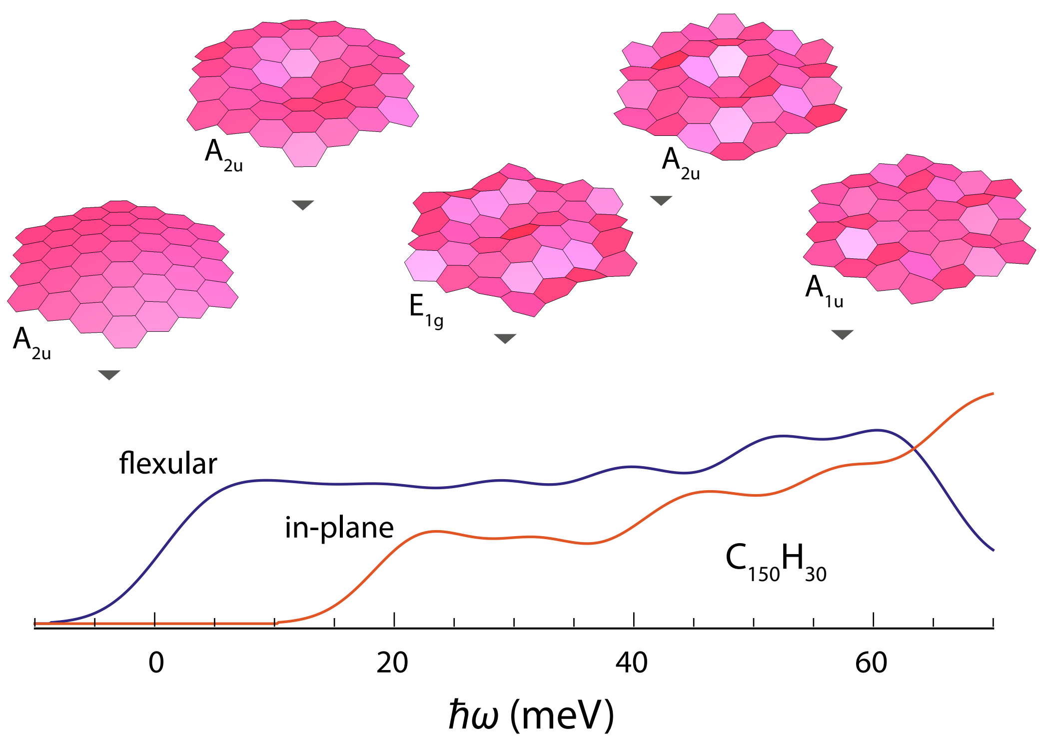
Outline

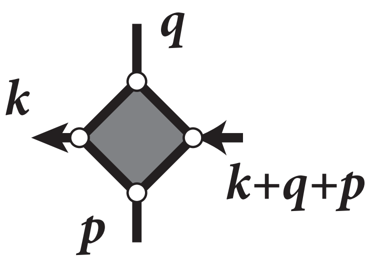
I. **KBEt^2*+nQ*^{2}**—Motivation:
   A. Scattering and dephasing
   B. Satellites
   C. Transient superconductivity

II. Functional approach
   A. Generalization of Hedin's eq.
   B. Sunrise, Debye-Waller, Fan-Migdal
   C. Pitfalls of non-equilibrium: $\langle Q \rangle$

III. Numerical results
   A. Single-site: linear vs. quadratic
   B. k-space: phonon window

I.A.Scattering and dephasing



$g(\boldsymbol{k},\boldsymbol{q},\boldsymbol{p}) \;=$ 

I.A. Scattering and dephasing

Flexural phonons in graphene:

- Long wavelength out-of-plane distortions from the elasticity theory (*Mariani and von Oppen, 2008*)
- Main mechanism limiting the resistivity in suspended graphene at small temperatures (*Castro et al., 2010*)
- Balance between linear and quadratic coupling can be influenced by the electrostatic gating (*Gunst et al., 2017*)

Large 2nd-order corrections in carbon materials—*ab initio* approach:

- Electron-phonon renormalization of the band gap in diamond (*Giustino, Louie, and Cohen, 2010*)
- Effect of the Quantum Zero-Point Atomic Motion on the Electronic Properties of Diamond and trans-Polyacetylene (*Cannuccia and Marini, 2011*)

Quadratic coupling of carriers in QD to acoustic phonons:

- Linear coupling generates satellites, but causes no Lorentzian broadening
- Polarization decay and exponential dephasing
- Cumulant expansion (*Muljarov and Zimmermann, 2004*)

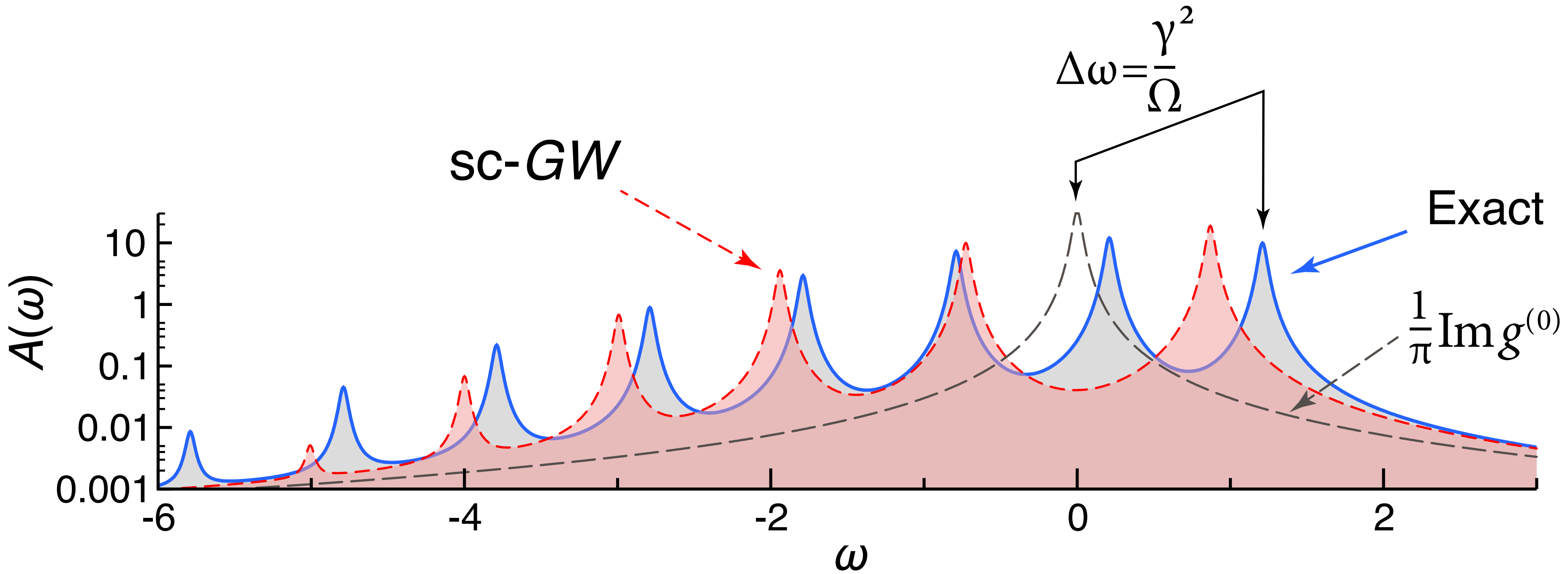
Nonlinear Holstein model:

- Quantum Monte Carlo approach (*Li, Nowadnick, and Johnston, 2015*)
- Momentum average approximation (*Adolphs and Berciu; 2013*)

Diagrammatic approach:

- *Marini, Poncé, and Gonze, 2015*
- *Giustino, 2017*

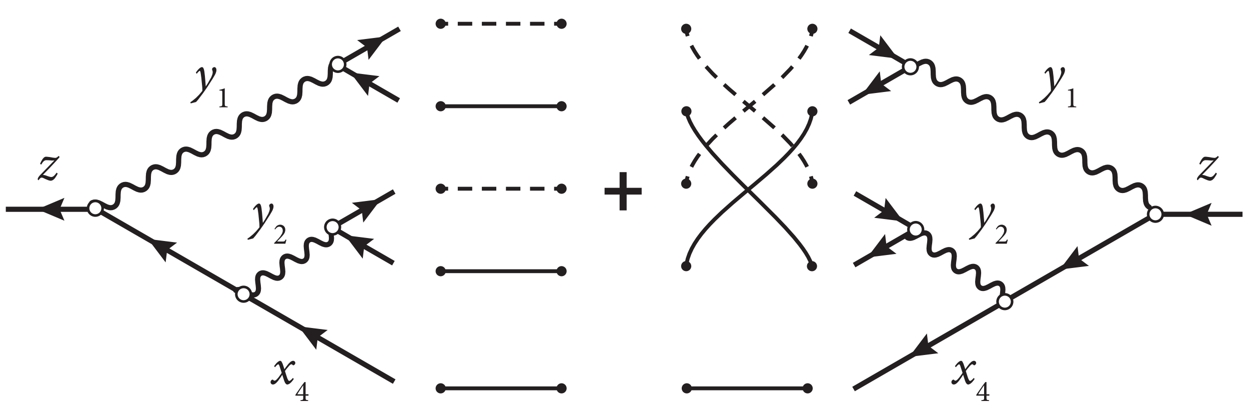
I.B.Satellites



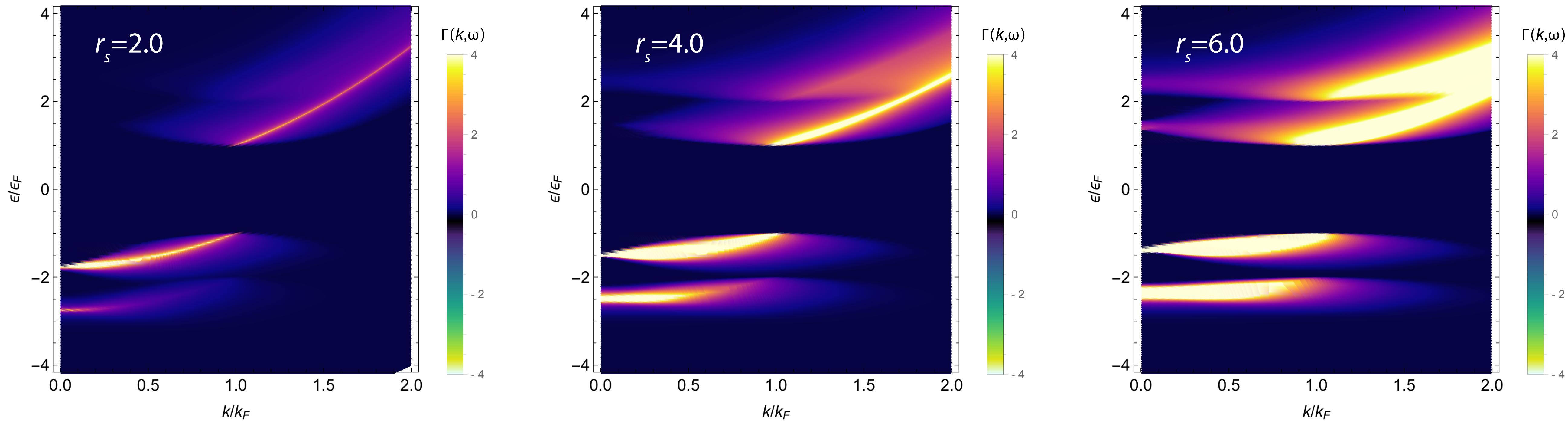
Y. Pavlyukh, *Padé resummation of many-body perturbation theories*, Sci.Rep. **7**, 41598 (2017)

I.B. Satellites

$\Sigma_{cc} + \Sigma_{c\bar{c}} =$

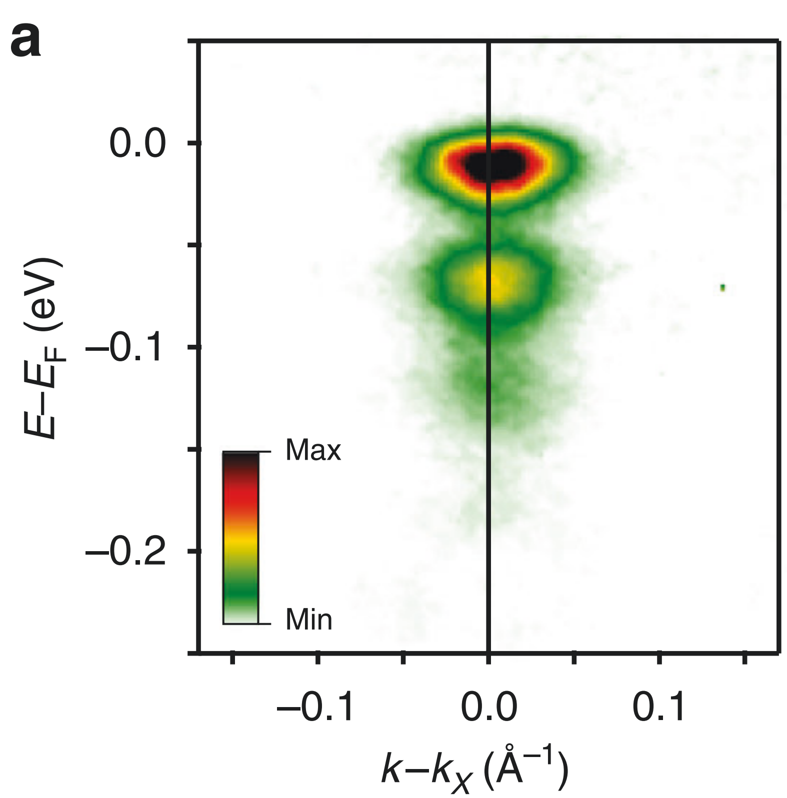


1. The Langreth solution (1970): *n*th order satellite results from the emission of *n* bosons—real or quasiparticle
2. Forget MBPT, **think of scattering processes**!
3. Sensitive to doping, can hybridise, is observable spectroscopically
4. Can we influence the strength and the position of satellites by external driving?



Y. P., G. Stefanucci & R. van Leeuwen, *in preparation*

I.B.Satellites



J.M. Riley, *et al.*, Spin-polarised electron gas in ferromagnetic EuO, Nature Commun. **9**:2305 (2018)

1. Langreth solution: *n*th order satellite results from the emission of *n* bosons—real or quasiparticle
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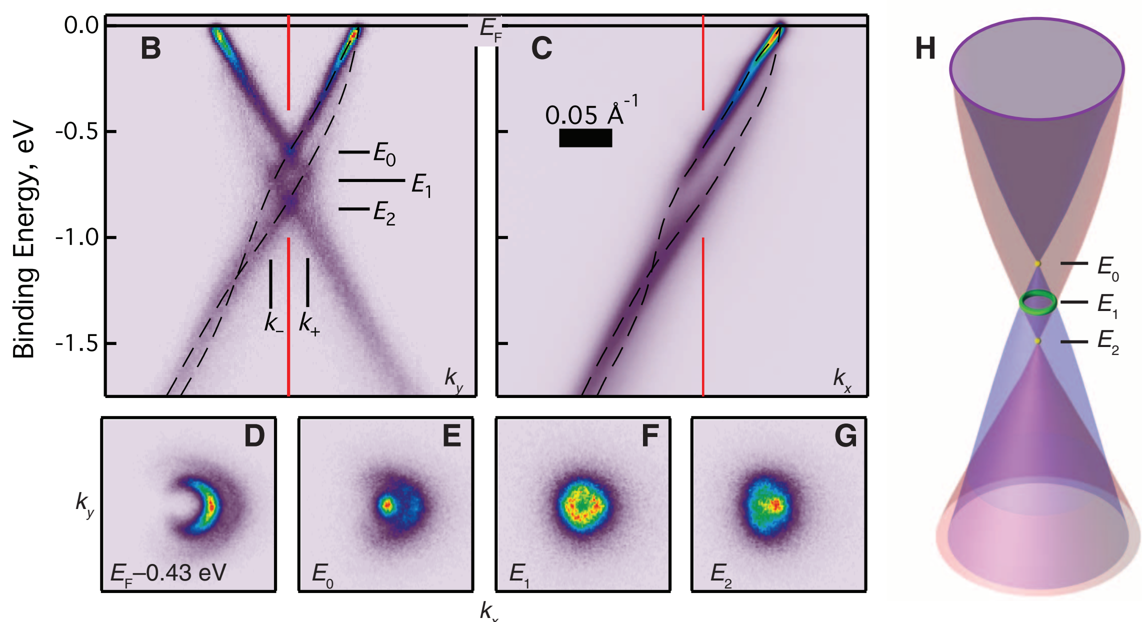
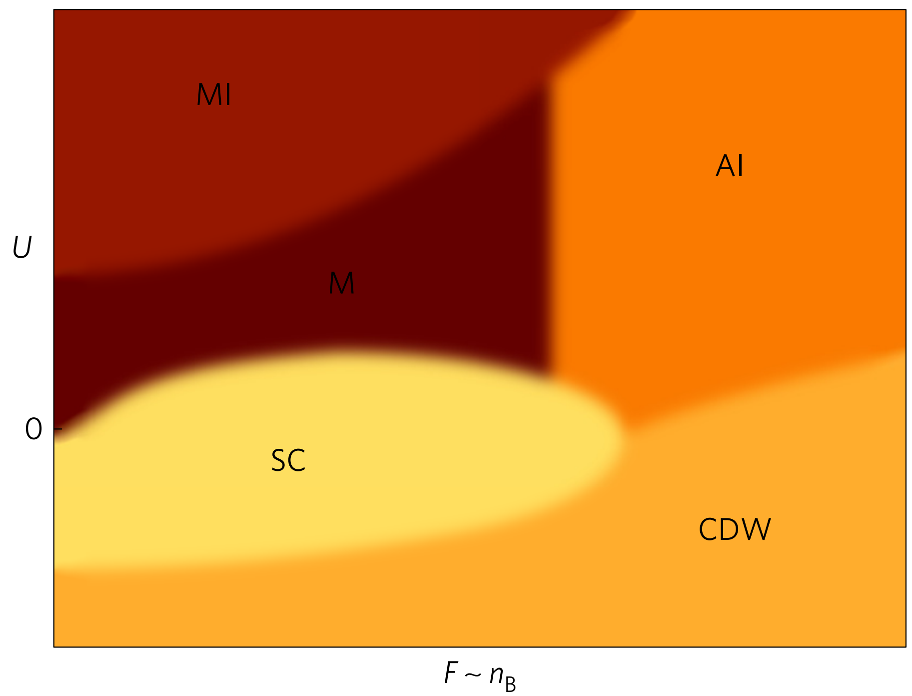


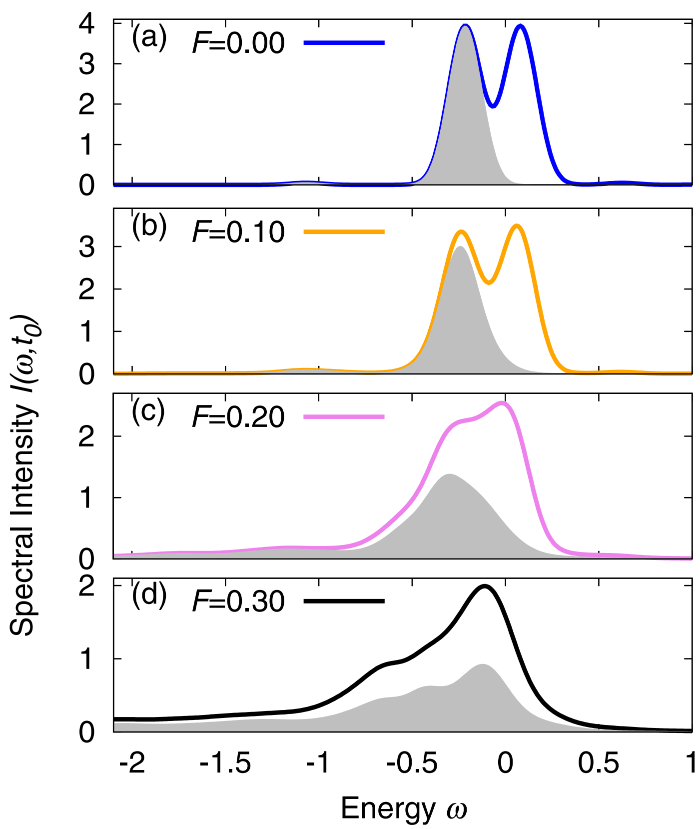
A. Bostwick *et al.*, Observation of Plasmarons in Quasi-Freestanding Doped Graphene, Science **328**, 999 (2010)

I.C. Transient superconductivity



D. M. Kennes, E. Y. Wilner, D. R. Reichman, and A. J. Millis, Nature Phys. **13**, 479 (2017)

1. Pumping the IR-active phonon modes
2. Solution by a canonical transformation
3. Effective hopping and Hubbard U depend on n_B—number of bosons in the system
4. Can we influence the strength and the position of satellites by external driving?



M.A.Sentef, Phys. Rev. B. **95**, 205111 (2017)

II.A. Functional approach— generalization of Hedin’s equations

Outline

- Bosons: photons, phonons, plasmons, etc.
- Specific features of the electron-boson (e-b) coupled systems
  - No Wick's theorem for bosons
  - 2nd-order equation-of-motion for bosonic Green's function
  - For certain scenarios higher-order diagrammatic theories can be constructed
  - No universal "electron-boson" interaction, specific form needs to be derived for each case of interest
- Method of functional derivatives
  - Allows to generate many-body perturbation theories even in absence of the Wick's theorem
  - Quick way to derive functional relations between the *dressed* correlators
  - Hedin's equations are derived in this way

Electrons

$$\left\{ \hat{\psi}^{\dagger}(\mathbf{x}), \hat{\psi}(\mathbf{y}) \right\} = \delta(\mathbf{x}-\mathbf{y}),$$
$$\left\langle \hat{\psi}(\mathbf{x}) \hat{\psi}(\mathbf{x}) \right\rangle = 0$$

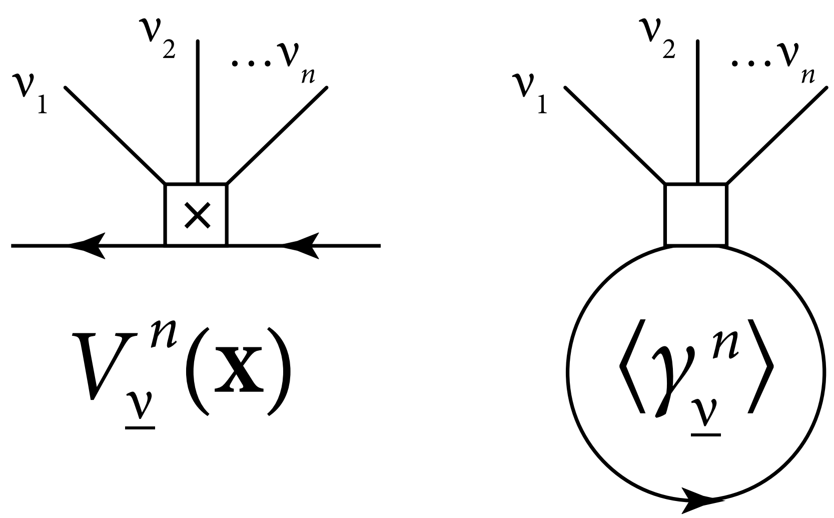
Bosons

$$\left[\widehat{Q}_{\mu}, \widehat{P}_{\nu}\right] = i\delta_{\mu\nu},$$
$$\left\langle \widehat{Q}_{\mu} \widehat{Q}_{\mu} \right\rangle \neq 0$$

- **Generalizations for nonlinear *e-b* interactions in the bosonic displacement**

General theory

Electrons ⟷ Bosons: photons, plasmons, phonons



Electron-boson interaction

$$\widehat{H}_{\text{e–b}} = \sum_{n,\underline{\nu}} \int d\mathbf{x}\, \hat{\psi}^{\dagger}(\mathbf{x})\, V_{\underline{\nu}}^{n}(\mathbf{x})\, \hat{\psi}(\mathbf{x})\, \widehat{Q}_{\underline{\nu}}^{n}$$

$$\hat{\gamma}_{\underline{\nu}}^{n} \equiv \int d\mathbf{x}\, \hat{\psi}^{\dagger}(\mathbf{x})\, V_{\underline{\nu}}^{n}(\mathbf{x})\, \hat{\psi}(\mathbf{x})$$

$$\widehat{H}_{\text{e–b}} = \sum_{n,\underline{\nu}} \hat{\gamma}_{\underline{\nu}}^{n}\, \widehat{Q}_{\underline{\nu}}^{n}$$

Hamiltonian and propagators

Total Hamiltonian

$$\hat{H}_{\mathrm{e}} = \int d\mathbf{x}\, \hat{\psi}^{\dagger}(\mathbf{x})\, h_e(\mathbf{x})\, \hat{\psi}(\mathbf{x})$$

$$\widehat{H}_{\mathrm{b}} = \frac{1}{2}\sum_{\nu} \Omega_{\nu} \left(\widehat{P}_{\nu}^{2} + \widehat{Q}_{\nu}^{2} \right)$$

$$\widehat{H}_{\mathrm{e-b}} = \sum_{n,\underline{\nu}} \hat{\gamma}_{\underline{\nu}}^{n} \widehat{Q}_{\underline{\nu}}^{n}$$

Propagators

$$G(1,2) = -i \left\langle \mathscr{T} \left\{ \hat{\psi}(1)\, \hat{\psi}^{\dagger}(2) \right\} \right\rangle$$

$$D_{\underline{\mu},\underline{\nu}}^{m,n}(z_1,z_2) = -i \left\langle \mathscr{T} \left\{ \Delta \widehat{Q}_{\underline{\mu}}^{m}(z_1)\, \Delta \widehat{Q}_{\underline{\nu}}^{n}(z_2) \right\} \right\rangle$$

with $\Delta \hat{\mathscr{O}} \equiv \hat{\mathscr{O}} - \langle \hat{\mathscr{O}} \rangle$

and $1 \equiv (\mathbf{x}_1, z_1)$

EOMs for operators

$$i \frac{d}{dz_1} \hat{\psi}(1) = \left[h_{\mathrm{e}}(1) + \sum_{n,\underline{\nu}} V_{\underline{\nu}}^{n}(\mathbf{x}_1)\, \widehat{Q}_{\underline{\nu}}^{n}(z_1) \right] \hat{\psi}(1)$$

$$\left[\frac{d^2}{dz_1^2} + \Omega_{\nu}^{2} \right] \widehat{Q}_{\nu}(z_1) = -\Omega_{\nu} \sum_{m,\underline{\mu}} m\, \hat{\gamma}_{\underline{\mu}\oplus\nu}^{m}(z_1)\, \widehat{Q}_{\underline{\mu}}^{m-1}(z_1)$$

Method of functional derivatives

Time-dependent Hamiltonian

$$\hat{H}_{\xi,\eta}(z) = \hat{H} + \sum_{n,\underline{\nu}} \xi^n_{\underline{\nu}}(z)\, \widehat{Q}^n_{\underline{\nu}} + \int d\mathbf{x}\, \eta(\mathbf{x},z)\, \hat{\rho}(\mathbf{x})$$

$$\left\langle \hat{\mathscr{O}}(z) \right\rangle_{\xi,\eta} = \frac{\mathrm{Tr}\left\{ \mathscr{T} \exp\left[-i \int_{\mathscr{C}} d\bar{z}\, \widehat{H}_{\xi,\eta}(\bar{z}) \right] \hat{\mathscr{O}}_{\xi,\eta}(z) \right\}}{\mathrm{Tr}\left\{ \mathscr{T} \exp\left[-i \int_{\mathscr{C}} d\bar{z}\, \widehat{H}_{\xi,\eta}(\bar{z}) \right] \right\}}$$

Timeline:

P.C. Martin and J. Schwinger (1959)

L. Hedin (1965), G. Strinati (1988)

R. van Leeuwen (2004), F. Giustino (2017)

Electrons

Actual vs. desired form

$$\left[i\frac{\partial}{\partial z_1} - h_\mathrm{e}(1) \right] G(1,2) = \delta(1,2) - i \sum_{n,\underline{\nu}} V^n_{\underline{\nu}}(\mathbf{x}_1) \times \left\langle \mathscr{T} \left\{ \hat{\psi}(1)\, \widehat{Q}^n_{\underline{\nu}}(z_1)\, \hat{\psi}^\dagger(2) \right\} \right\rangle$$

$$\left[i\frac{\partial}{\partial z_1} - h_\mathrm{e}(1) - \Phi(1) \right] G(1,2) = \delta(1,2) + \int d3\, \Sigma(1,3)\, G(3,2)$$

Self-energy and mean-field potential

Exploitation of variational derivatives

$$-i \left\langle \mathscr{T} \hat{\psi}(1)\, \widehat{Q}^n_{\underline{\nu}}(z_1)\, \hat{\psi}^\dagger(2) \right\rangle = \left[i\frac{\delta}{\delta \xi^n_{\underline{\nu}}(z_1)} + \left\langle \widehat{Q}^n_{\underline{\nu}}(z_1) \right\rangle \right] G(1,2)$$

Method of functional derivatives

Time-dependent Hamiltonian

$$\hat{H}_{\xi,\eta}(z) = \hat{H} + \sum_{n,\underline{\nu}} \xi^n_{\underline{\nu}}(z)\,\widehat{Q}^n_{\underline{\nu}} + \int d\mathbf{x}\,\eta(\mathbf{x},z)\,\hat{\rho}(\mathbf{x})$$

$$\left\langle \hat{\mathscr{O}}(z) \right\rangle_{\xi,\eta} = \frac{\mathrm{Tr}\left\{ \mathscr{T} \exp\left[-i \int_{\mathscr{C}} d\bar{z}\, \widehat{H}_{\xi,\eta}(\bar{z}) \right] \hat{\mathscr{O}}_{\xi,\eta}(z) \right\}}{\mathrm{Tr}\left\{ \mathscr{T} \exp\left[-i \int_{\mathscr{C}} d\bar{z}\, \widehat{H}_{\xi,\eta}(\bar{z}) \right] \right\}}$$

Timeline:

P.C. Martin and J. Schwinger (1959)

L. Hedin (1965), G. Strinati (1988)

R. van Leeuwen (2004), F. Giustino (2017)

In short, the perturbation framework developed by Julian is superior to the conventional scheme in that:

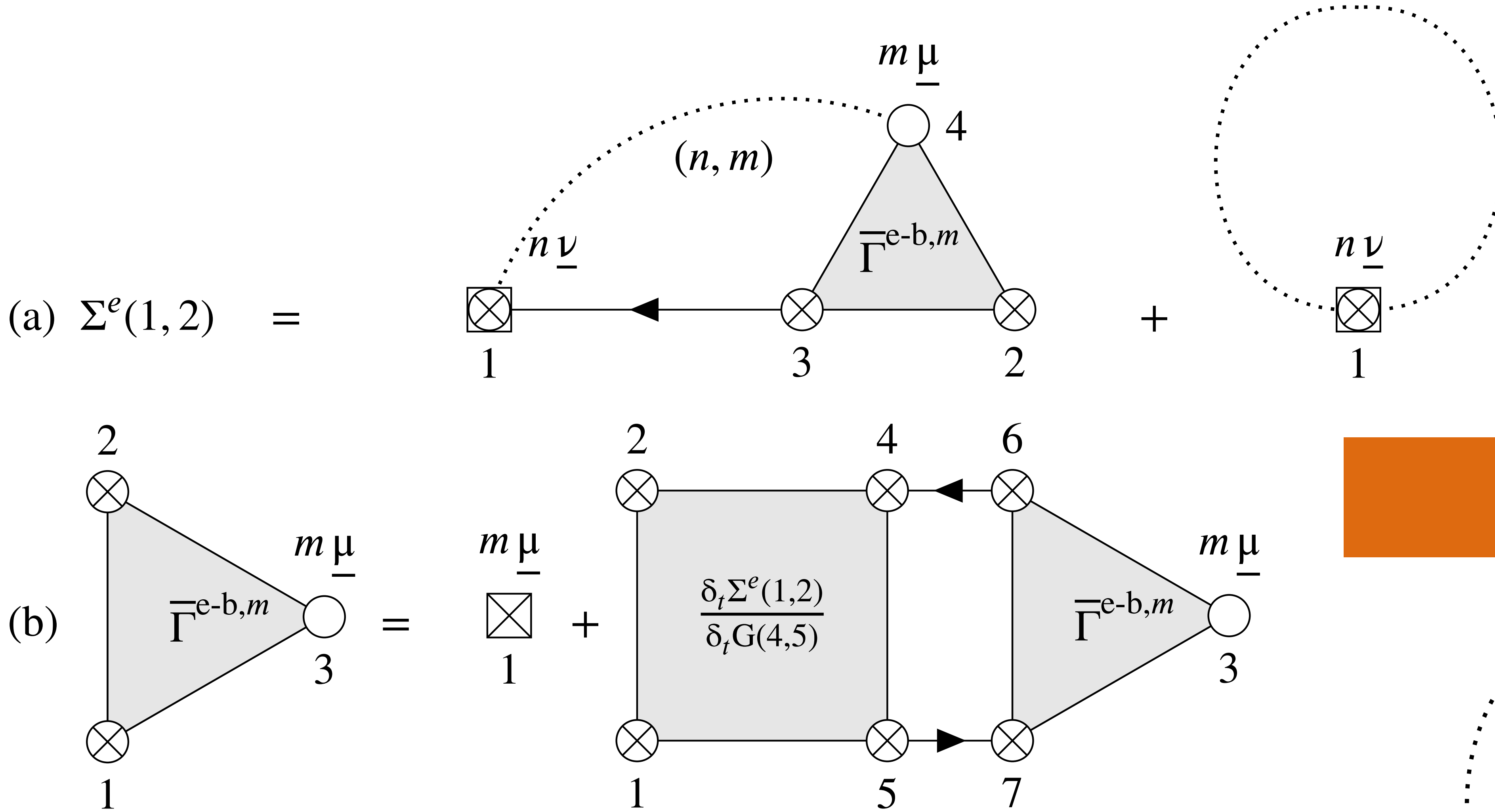
1) It allows for and "insists upon" the possibility for anomalous propagators. This possibility arises naturally because the theory is phrased entirely in terms of "true", rather than "bare", propagators.

2) It makes no "adiabatic" perturbative assumption, and thus allows naturally for self-consistent solutions.

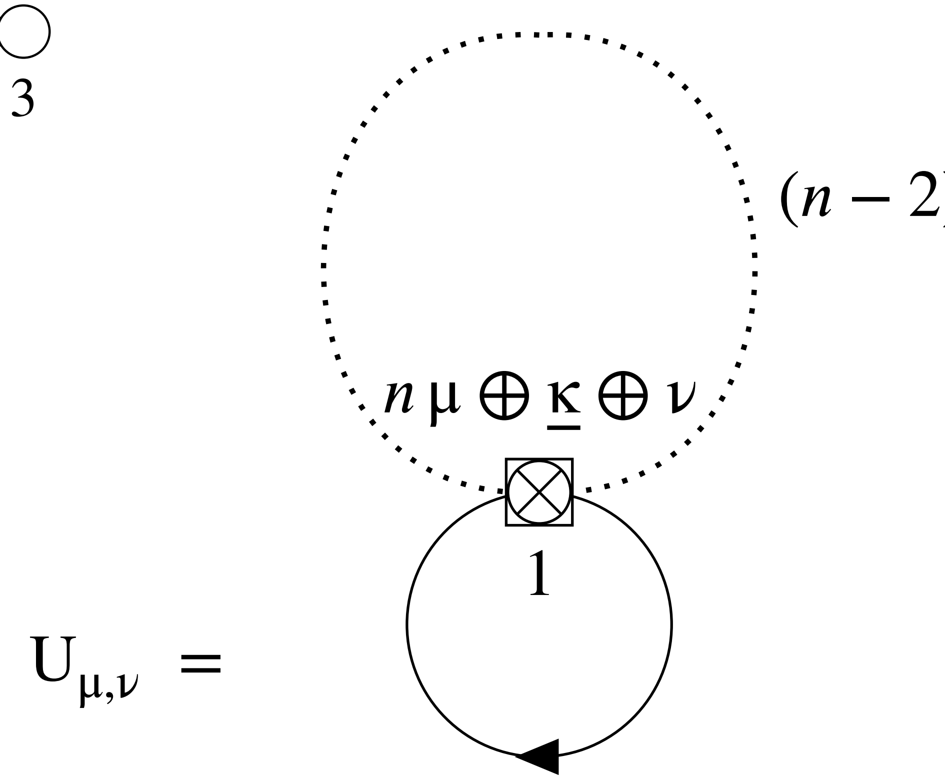
3) At no stage does it entail unphysical "unlinked diagrams." Their absence does not rest on a "Wick theorem" (which does not hold for operators that do not satisfy canonical commutation relations).

Paul C. Martin, Schwinger and statistical physics, Physica 96A, 70-88 (1979)

Mean-field potentials



Electrons



Bosons

Mean-field potentials

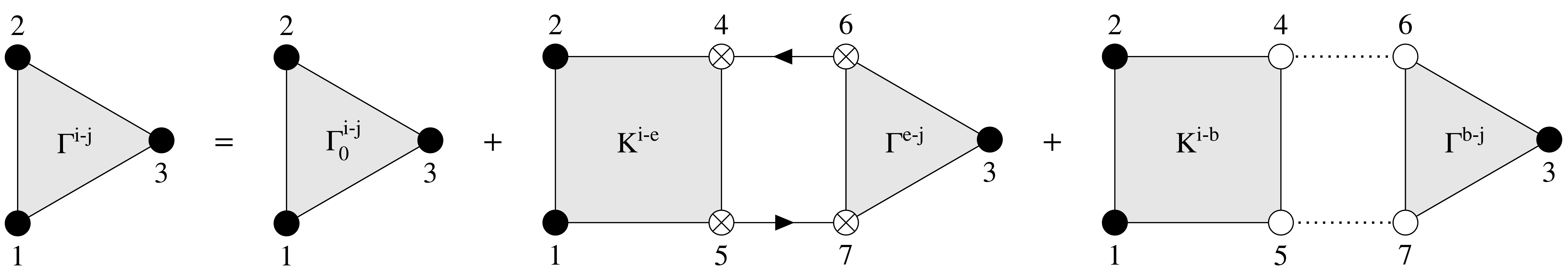
$$\Phi^n_{\mathrm{DW}}(1) = \sum_{n,\underline{\nu}} V^n_{\underline{\nu}}(\mathbf{x}_1)\left\langle \widehat{Q}^n_{\underline{\nu}}(z_1)\right\rangle$$

$$U_{\mu,\nu}(z_1) = \sum_{n,\underline{\kappa}} n\,\gamma^n_{\mu\oplus\underline{\kappa}\oplus\nu}(\mathbf{x}_1)\left\langle \widehat{Q}^{n-2}_{\underline{\kappa}}(z_1)\right\rangle$$

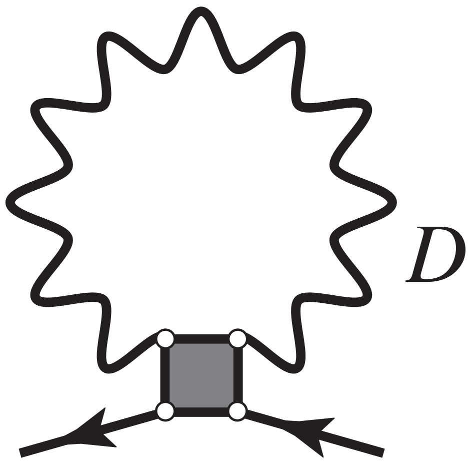
The generalized BSE

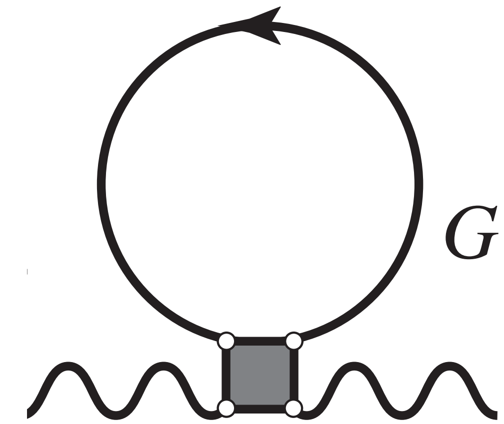
Cross-channel correlations

$$\Gamma^{\text{i-j}}(1,2;3) = \Gamma_0^{\text{i-j}}(1,2;3) + K^{\text{i-e}}(1,5;4,2)\,G(4,6)\,\Gamma^{\text{e-j}}(6,7;3)\,G(7,5)$$
$$+ K^{\text{i-b}}(1,5;4,2)\,D_{\phi,\eta}(4,6)\,\Gamma^{\text{b-j}}_{\eta,\xi}(6,7;3)\,D_{\xi,\psi}(7,5)$$



II.B. Sunrise, Debye-Waller, Fan-Migdal

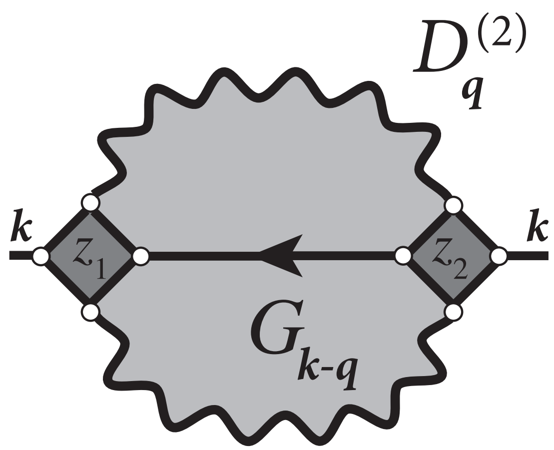




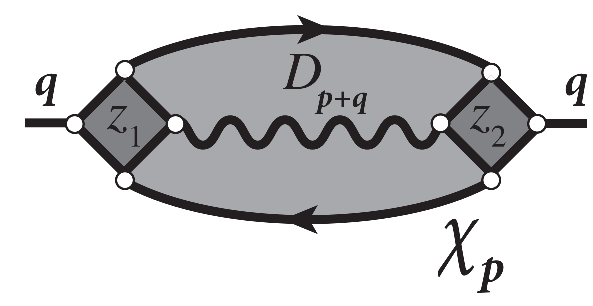
$$\phi^{\mathrm{DW}}_{\mathbf{k}}(z) = \frac{g}{N_k}\sum_{\mathbf{q}} \langle \hat{Q}_{\mathbf{q}}(z)\hat{Q}_{-\mathbf{q}}(z)\rangle.$$

$$u_{\mathbf{q}}(z) = g\sum_{\mathbf{k}} \langle \hat{c}^{\dagger}_{\mathbf{k}}\hat{c}_{\mathbf{k}}\rangle = -\mathrm{i}g\sum_{\mathbf{k}} G_{\mathbf{k}}(z, z^{+}),$$

$\Sigma_k(z_1, z_2) =$



$\Pi_q(z_1, z_2) =$



$$\Sigma_{\mathbf{k}}(z, z') = \mathrm{i}\frac{g^2}{N_k}\sum_{\mathbf{q}} G_{\mathbf{k}-\mathbf{q}}(z, z')D^{(2)}_{\mathbf{q}}(z, z')\ ,$$

$$\Pi_{\mathbf{q}}(z_1, z_2) = \mathrm{i}\frac{g^2}{N_k}\sum_{\mathbf{p}} D_{\mathbf{q}+\mathbf{p}}(z_1, z_2)\chi_{\mathbf{p}}(z_1, z_2).$$

II.C. Pitfalls of non-equilibrium

Mean-field potentials

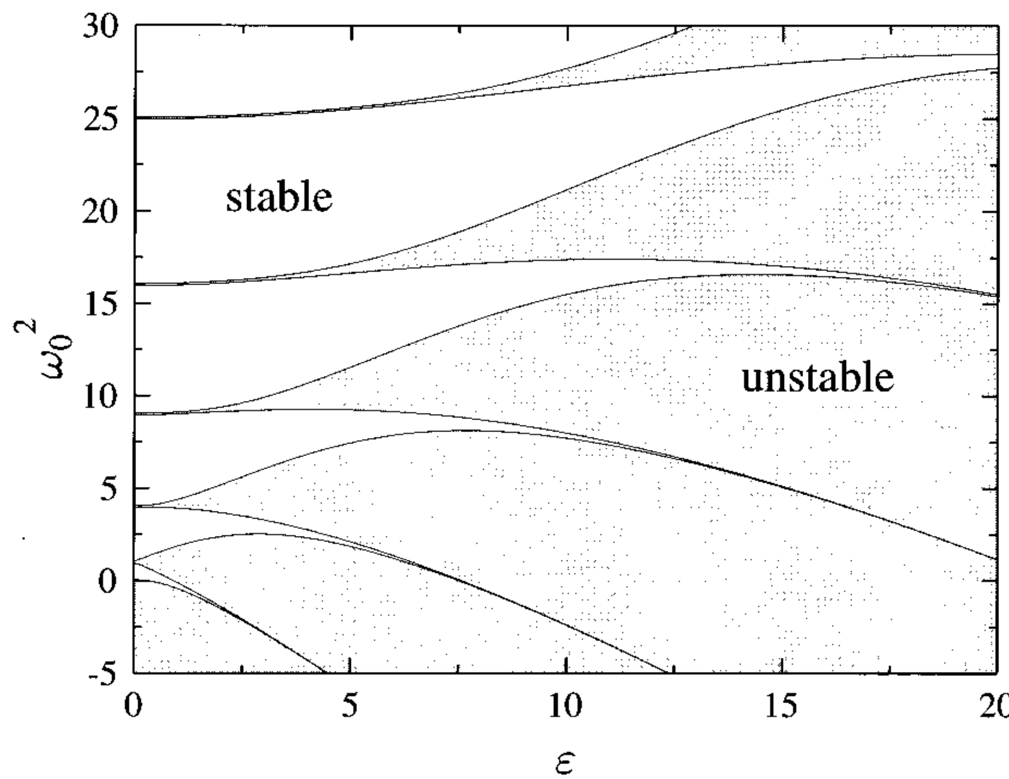
$$\Phi^n_{\mathrm{DW}}(1) = \sum_{n,\underline{\nu}} V^n_{\underline{\nu}}(\mathbf{x}_1)\left\langle \widehat{Q}^n_{\underline{\nu}}(z_1)\right\rangle$$

$$U_{\mu,\nu}(z_1) = \sum_{n,\underline{\kappa}} n\,\gamma^n_{\mu\oplus\underline{\kappa}\oplus\nu}(\mathbf{x}_1)\left\langle \widehat{Q}^{n-2}_{\underline{\kappa}}(z_1)\right\rangle$$

Correlation functions alone are not sufficient to describe dynamics

$$\left[\frac{d^2}{dz_1^2} + \Omega^2_\nu\right]\widehat{Q}_\nu(z_1) = -\Omega_\nu \sum_{m,\underline{\mu}} m\,\hat{\gamma}^m_{\underline{\mu}\oplus\nu}(z_1)\,\widehat{Q}^{m-1}_{\underline{\mu}}(z_1)$$

The Mathieu oscillator



Mean-field electron dynamics—DW potential:

1. m=1,2 ➩ propagation of $\langle Q\rangle$ is needed!
2. m=1 ➩ driven oscillator
3. m=2 ➩ parametric oscillator

$$k(t) = m(\omega_0^2 + \varepsilon\cos\Omega t)$$

II.C. Pitfalls of non-equilibrium

Decoupling in equilibrium

$$D^{2,2}_{\underline{\mu},\underline{\nu}}(z_1,z_2) = \frac{\delta\langle \widehat{Q}^2_{\underline{\mu}}(z_1)\rangle}{\delta \xi^2_{\underline{\nu}}(z_2)} = i\frac{\delta D_{\underline{\mu}}(z_1,z_1)}{\delta \xi^2_{\underline{\nu}}(z_2)}$$

$$= -i\sum_{\zeta\xi}\int dz dz'\, D_{\mu_1\zeta}(z_1,z)\frac{\delta D^{-1}_{\zeta\xi}(z,z')}{\delta \xi^2_{\underline{\nu}}(z_2)} D_{\xi\mu_2}(z',z_1)$$

$$\approx iD_{\mu_1\nu_1}(z_1,z_2)D_{\nu_2\mu_2}(z_2,z_1).$$

Decoupling out of equilibrium

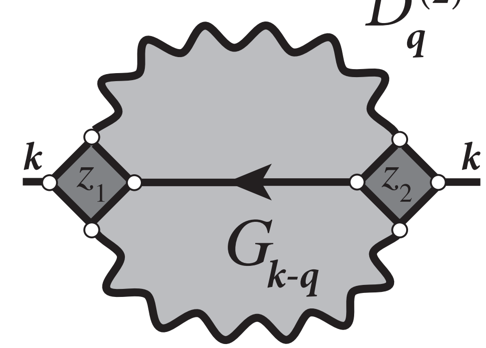
$$D^{2,2}_{\underline{\mu},\underline{\nu}}(z_1,z_2) = i\frac{\delta D_{\underline{\mu}}(z_1,z_1)}{\delta \xi^2_{\underline{\nu}}(z_2)} + \frac{\delta\left\{\langle \widehat{Q}_{\mu_1}(z_1)\rangle\langle \widehat{Q}_{\mu_2}(z_1)\rangle\right\}}{\delta \xi^2_{\underline{\nu}}(z_2)}.$$

In equilibrium:

coupled RPA equations for $D^{(2)}$ and χ

Out of equilibrium:

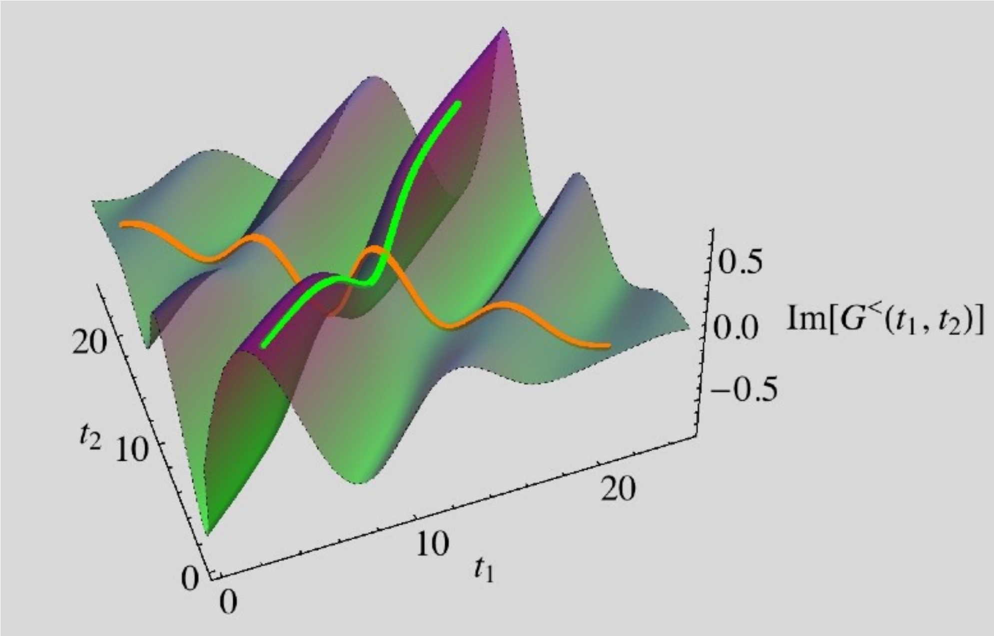
extra terms



Outlook:

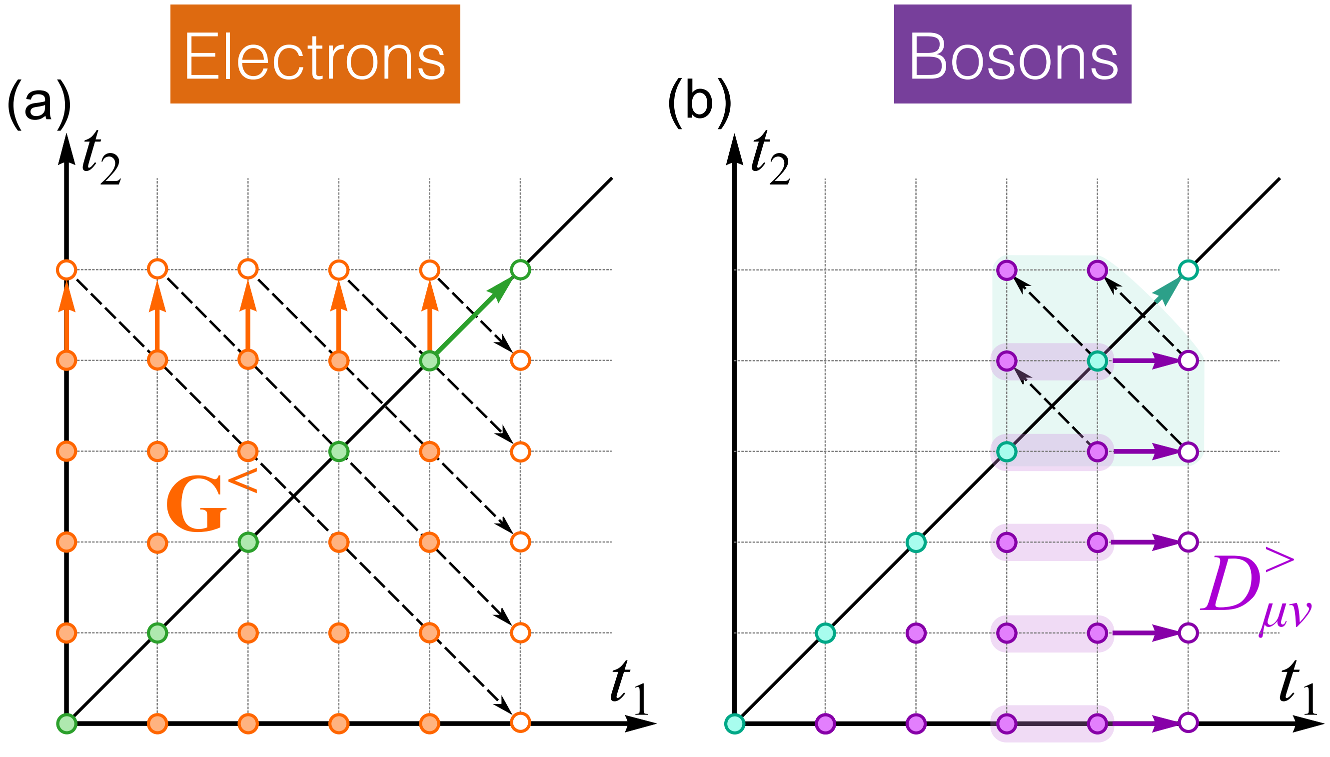
1. Theory becomes too complicated when $\langle Q\rangle \neq 0$
2. Assumption $\langle Q\rangle = 0$ is justified when there is no linear coupling ➪ used in our first implementation

III. Numerical results



1. One site, linear coupling
2. One site, quadratic coupling
3. *k*-space, linear coupling, relaxation

Nonequilibrium *e-pl* dynamics

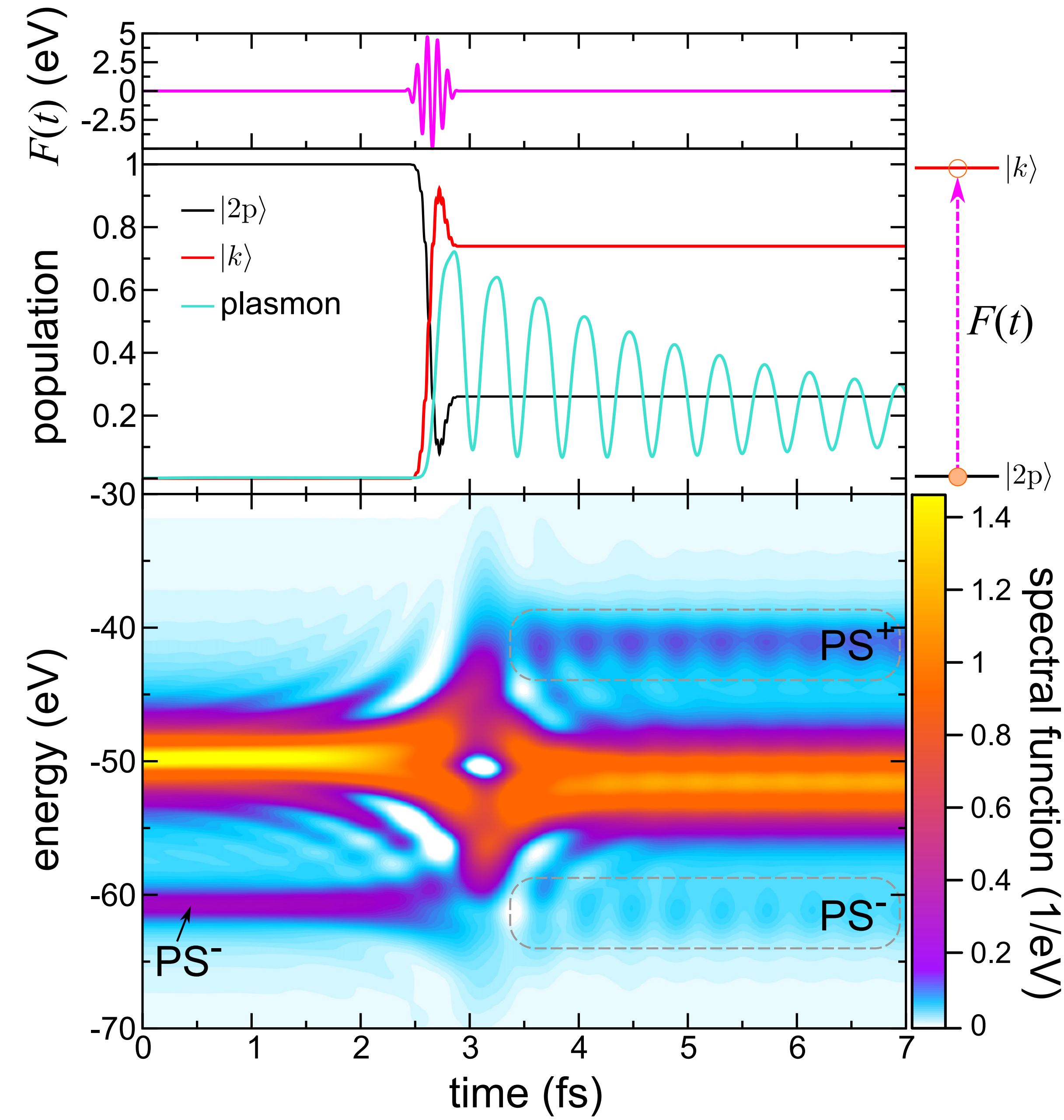


Bosonic EOM

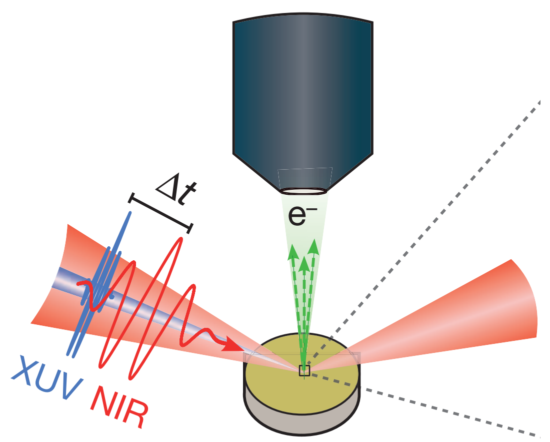
$$-\frac{1}{\Omega_\nu}\left(\frac{\partial^2}{\partial z_1^2}+\Omega_\nu^2\right)D_{\mu\nu}(z_1,z_2)=\delta_{\mu\nu}\delta(z_1,z_2)$$
$$+\sum_\xi\int_C \mathrm{d}z_3\,\Pi_{\mu\xi}(z_1,z_3)D_{\xi\nu}(z_3,z_2)\ .$$

M. Schüler, J. Berakdar, Y. Pavlyukh, *Time-dependent many-body treatment of electron-boson dynamics: Application to plasmon-accompanied photoemission* Phys. Rev. B **93**, 054303 (2016)

$A(T,\mathscr{E})$ of Mg/W(110)

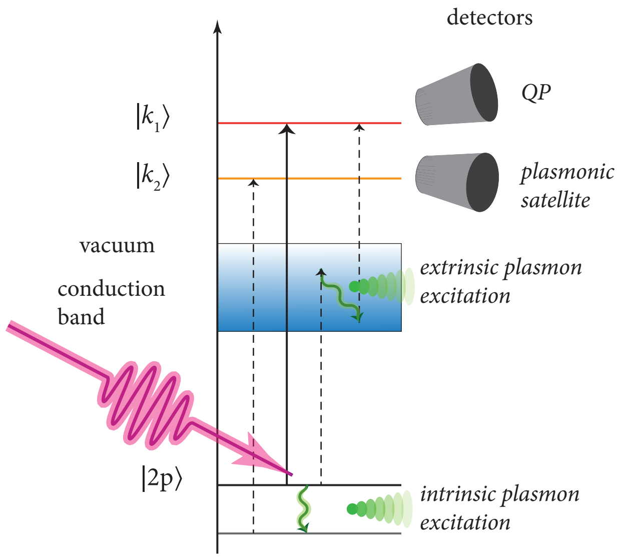


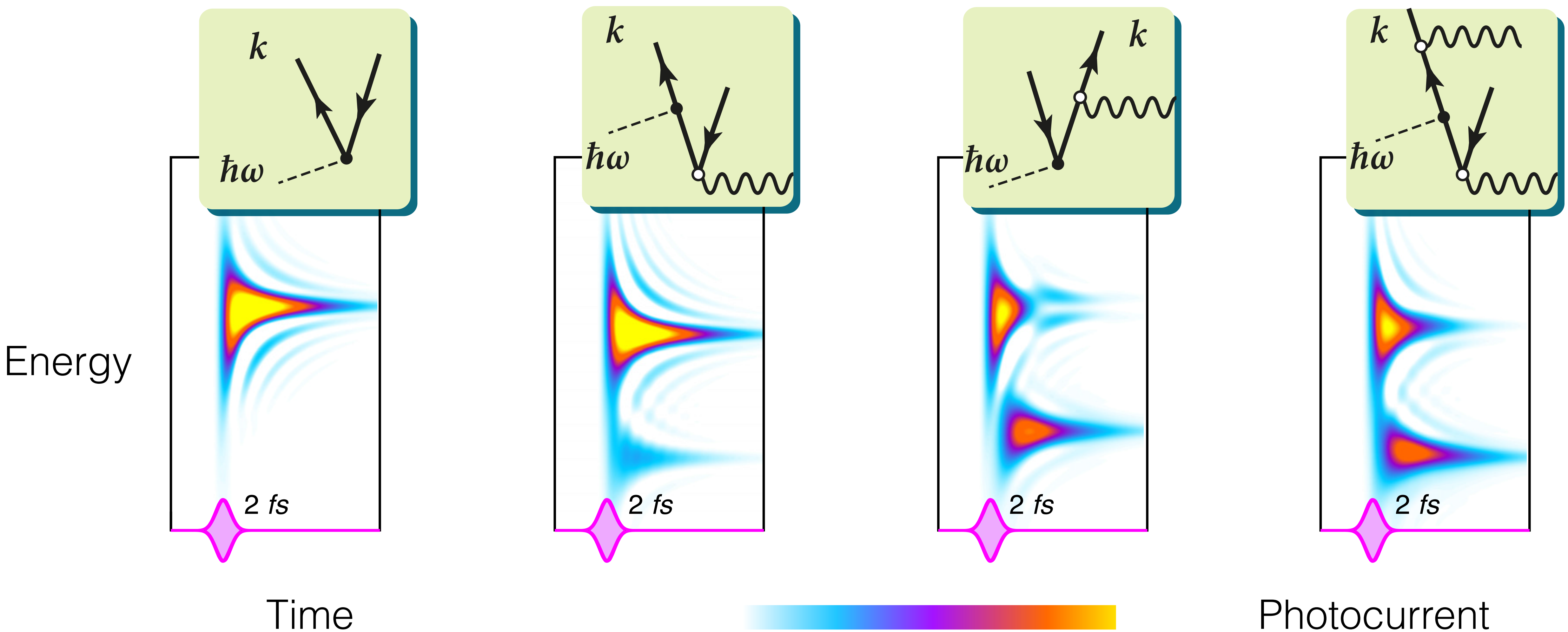
Atto-second time-delays in photoemission



Zooming into the energy range of 2p peak

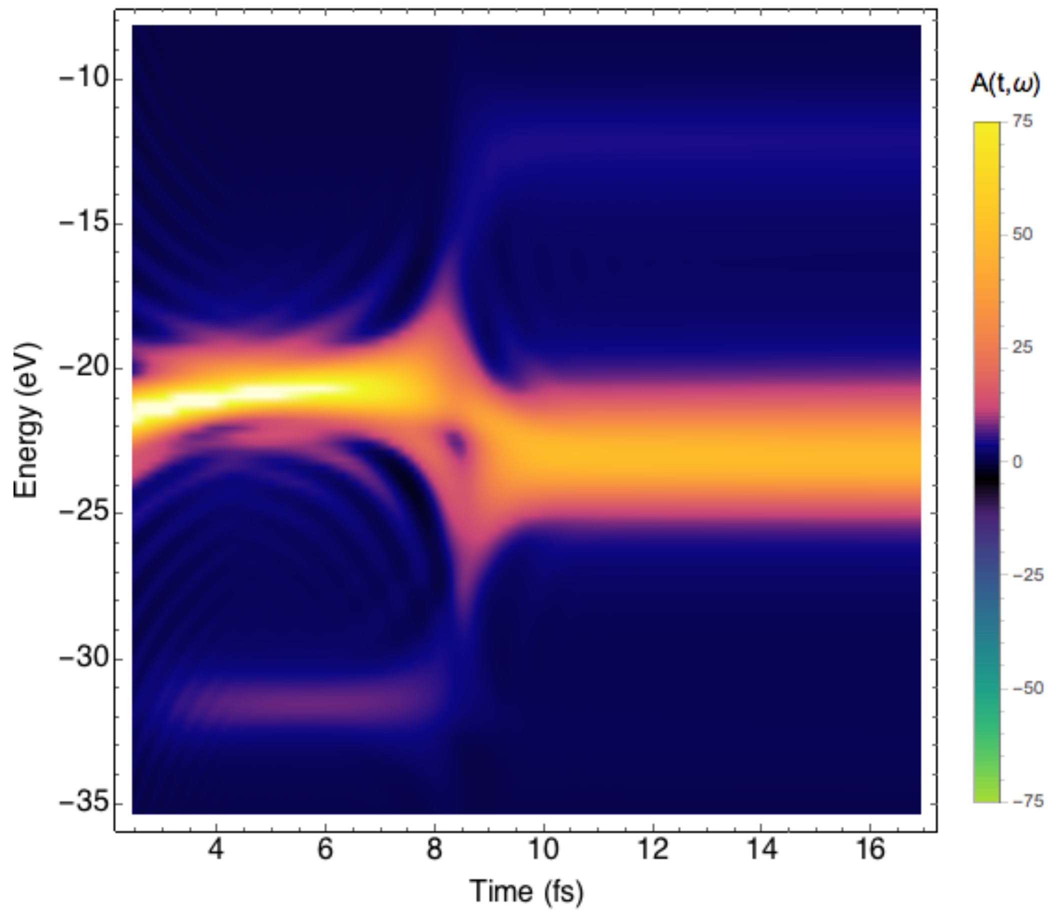
C. Lemell *et al.*, *Real-time observation of collective excitations in photoemission*, Phys. Rev. B **91**, 241101 (2015)

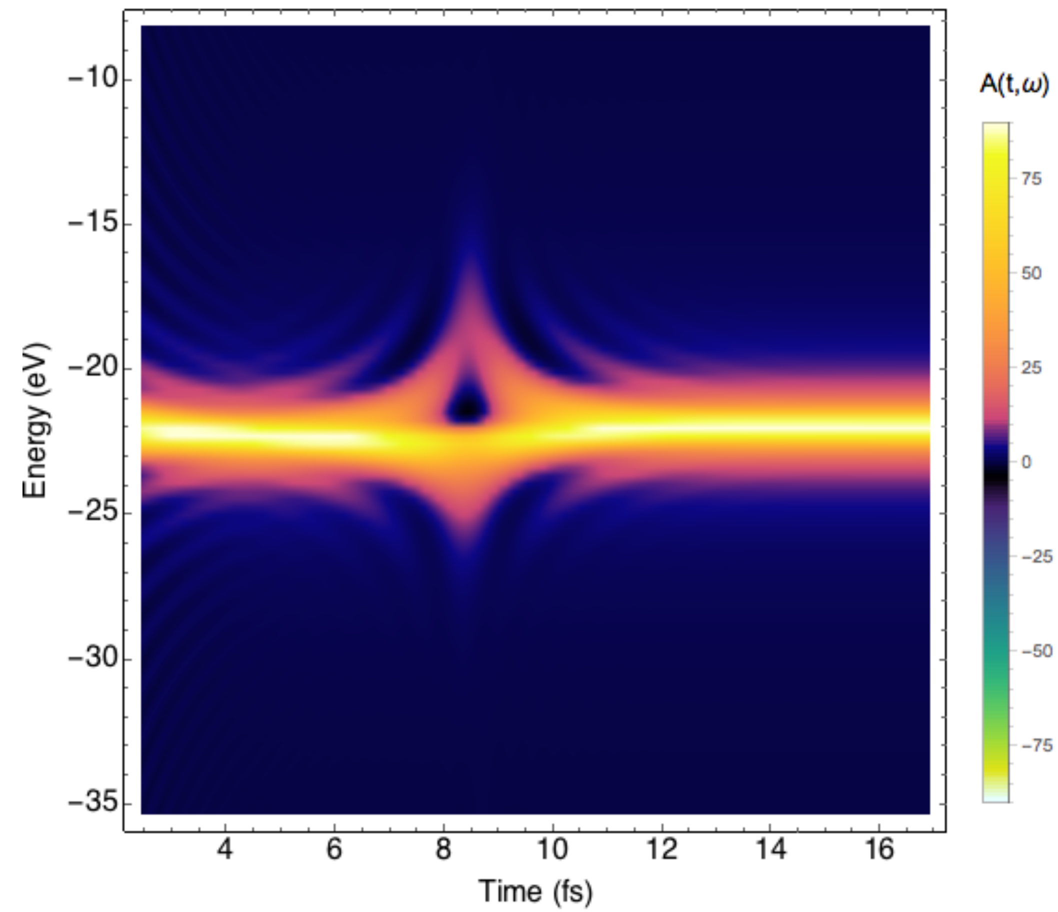


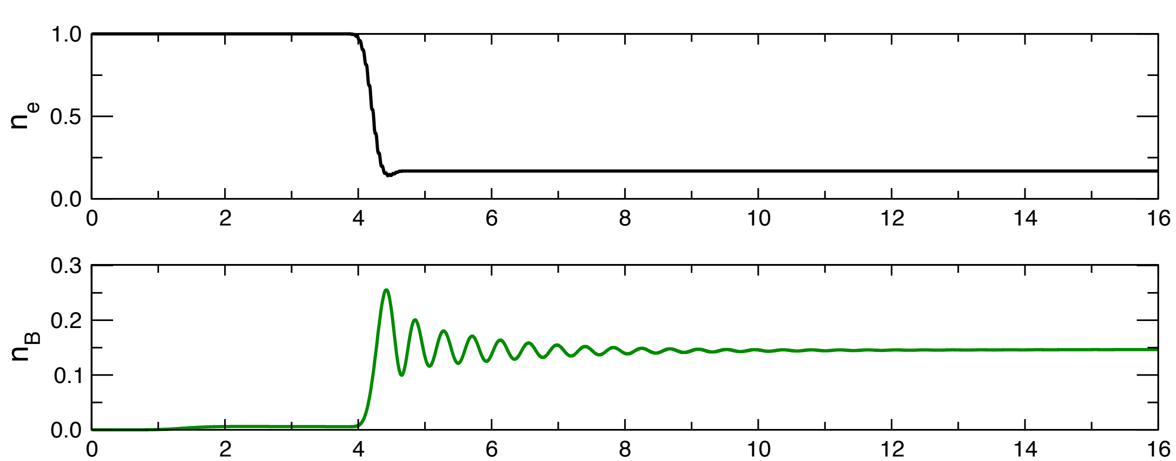


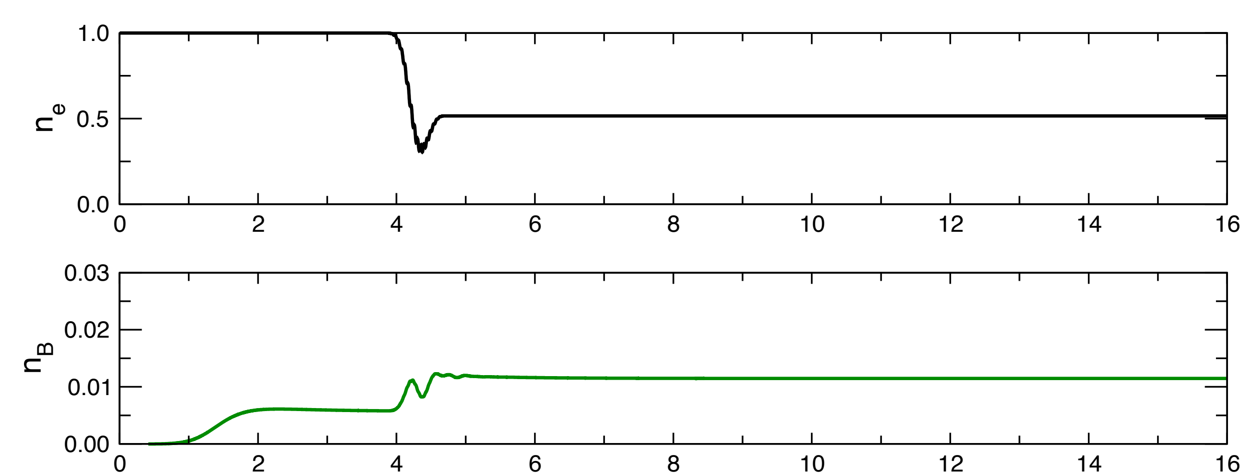
Linear vs. quadratic coupling

1. Two-level system, **short** resonant XUV pulse (44 eV)
2. Coupling to a single plasmon (Ω=10 eV), *g*=5 eV
3. Transient spectral function



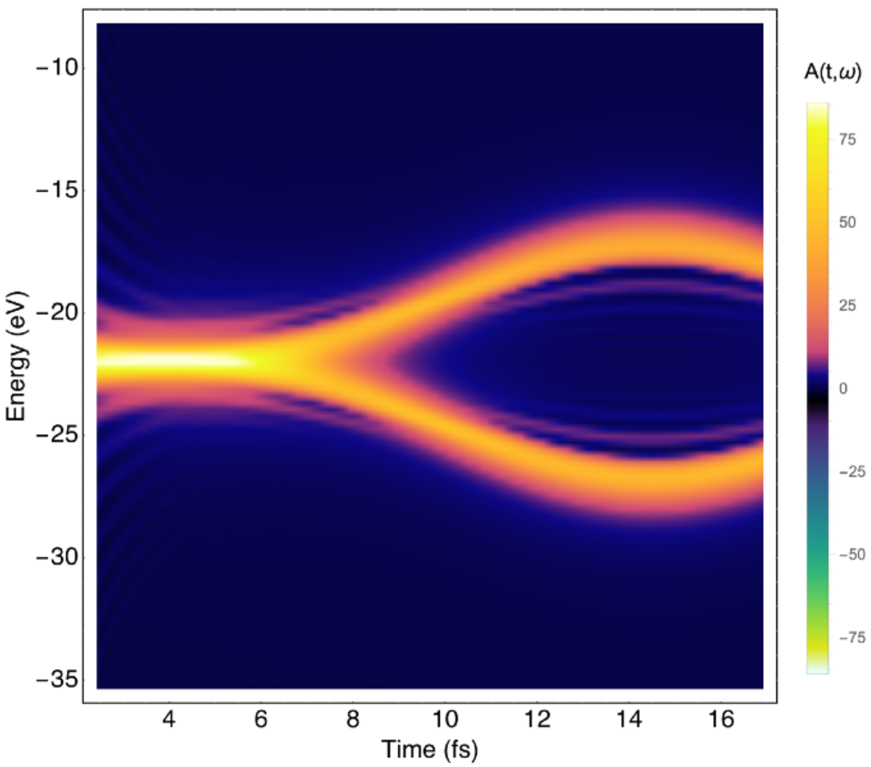




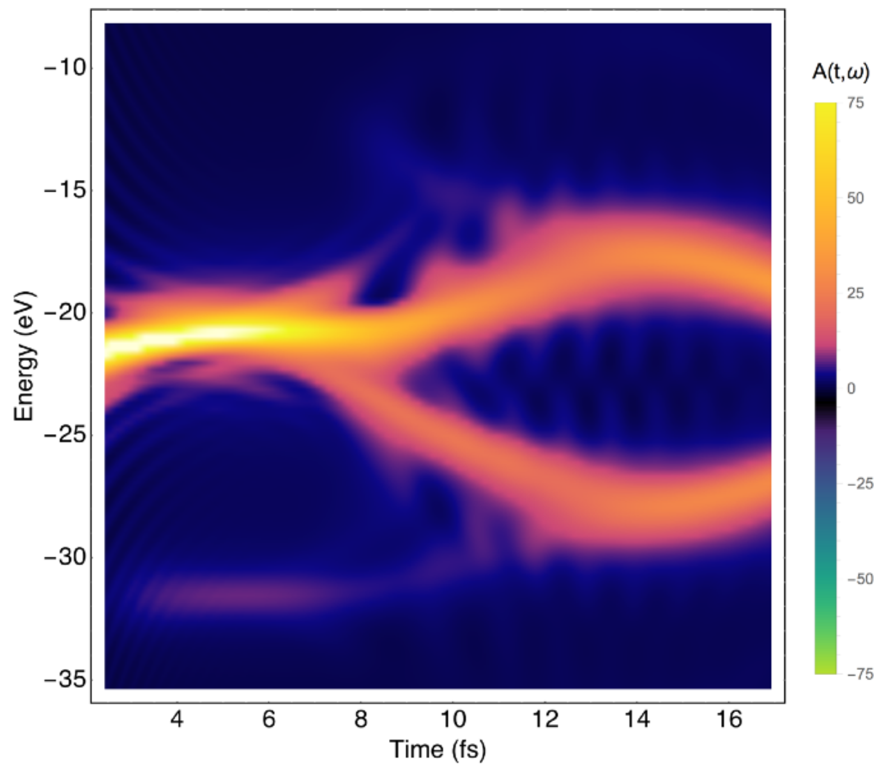


Linear vs. quadratic coupling

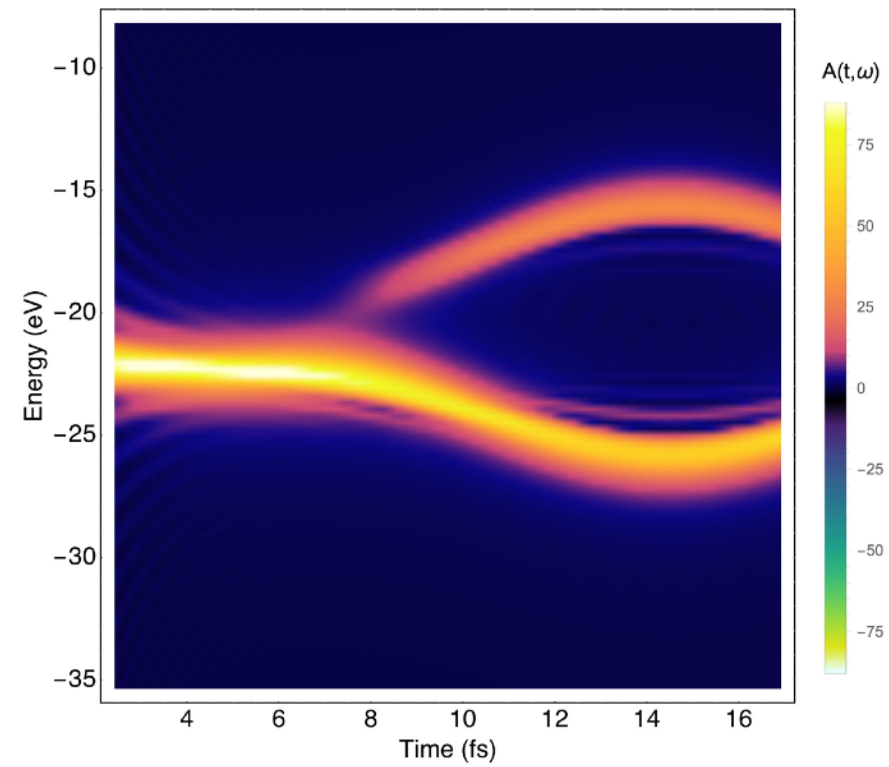
1. Two-level system, **long** resonant XUV pulse (44 eV)
2. Coupling to a single plasmon (Ω=10 eV, g=5 eV)
3. Transient spectral function



1. **No coupling**
2. Autler-Townes splitting



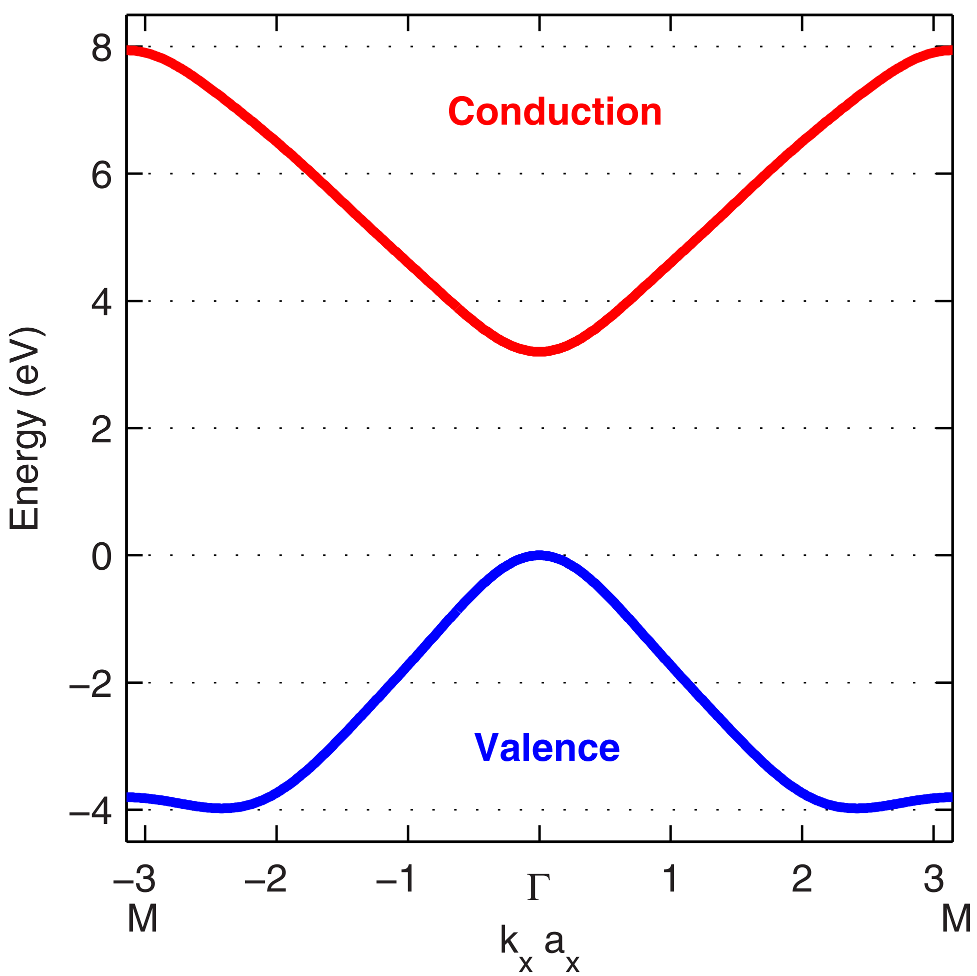
1. **Linear coupling**
2. Self-consistent Fan-Migdal
3. Transient *pl*-satellite dynamics



1. **Quadratic coupling**
2. Sunrise self-energy
3. Spectral weight re-distribution

Tight-binding model

Setup



[Vampa et al., PRB 91, 064302 (2015)]

- TB model of ZnO (1D)
- Holstein model for el-ph interactions

$$\hat{H} = \sum_{\mathbf{k}} \sum_{nn'} h_{nn'}(\mathbf{k},t)\hat{c}^\dagger_{\mathbf{k}n}\hat{c}_{\mathbf{k}n'} + g \sum_{\mathbf{k},n} \sum_{\mathbf{q}} \hat{c}^\dagger_{\mathbf{k+q}n}\hat{c}_{\mathbf{k}n}\hat{Q}_{\mathbf{q}} + \frac{\omega_0}{2}\sum_{\mathbf{q}}\left(\hat{P}^2_{\mathbf{q}} + \hat{Q}^2_{\mathbf{q}}\right)$$

- Light-matter interaction by generalized Peierls substitution:

$$h_{nn'}(\mathbf{k},t) = h^{(0)}_{nn'}(\mathbf{k}-\mathbf{A}(t)) - \mathbf{E}(t)\cdot\mathbf{D}_{nn'}(\mathbf{k}-\mathbf{A}(t))$$

- Levels of approximation:

non-selfconsistent (local) Migdal

$$\Sigma(z,z') = ig^2 G_{\rm loc}(z,z')D^{(0)}(z,z')$$

self-consistent (local) Migdal

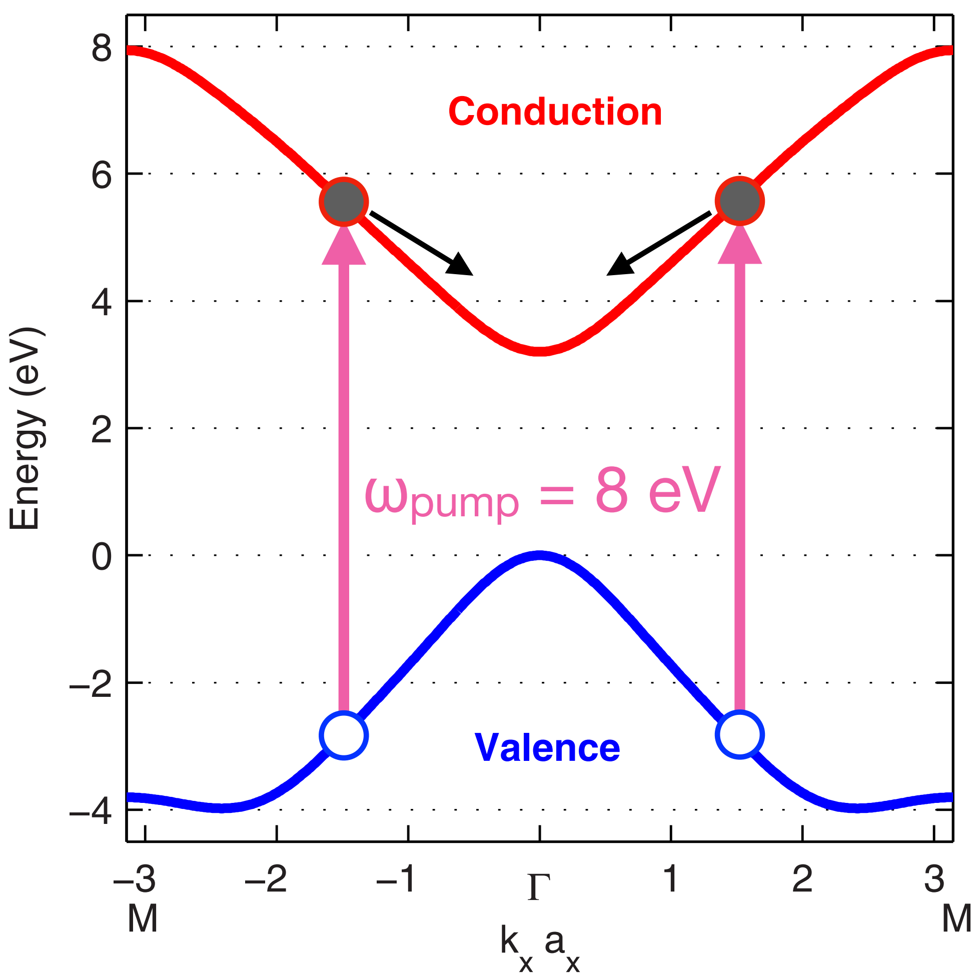
$$\Sigma(z,z') = ig^2 G_{\rm loc}(z,z')D(z,z')$$

Phonon window effect

J. Rameau *et al.*, Nature Commun. **7**, 13761 (2016)

Tight-binding model

Setup



[Vampa et al., PRB 91, 064302 (2015)]

(Ω=0.2 eV, *g*=0.2 eV)

- TB model of ZnO (1D)
- Holstein model for el-ph interactions

$$\hat{H} = \sum_{\mathbf{k}} \sum_{nn'} h_{nn'}(\mathbf{k},t)\hat{c}^\dagger_{\mathbf{k}n}\hat{c}_{\mathbf{k}n'} + g\sum_{\mathbf{k},n}\sum_{\mathbf{q}} \hat{c}^\dagger_{\mathbf{k}+\mathbf{q}n}\hat{c}_{\mathbf{k}n}\hat{Q}_{\mathbf{q}} + \frac{\omega_0}{2}\sum_{\mathbf{q}}\left(\hat{P}^2_{\mathbf{q}} + \hat{Q}^2_{\mathbf{q}}\right)$$

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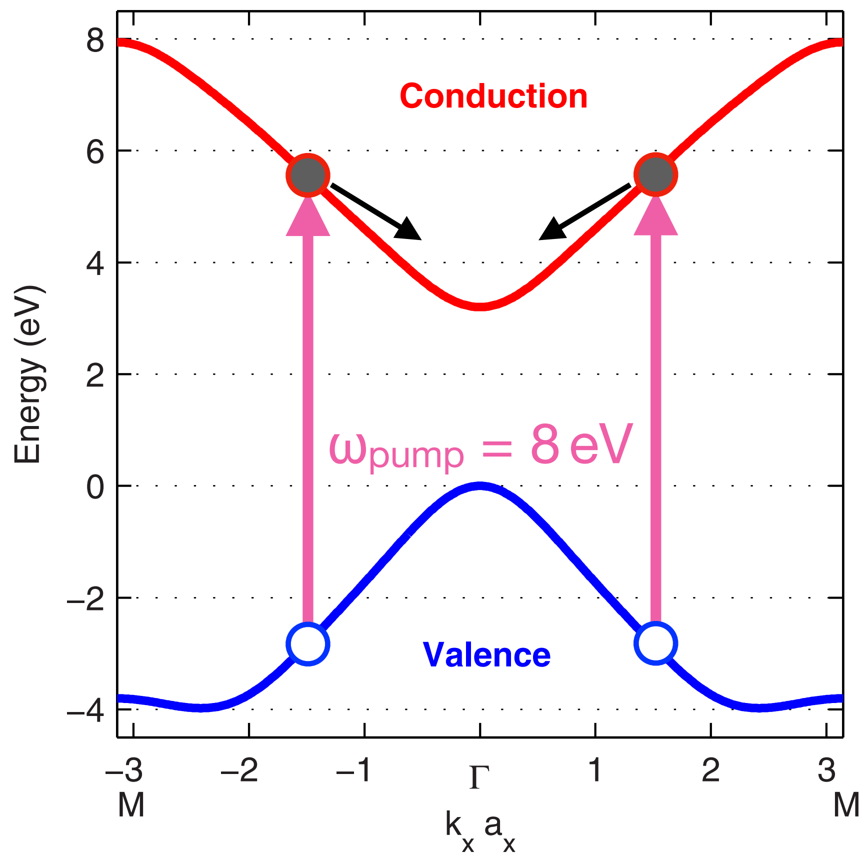
self-consistent (local) Migdal

$$\Sigma(z,z') = ig^2 G_{\text{loc}}(z,z')D(z,z')$$

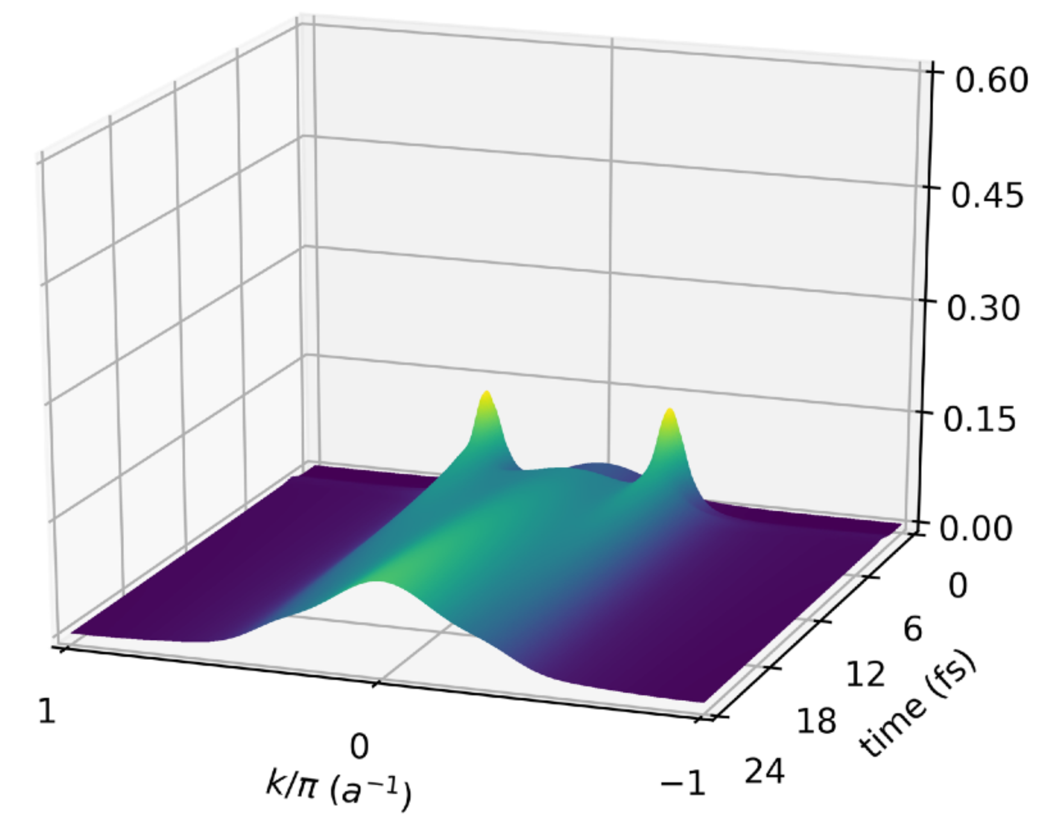
Phonon window effect

J. Rameau *et al.*, Nature Commun. **7**, 13761 (2016)

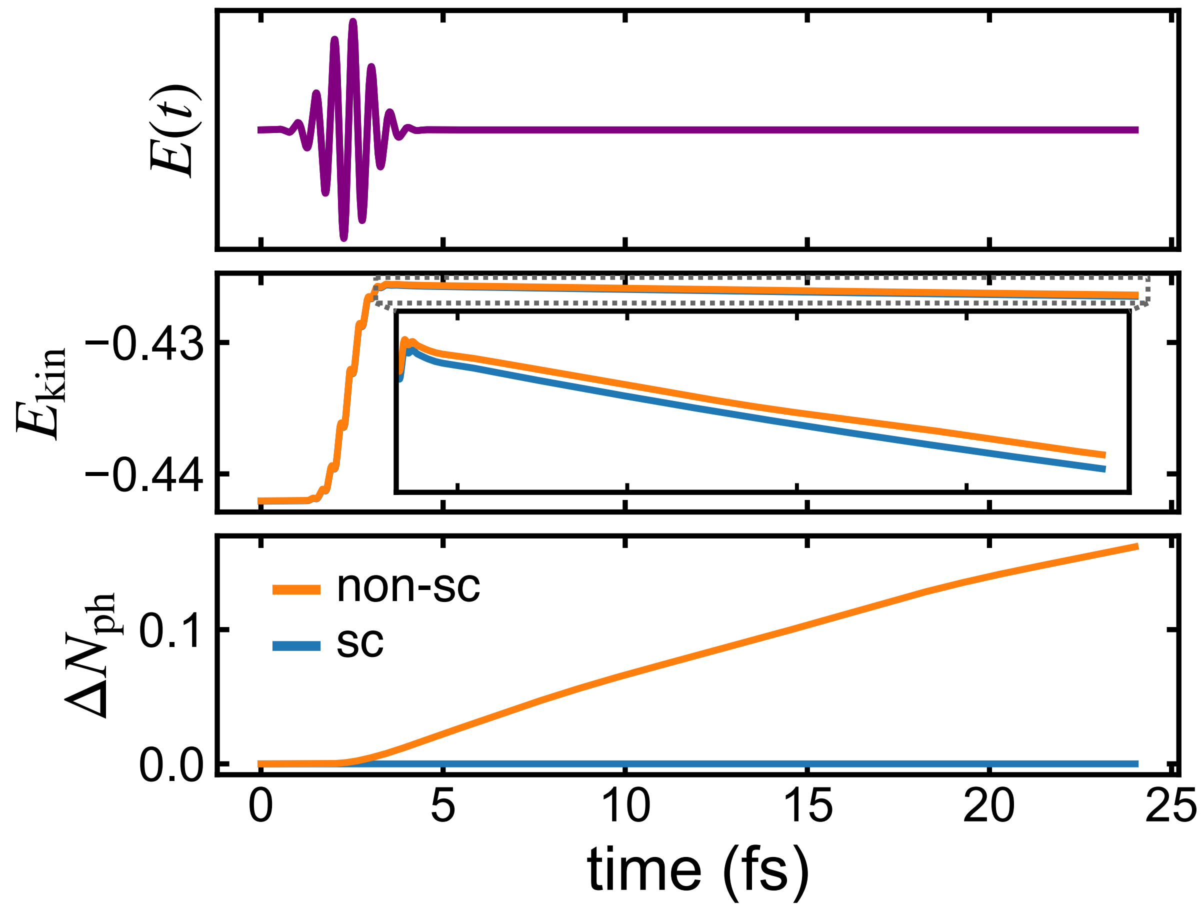
Weak pump



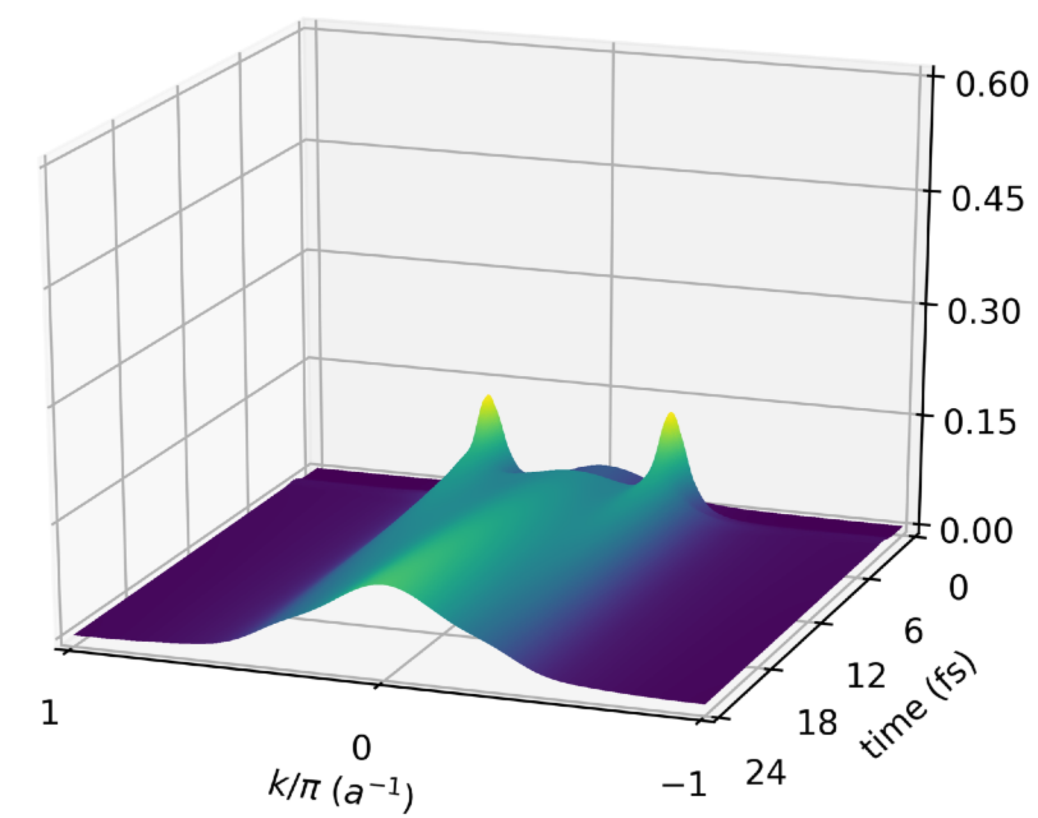
8
6
4
2
0
−2
−4
Energy (eV)
Conduction
Valence
ωpump = 8 eV
−3
M
−2
−1
Γ
1
2
3
M
kx ax



0.60
0.45
0.30
0.15
0.00
0
6
12
18
24
time (fs)
1
0
−1
k/π (a−1)

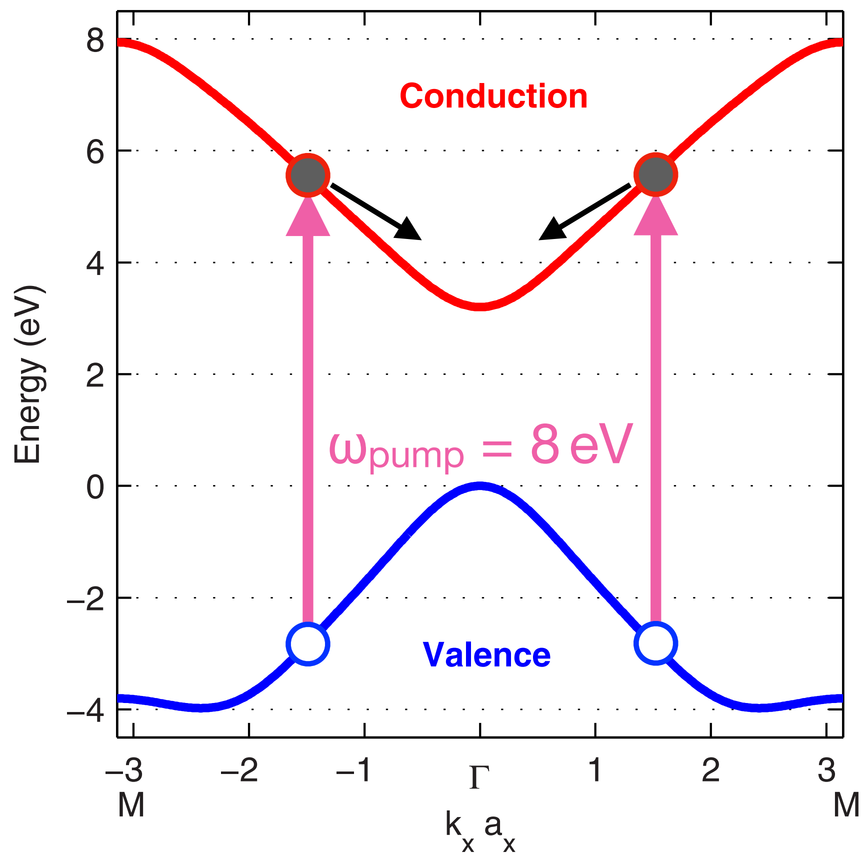


E(t)
Ekin
−0.43
−0.44
ΔNph
0.1
0.0
non-sc
sc
0
5
10
15
20
25
time (fs)

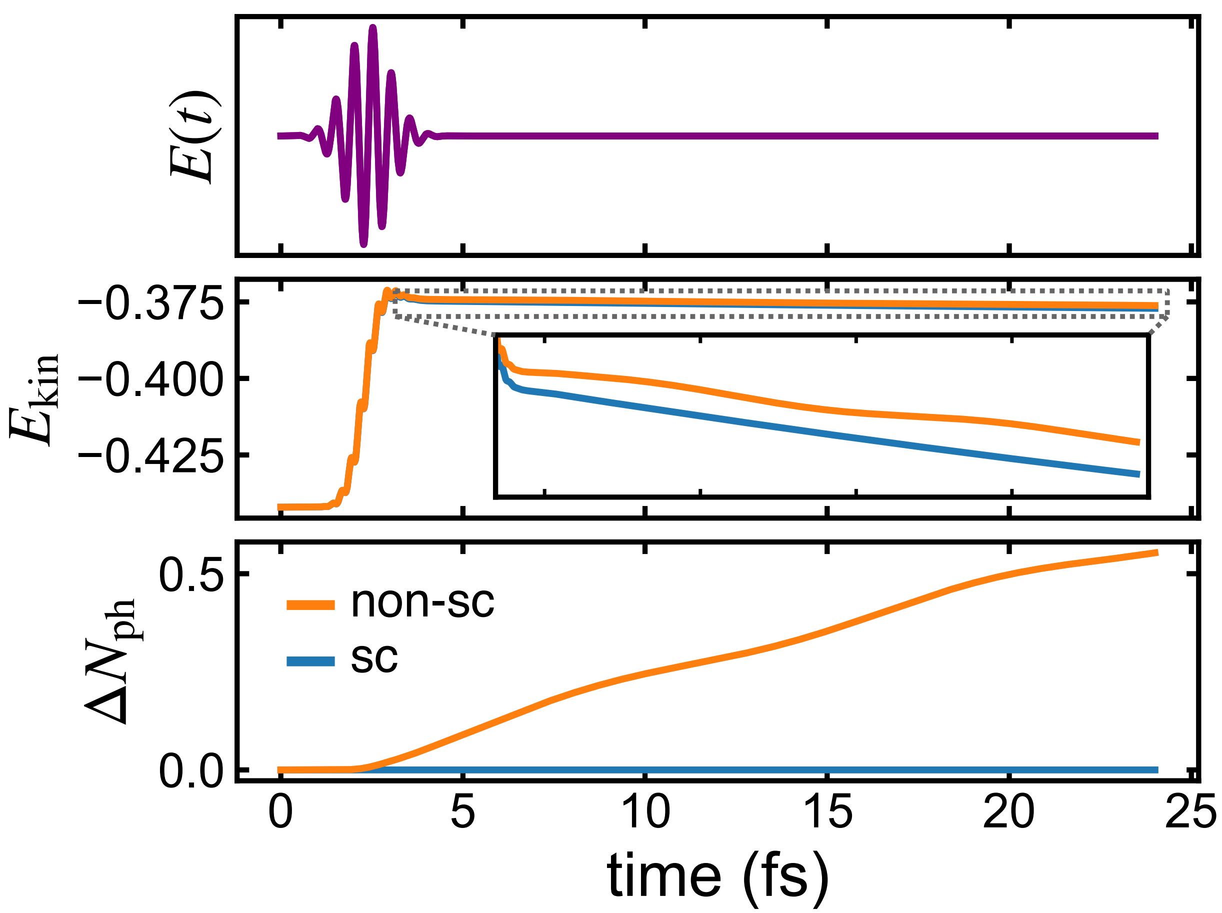


0.60
0.45
0.30
0.15
0.00
0
6
12
18
24
time (fs)
1
0
−1
k/π (a−1)

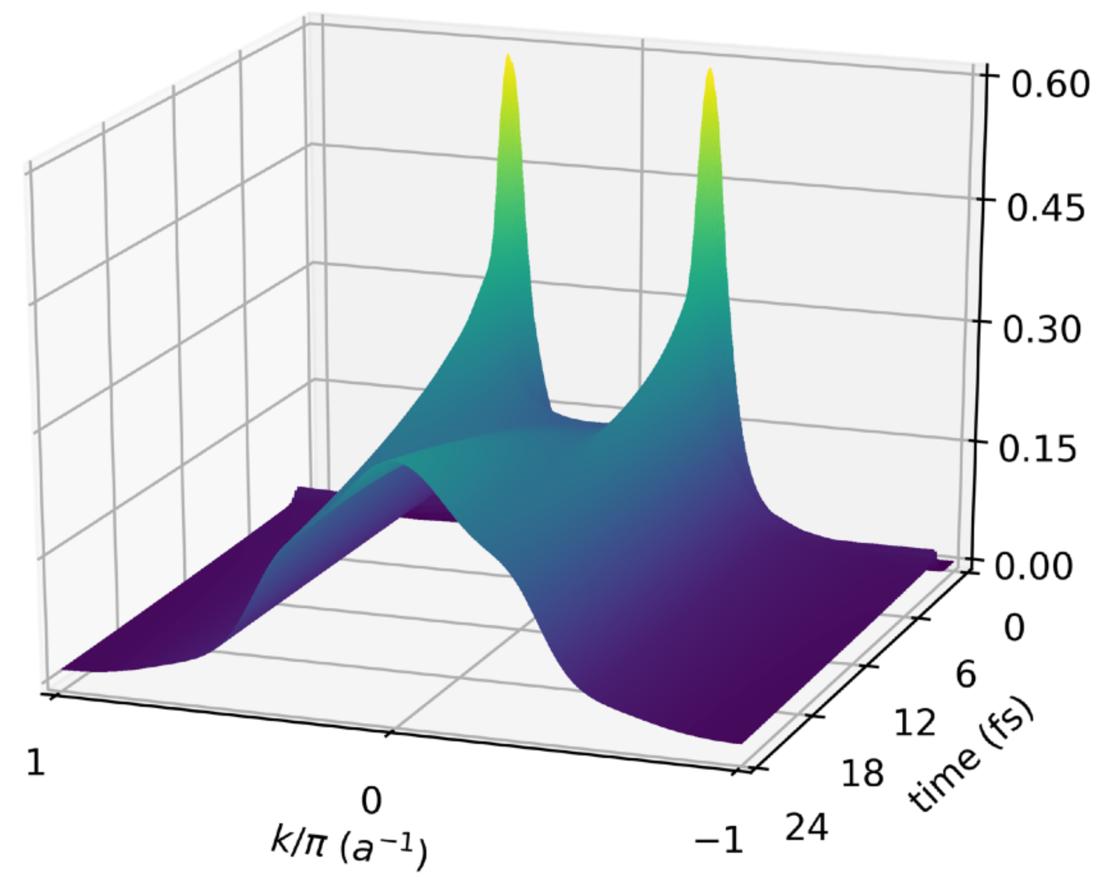
Strong pump



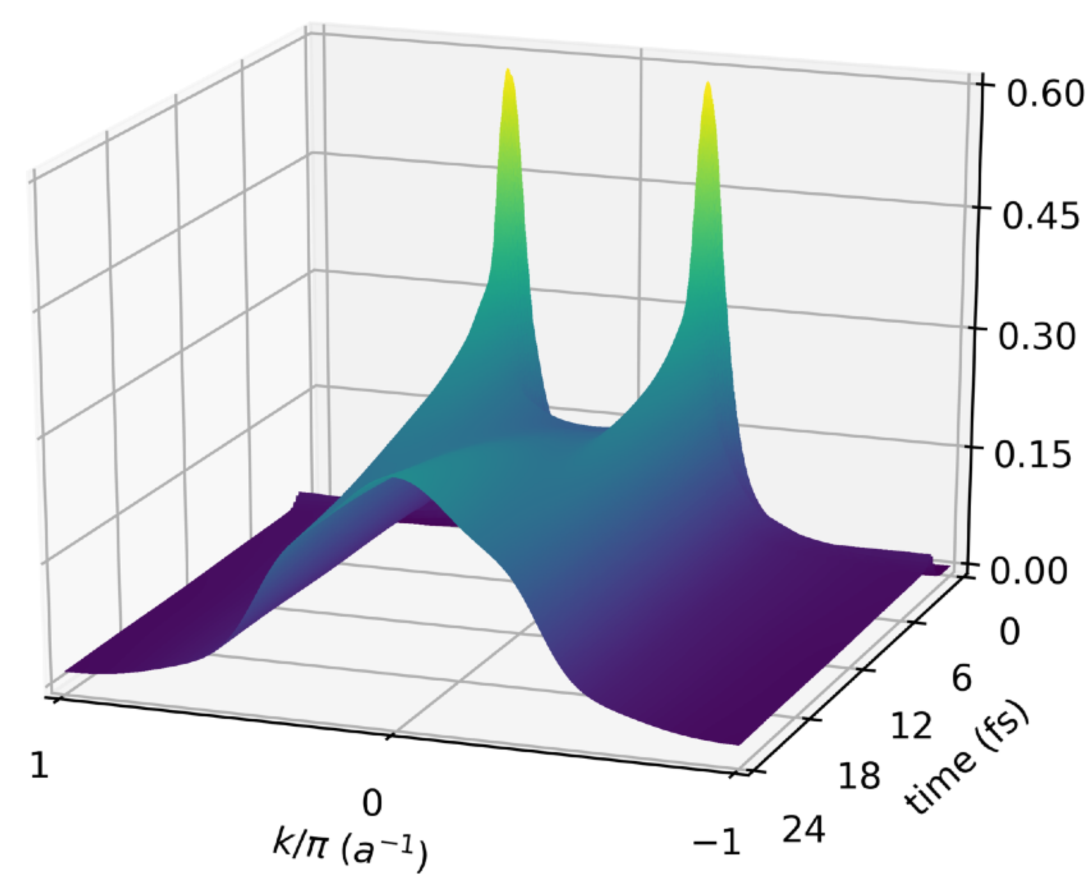
Conduction
Valence
$\omega_{pump} = 8\,eV$
Energy (eV)
8
6
4
2
0
−2
−4
−3
M
−2
−1
Γ
1
2
3
M
$k_x a_x$



$E(t)$
E_{kin}
−0.375
−0.400
−0.425
ΔN_{ph}
0.5
0.0
non-sc
sc
0
5
10
15
20
25
time (fs)



0.60
0.45
0.30
0.15
0.00
0
6
12
18
24
time (fs)
1
0
−1
k/π (a^{-1})



0.60
0.45
0.30
0.15
0.00
0
6
12
18
24
time (fs)
1
0
−1
k/π (a^{-1})

Numerical details

Gregory quadrature

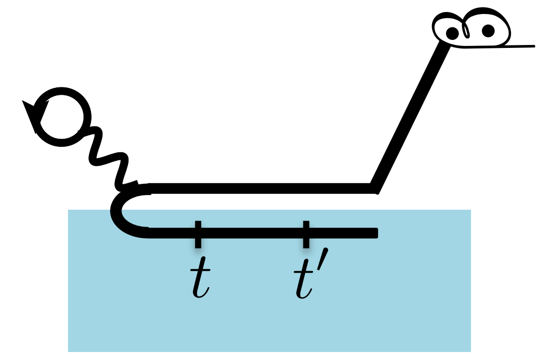
$\mathcal{I}(t) = \int_0^t dt'\, y(t')$ Error ~ $\mathcal{O}(\Delta t^7)$ also for small t

Matsubara

$G(\tau) = G_0(\tau) + \int_0^\beta d\tau'\, K(\tau - \tau')G(\tau')$ av. error ~ $\mathcal{O}(\Delta\tau^7)$

Solved as integral equation using Newton's method

Open source library **NESSY** available soon!



Kadanoff-Baym equations

$\left(i\partial_z - h(z)\right) G(z, z') = \delta_C(z, z') + \int_C d\bar{z}\, \Sigma(z, \bar{z})G(\bar{z}, z')$ av. error ~ $\mathcal{O}(\Delta t^6)$

Solved by Adams predictor-corrector method

Volterra integral equations

$G(z, z') = G_0(z, z') + \int_C d\bar{z}\, K(z, \bar{z})G(\bar{z}, z')$ av. error ~ $\mathcal{O}(\Delta t^7)$

Parallelization

Hybrid MPI (**k**-space) + OpenMP (time)

Conclusions

I. Quadratic electron-phonon coupling contains a lot of interesting physics
II. First calculations with sunrise self-energy
III. Plans:
   A. Renormalization of constituent response functions ➪ coupled RPA equations for $D^{(2)}$ and χ
   B. IR-active phonons, driving, $\langle Q(t) \rangle \neq 0$
   C. Dynamics in k-space

Thank you for your attention