Stability of the long-range corrected exchange-correlation functional in TDDFT

Carsten A. Ullrich
University of Missouri

TDDFT school and workshop
Benasque
April 14, 2025

Motivation/Overview

PHYSICAL REVIEW LETTERS **127,** 077401 (2021)

Real-Time Exciton Dynamics with Time-Dependent Density-Functional Theory

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Goal: simulate exciton dynamics with RT-TDDFT
→ ultrafast pump-probe experiments, transient absorption, HHG, ...

We used time-dependent LRC approach.
→ Good for weakly bound excitons, but numerically unstable for strongly bound excitons. Why??

Motivation/Overview

PHYSICAL REVIEW B **111**, L060302 (2025)

Letter

Kohn-Sham-Proca equations for ultrafast exciton dynamics

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S. Sharma*
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Sharma et al. proposed simple numerical fix which seems to work quite well.
→ But physical reason is not completely clear!

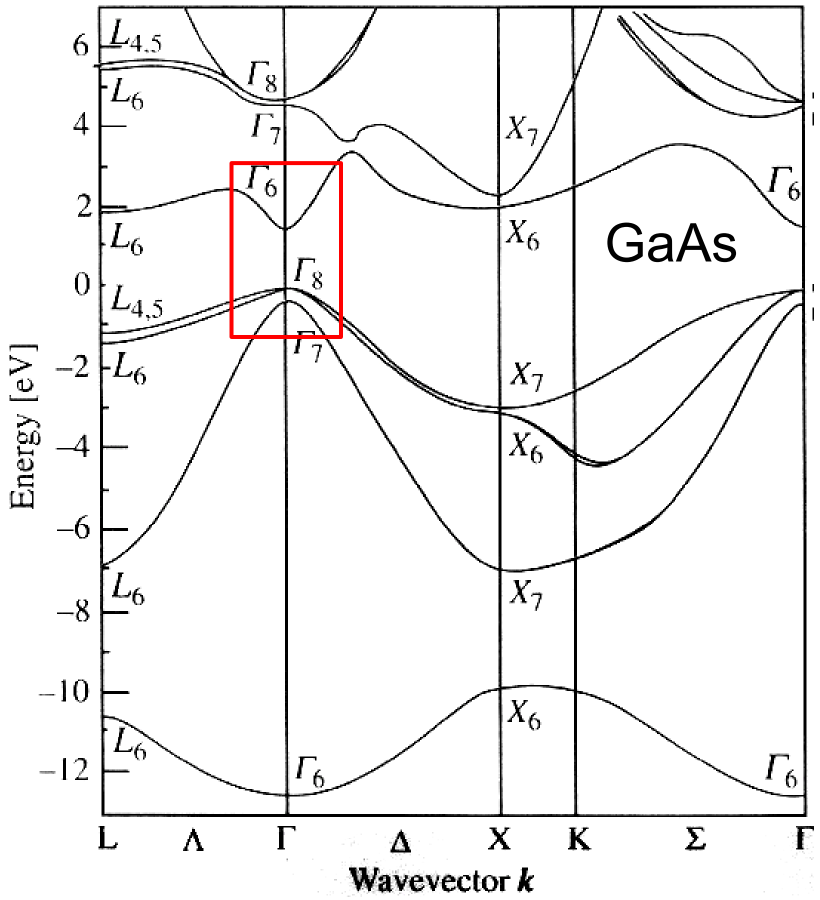
This talk:
→ Explanation how RT-TDDFT for excitons works
→ Physical reason for the instability and how to fix it.

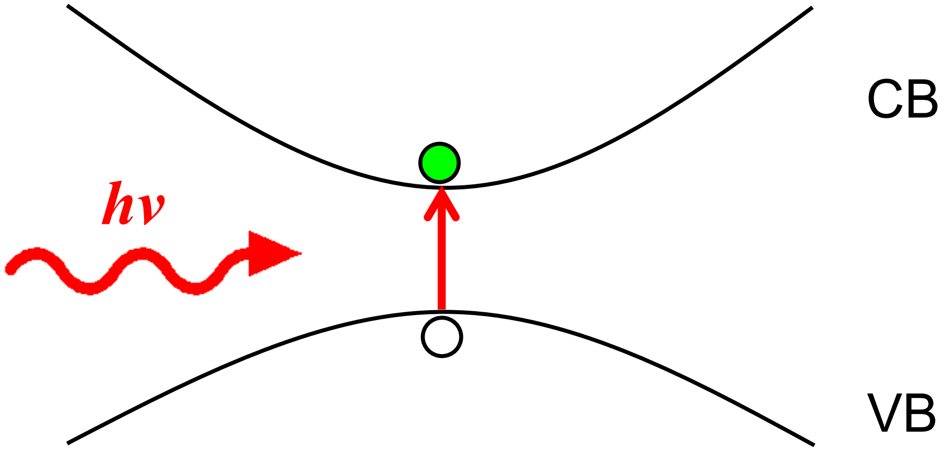
J. R. Williams and C. A. Ullrich, arXiv:2501.13290
(to appear in JCTC)

Outline

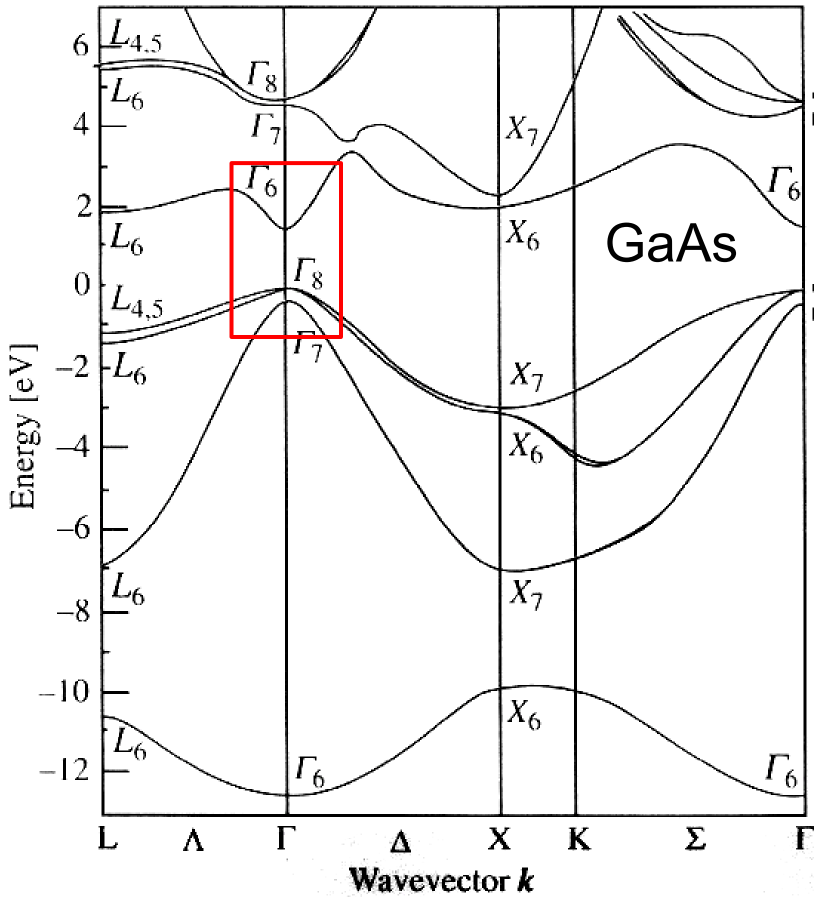
- **Excitons with TDDFT: the LRC kernel**
- **real-time TDDFT with LRC**
- **The "Kohn-Sham-Proca" approach: Sangeeta's slides**
- **Stability analysis of TDLRC: why it works**

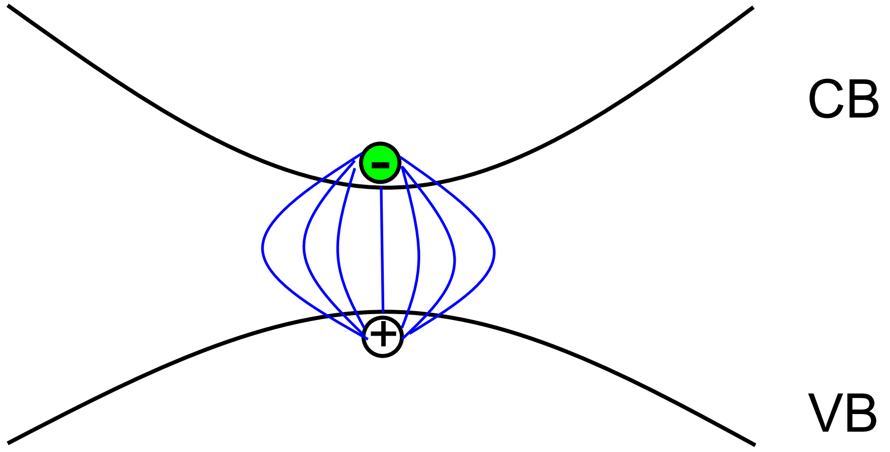
Absorption of light across the band gap





Absorption of light across the band gap





Excitons: bound e-h pairs

Linear-response (LR) TDDFT

$$\delta n(\mathbf{r},\omega) = \int d\mathbf{r}' \chi(\mathbf{r},\mathbf{r}',\omega)\delta V(\mathbf{r}',\omega)$$

$$\chi(\mathbf{r},\mathbf{r}',\omega) = \chi_s(\mathbf{r},\mathbf{r}',\omega) + \int d\mathbf{x}\int d\mathbf{x}' \chi_s(\mathbf{r},\mathbf{x},\omega)\left\{\frac{1}{|\mathbf{x}-\mathbf{x}'|} + f_{xc}(\mathbf{x},\mathbf{x}',\omega)\right\}\chi(\mathbf{x}',\mathbf{r}',\omega)$$

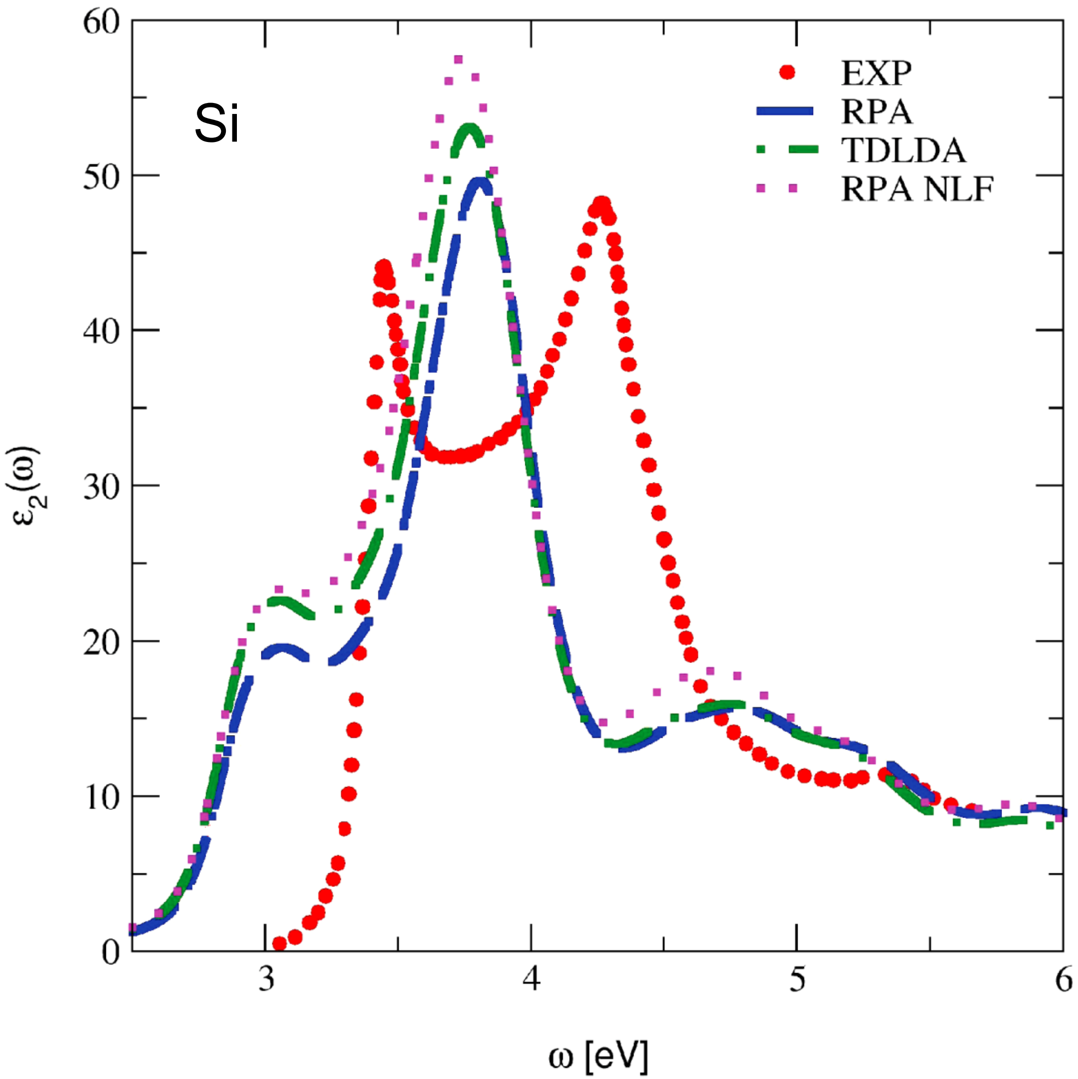
dielectric function in a periodic system:

$$\varepsilon^{-1}_{\mathbf{GG}'}(\mathbf{q},\omega) = \delta_{\mathbf{GG}'} + \frac{4\pi}{|\mathbf{q}+\mathbf{G}|}\chi_{\mathbf{GG}'}(\mathbf{q},\omega)$$

macroscopic dielectric function (determines optical absorption):

$$\varepsilon_{mac}(\omega) = 1 - \lim_{q\to 0}\frac{4\pi}{q^2}\bar{\chi}_{00}(\mathbf{q},\omega)$$

Failure of the ALDA/GGA



Why do ALDA/GGA fail??

- ► gap too small (use scissors)
- ► no excitonic binding
- ► need xc functionals with spatial long range

G. Onida, L. Reining, A. Rubio, RMP **74**, 601 (2002)
S. Botti, A. Schindlmayr, R. Del Sole, L. Reining, Rep. Prog. Phys. **70**, 357 (2007)

Which exchange-correlation functional to choose?

No excitons with standard functionals (LDA, GGA)!

Long-range corrected (LRC):

$$f_{xc}^{LRC}(\mathbf{r},\mathbf{r}') = -\frac{\alpha}{4\pi|\mathbf{r}-\mathbf{r}'|}$$

- ▶ model parameters/empirical fitting
- ▶ Other functionals reduce to same basic type
- ▶ Qualitatively correct excitonic physics
- ▶ Computationally cheap, but less accurate

Botti *et al.*, PRB **69**, 155112 (2004)
Sharma, Dewhurst, Sanna & Gross, PRL **107**, 186401 (2011)
Rigamonti et al., PRL **114**, 146402 (2015)
Trevisanutto *et al.*, PRB **87**, 205143 (2013)
Berger, PRL **115**, 137402 (2015)
Cavo, Berger & Romaniello, PRB **101**, 115109 (2020)
Byun, Sun & Ullrich, Electron. Struct. **2**, 023002 (2020)

Screened hybrid:

$$K_{xc}^{hybrid} = \gamma K_{x}^{XX} + (1-\gamma)K_{xc}^{ALDA}$$

- ▶ Generalized TDDFT (includes nonlocal exchange)
- ▶ Computationally more demanding
- ▶ More accurate (comparable to BSE)

Refaely-Abramson *et al.*, PRB **92**, 081204 (2015)
Wing *et al.*, PRMat **3**, 064603 (2019)
Tal, Liu, Kresse & Pasquarello, PRRes **2**, 032019 (2020)
Zivkovic *et al.*, JPC C **124**, 24995 (2020)
Sun, Li & Liang, PCCP **21**, 16296 (2021)
Sun, Yang & Ullrich, PRRes. **2**, 013091 (2020)
Alam, Sun & Ullrich, arXiv:2502.20683 (→ PRB)

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- Excitons with TDDFT: the LRC kernel
- **real-time TDDFT with LRC**
- The “Kohn-Sham-Proca” approach: Sangeeta’s slides
- Stability analysis of TDLRC: why it works

Excitons with real-time TDDFT

$$i\frac{\partial}{\partial t}\varphi_j(\mathbf{r},t) = \left[\frac{1}{2}\left(\frac{\nabla}{i} + \mathbf{A}_{ext}(\mathbf{r},t) + \mathbf{A}_{xc}(\mathbf{r},t)\right)^2 + V_{nuc}(\mathbf{r}) + V_{Hxc}(\mathbf{r},t)\right]\varphi_j(\mathbf{r},t)$$

$$f_{xc}^{LRC}(\mathbf{r},\mathbf{r}') = -\frac{\alpha}{4\pi|\mathbf{r}-\mathbf{r}'|} \Rightarrow V_{xc}^{LRC}(\mathbf{r},t) = -\int f_{xc}^{LRC}(\mathbf{r},\mathbf{r}')\delta n(\mathbf{r}',t)d\mathbf{r}'$$

Long-range part is ill defined!
Make gauge transformation:

$$\nabla\cdot\mathbf{j} = -\dot{n} \qquad -\nabla V_{xc}^{LRC} = \dot{\mathbf{A}}_{xc}^{LRC}$$

$$\mathbf{A}_{xc}^{LRC}(\mathbf{r},t) = -\frac{\alpha}{4\pi}\int_0^t dt'\int_0^{t'} dt''\nabla\int d\mathbf{r}'\frac{\nabla'\cdot\mathbf{j}(\mathbf{r}',t'')}{|\mathbf{r}-\mathbf{r}'|}$$

Head-only approximation:

$$\frac{d^2}{dt^2}\mathbf{A}_{xc,\mathbf{G}=0}^{LRC}(t) = \alpha\mathbf{j}_0(t)$$

TDLRC approach

$$i\frac{\partial}{\partial t}\varphi_j(\mathbf{r},t) = \left[\frac{1}{2}\left(\frac{\nabla}{i} + \mathbf{A}_{ext}(t) + \mathbf{A}_{xc}^{LRC}(t)\right)^2 + V_{nuc}(\mathbf{r}) + V_{Hxc}(\mathbf{r},t)\right]\varphi_j(\mathbf{r},t)$$

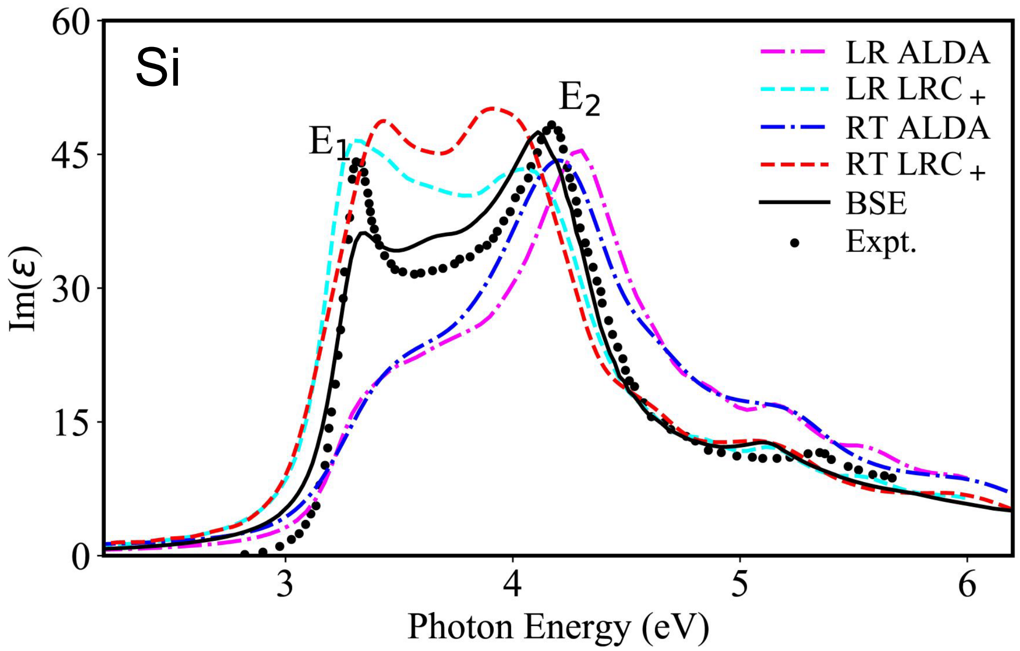
$$\frac{d^2}{dt^2}\mathbf{A}_{xc}^{LRC}(t) = \alpha \mathbf{j}_0(t)$$

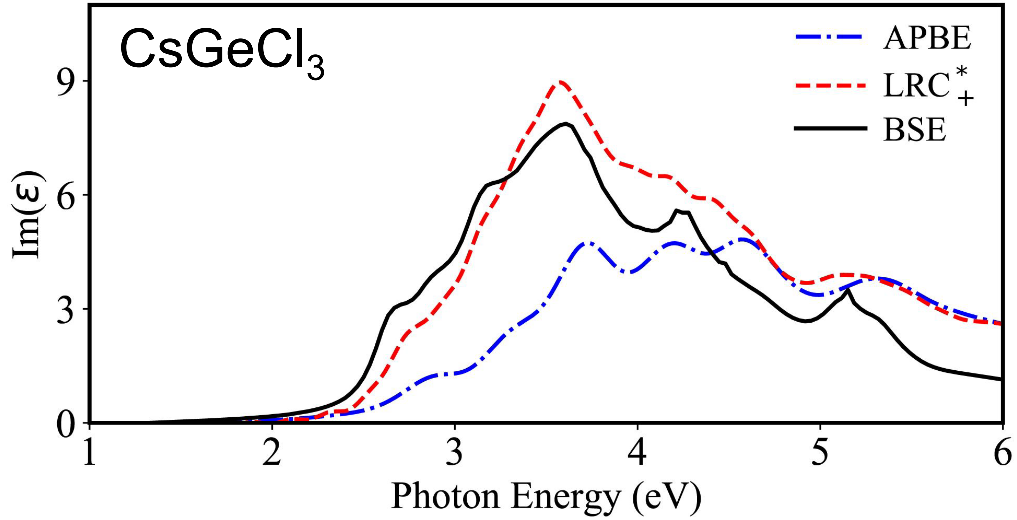
Macroscopic current: Implicit and explicit feedback on $\mathbf{A}_{xc}$

$$\mathbf{j}_0(t) = 2\sum_{l}^{N/2}\sum_{\mathbf{k},\mathbf{G}} \mathbf{G}\,|C_{l,\mathbf{k}-\mathbf{G}}(t)|^2 + N\left[\mathbf{A}(t) + \mathbf{A}_{xc}^{LRC}(t)\right]$$

where $\varphi_{l\mathbf{k}}(\mathbf{r},t) = \sum_{\mathbf{G}} C_{l,\mathbf{k}-\mathbf{G}}(t)e^{-i(\mathbf{k}-\mathbf{G})\cdot\mathbf{r}}$

Optical spectra from TDLRC





Calculations done using Qb@ll code

delta-kick: $V(\mathbf{r},t) = \mathbf{E}_0 \cdot \mathbf{r}\delta(t-t_0)$

$$\Rightarrow \mathbf{A}(t) = \mathbf{E}_0\theta(t-t_0)$$

conductivity:

$$\sigma_{ij}(\omega) = -\frac{c}{A_j}\int_0^T e^{i\omega t} f(t) j_{0,i}(t)dt$$

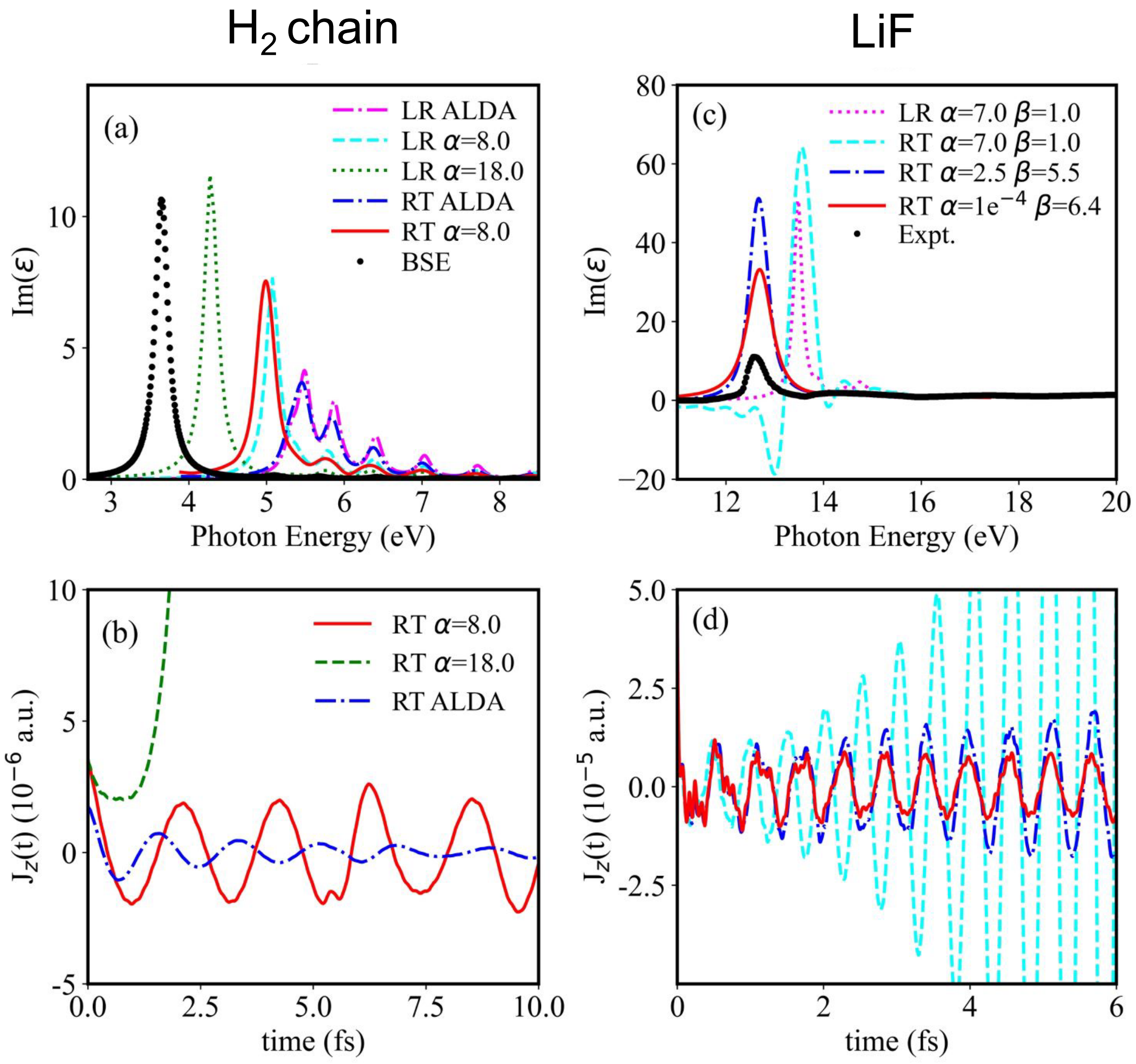
dielectric function:

$$\varepsilon_{mac}(\omega) = 1 + \frac{4\pi i\sigma(\omega)}{\omega}$$

Works well for weakly bound excitons!

Sun, Lee, Kononov, Schleife & Ullrich, PRL **127**, 077401 (2021)

Strongly-bound excitons from TDLRC



► Strongly bound excitons: TDLRC develops **instabilities.**

► **quick and dirty fix:** e-h binding through local-field effects

► **Questions:**
- **Could it be numerics?**
- **Can TDLRC be stabilized?**

Sun, Lee, Kononov, Schleife & Ullrich, PRL **127**, 077401 (2021)

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- Stability analysis of TDLRC: why it works

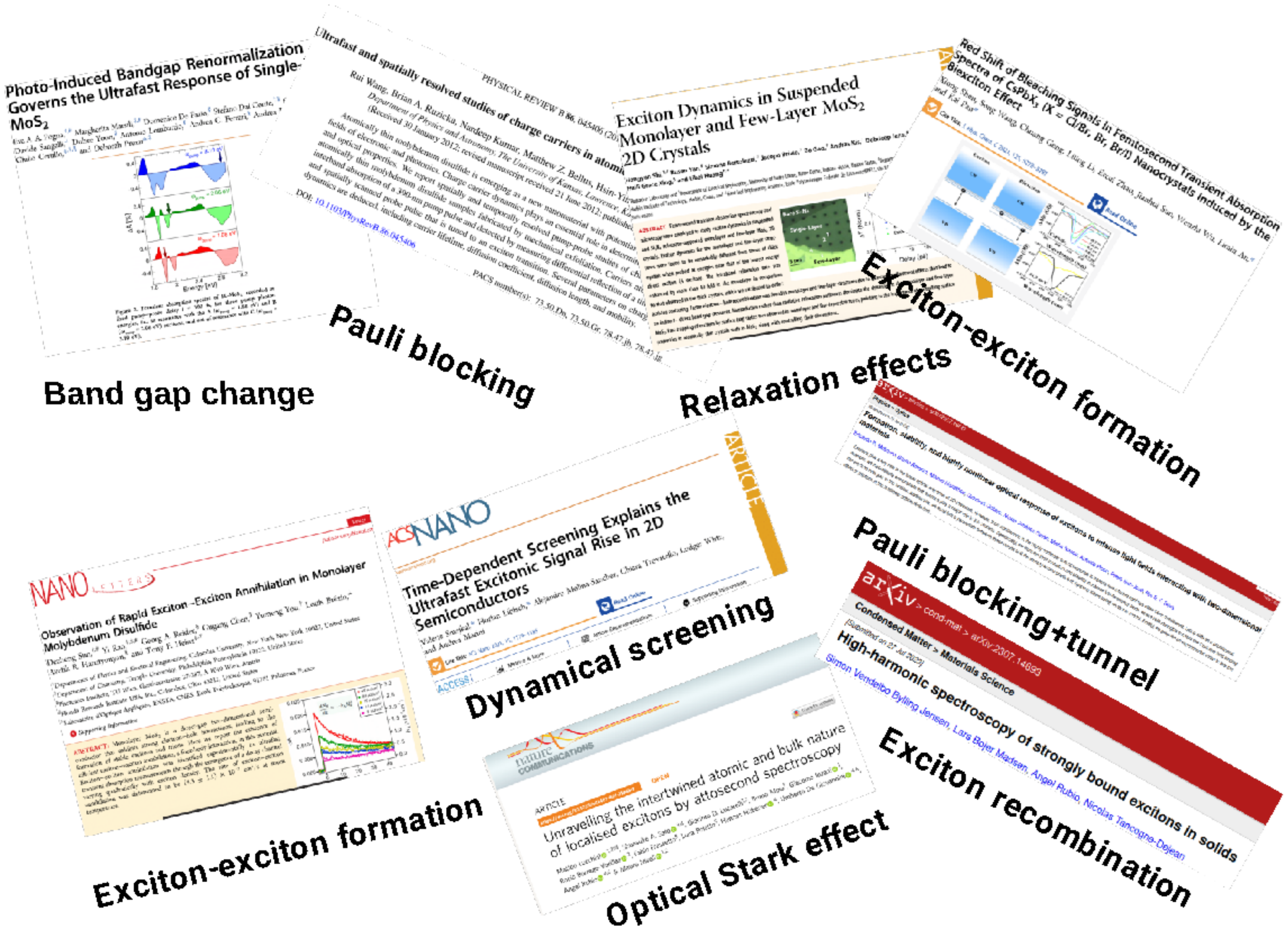
Ultrafast light dressed excitons

D. Gill, S. Shallcross, J. K. Dewhurst and S. Sharma

Max-Born Institute, Berlin, Germany
Freie University Berlin, Germany
Max Planck Institute Halle, Germany

J. K. Dewhurst, D. Gill, S. Shallcross, and S. Sharma, PRB **111**, L060302 (2025)
D. Gill, S. Shallcross, W. Chen, J. K. Dewhurst, and S. Sharma, arXiv2504.04476 (2025)

Different Physics underpinning similar observation?



Light dressed excitons:

Same experimental observation different theoretical explanations:
ab-initio theory missing!!

Proca equation as functional generator

Time-Dependent Kohn-Sham Equation

$$i\frac{\partial}{\partial t}\psi_j(\mathbf{r},t) = \left[\frac{1}{2}\left(-i\nabla - \frac{1}{c}\left[\mathbf{A}(t) + \mathbf{A}_{\mathbf{xc}}(t)\right]\right)^2 + v_s(\mathbf{r},t)\right]\psi_j(\mathbf{r},t)$$

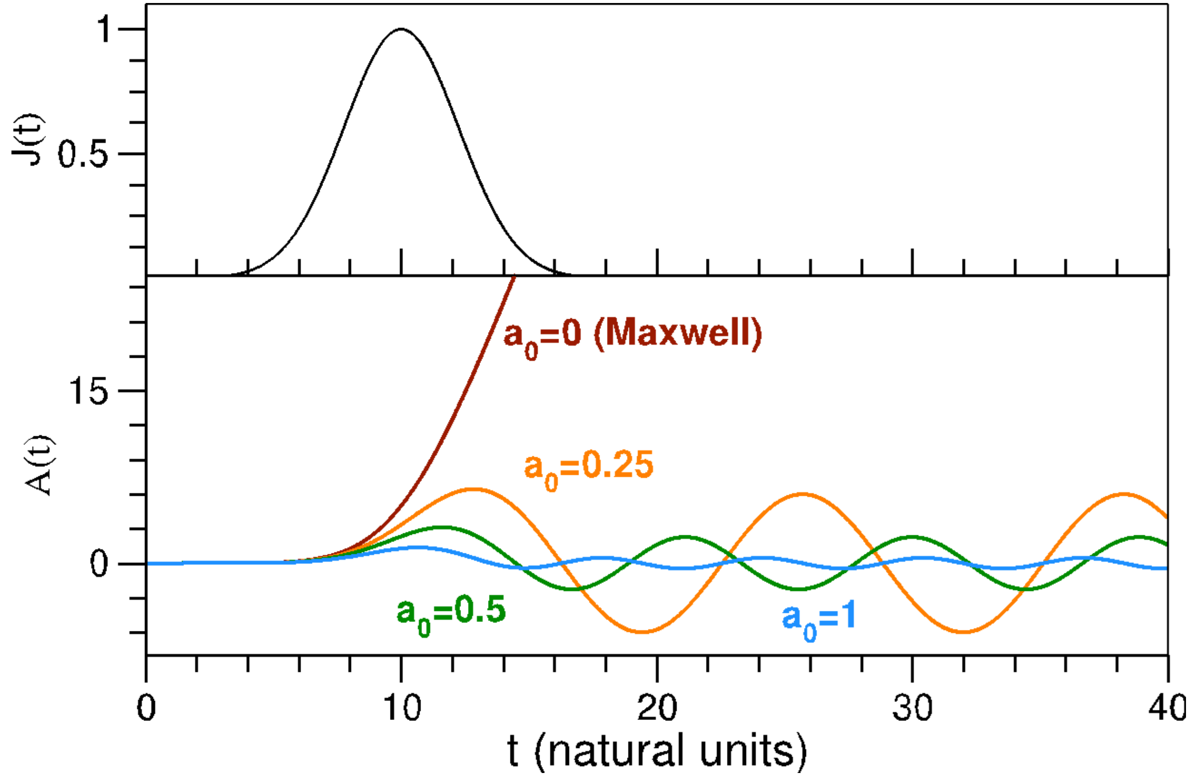
$$\mathbf{j}(\mathbf{r},t) = \Im\sum_j^{\mathrm{occ}} \psi_j(\mathbf{r},t)^* \nabla\psi_j(\mathbf{r},t) - \frac{1}{c}\left[\mathbf{A}(t) + \mathbf{A}_{\mathrm{xc}}(t)\right]\rho(\mathbf{r},t)$$

$$a_2\frac{\partial^2}{\partial t^2}\mathbf{A}_{\mathbf{xc}}(t) = 4\pi\mathbf{J}(t) - a_0\mathbf{A}_{\mathbf{xc}}(t)$$

Effective Proca's Equation

Proca equation as functional generator

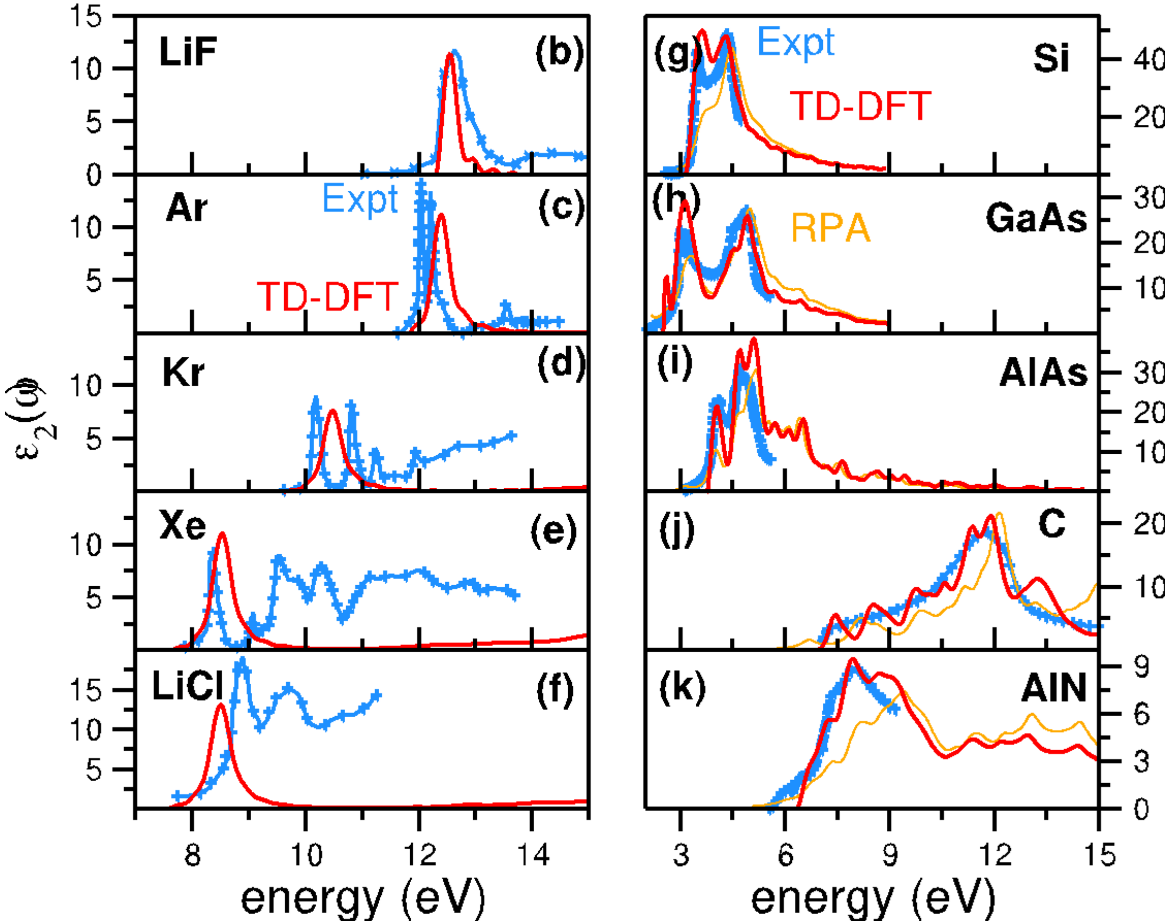
$$a_2 \frac{\partial^2}{\partial t^2} A_{xc}(t) = 4\pi J(t) - a_0 A_{xc}(t)$$



$A_{xc}(t)$ oscillates at a characterstic frequency of the exciton resonance

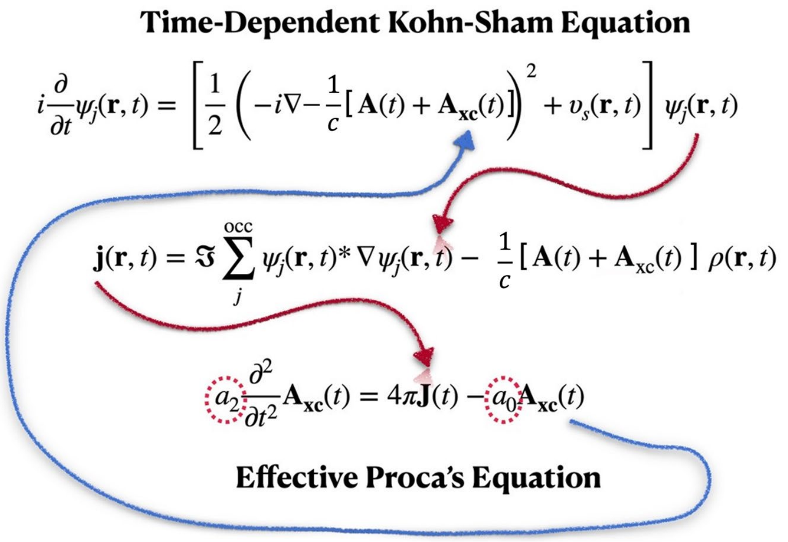
Mass term leads to memory $A_{xc}(t) = \int_{-\infty}^{t} E(t')dt'$

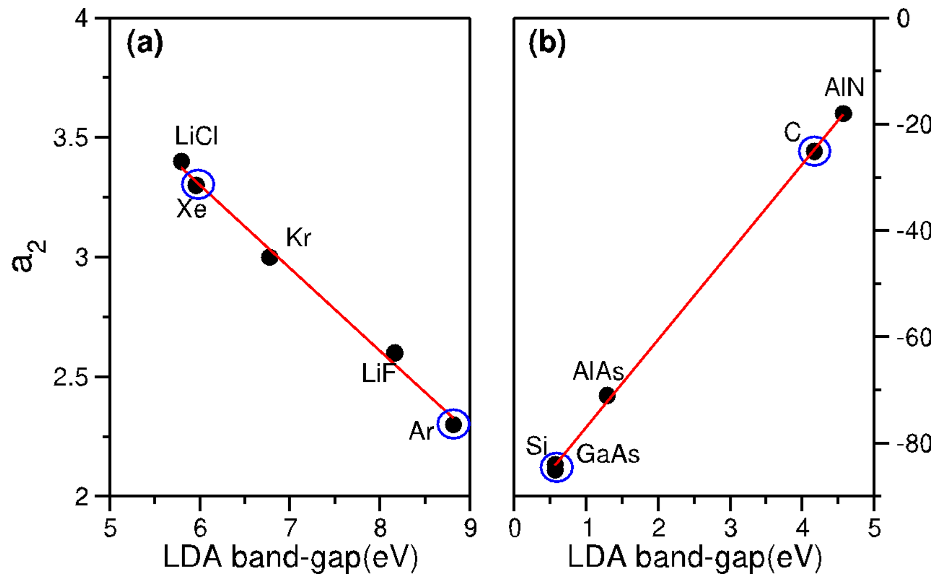
Weakly and strongly bound excitons in solids



- ❑ Describes excitonic response in weak pumping regime.
- ❑ Rydberg series, i.e. excited state of excitons is missing

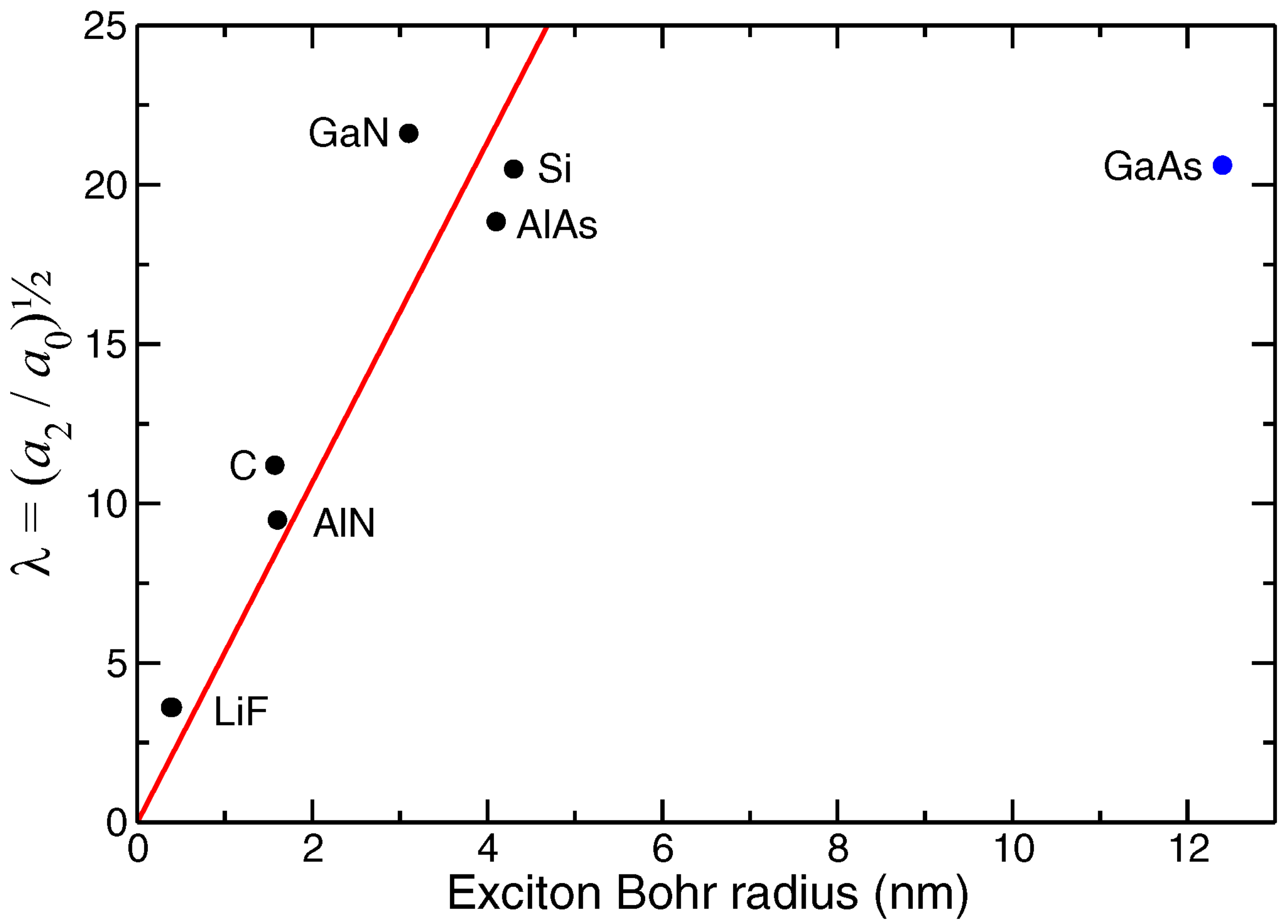
Universality of the functional





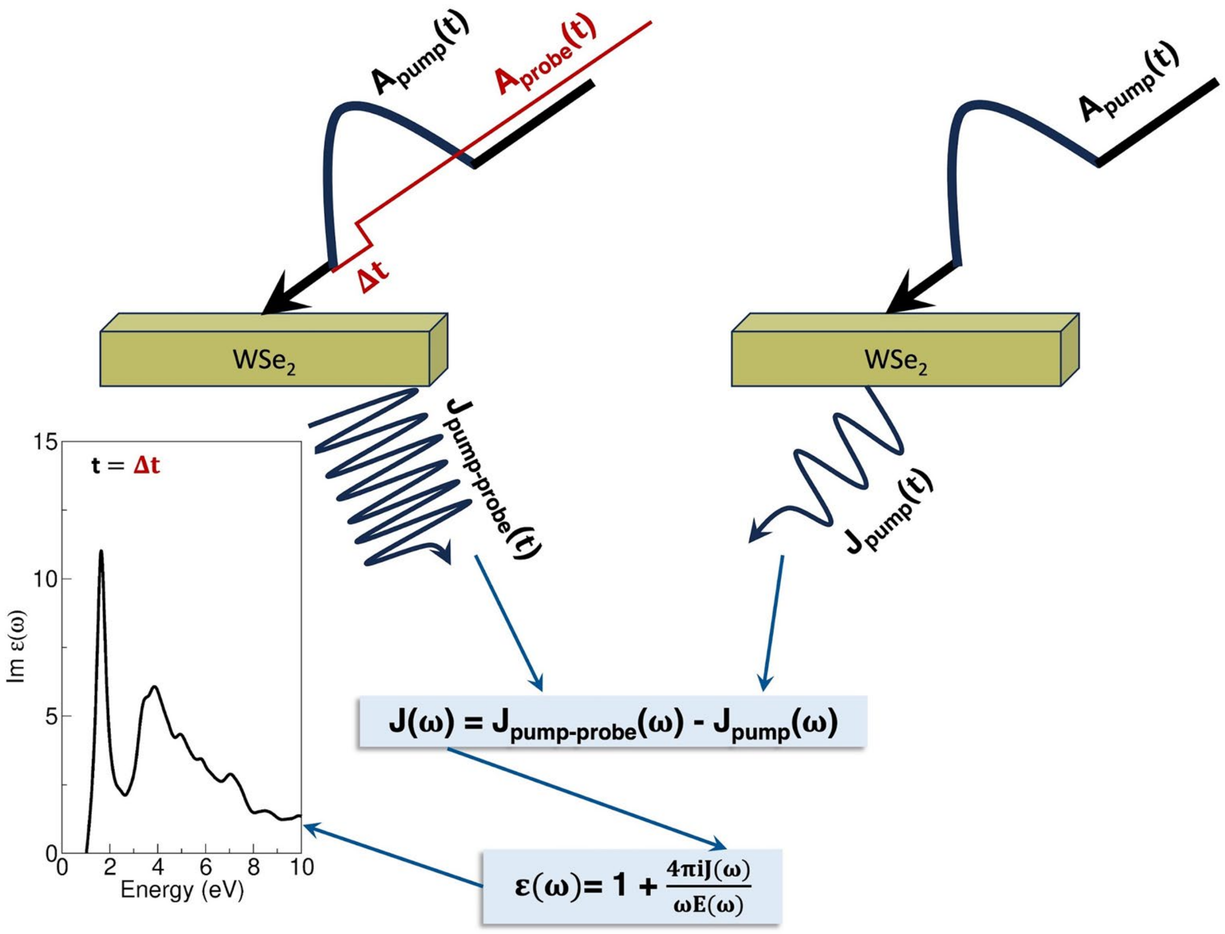
- Parameters are universal for a class (keeping the method ab-initio)
- $a_0 = -0.2$ for weakly bound and $a_0 = 0.2$ for strongly bound excitons
- a_2 is linear wrt the gap
- memory dependent functional

Excitonic radius in solids



- ❑ Exciton radius can also be determined
- ❑ GaAs is an outlier

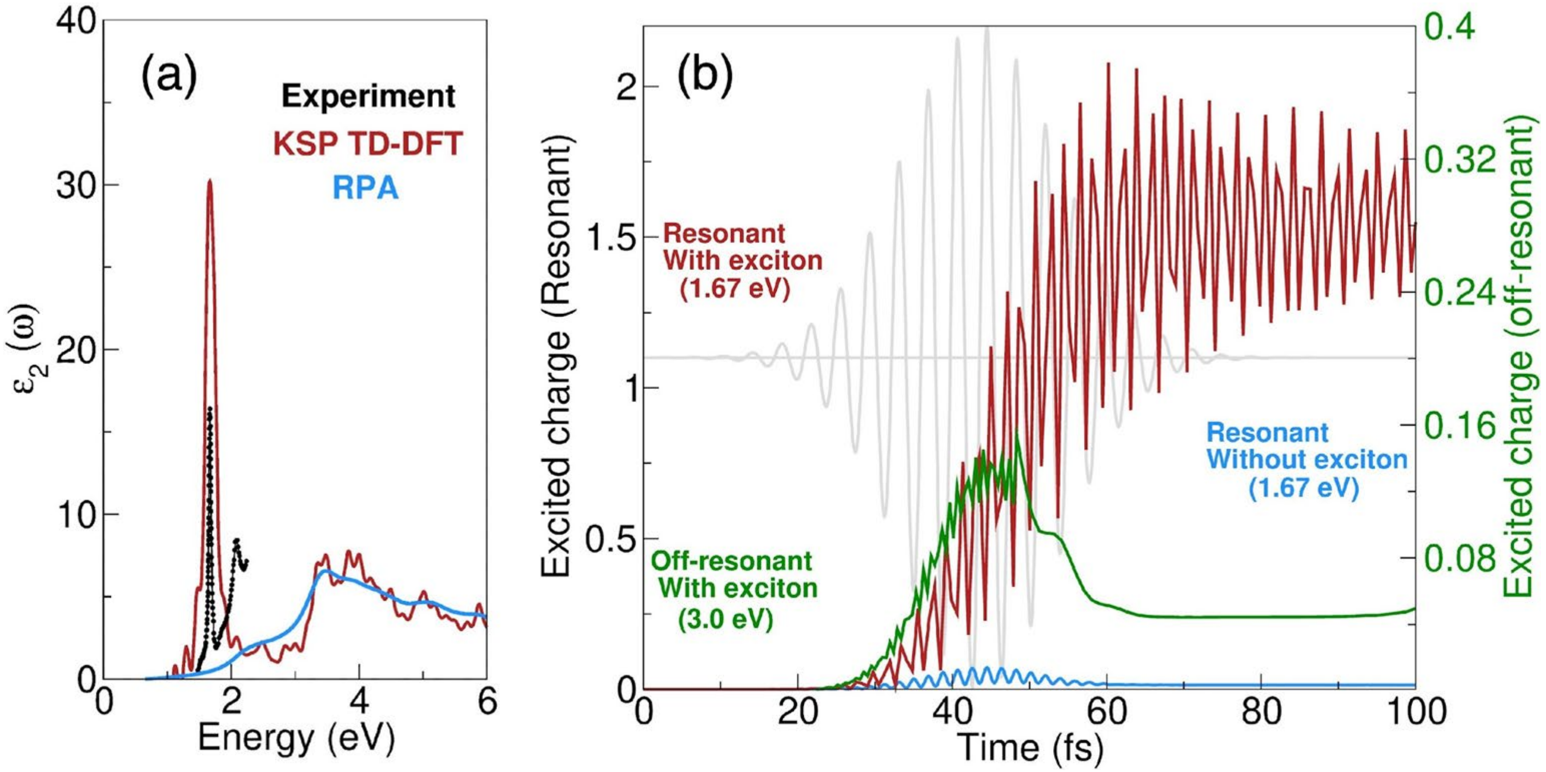
Response: pump-probe spectroscopy



- ❑ Pump pulse can be strong or weak
- ❑ Can probe the response at any time

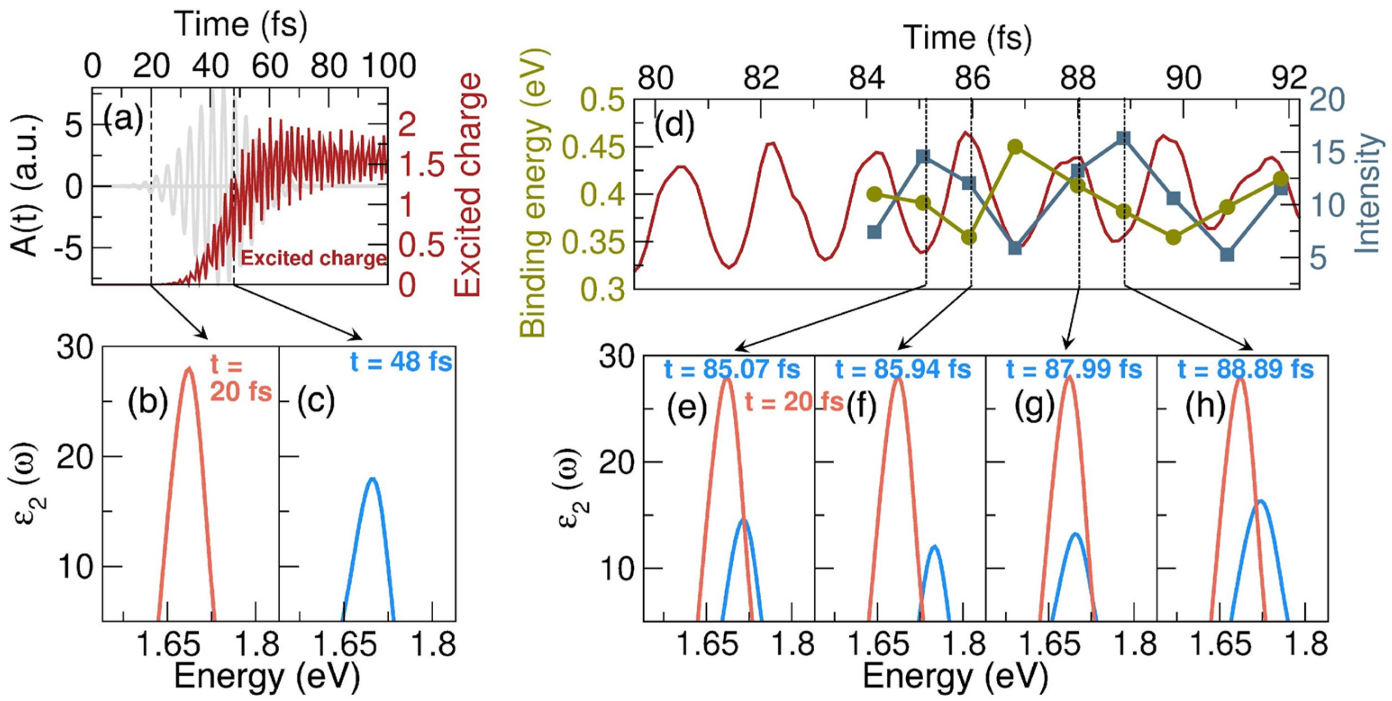
Light dressed excitons: free carrier dynamics

WSe$_2$



- ❑ Accurate description of excitons in 2d materials.
- ❑ Free carrier excitation enhanced 10 times when pumped at excitonic frequency.
- ❑ Free carrier dynamics strongly correlated with exciton dynamics and light.
- ❑ Free carrier excitation suppressed when pumped with frequency > gap.

Light dressed excitons: exciton dynamics



- ❑ Excitons are formed by the pump pulse
- ❑ Excitons are destroyed by the pump pulse
- ❑ Exciton-exciton interaction destroys excitons
- ❑ Free carrier number increases
- ❑ Excitons are screened: binding energy changes
- ❑ Some free carriers form new excitons

Elk code: full potential LAPW method

Science 351, 6280 (2016)

		AE							
		Elk	exciting	FHI-aims/tier2	FLEUR	FPLO/T+F+s	RSPt	WIEN2k/acc	average <Δ>
AE	Elk		0.3	0.3	0.6	1.0	0.9	0.3	0.6
	exciting	0.3		0.1	0.5	0.9	0.8	0.2	0.5
	FHI-aims/tier2	0.3	0.1		0.5	0.9	0.8	0.2	0.5
	FLEUR	0.6	0.5	0.5		0.8	0.6	0.4	0.6
	FPLO/T+F+s	1.0	0.9	0.9	0.8		0.9	0.9	0.9
	RSPt	0.9	0.8	0.8	0.6	0.9		0.8	0.8
	WIEN2k/acc	0.3	0.2	0.2	0.4	0.9	0.8		0.5
PAW	GBRV12/ABINIT	0.9	0.8	0.8	0.9	1.3	1.1	0.8	0.9
	GPAW09/ABINIT	1.3	1.3	1.3	1.3	1.7	1.5	1.3	1.4
	GPAW09/GPAW	1.5	1.5	1.5	1.5	1.8	1.7	1.5	1.6
	JTH02/ABINIT	0.6	0.6	0.6	0.6	0.9	0.7	0.5	0.6
	PSlib100/QE	0.9	0.8	0.8	0.8	1.3	1.1	0.8	0.9
	VASPGW2015/VASP	0.5	0.4	0.4	0.6	1.0	0.9	0.4	0.6

Gold standard for electronic structure of solids. Features include:

- ❑ Ground state
- ❑ Most single particle observables
- ❑ Structural optimization
- ❑ Many-body methods: GW and beyond, RDMFT, BSE ...
- ❑ Response functions: magnons, phonons, plasmons, excitons ...
- ❑ Wannier90 interface
- ❑ Tensor moments
- ❑ Non-equilibrium spin dynamics
- ❑ Superconductivity: calculation of Tc, Eliashberg

J. K. Dewhurst, S. Sharma, L. Nordström and E. K. U. Gross ....

http://elk.sourceforge.net/

Summary

- ❑ Time (and memory) dependent functional generated for ab-initio description of light dressed excitons
- ❑ Its now possible to couple excitons, spins and phonons.
- ❑ **Resonant pumping**:
  - large amount of free carriers excited
  - Exciton creation and dissociation
  - Strongly coupled dynamics of excitons, laser pulse and free-carriers
- ❑ **Off-resonant pumping**:
  - Free carrier excitations are small
  - Coupling between excitons and light is suppressed.

J. K. Dewhurst, D. Gill, S. Shallcross, and S. Sharma, PRB **111**, L060302 (2025)
D. Gill, S. Shallcross, W. Chen, J. K. Dewhurst, and S. Sharma, arXiv2504.04476 (2025)

Why KSP: pros and cons

	TD-DFT	MBPT
Efficiency	😊	😒
Probe pulse effects	😊	😒
Multi pulse effects	😊	😒
Exciton visualization	😒	😊
Rydberg series	😒	😊
Non-linear effects	😊	😒
Strong field effects	😊	😒
Exact and controlled	😒	😊

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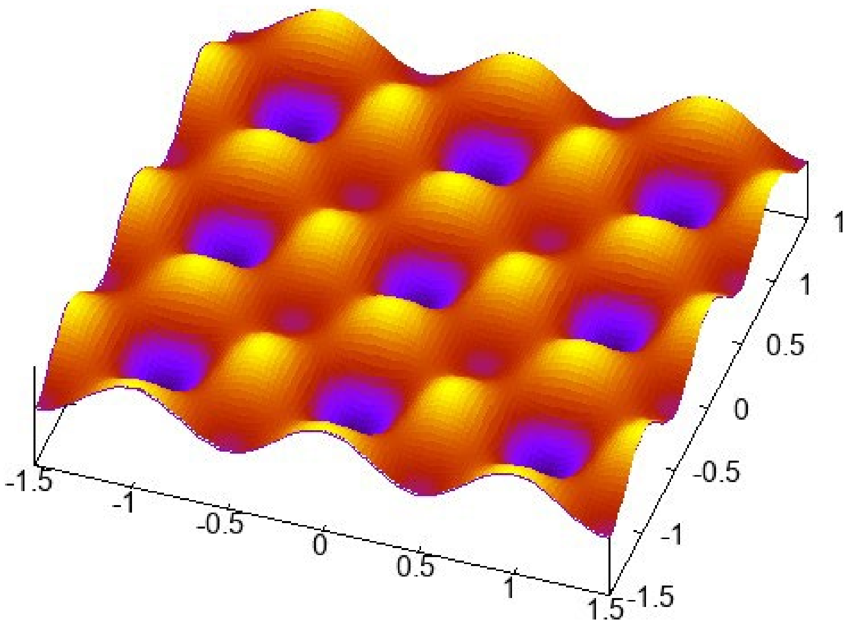
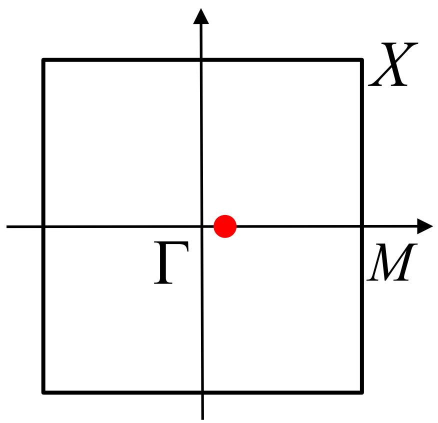
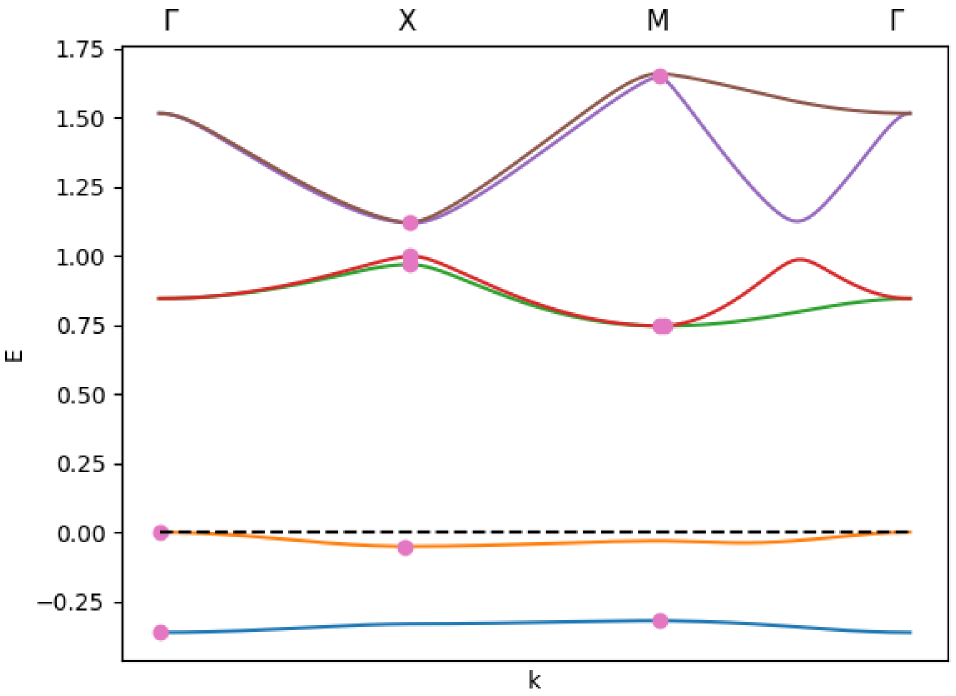
2D model solid to study LR- and RT-TDDFT





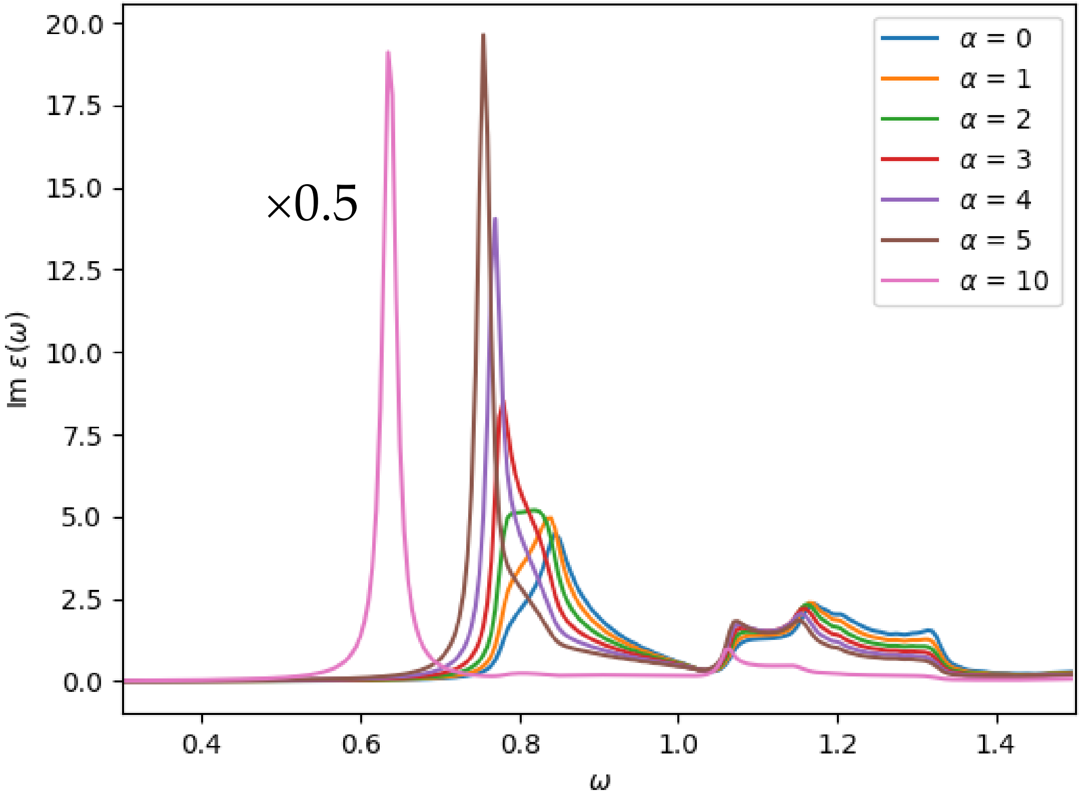


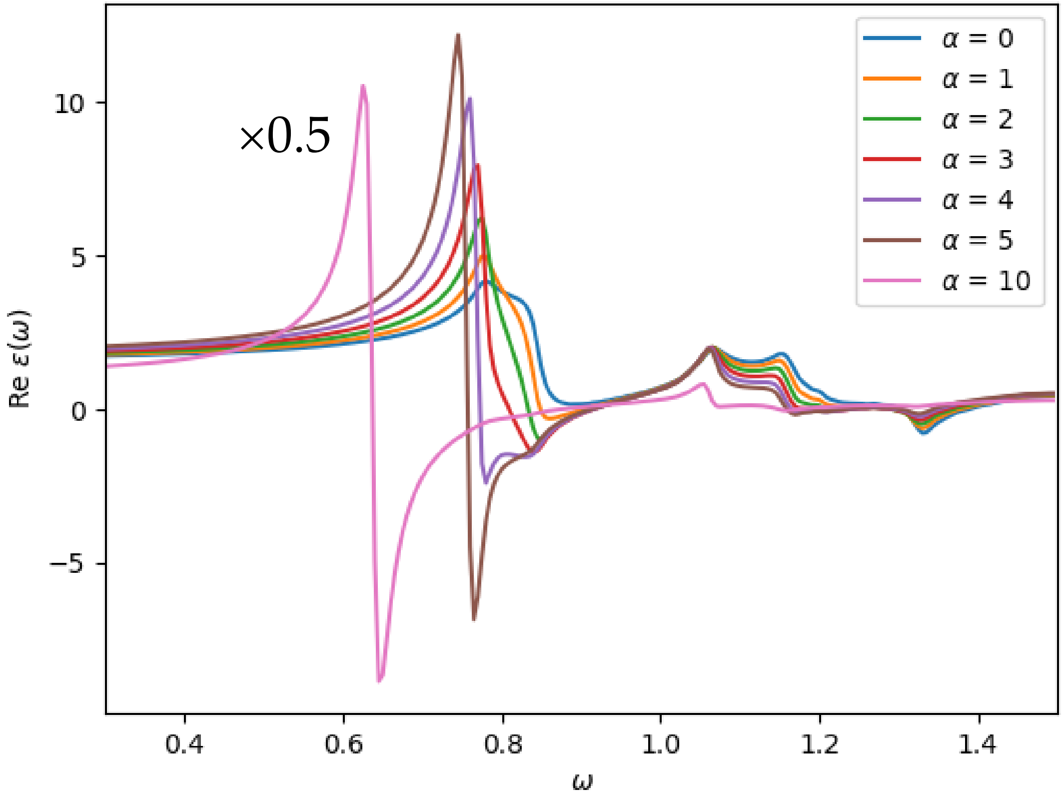
$A = 1, B = 0.9, c = 5$

$$V(x,y) = -4A\cos^2\left(\frac{\pi x}{c}\right)\cos^2\left(\frac{\pi y}{c}\right) + 4B\sin^2\left(\frac{\pi x}{c}\right)\sin^2\left(\frac{\pi y}{c}\right)$$

- N electrons per unit cell
- Potential parameters A,B
- Simple plane-wave basis
- 2D Coulomb interaction
- Dielectric function at finite q
- ALDA, LRC and screened HF

Dielectric function with linear-response LRC



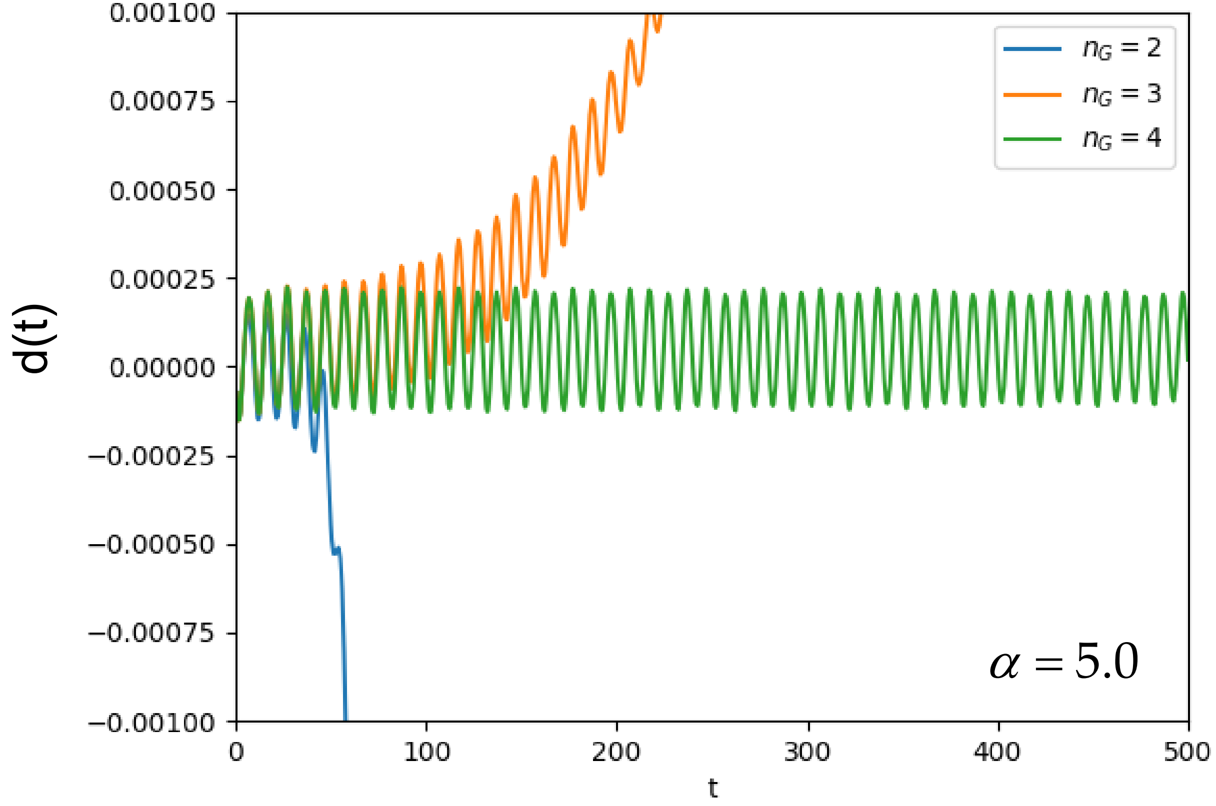


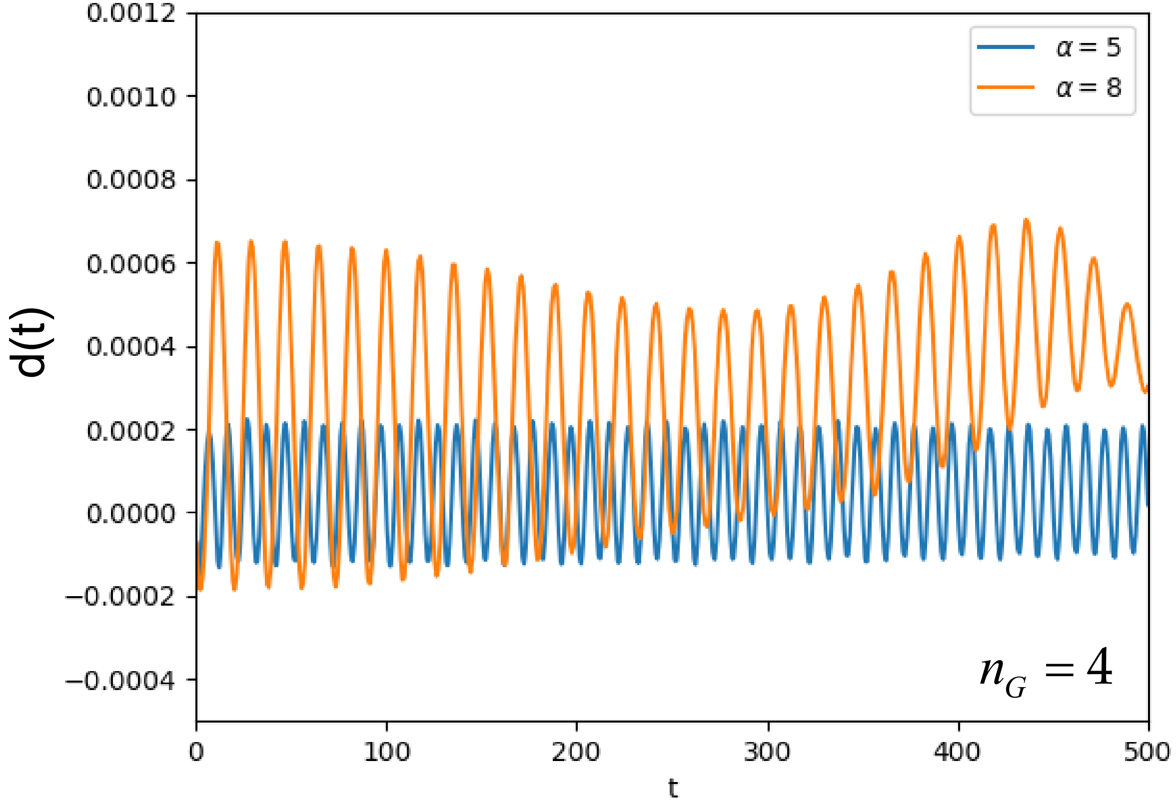
$$f_{xc}^{LRC}(\mathbf{r},\mathbf{r}') = -\frac{\alpha}{4\pi|\mathbf{r}-\mathbf{r}'|}$$

- ► **Strongly bound excitons if α is large**
- ► **But, LRC behaves unphysically:**
  - **●Excitons have huge oscillator strength**
  - **●Rydberg series condensed in 1 peak**

Byun, Sun & Ullrich, Electron. Struct. **2**, 023002 (2020)

TDLRC: instability of time-dependent dipole moment





Increasing the number of **G**-vectors helps somewhat

of **G**-vectors: $(2n_G + 1)^2$

But d(t) eventually becomes unstable if α is large enough.

Increasing n_G doesn't help.

Numerical stabilization of TDLRC

DGSS ("Proca") equation of motion: Dewhurst, Gill, Shallcross & Sharma, PRB **111**, L060302 (2025)

$$\left[\frac{d^2}{dt^2} + \beta\frac{d}{dt} + \gamma\right]\mathbf{A}_{xc,0}^{DGSS}(t) = \alpha\,\mathbf{j}_0(t)$$

damping term

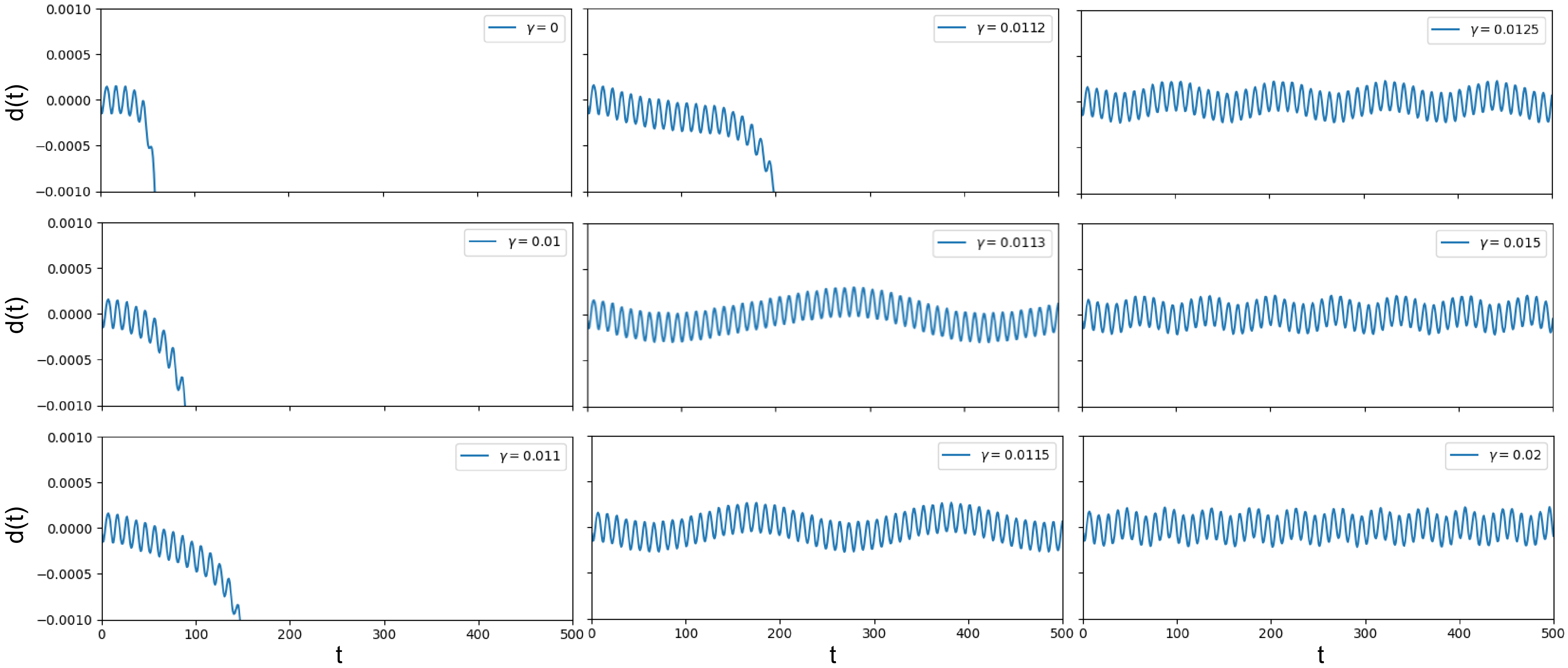
generalized spring constant

careful with numerics:

$$t_j \rightarrow t_{j+1}$$

requires $\mathbf{A}_{xc,0}^{DGSS}(t_{j+1/2})$

Numerical stabilization of TDLRC

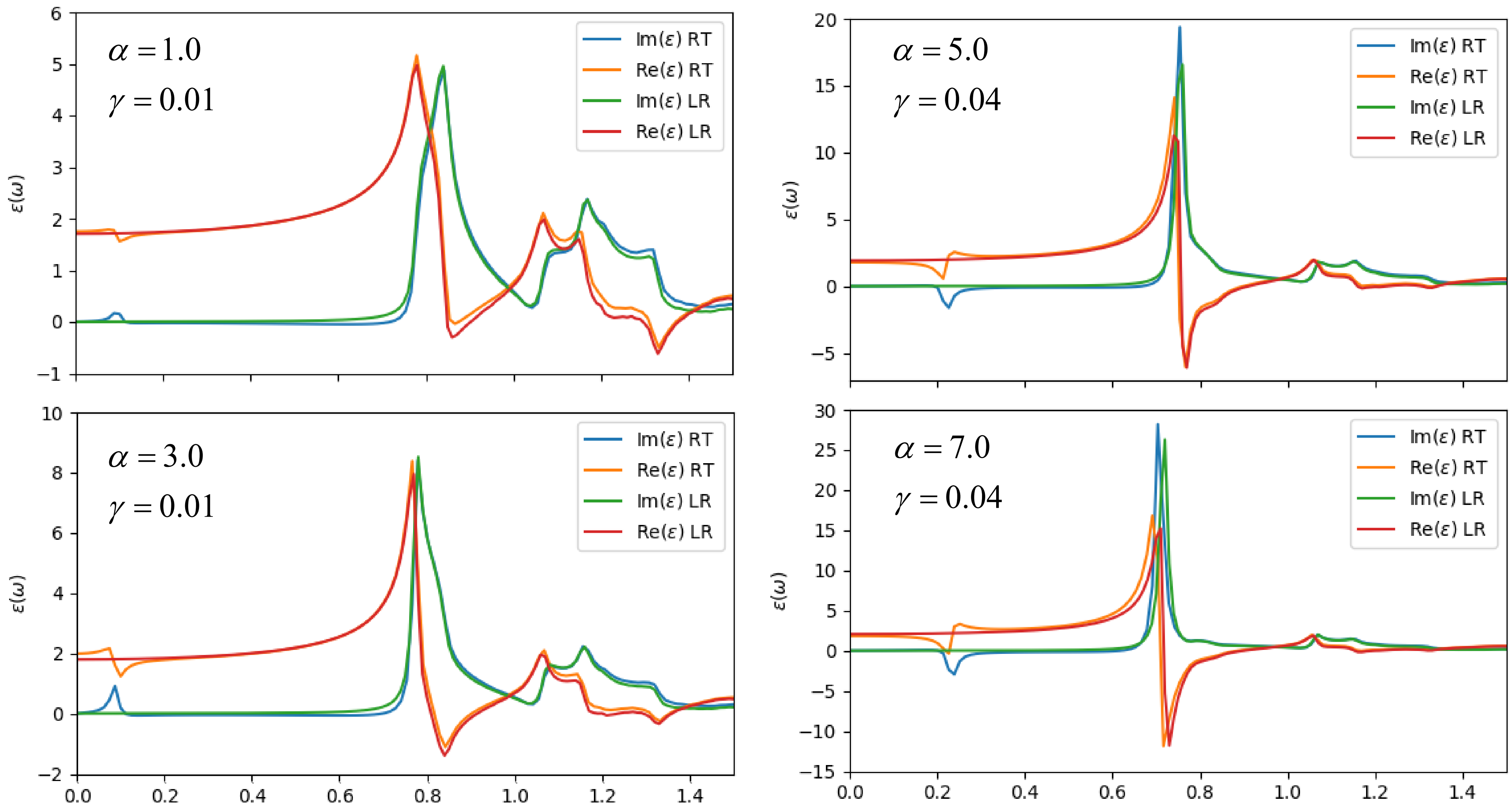


Dipole oscillations stabilize for γ > 0.01125

$$\alpha = 5.0$$

$$n_G = 2$$

Numerical stabilization of TDLRC



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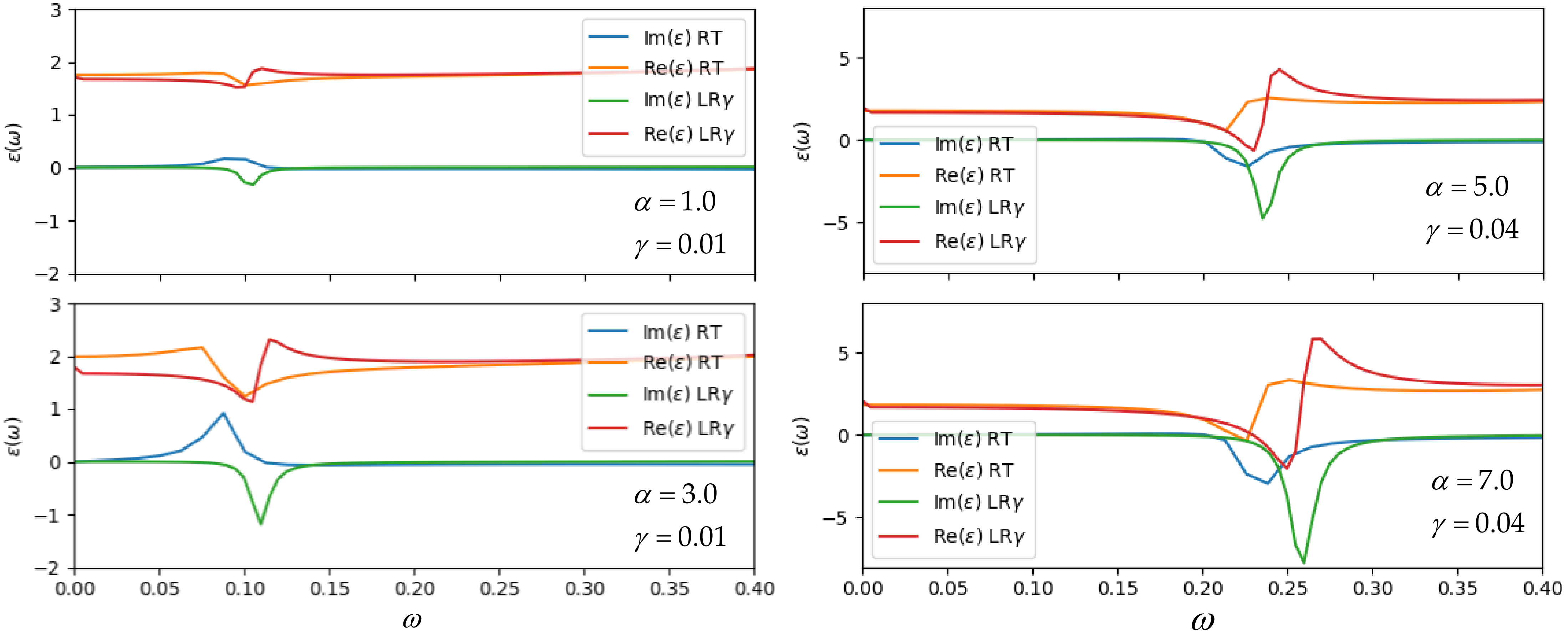


Additional features at low frequency:
ω-dependent xc kernel

$$f_{xc}^{DGSS}(\mathbf{r},\mathbf{r}',\omega) = \frac{\omega^2 f_{xc}^{LRC}(\mathbf{r},\mathbf{r}')}{\omega^2 + i\omega\beta - \gamma}$$

How does TDLRC work?

xc vector potential drives the excitonic dipole oscillations:

$$\ddot{\mathbf{A}}_{xc,0}^{LRC}(t) = \alpha \mathbf{j}_0(t) \equiv -\omega_{LRC}^2 A_{xc,0}^{LRC}$$

depends on A_{xc}

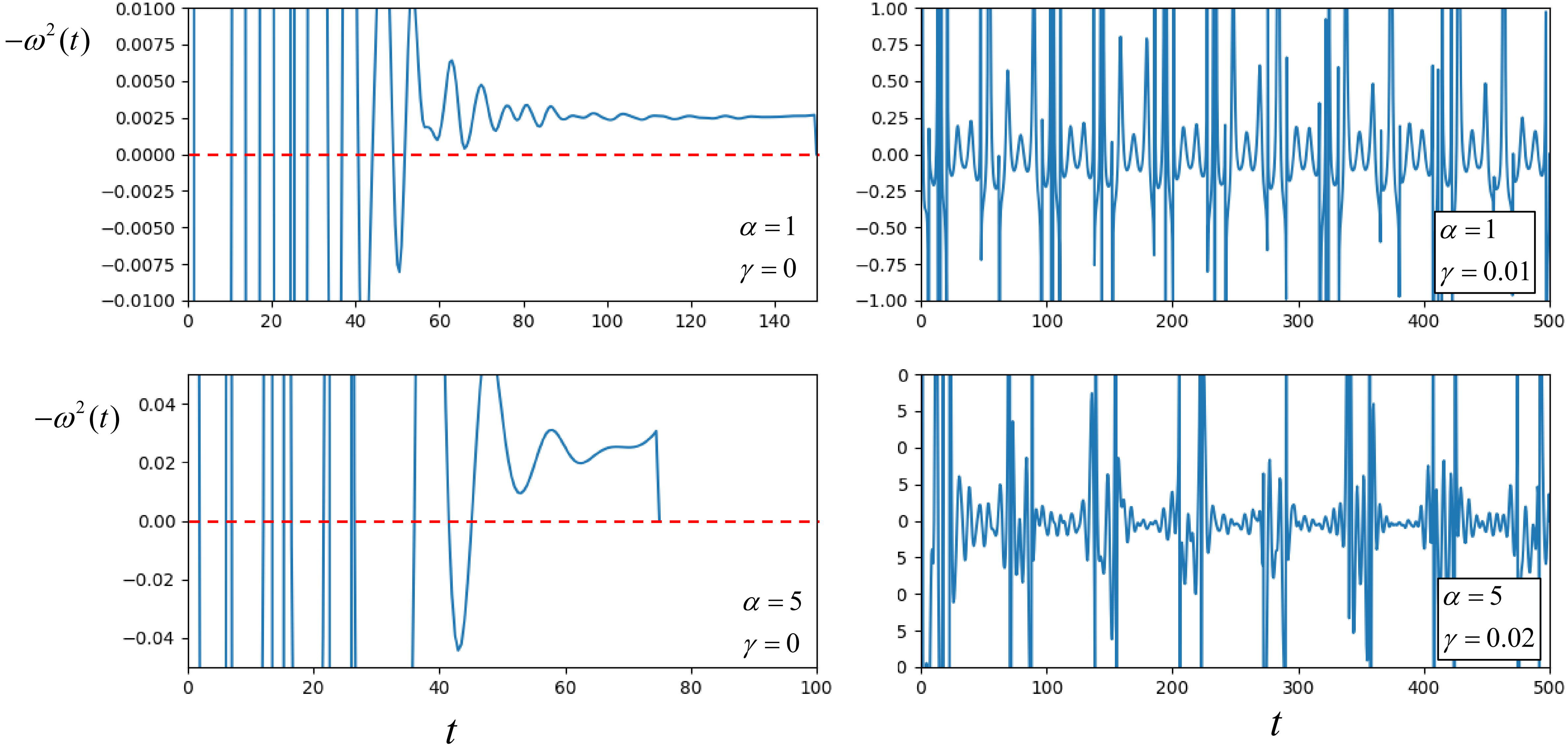
We define:

$$\frac{\ddot{\mathbf{A}}_{xc,0}^{LRC}(t)}{\mathbf{A}_{xc,0}^{LRC}(t)} = -\omega_{LRC}^2(t)$$

The equation of motion is that of a parametric oscillator:

$$\ddot{\mathbf{A}}_{xc,0}^{LRC}(t) + \omega^2(t)\mathbf{A}_{xc,0}^{LRC}(t) = 0$$

Parametric oscillators are known to have regions of stability/instability.



finite offset in $\omega(t)$ → parametric oscillator diverges

zero offset → parametric oscillator stable

Zero-force theorem: violation and restoration

$$\int dr\; n(\mathbf{r},t)\nabla V_{xc}^{approx}(\mathbf{r},t) = \mathbf{F}(t)$$

approximate xc potential can violate ZFT and give finite net force

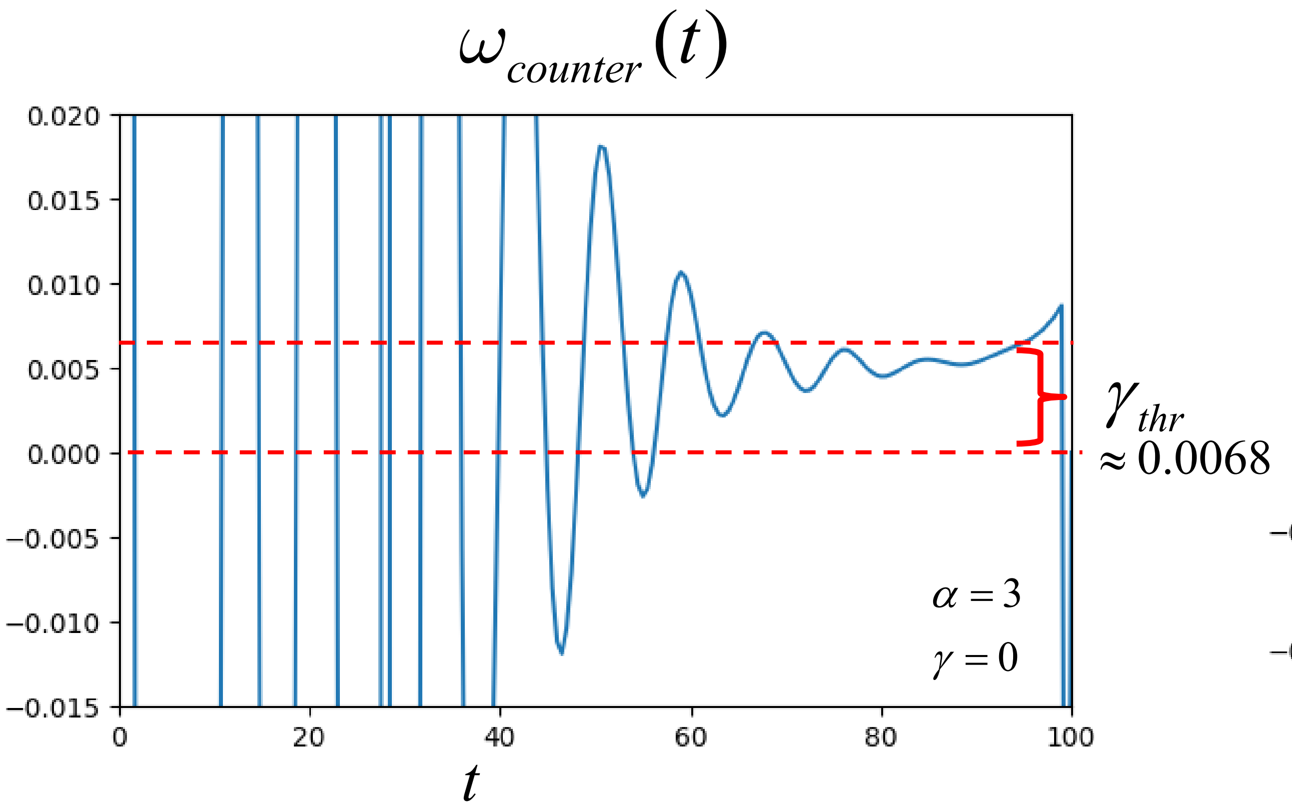
Counter-force to restore ZFT: $\int dr\; n(\mathbf{r},t)\mathbf{f}(\mathbf{r},t) = -\mathbf{F}(t)$ where $\left\|\mathbf{f}^2(t)\right\| = \min$

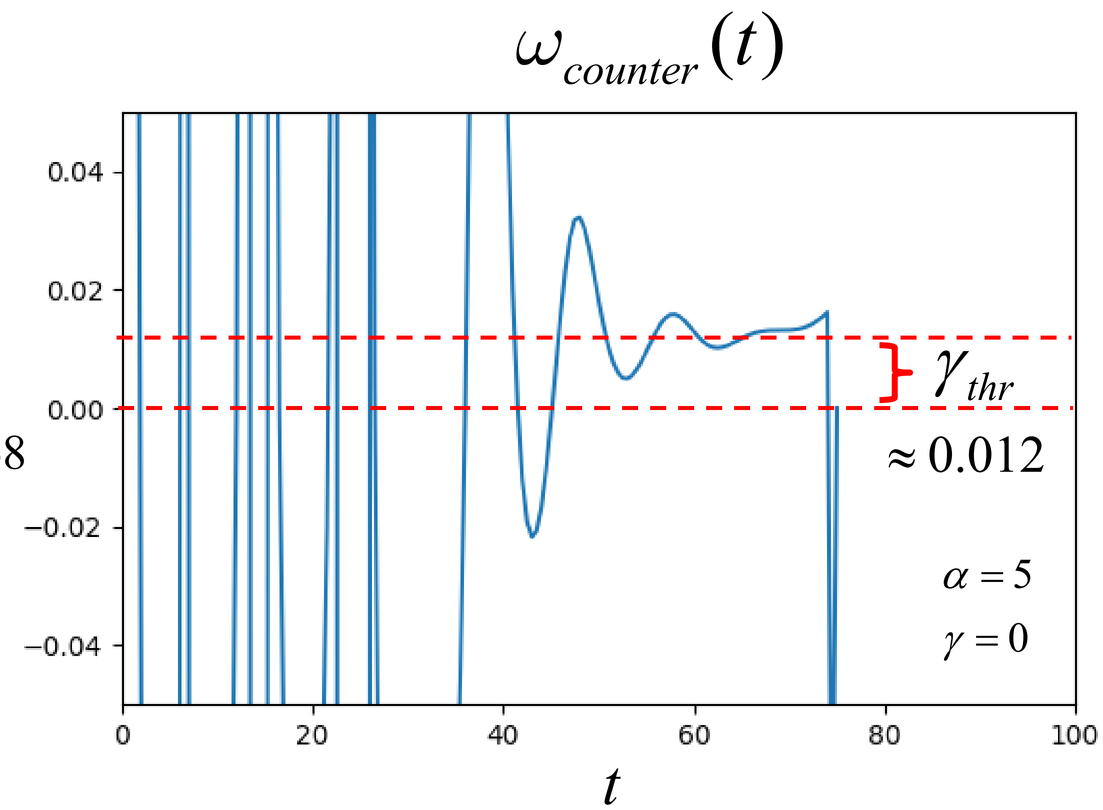
One finds $\mathbf{f}(\mathbf{r},t) = -\dfrac{\mathbf{F}(t)n(\mathbf{r},t)}{\left\|n^2(t)\right\|}$ where $\mathbf{F}_{LRC}(t) = \alpha N \int_0^t dt'\; \mathbf{j}_0(t')$

We define: $$\omega_{counter}^2(t) = \frac{\ddot{\mathbf{A}}_{xc,0}^{counter}(t)}{\mathbf{A}_{xc,0}^{LRC}(t)}$$

$$\dot{\mathbf{A}}_{xc,\mathbf{G}}^{counter}(t) = -\frac{\mathbf{F}_{LRC}(t)n_{\mathbf{G}}(t)}{\left\|n^2(t)\right\|}$$

Stabilizing TDLRC by average counter force

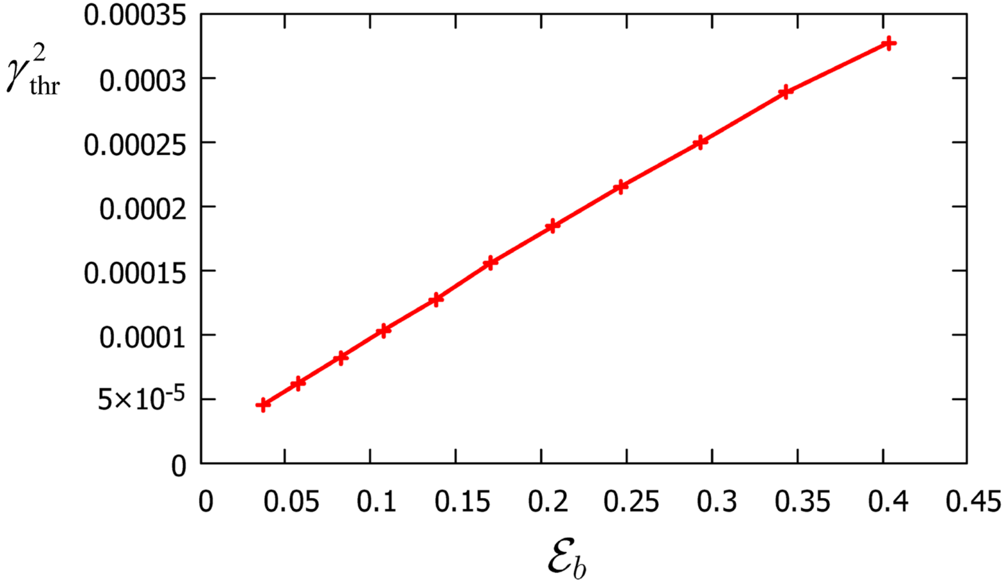




$$\gamma_{thr} = \left\langle \omega_{counter}^{2}(t) \right\rangle$$

- ► We obtain the threshold value for γ which stabilizes TDLRC
- ► This explains the choice of γ in DGSS

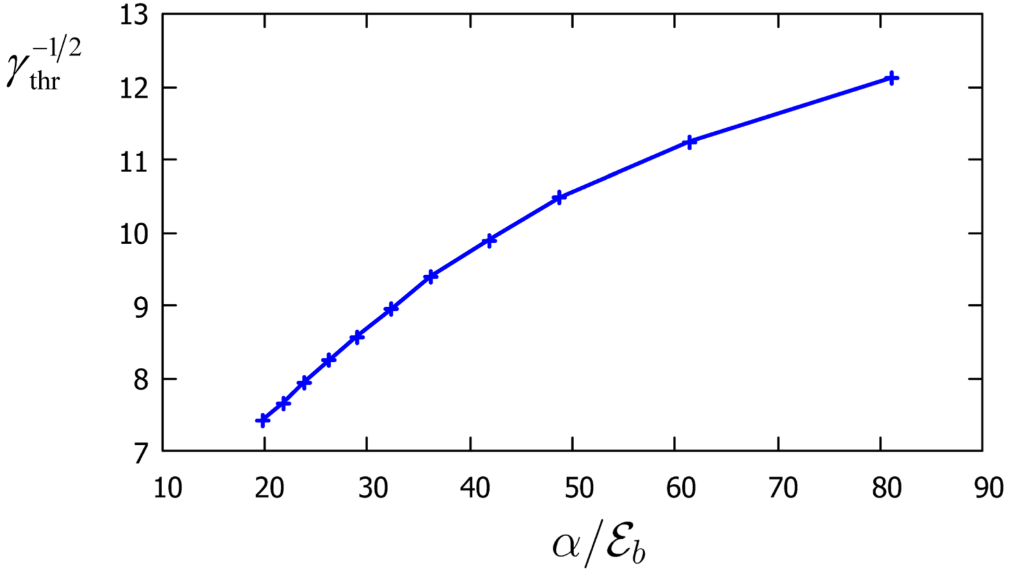
Connection between γ and exciton characteristics

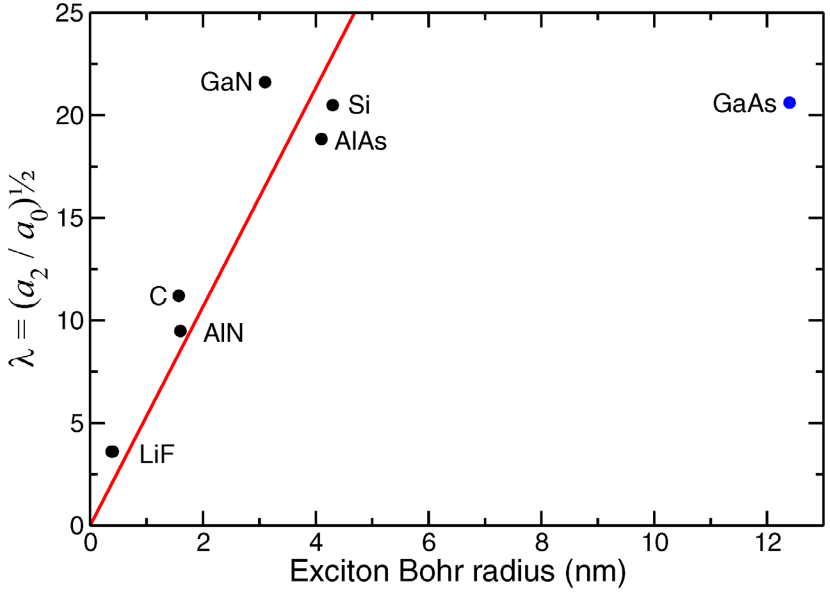


$$\gamma_{thr}^2 \sim \text{Exciton binding energy}$$

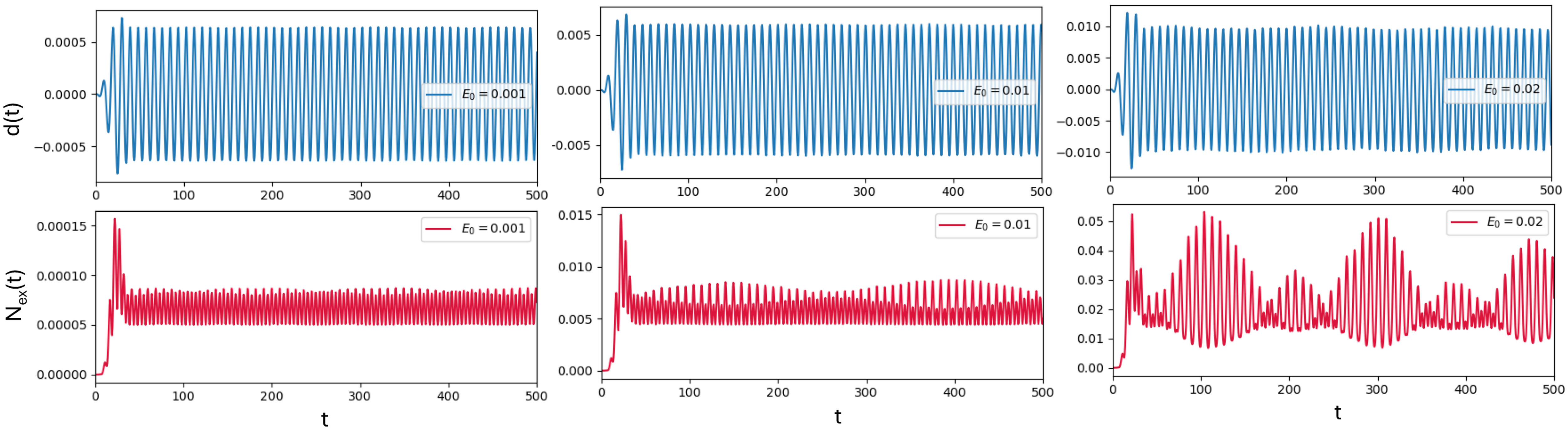
$$\frac{1}{\sqrt{\gamma_{thr}}} \sim \text{Exciton radius}$$

(Explains data from DGSS)





Stabilization persists into the nonlinear regime



$$\alpha = 4, \ \gamma = 0.009$$

3-cycle laser pulses with intensities $3.5\times10^{10}, 3.5\times10^{12}, 1.4\times10^{13}\ \mathrm{W/cm^2}$

No longer stable if $I > 2\times10^{13}\ \mathrm{W/cm^2}\ \ (N_{ex} > 0.1)$

Summary

- ►TDLRC operates by violating the zero-force theorem (because it is a non-variational theory).
- ►If stable, the ZFT is obeyed on average. TDLRC then creates excitons like a stable **parametric oscillator**.
- ►If unstable, TDLRC causes a net force on average. This causes exponential instability.
- ►"Proca" works by making sure that the parametric oscillations do not exponentially diverge. **The ZFT is enforced on average**. Enforcing the ZFT at each time t would spoil the effect.
- ►Also works in the nonlinear regime.

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