Ab initio few-mode theory

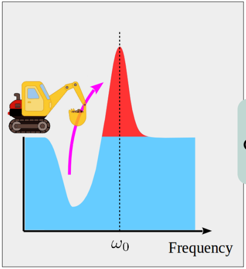
for quantum potential scattering problems

Dominik Lentrodt, Kilian P. Heeg,
Christoph H. Keitel and Jörg Evers

Max-Planck-Institut für Kernphysik, Heidelberg

https://xkcd.com/1070/

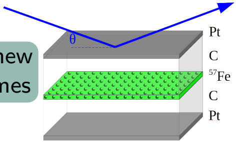
Background & Motivation



Coherent control of x-rays and nuclei

Nuclear quantum optics

X-rays excite new quantum regimes



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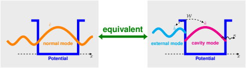
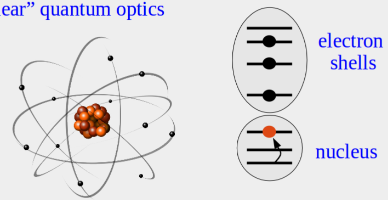


"Nuclear" quantum optics



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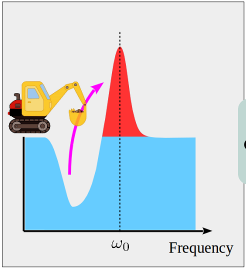

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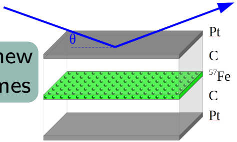

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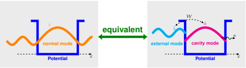

Mössbauer transitions as extreme qubits

- Tiny decoherence ($Q = 10^{12}$ to 10^{24})
- Room temperature
- Solid state (no vacuum necessary)
- Large coherently interacting ensembles

Motivations: metrology, spectroscopy,. . .

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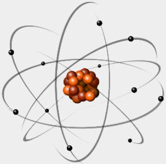

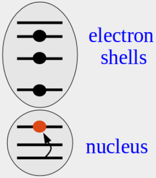

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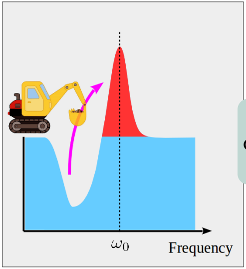

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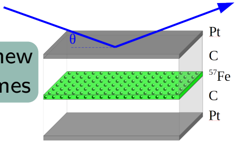

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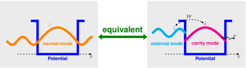

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Heeg & Evers *Phys. Rev. A* **88**, 043828 (2013)
Heeg et. al. *Phys. Rev. Lett.* **111** 073601 (2013)
Heeg et. al. *Phys. Rev. Lett.* **114** 203601 (2015)
Heeg et al. *Phys. Rev. Lett.* **114**, 207401 (2015)
Haber et. al. *Nature Photonics* **10** 445 (2016)
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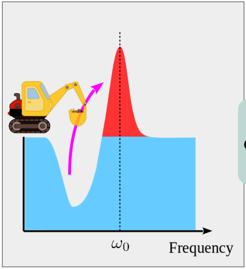

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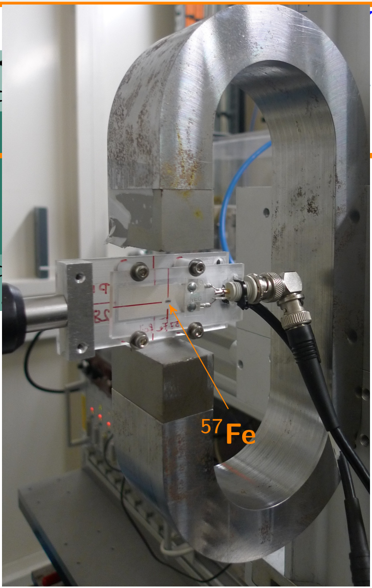

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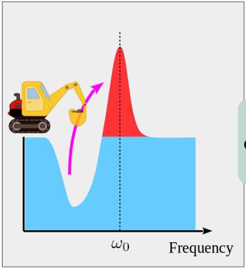

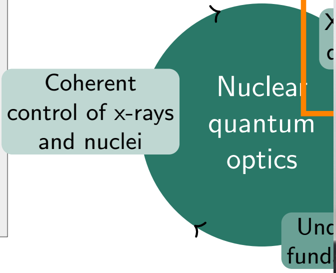

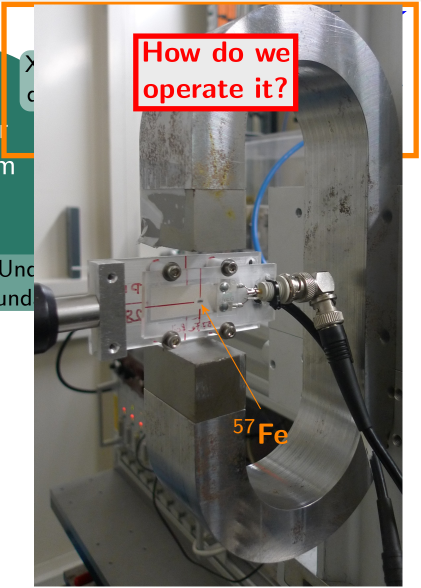

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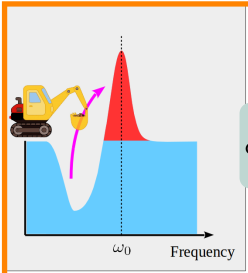

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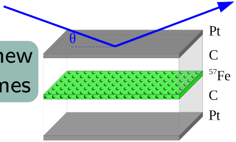

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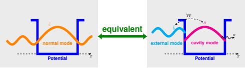

New X-ray sources

- 4th generation synchrotrons
- X-ray free electron lasers
- Lab-based X-ray sources

Control techniques

- Pulse shaping
- Coherent excitation control

Shvyd'ko et. al. *Phys. Rev. Lett.* **77**, 3232 (1996)
Bürvenich, Evers, Keitel *Phys. Rev. Lett.* **96** *142* (2006)
Pálffy et. al. *Phys. Rev. Lett.* **103** 017401 (2009)
Adams et. al. *J. Mod. Opt.* **60** 2 (2013)
Vagizov et. al. *Nature* **508**, 80 (2014)
Heeg et. al. *Science* **357** 6349 (2017)
Heeg et. al. arXiv:1607.04116 [quant-ph]
Goerttler et. al. *Phys. Rev. Lett.* **123**, 153902 (2019)
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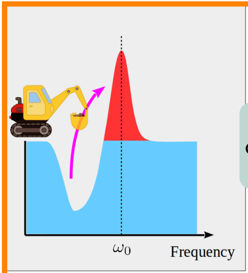

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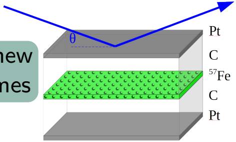

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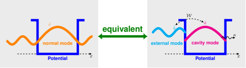

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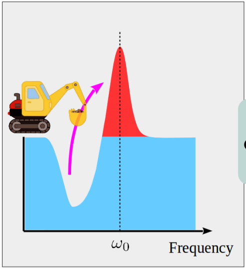

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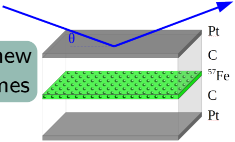

today

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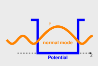
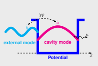


equivalent



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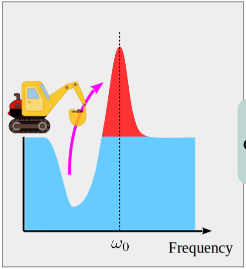

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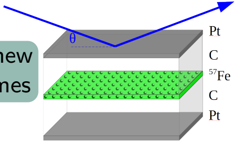

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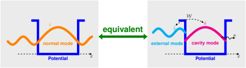

Extreme regimes
⇒ New theoretical challenges

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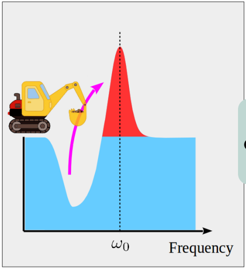

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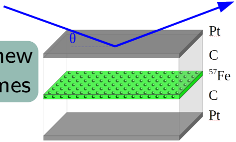

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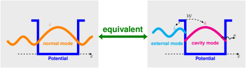

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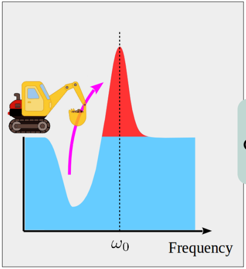

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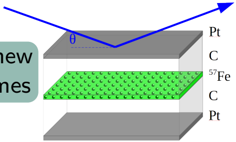

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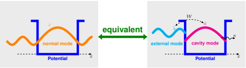

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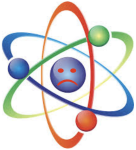
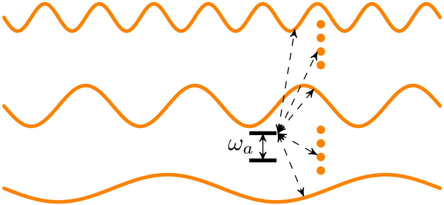


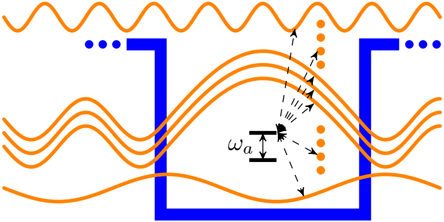
Extreme **atomic** systems

Overview

Continuum coupling



Structured continuum featuring resonances



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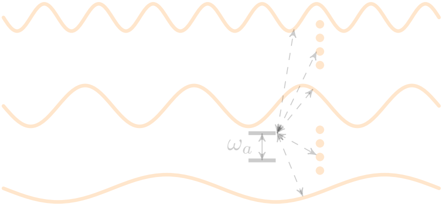
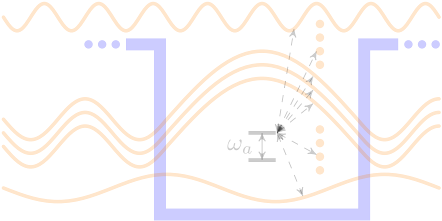
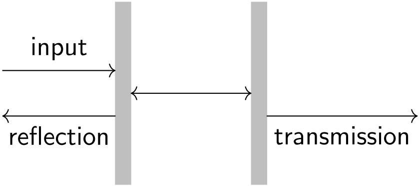


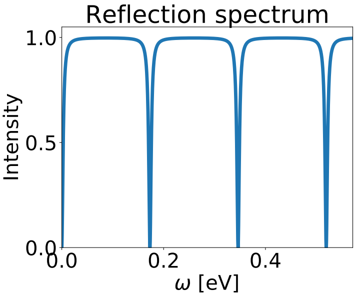
Can we extract **relevant** degrees of freedom from a continuum?

Structured continuum featuring resonances



Example: Fabry-Perot cavity





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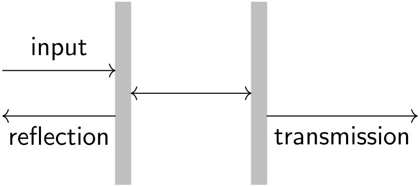

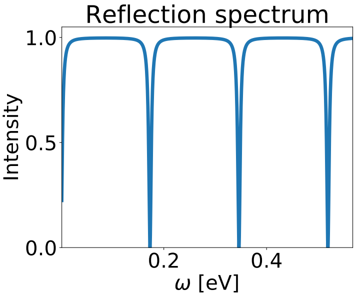

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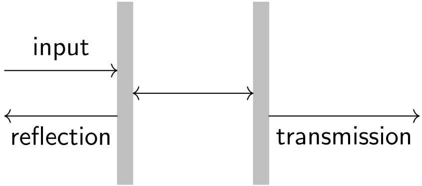

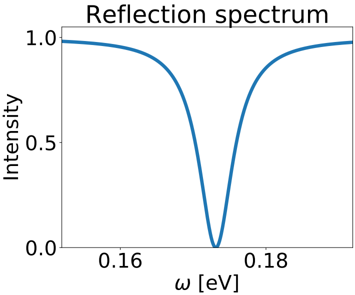

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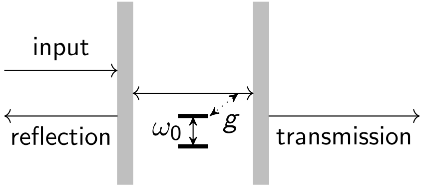

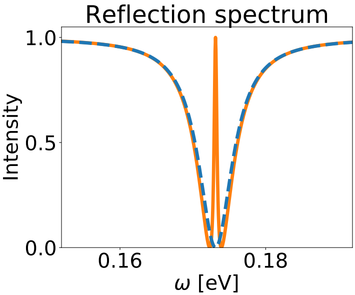

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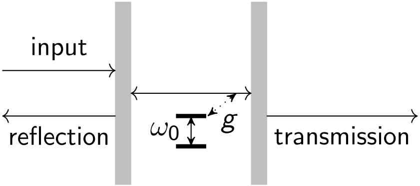
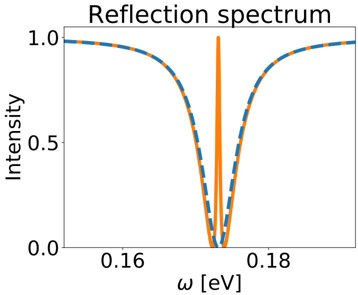
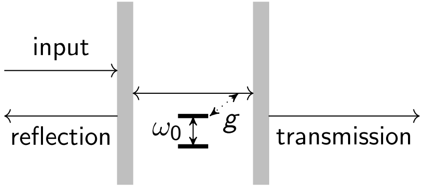
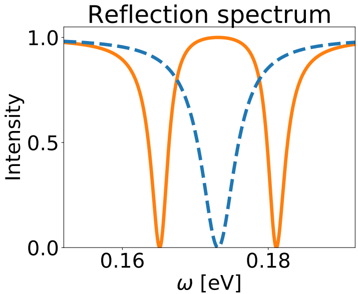




$\rightarrow$ Weak coupling: Purcell effect

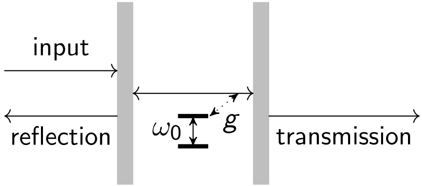
Example: Fabry-Perot cavity

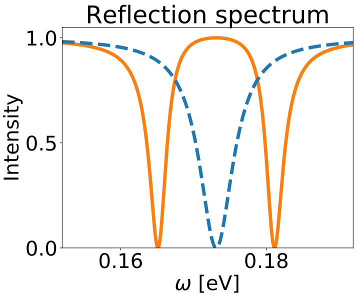




→ Strong coupling: Vacuum Rabi-splitting

Example: Fabry-Perot cavity

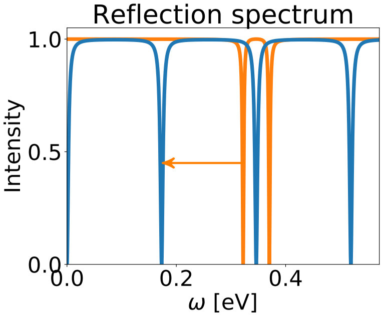




$\Rightarrow$ Quantum effects via strong light-matter interactions!

Extreme regimes

- Multi-mode strong coupling



Türeci et al. *Science* **320**, 643 (2008)
Krimer et al. *Phys. Rev. A* **89**, 033820 (2014)
Sundaresan et al. *Phys. Rev. X* **5**, 021035 (2015)
. . . and many more . . .

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- Multi-mode strong coupling
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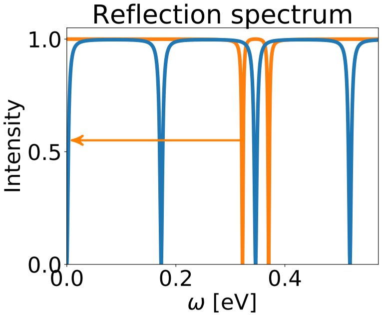
- Deep-strong coupling



Recent reviews:
Carusotto & Ciuti *Rev. Mod. Phys.* **85**, 299 (2013)
Frisk Kockum et al. *Nat. Rev. Phys.* **1**, 19 (2019)
Forn-Díaz et al. *Rev. Mod. Phys.* **91**, 025005 (2019)
Experimental:
Niemczyk et al. *Nat. Phys.* **6**, 772 (2010)
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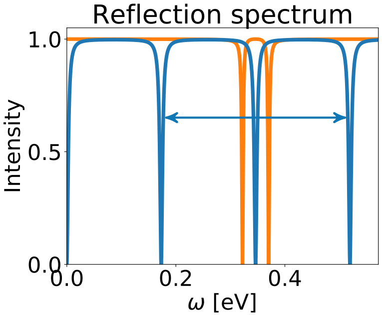
- Multi-mode strong coupling
- Ultra-strong coupling
- Deep-strong coupling
- Overlapping modes



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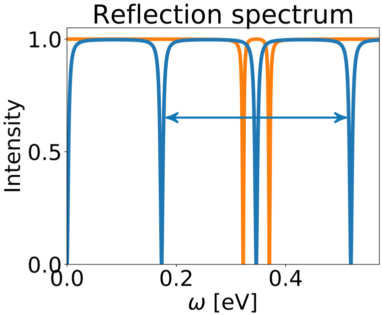

e.g. non-Hermitian photonics

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I. Rotter *J. Phys. A: Mathematical and Theoretical* **45**, 15 (2009)
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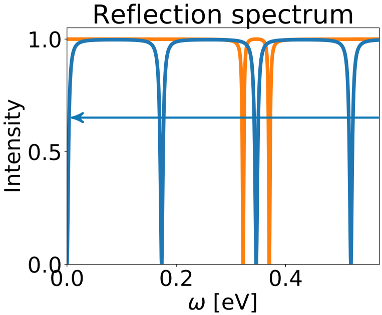
. . . and many more . . .

Extreme regimes

- Multi-mode strong coupling
- Ultra-strong coupling
- Deep-strong coupling
- Overlapping modes
- Large leakage



Experimentally relevant:
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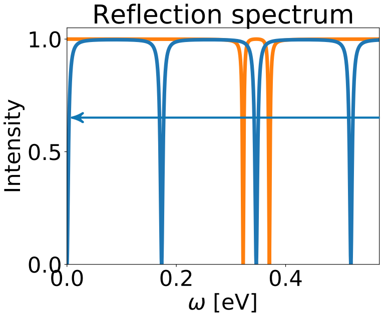
Extreme openness



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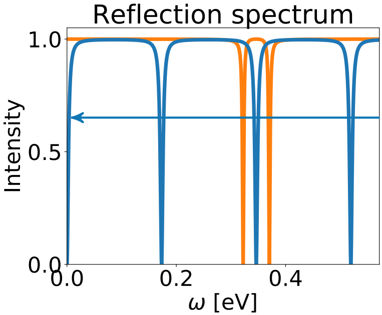
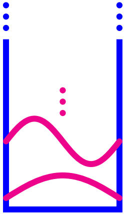


Extreme complexity
(e.g. many-body)

From closed to open boxes



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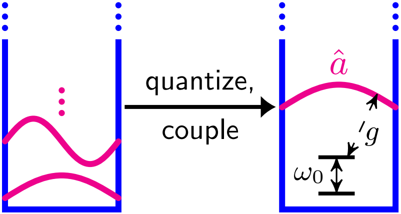
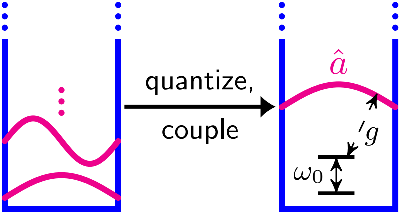


Jaynes-Cummings & friends

$$H = H_{\text{atom}} + H_{\text{cav}} + g\,\hat{a}\hat{\sigma}^{+} + h.c.$$

$\rightarrow$ **few-mode concept**

From closed to open boxes



- discrete eigenstates
- closed system
  - × no leakage
  - × no driving
  - × no scattering
  - × no external detection

Jaynes-Cummings & friends

$$H = H_{\mathrm{atom}} + H_{\mathrm{cav}} + g\hat{a}\hat{\sigma}^{+} + h.c.$$

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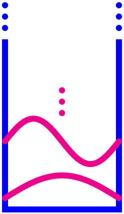
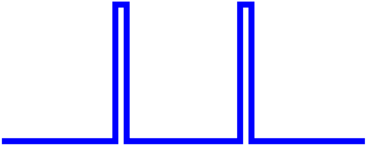
From closed to open boxes

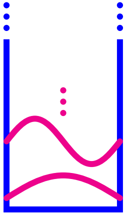
open system

- ✓ leakage
- ✓ driving
- ✓ scattering





From closed to open boxes



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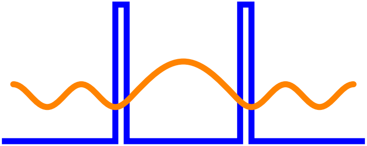
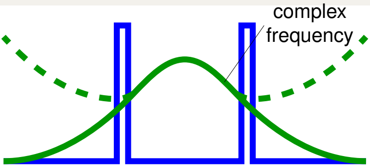


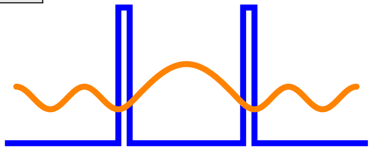
continuum eigenstates

☹ few-mode concept is lost

From closed to open boxes



resonant modes



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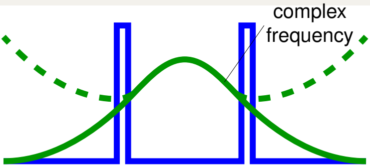

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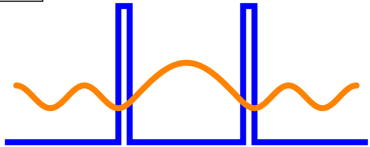

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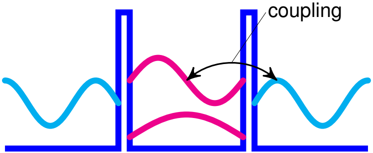
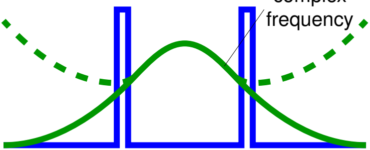


few-mode + input-output

From closed to open boxes



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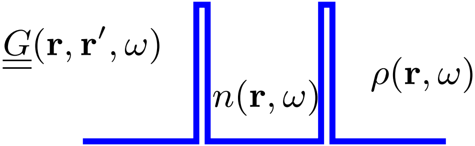
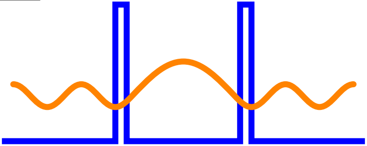


Green fns, LDOS, Master eqs.



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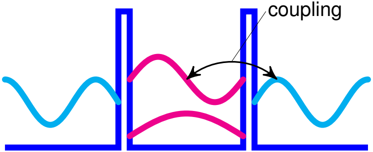

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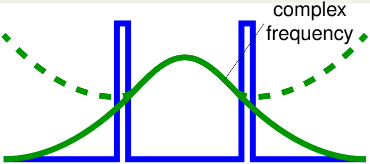

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Ching et al. *Rev. Mod. Phys.* **70**, 1545 (1998)
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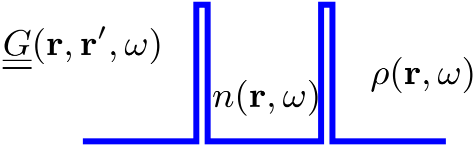

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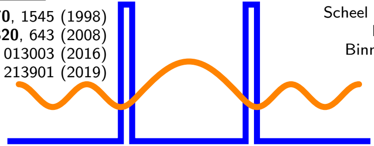

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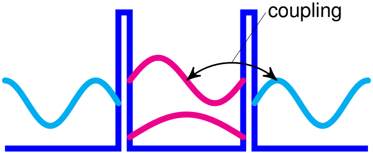

few-mode + input-output

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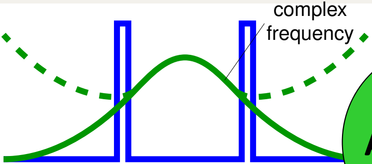

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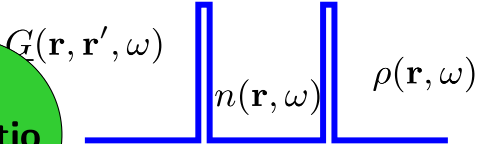
Ab initio



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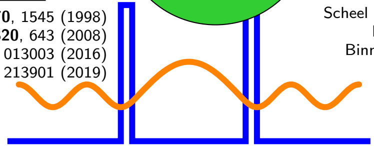

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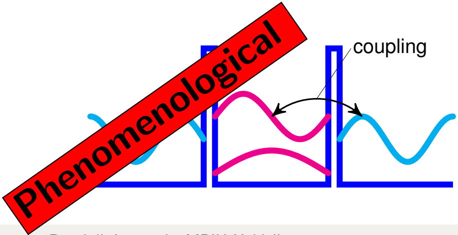

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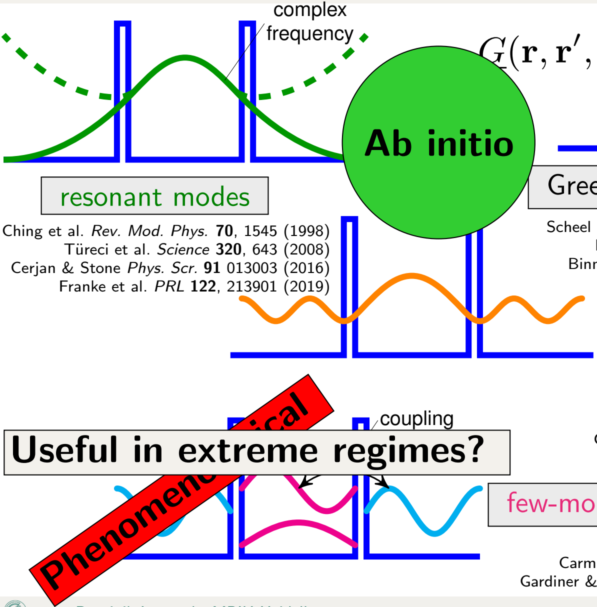

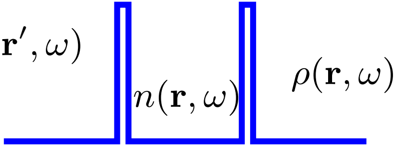

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Useful in extreme regimes?

few-mode + input-output

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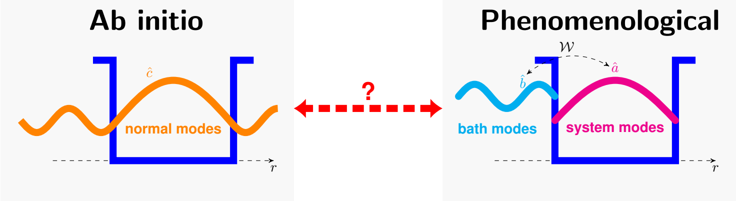
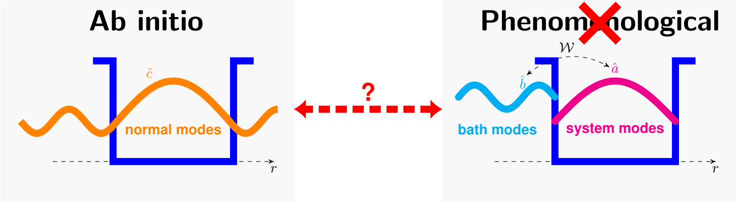
The problem


Ab initio
$\hat{c}$
normal modes
r
?
Phenomenological
$\mathcal{W}$
$\hat{b}$
$\hat{a}$
bath modes
system modes
r

The problem



How to make

- **few-mode**

and

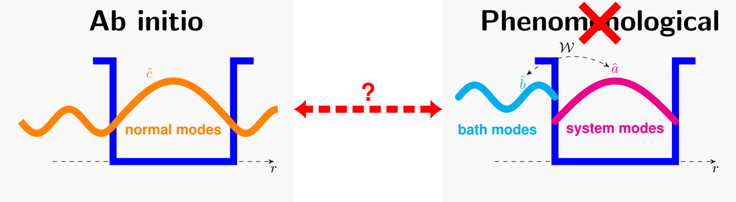
- **input-output**

ab initio?

?

DL & J. Evers, *Phys. Rev. X* **10**, 011008 (2020)

The problem



How to make

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and

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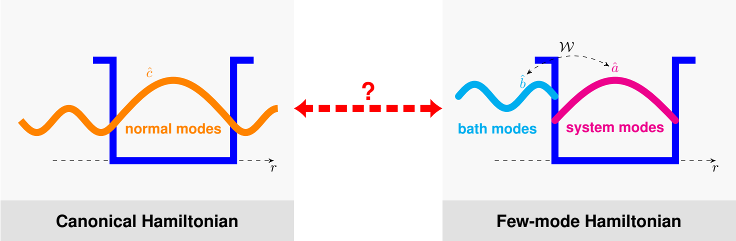
ab initio?

?

$\Rightarrow$ **Ab initio few-mode theory**

DL & J. Evers, *Phys. Rev. X* **10**, 011008 (2020)

Ab initio few-mode Hamiltonians



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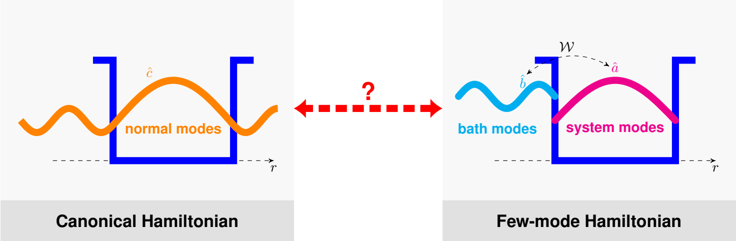

$$\overbrace{\boxed{\hat{c}(\omega)}}^{\text{normal modes}} = \overbrace{\boxed{\sum_\lambda \alpha_\lambda(\omega)\hat{a}_\lambda}}^{\text{discrete modes}} + \overbrace{\boxed{\int d\omega' \beta(\omega,\omega')\hat{b}(\omega')}}^{\text{external continuum}}$$ [1,2]

[1] Viviescas & Hackenbroich, *Phys. Rev. A* **67**, 013805 (2003)
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[3] DL & J. Evers, *Phys. Rev. X* **10**, 011008 (2020)

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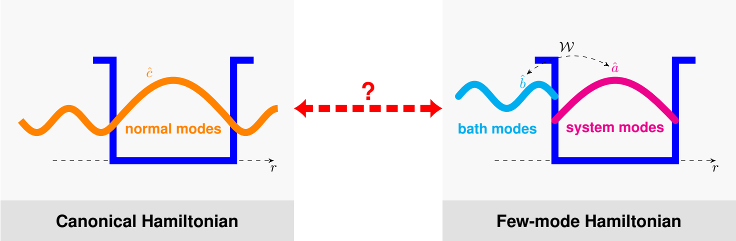

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$\Rightarrow$ select resonant states as few-mode basis[3]

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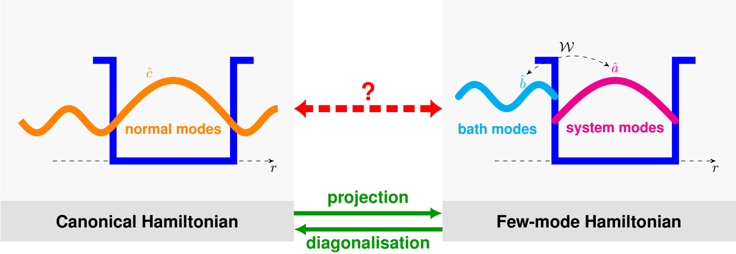
Ab initio few-mode Hamiltonians



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⇒ select resonant states as few-mode basis[3]

⇒ **ab initio few-mode Hamiltonians** ☺ [3]

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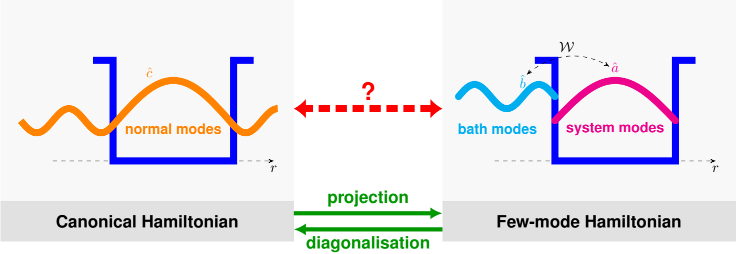
Few-mode scattering



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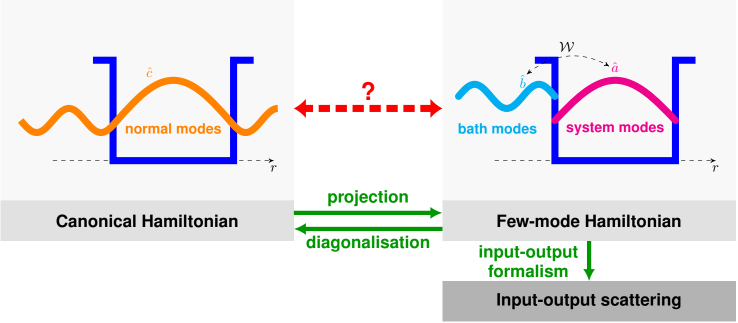

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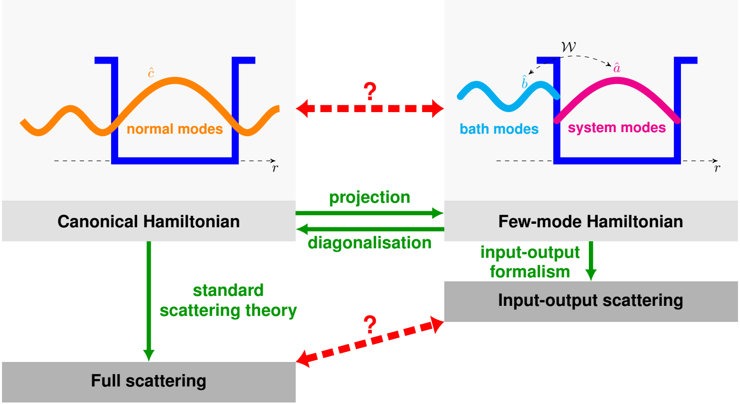

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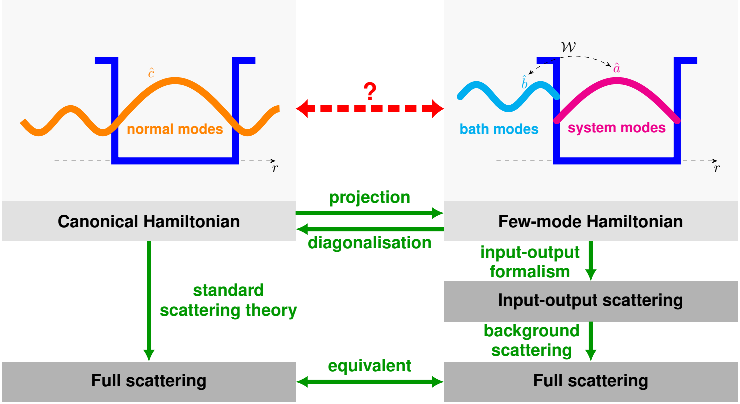
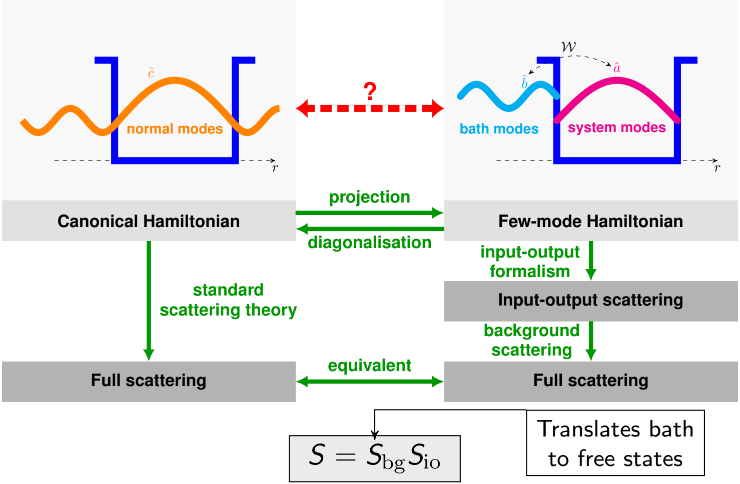


$$\boxed{S = S_{\mathrm{bg}} S_{\mathrm{io}}}$$

DL & J. Evers, *Phys. Rev. X* **10**, 011008 (2020)

Few-mode scattering



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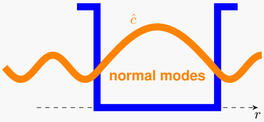
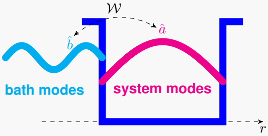


equivalent



Canonical Hamiltonian — projection → **Few-mode Hamiltonian**

Few-mode Hamiltonian — diagonalisation → **Canonical Hamiltonian**

Canonical Hamiltonian — standard scattering theory → **Full scattering**

Few-mode Hamiltonian — input-output formalism → **Input-output scattering**

Input-output scattering — background scattering → **Full scattering**

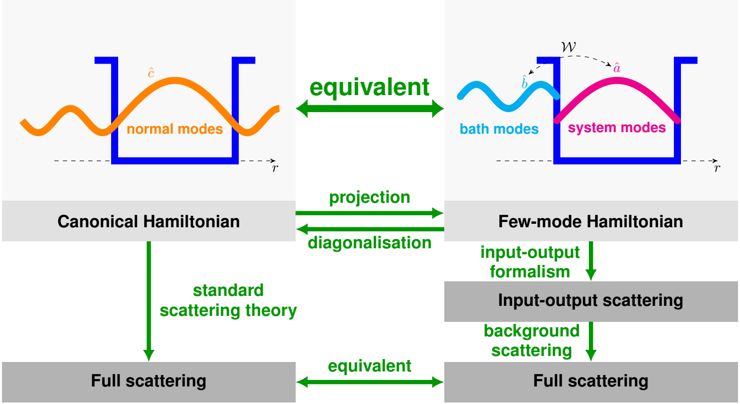
Full scattering ↔ equivalent ↔ **Full scattering**

$$S = S_{\mathrm{bg}} S_{\mathrm{io}}$$

Translates bath to free states

DL & J. Evers, *Phys. Rev. X* **10**, 011008 (2020)

Few-mode scattering



$$\boxed{S = S_{\mathrm{bg}} S_{\mathrm{io}}}$$

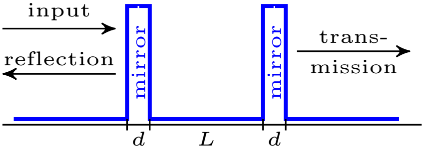
Translates bath to free states

⇒ Few-mode theory can apply in extreme regimes!

DL & J. Evers, *Phys. Rev. X* **10**, 011008 (2020)

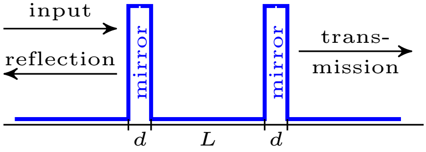
Illustrative example

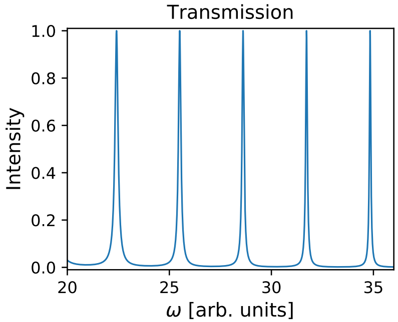
Example: Two-sided Fabry-Perot cavity

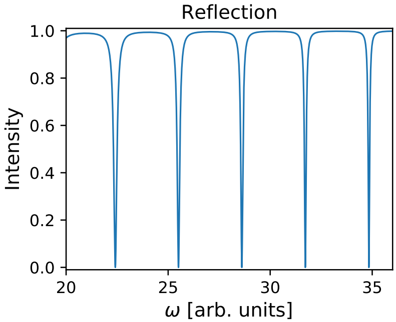


Ley & Loudon *J. Mod. Opt.* **34**, 227-255 (1987)

Example: Two-sided Fabry-Perot cavity







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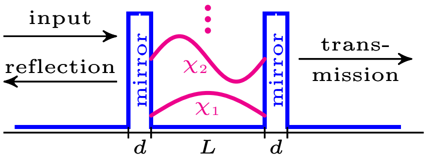
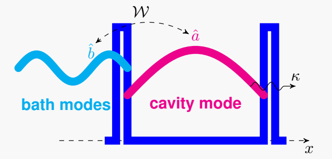
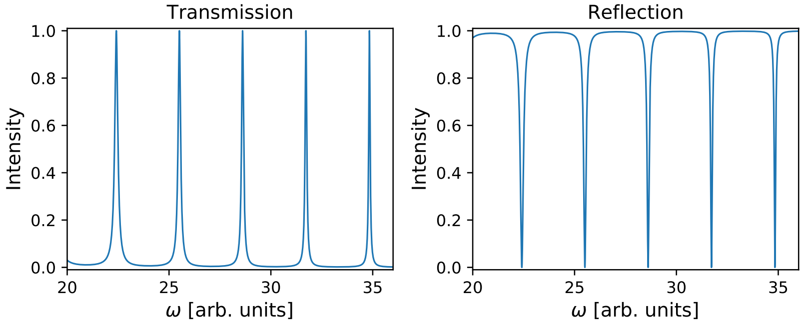
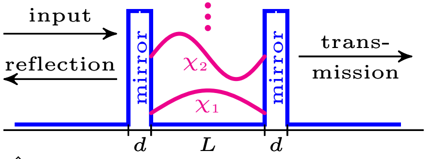
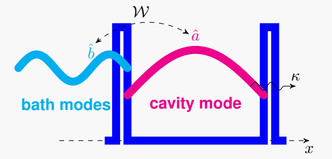


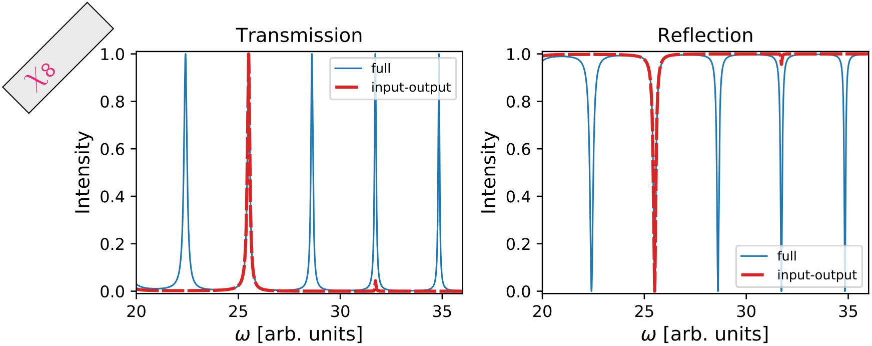




Example: Two-sided Fabry-Perot cavity

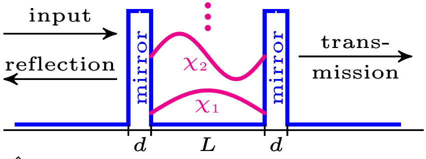


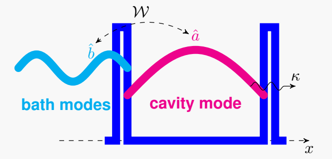




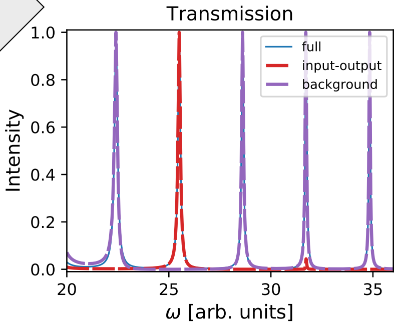
$\Rightarrow$ ab initio, not a fit!

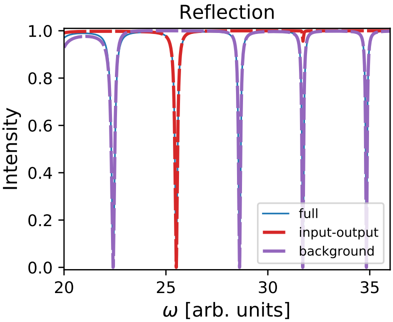
Example: Two-sided Fabry-Perot cavity





χ_8





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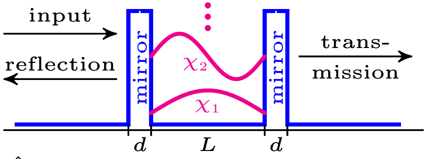
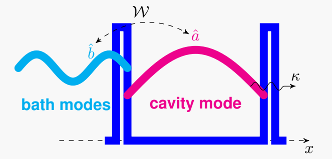
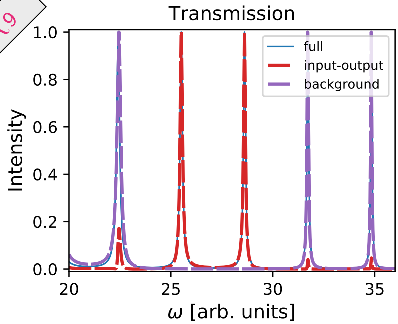
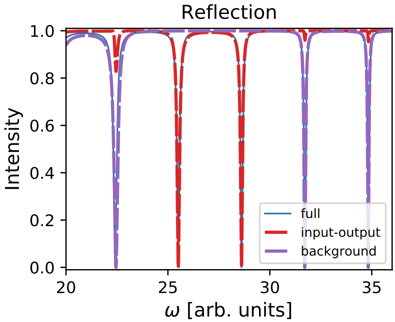




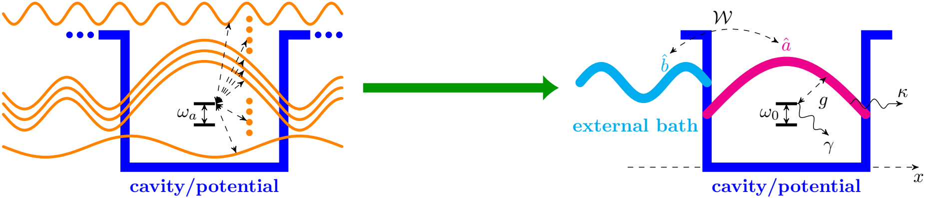
χ_8, χ_9



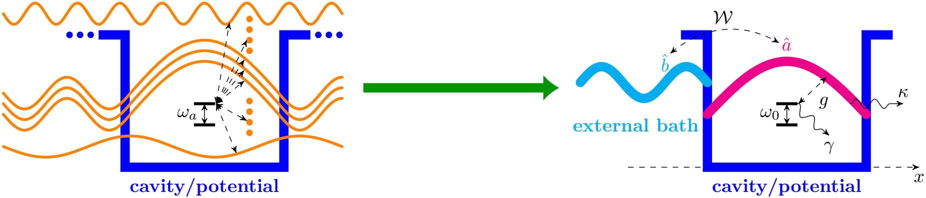


$\Rightarrow$ extract resonant dynamics

Interacting systems

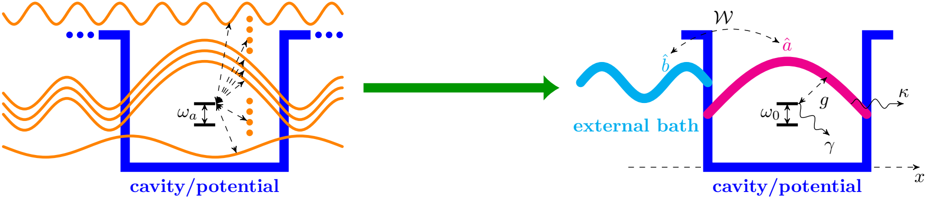


Interacting systems



- Many degrees of freedom
- Often difficult!

Interacting systems



- Many degrees of freedom
- Often difficult!

- Much easier to solve!
- Many methods already exist![1,2,3]
- Advantages to model version

$\Rightarrow$ Non-interacting system exact!

[1] Carmichael, *Statistical Methods in Quantum Optics 1* (1999)
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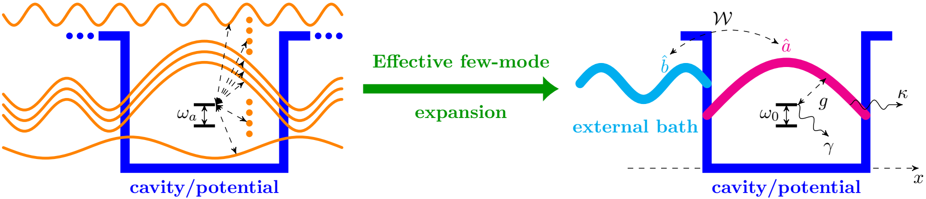
[3] Kirton et al. *Adv. Quantum Technol.* **2**, 1800043 (2019)

Interacting systems



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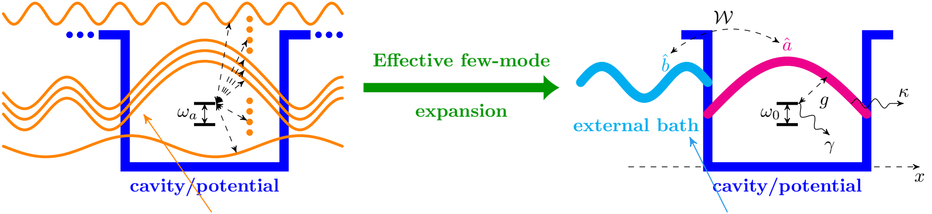

non-perturbative/non-Markovian

perturbative/Markovian

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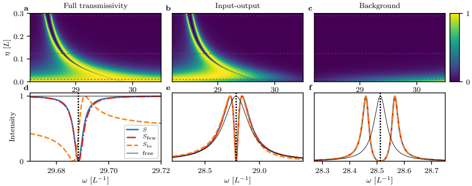
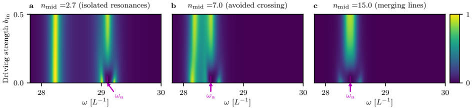
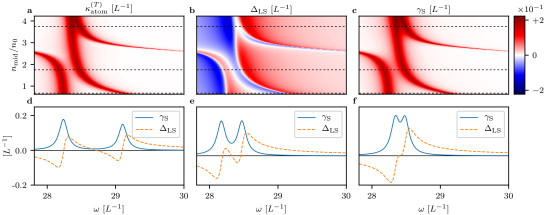
Benchmarks and advantages



- ✓ Benchmarked in linear regime
- ✓ Highly open systems

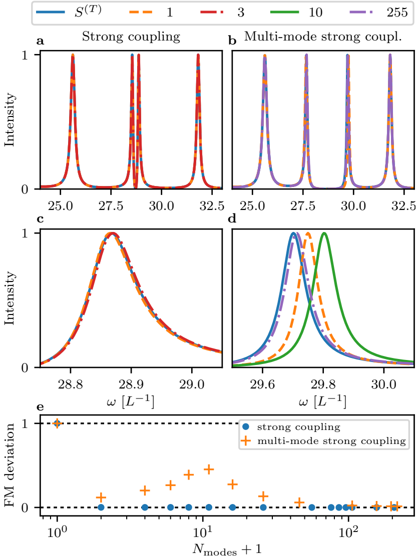


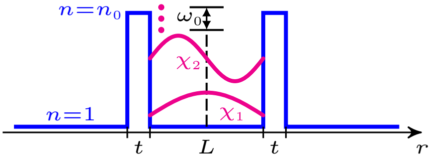
- ✓ Non-linear effects
- ✓ Overlapping modes features
  - ⇒ Non-trivial bath effects!
- ✓ Ab initio calculation of quantum couplings



DL & J. Evers, *Phys. Rev. X* **10**, 011008 (2020)

Convergence and extreme regimes





DL & J. Evers, *Phys. Rev. X* **10**, 011008 (2020)

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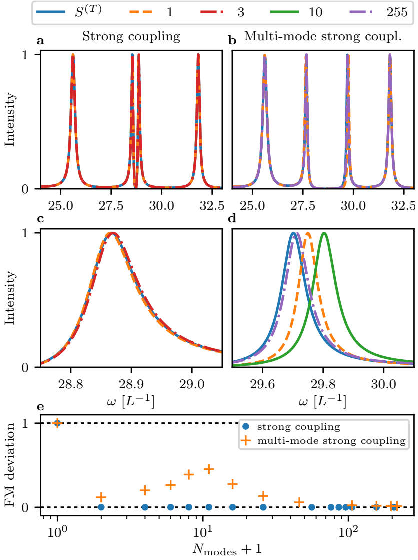
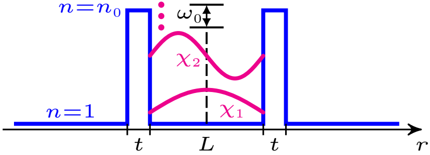




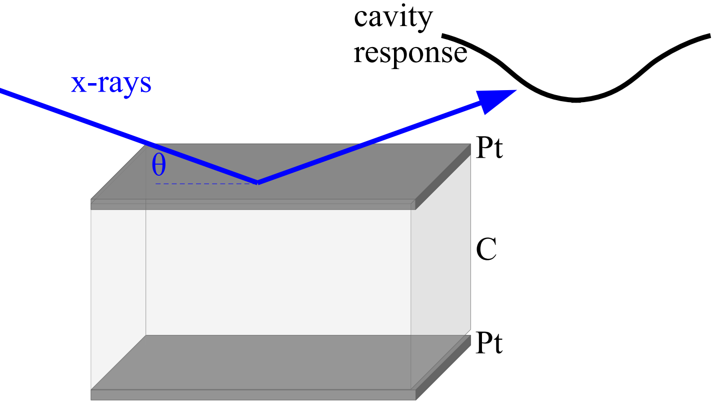
Convergence of light-matter coupling models is non-trivial![1]

[1] e.g. Krimer et al. *Phys. Rev. A* **89**, 033820 (2014)
Malekakhlagh, Petrescu, Türeci *Phys. Rev. Lett.* **119**, 073601 (2017)
Gely et al. *Phys. Rev. B* **95**, 245115 (2017)

DL & J. Evers, *Phys. Rev. X* **10**, 011008 (2020)

X-ray cavity QED

New experimental platform:



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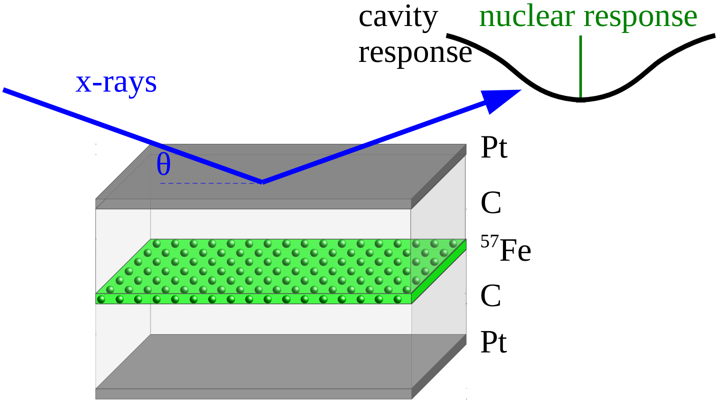
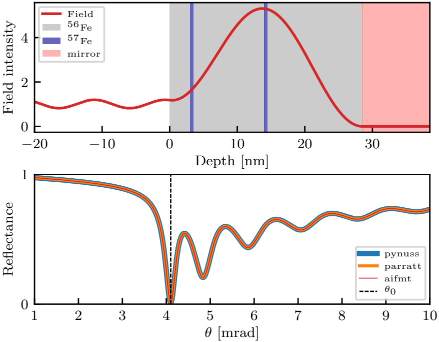
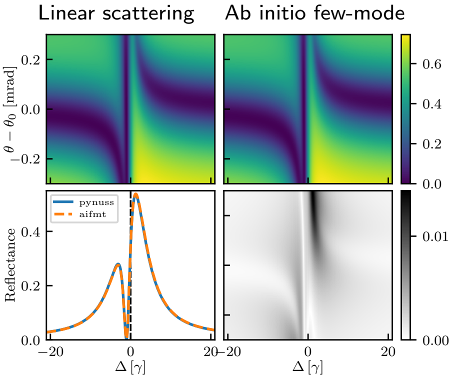


Fabry-Perot + Many-body ensemble

Ab initio few-mode theory for X-ray cavity QED





DL, Heeg, Keitel & Evers, *to be submitted*

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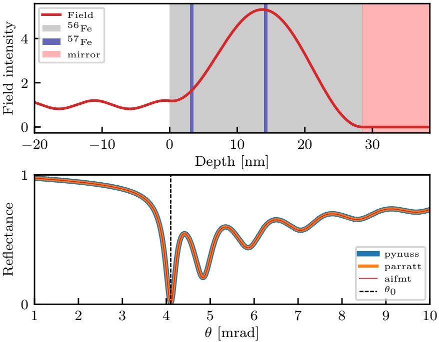
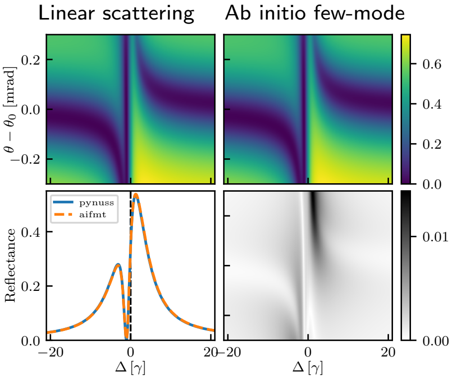


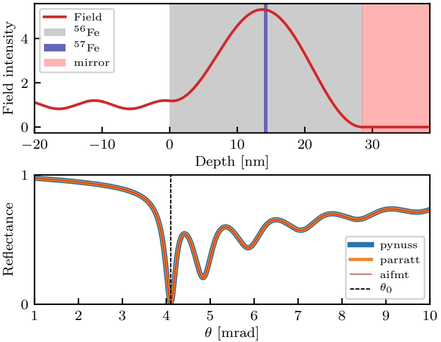


DL, Heeg, Keitel & Evers, *to be submitted*

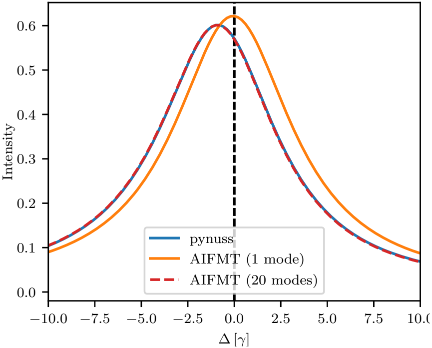
⇒ improves successful phenomenological model[1,2]

[1]Heeg & Evers *PRA* (2013)
[2]Heeg & Evers *PRA* (2015)

Overlapping modes effects beyond input-output models



Collective Lamb shift[1]



[1] Röhlsberger et. al. *Science* **328** 5983 (2010)

DL, Heeg, Keitel & Evers, *to be submitted*

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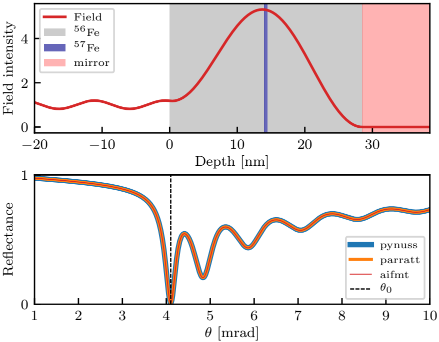

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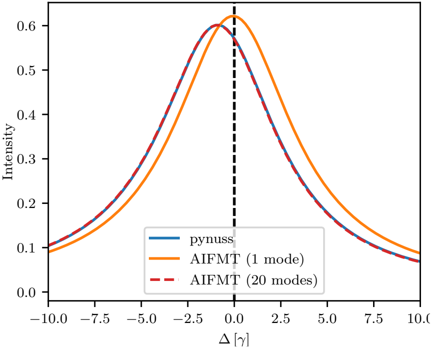

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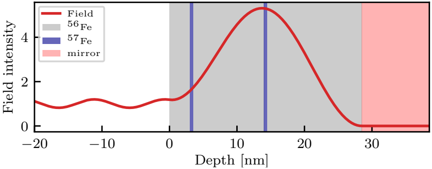
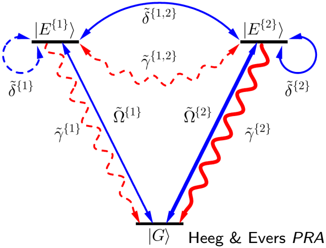
$\Rightarrow$ **overlapping modes effect**

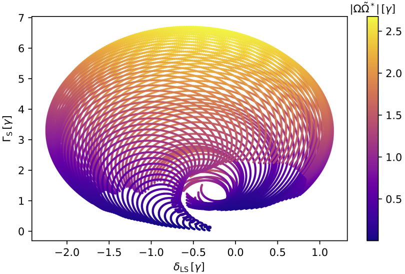
DL, Heeg, Keitel & Evers, *to be submitted*

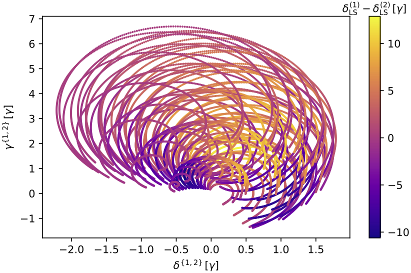
Towards designing nuclear level schemes





Heeg & Evers *PRA* (2015)





DL, Heeg, Keitel & Evers, *in preparation*

Conclusion

- ✓ Rigorous construction of few-mode Hamiltonians
- ✓ Exact scattering theory via input-output formalism
- ✓ Non-perturbative expansion scheme for interactions
- ✓ Linking ab initio theory and models in cavity QED
  - $\Rightarrow$ Access to new regimes!

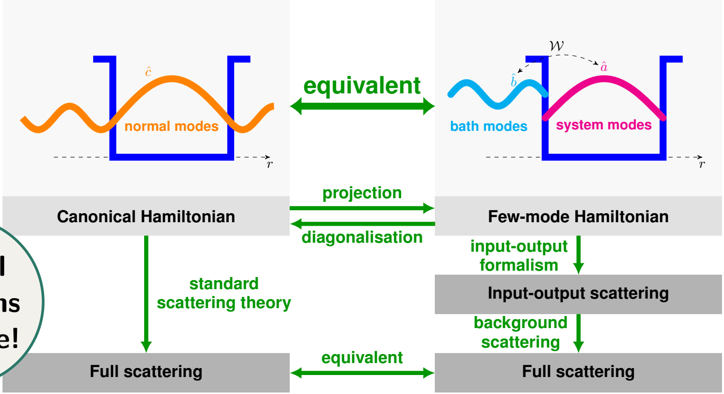
- !! Explore quantum effects in X-ray cavities
  - $\Rightarrow$ In progress: non-linear and correlation effects at XFELs
- ?! Extreme regimes of open quantum dynamics

Thank you for your attention!

Jörg Evers

Kilian P. Heeg

Christoph H. Keitel



Critical questions welcome!

DL & J. Evers, *Phys. Rev. X* **10**, 011008 (2020)