Ab initio few-mode theory

for quantum potential scattering problems

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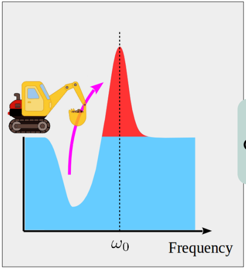
Christoph H. Keitel and Jörg Evers

Max-Planck-Institut für Kernphysik, Heidelberg

https://xkcd.com/1070/

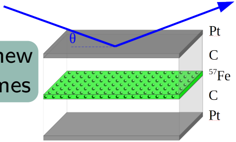
Background & Motivation



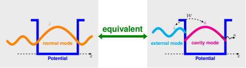
Coherent control of x-rays and nuclei

Nuclear quantum optics

X-rays excite new quantum regimes



Understand fundamentals



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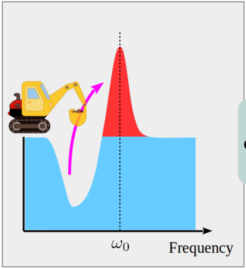
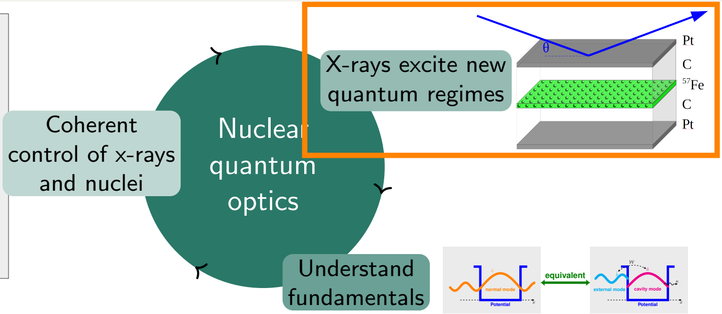
Project B02

Background & Motivation





Nuclear transitions as extreme qubits

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

Other motivations: metrology. . .

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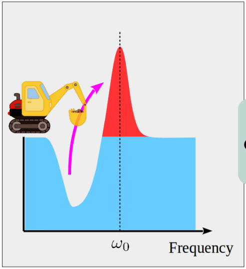

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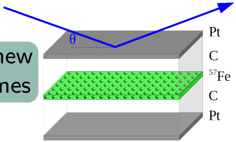

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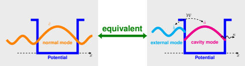

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Heeg & Evers *Phys. Rev. A* **88**, 043828 (2013)
Heeg et. al. *Phys. Rev. Lett.* **111** 073601 (2013)
Heeg et. al. *Phys. Rev. Lett.* **114** 203601 (2015)
Heeg et al. *Phys. Rev. Lett.* **114**, 207401 (2015)
Haber et. al. *Nature Photonics* **10** 445 (2016)
Haber et. al. *Nature Photonics* **11** 720 (2017)
...

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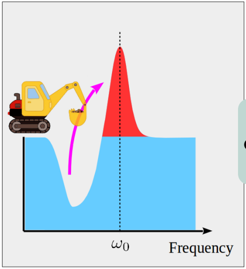

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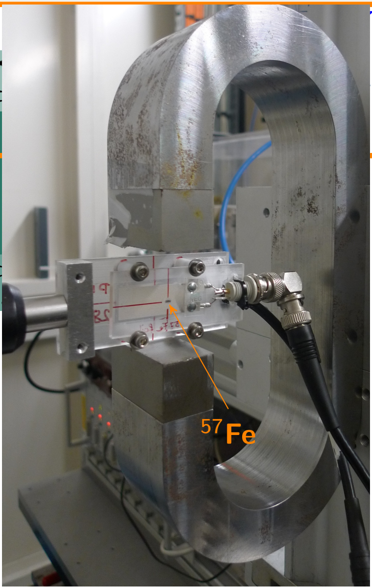

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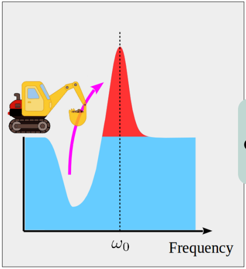

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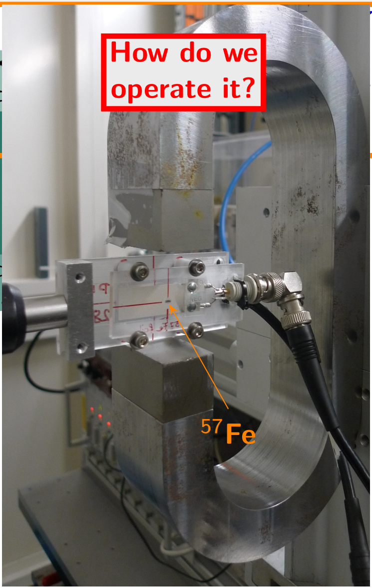

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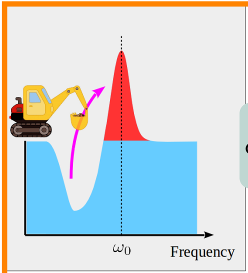

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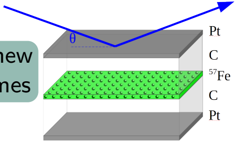

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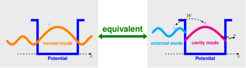

New X-ray sources

- 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]
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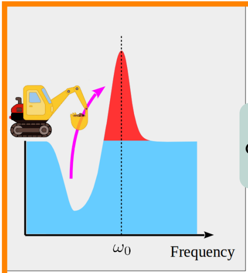

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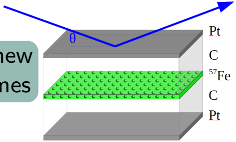

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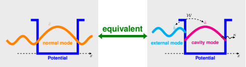

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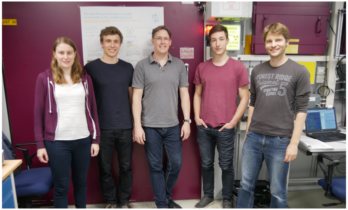

Heeg, Kaldun, Strohm, Reiser, Ott, Subramanian, DL, Haber, Wille, Goerttler, Rüffer, Keitel, Röhlsberger, Pfeifer, Evers, *Science* **357**, 375 (2017) + *submitted*

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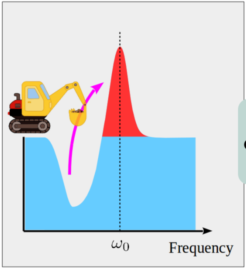

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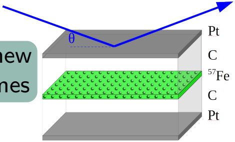
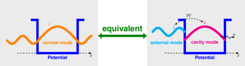


today

Understand fundamentals



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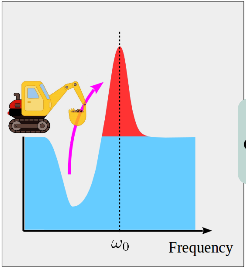

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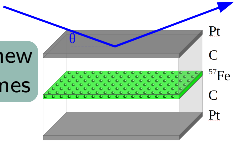

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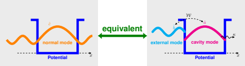
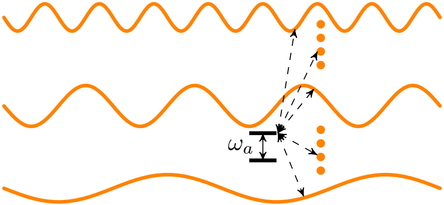


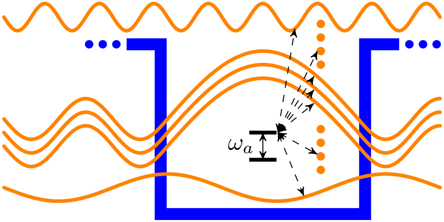
Extreme regimes
⇒ New theoretical challenges

Overview

Continuum coupling



Structured continuum featuring resonances



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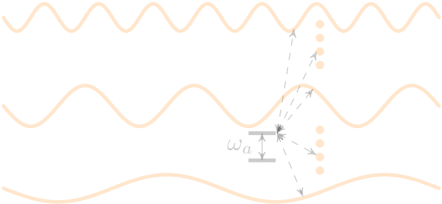
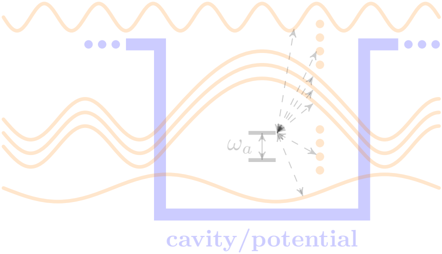
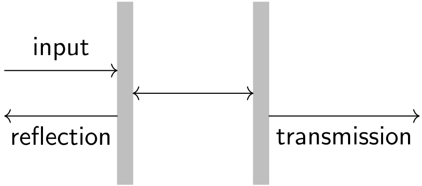


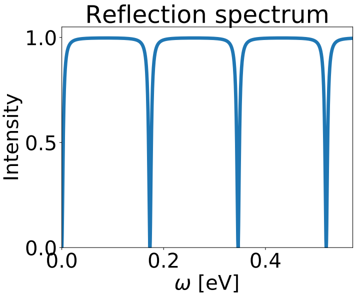
How to extract **relevant** degrees of freedom from a continuum?

Structured continuum featuring resonances



Example: Fabry-Perot cavity





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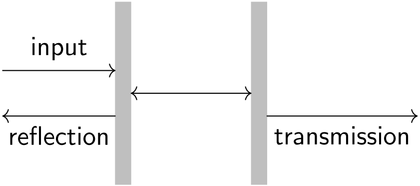

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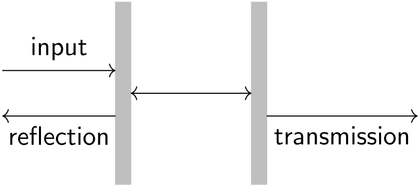

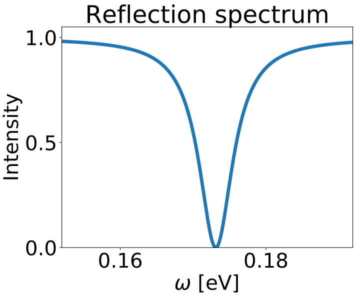

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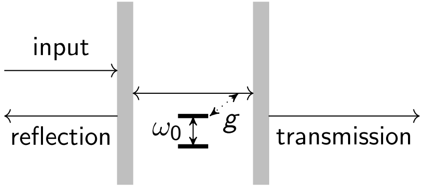

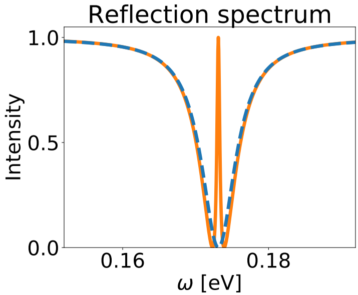

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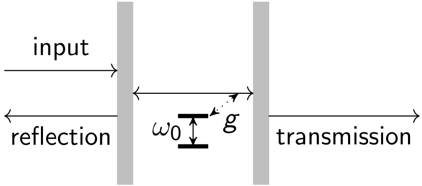
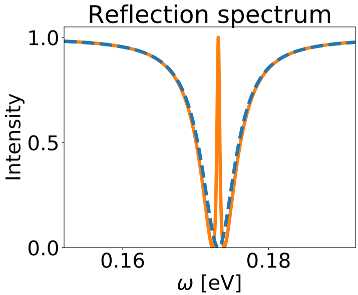
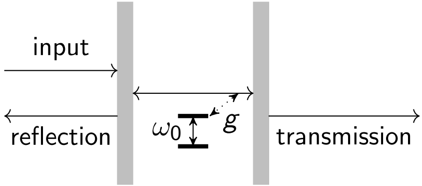
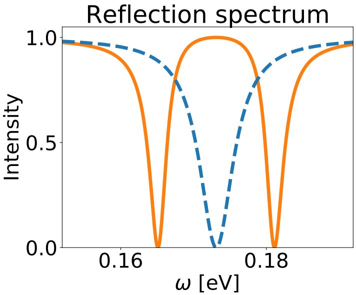




$\rightarrow$ Weak coupling: Purcell effect

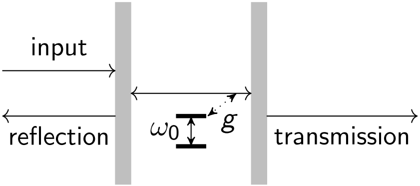
Example: Fabry-Perot cavity

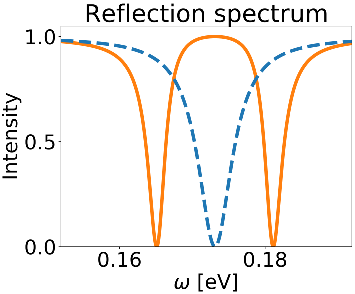




$\rightarrow$ Strong coupling: Vacuum Rabi-splitting

Example: Fabry-Perot cavity

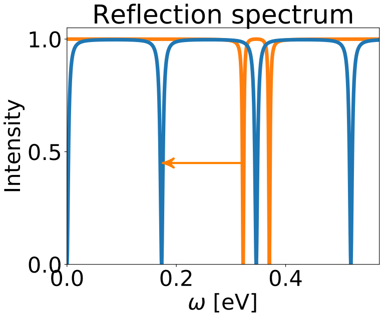




$\boxed{\Rightarrow \text{Quantum effects via strong light-matter interactions!}}$

Extreme regimes

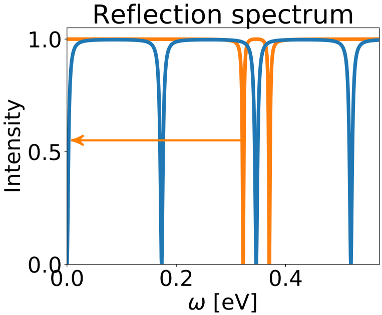
- Multi-mode strong coupling



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 . . .

Extreme regimes

- Multi-mode strong coupling
- Ultra-strong coupling
- 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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Extreme regimes

- Multi-mode strong coupling
- Ultra-strong coupling
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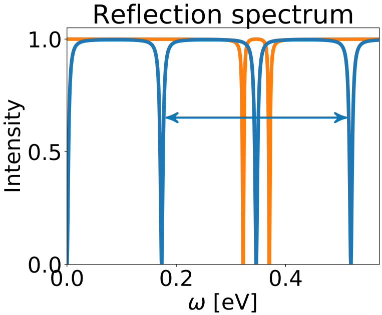
- Overlapping modes



Petermann *IEEE J. Quantum Electron.* **15**, 566 (1979)
Hackenbroich, Viviescas & Haake *Phys. Rev. Lett.* **89**, 083902 (2002)
I. Rotter *J. Phys. A: Mathematical and Theoretical* **45**, 15 (2009)
Heeg et al. *Phys. Rev. Lett.* **114**, 207401 (2015)
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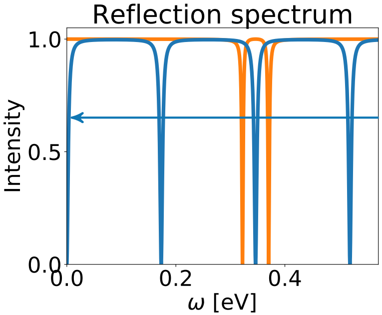
Extreme regimes

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



Experimentally relevant:

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Savage et al. *Nature* **491**, 574577 (2012)

Esteban et al. *Nat. Comm.* **3**, 825 (2012)

Tame et al. *Nat. Phys.* **9**, 329340 (2013)

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Extreme regimes

Extreme coupling

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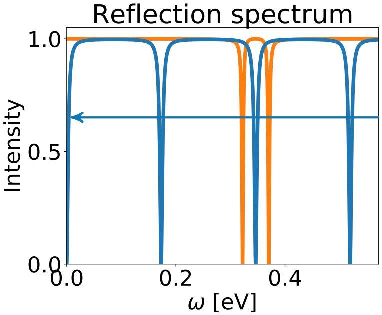
Extreme openness



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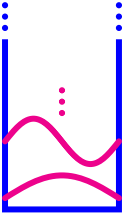
From closed to open boxes



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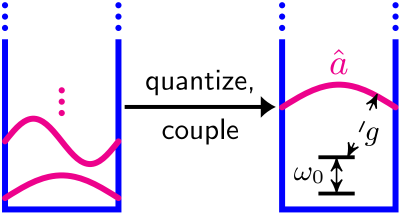
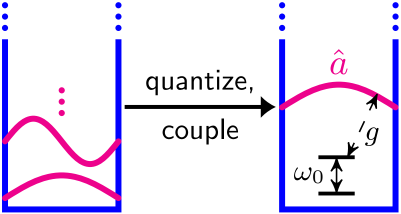


Jaynes-Cummings & friends

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

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

From closed to open boxes



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

Jaynes-Cummings & friends

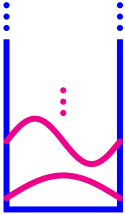
$$H = H_{\text{atom}} + H_{\text{cav}} + g\hat{a}\hat{\sigma}^{+} + h.c.$$

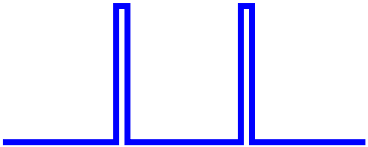
→ **few-mode concept**

From closed to open boxes

open system

- ✓ leakage
- ✓ driving
- ✓ scattering





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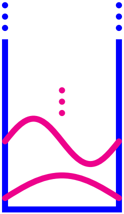

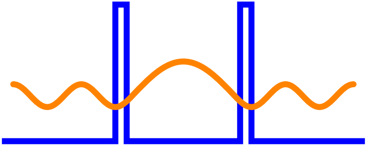

continuum eigenstates

☹ few-mode concept is lost

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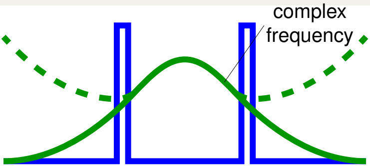
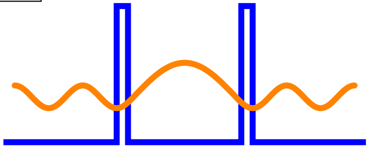


resonant modes



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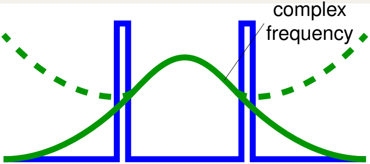
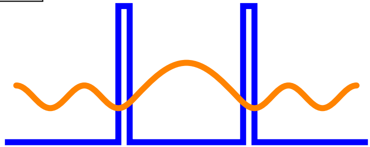
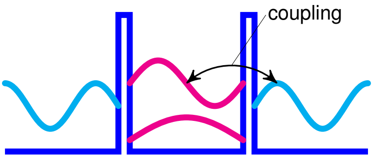


resonant modes



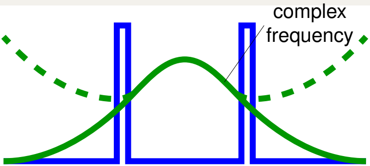
continuum eigenstates

☹ few-mode concept is lost

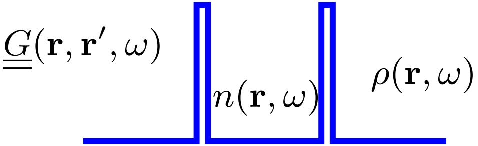


few-mode + bath

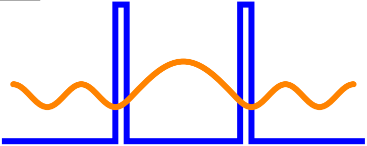
From closed to open boxes



resonant modes



Green fns, LDOS, lin. disp. theory



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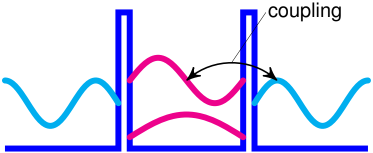

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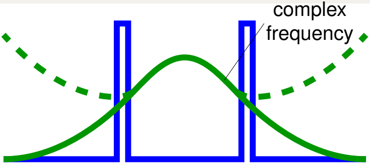

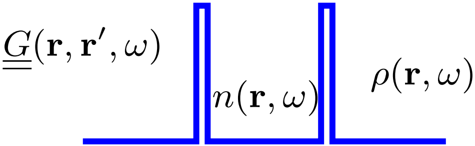

resonant modes

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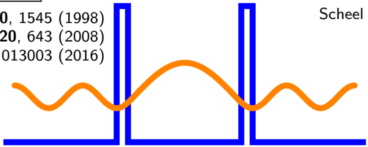

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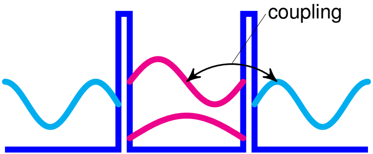

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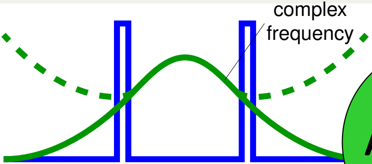

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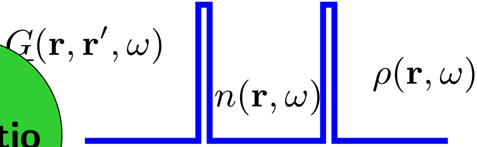

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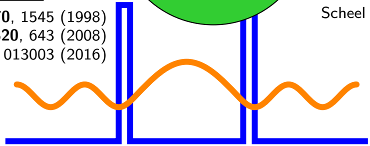

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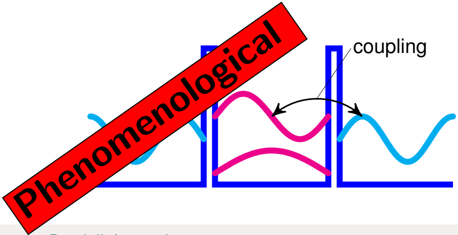

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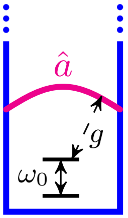
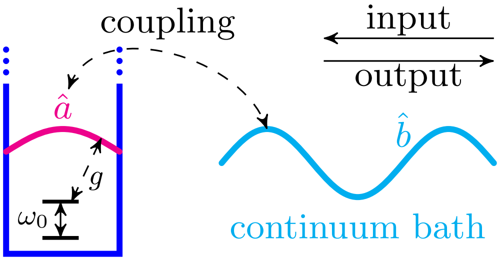
Phenomenological few-mode theory



Jaynes-Cummings & friends

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

Phenomenological few-mode theory



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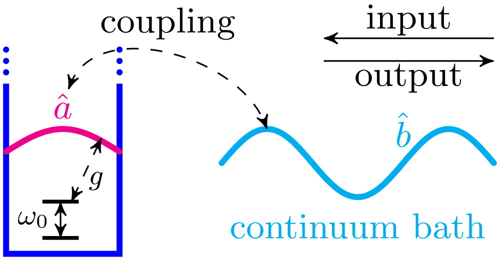

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System-bath Hamiltonian

$$H_{\mathrm{cav}} = H_{\mathrm{syst}} + H_{\mathrm{bath}} + \mathcal{W}\hat{a}\hat{b}^{\dagger} + h.c.$$

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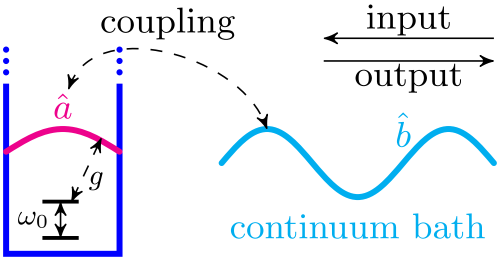

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Input-output theory

$$\hat{b}_{\mathrm{out}} = \hat{b}_{\mathrm{in}} + \kappa\hat{a}$$

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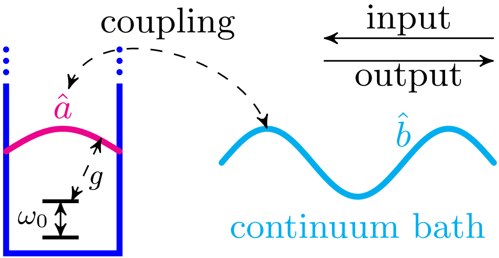

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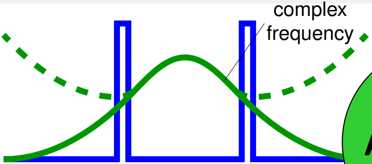
$\rightarrow$ **few-mode concept**

$\rightarrow$ **scattering**

$\Rightarrow$ **Big tool box for quantum dynamics!**

From closed to open boxes



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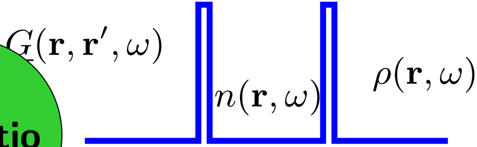

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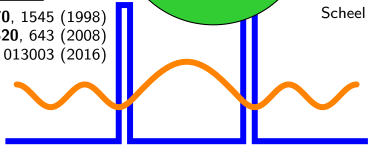

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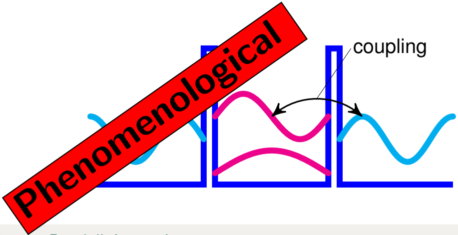

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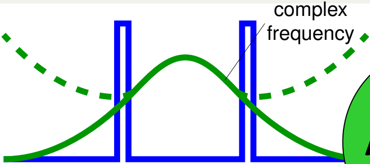

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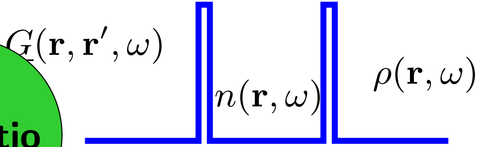

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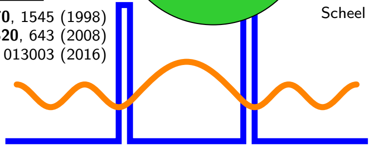

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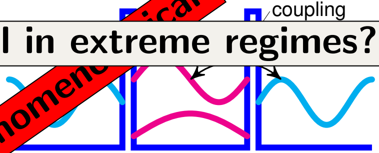

Phenomenological

Useful in extreme regimes?

few-mode + bath

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Carmichael *Quantum Optics* (1991)
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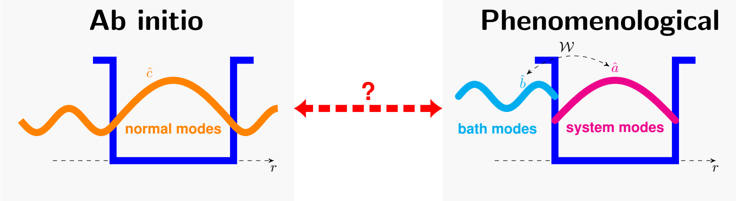
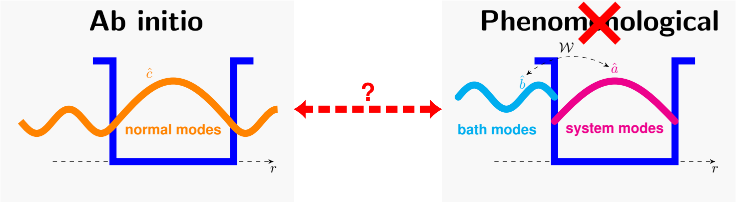
The problem



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**

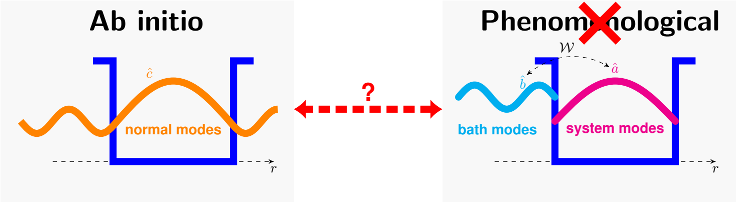
and

- **input-output**

ab initio?

?

The problem



How to make

- **few-mode**

and

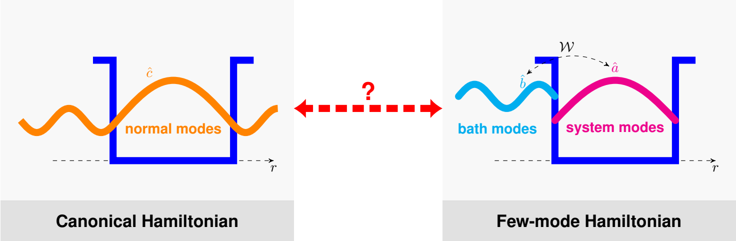
- **input-output**

ab initio?

?

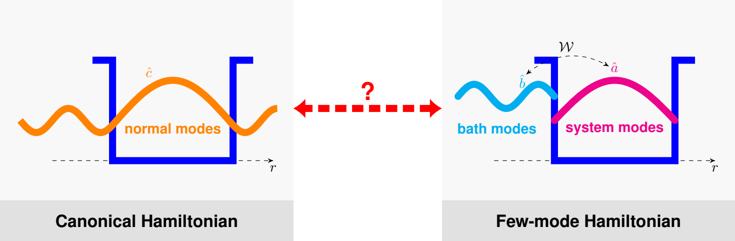
$\Rightarrow$ **Ab initio few-mode theory**

Ab initio few-mode Hamiltonians



Glauber & Lewenstein, *Phys. Rev. A* **43**, 467 (1991)
Gardiner & Collett, *Phys. Rev. A* **31**, 3761 (1985)

Ab initio few-mode Hamiltonians



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

[1] Viviescas & Hackenbroich, *Phys. Rev. A* **67**, 013805 (2003)
[2] Domcke, *Phys. Rev. A* **28**, 2777 (1982)
[3] DL & J. Evers, arXiv:1812.08556 [quant-ph]

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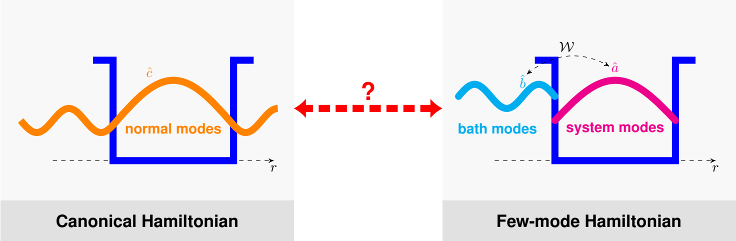

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⇒ select resonant states as few-mode basis[3]

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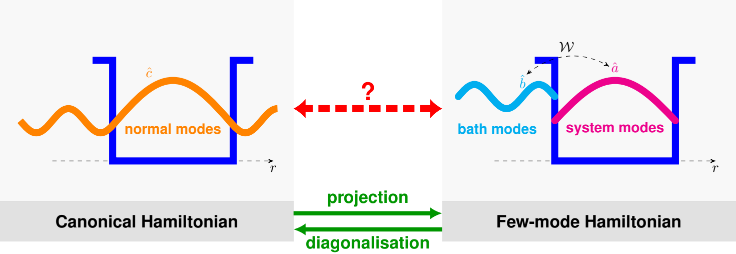

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⇒ **ab initio few-mode Hamiltonians** ☺ [3]

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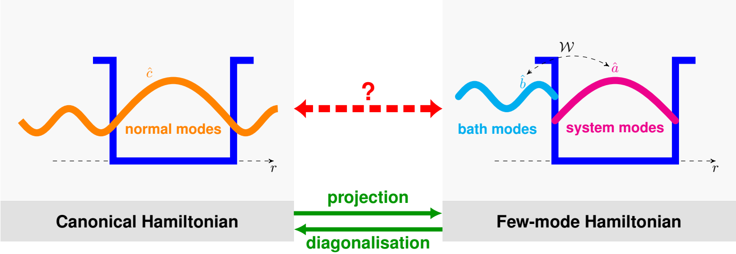
Few-mode scattering



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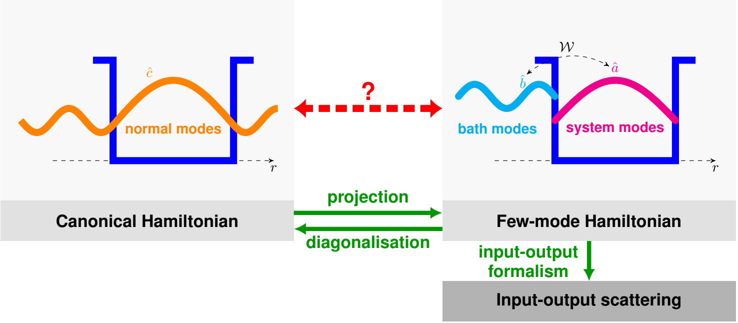

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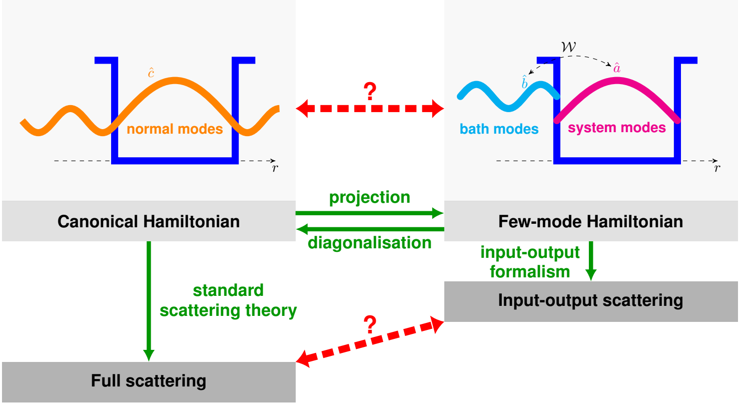

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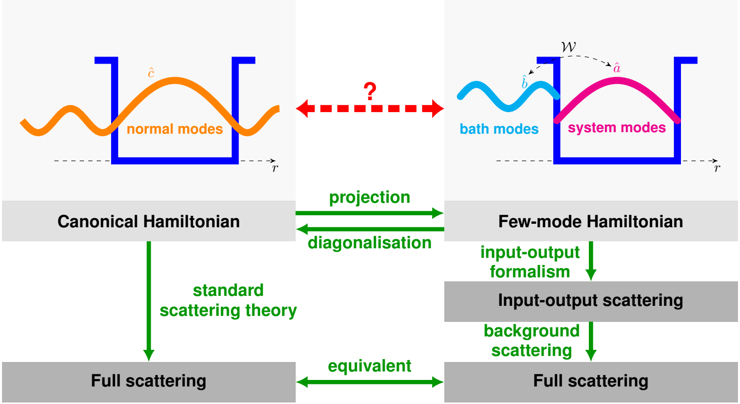

$$\boxed{S = S_{\text{bg}} S_{\text{io}}}$$

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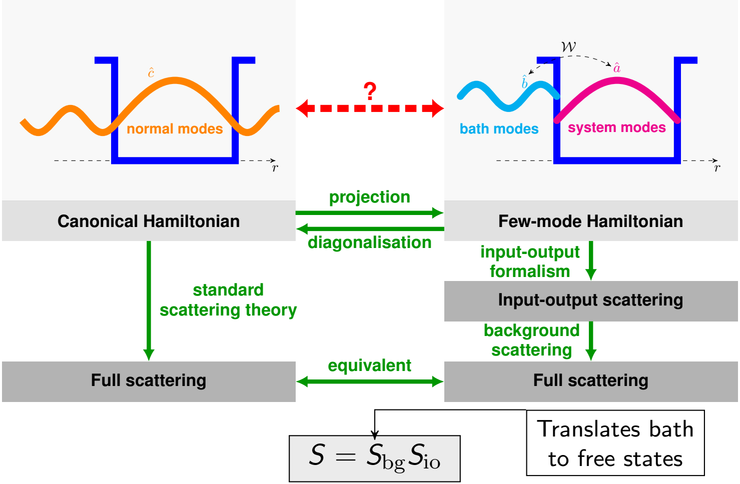
Few-mode scattering



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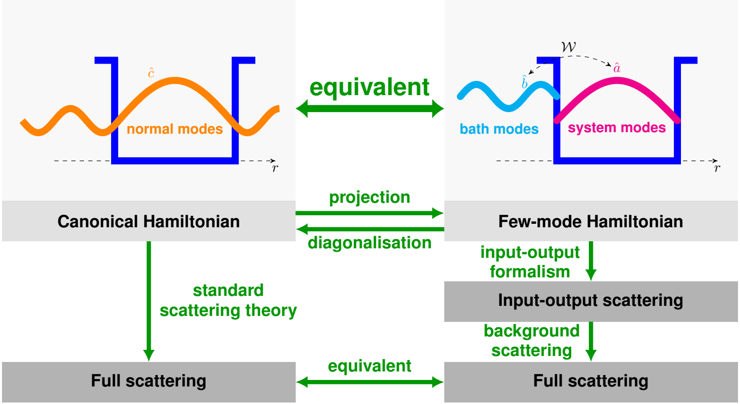
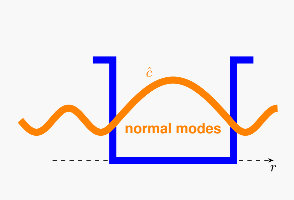


$$S = S_{\mathrm{bg}} S_{\mathrm{io}}$$

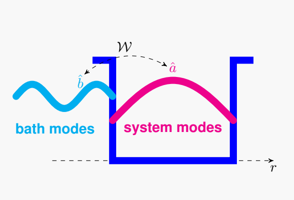
Translates bath to free states

DL & J. Evers, arXiv:1812.08556 [quant-ph]

Few-mode scattering



equivalent



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

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

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

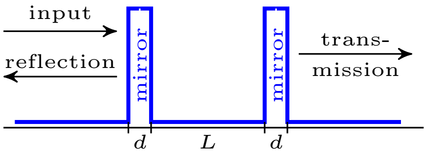
Translates bath to free states

$\Rightarrow$ Few-mode theory can apply in extreme regimes!

DL & J. Evers, arXiv:1812.08556 [quant-ph]

Illustrative example

Example: Two-sided Fabry-Perot cavity



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

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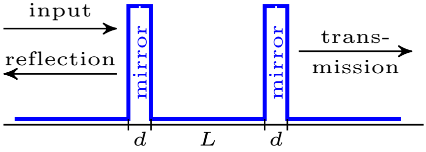

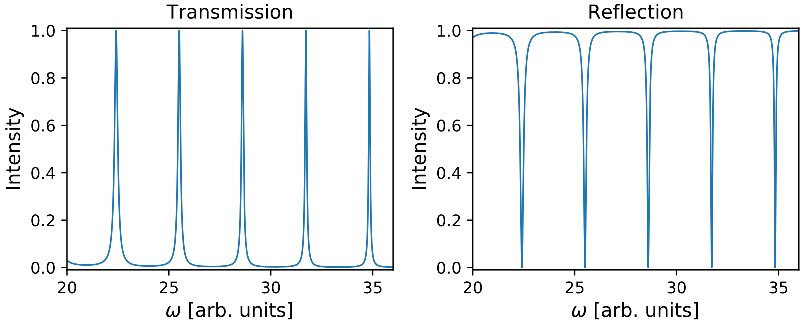

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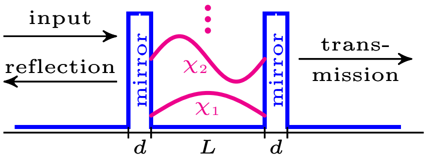

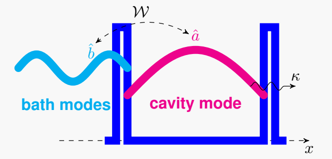

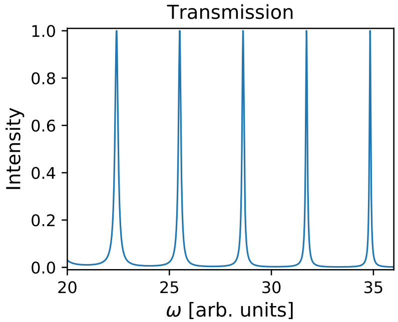

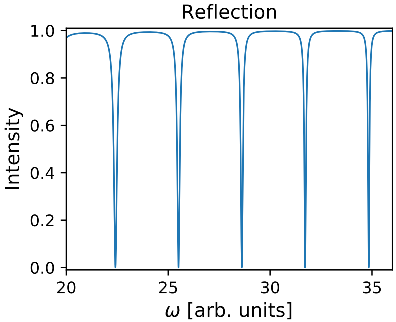

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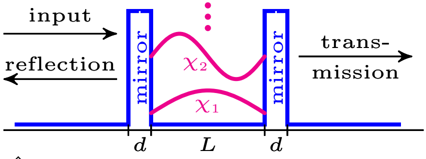
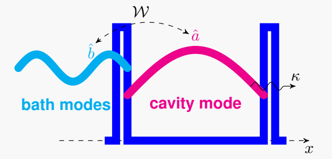
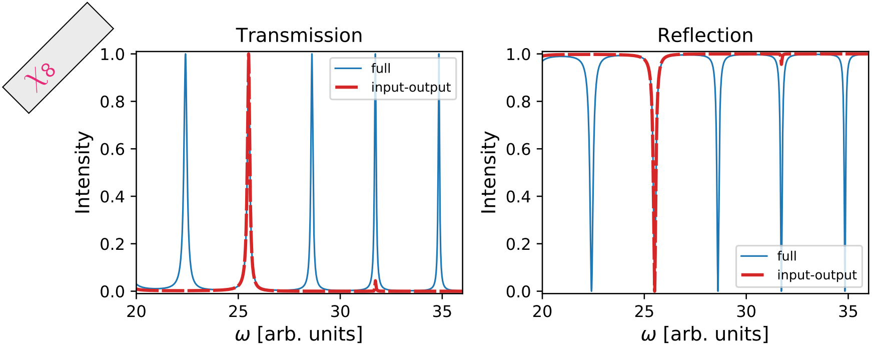
Example: Two-sided Fabry-Perot cavity







$\Rightarrow$ ab initio, not a fit!

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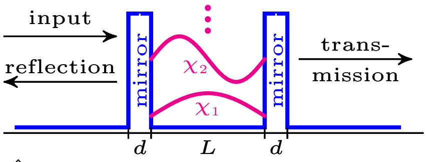

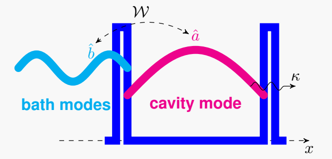

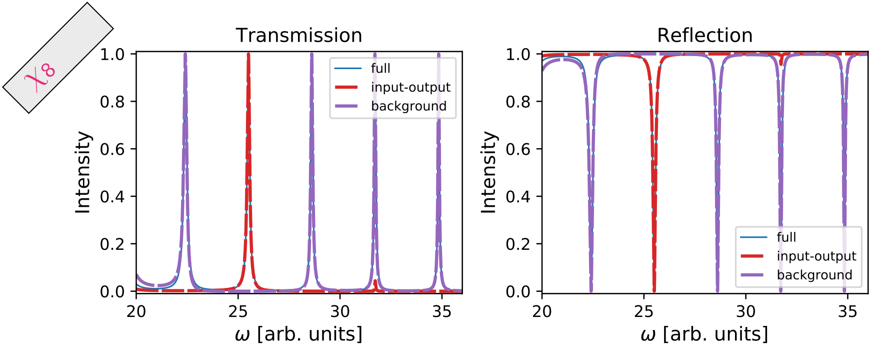

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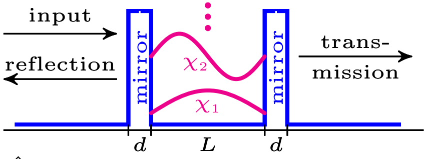
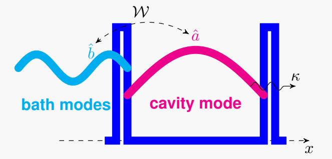
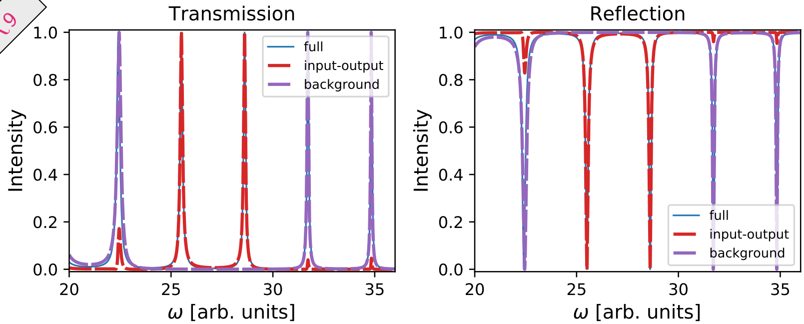




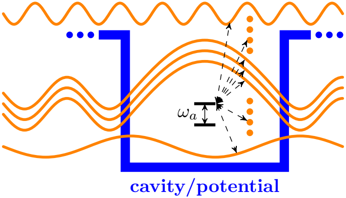
χ_8, χ_9

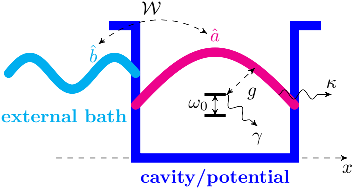


$\Rightarrow$ extract resonant dynamics

DL & J. Evers, arXiv:1812.08556 [quant-ph]

Interacting systems





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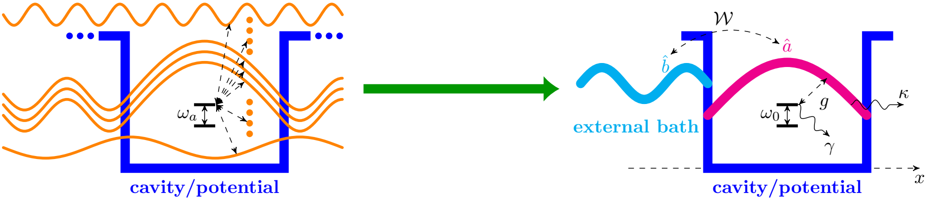
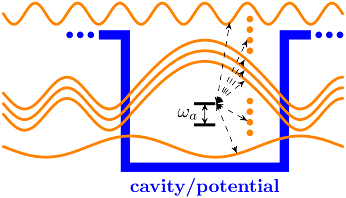
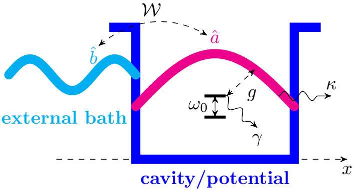


- Many degrees of freedom
- Often difficult!

Interacting systems



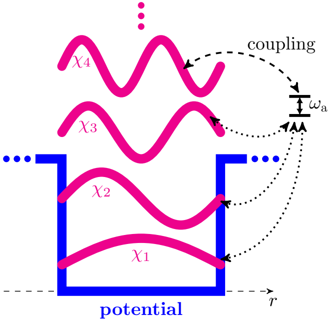


- Many degrees of freedom
- Often difficult!

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

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

Effective few-mode expansions



Recipe:

1. choose few-mode basis
2. perform few-mode approximation in interaction
3. include more modes if necessary

$\Rightarrow$ **Non-perturbative expansion scheme**

DL & J. Evers, arXiv:1812.08556 [quant-ph]

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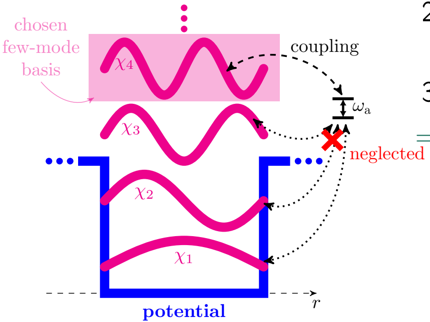

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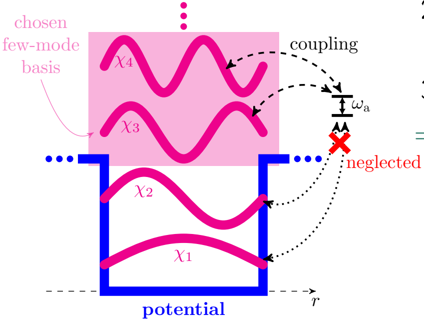

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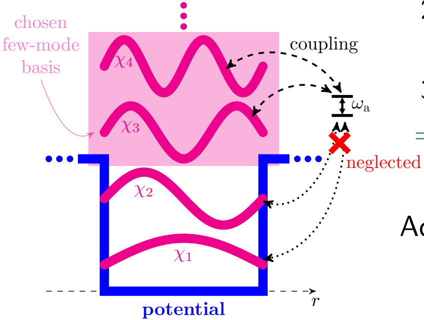

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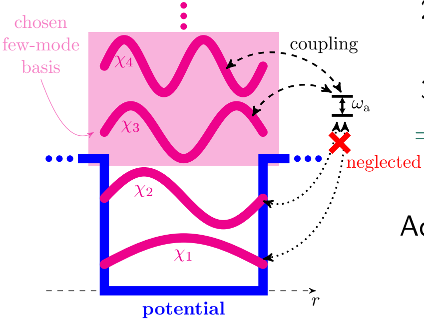
Advantages of ab initio few-mode theory

- Non-interacting part treated *exactly*
- Disentangles approximations
- Connects to existing toolbox

DL & J. Evers, arXiv:1812.08556 [quant-ph]

Effective few-mode expansions



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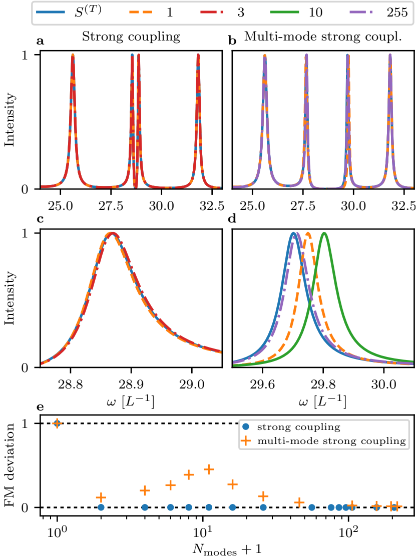
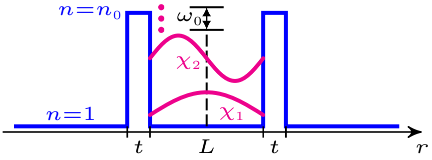
$\Rightarrow$ **Applies in extreme regimes!**

DL & J. Evers, arXiv:1812.08556 [quant-ph]

Convergence and extreme regimes





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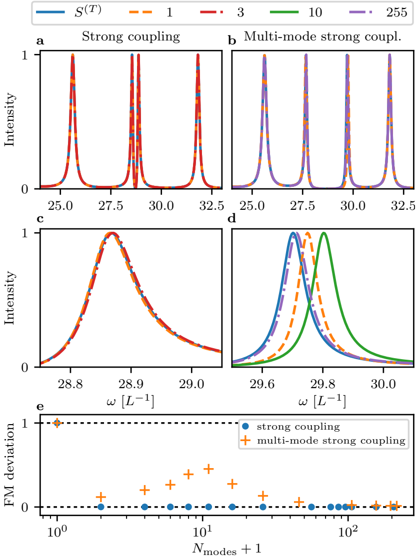

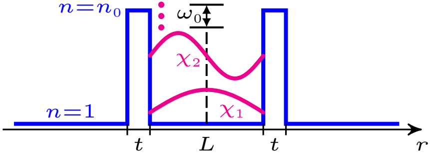

Convergence of light-matter coupling models is non-trivial![1]

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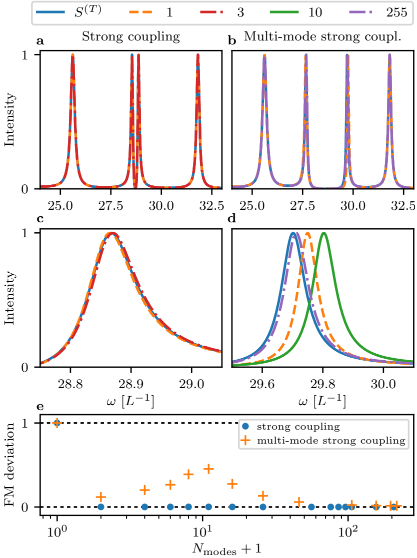
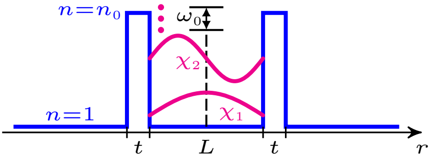


Convergence can also be shown analytically!



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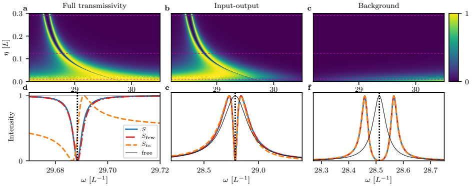
Benchmarks and more advantages

- ✓ Benchmarked in linear regime
- ✓ Highly open systems



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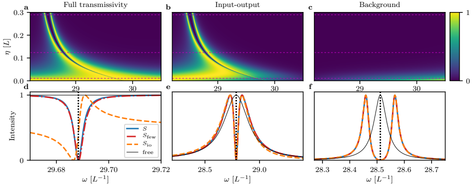

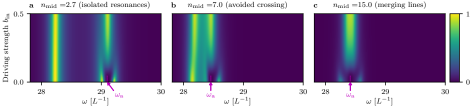

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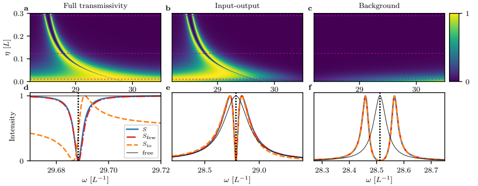

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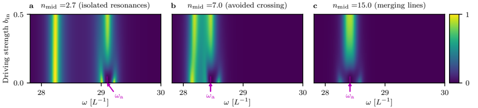
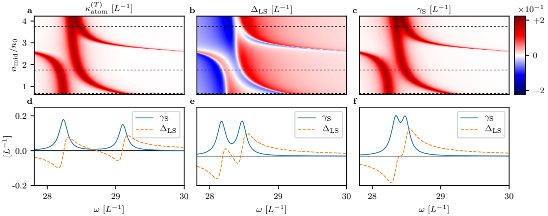


- ✓ Overlapping modes features
  - ⇒ Non-trivial bath effects!
- ✓ Ab initio calculation of quantum couplings



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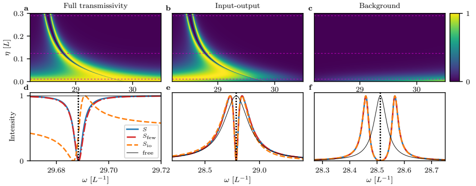

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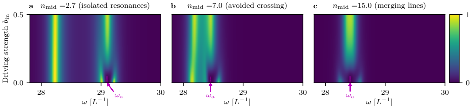

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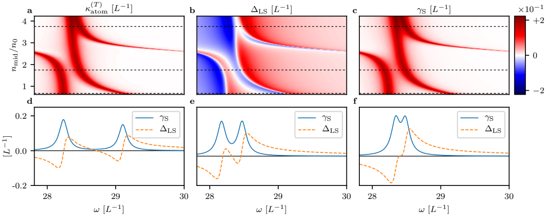
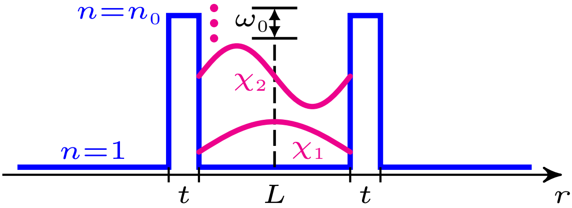
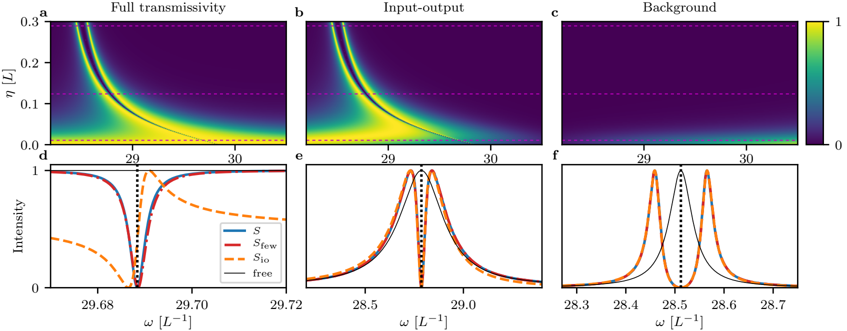


Poster tonight!

From strong coupling to free space





DL & J. Evers, arXiv:1812.08556 [quant-ph]

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

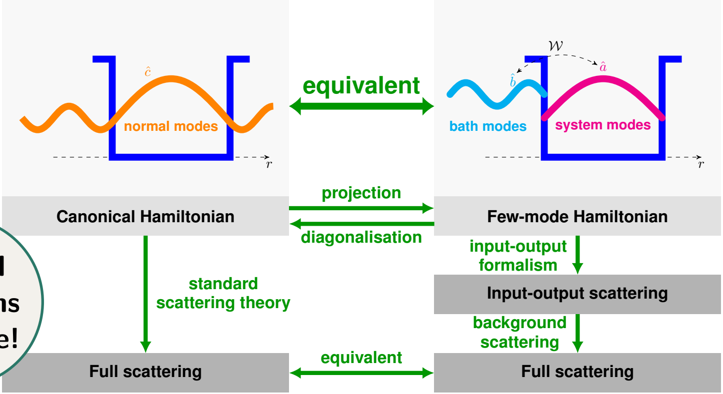
?! Applications in extreme regimes of open quantum dynamics

Thank you for your attention!

Jörg Evers

Kilian P. Heeg

Christoph H. Keitel



Critical questions welcome!

DL & J. Evers, arXiv:1812.08556 [quant-ph]