

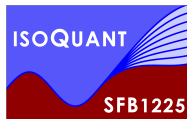


# Ab initio **few-mode** theory

for quantum potential scattering problems

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

Max-Planck-Institut für Kernphysik, Heidelberg



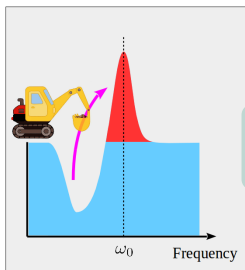
JUST TO CLEAR THINGS UP:

<b>A FEW</b>	ANYWHERE FROM 2 TO 5
A HANDFUL	ANYWHERE FROM 2 TO 5
SEVERAL	ANYWHERE FROM 2 TO 5
A COUPLE	2 (BUT SOMETIMES UP TO 5)

<https://xkcd.com/1070/>



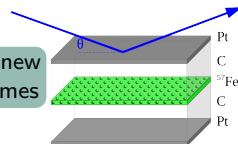
# Group of Jörg Evers at MPIK in Heidelberg



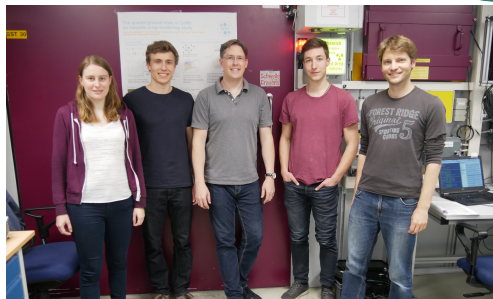
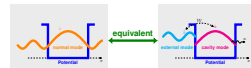
Coherent  
control of x-rays  
and nuclei

Nuclear  
quantum  
optics

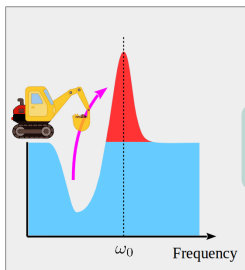
X-rays excite new  
quantum regimes



Understand  
fundamentals



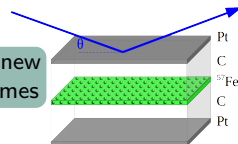
# Group of Jörg Evers at MPIK in Heidelberg



Coherent  
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and nuclei

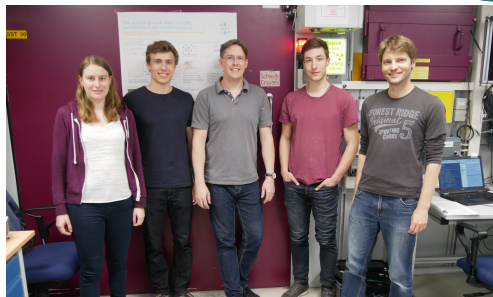
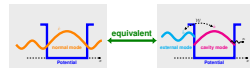
Nuclear  
quantum  
optics

X-rays excite new  
quantum regimes

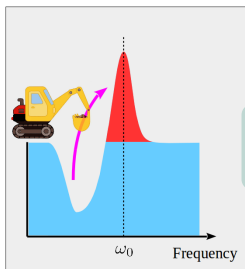


today

Understand  
fundamentals



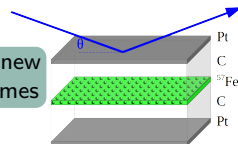
# Group of Jörg Evers at MPIK in Heidelberg



Coherent  
control of x-rays  
and nuclei

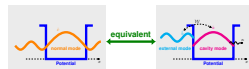
Nuclear  
quantum  
optics

X-rays excite new  
quantum regimes



today

Understand  
fundamentals

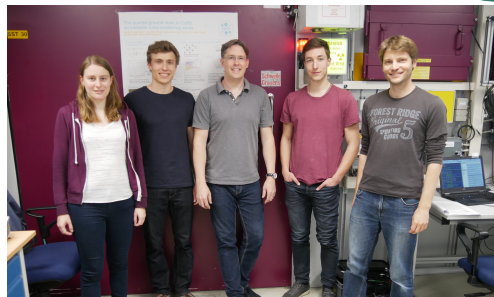


Open quantum  
systems

Light-matter  
interactions

Cavity QED,  
Circuit QED

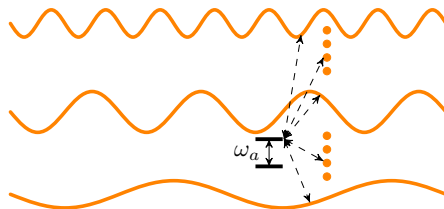
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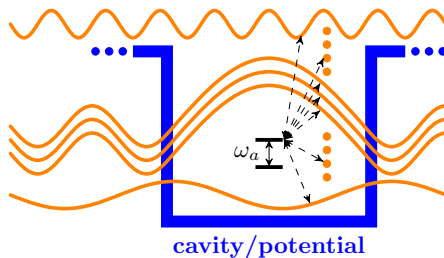


# Overview

Matter-continuum  
coupling

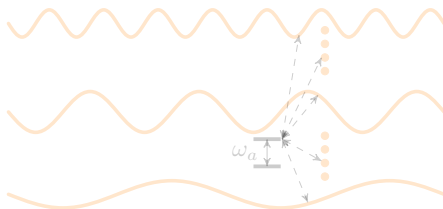


Structured continuum  
featuring resonances



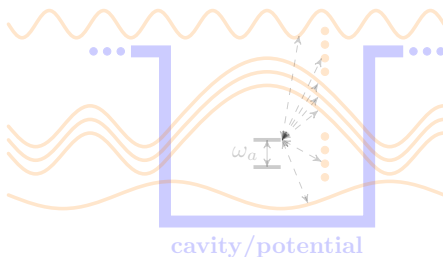
# Overview

Matter-continuum  
coupling

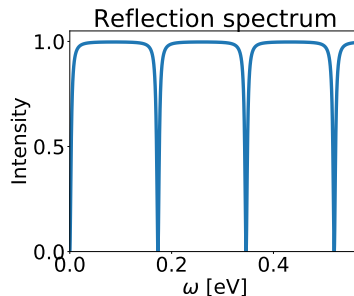
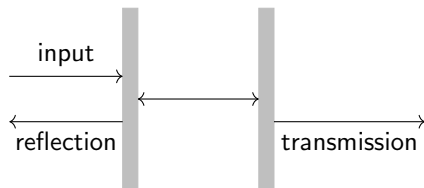


Can we extract **relevant degrees of freedom** from a continuum?

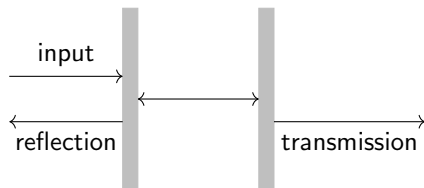
Structured continuum  
featuring resonances



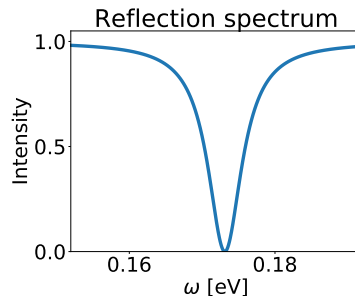
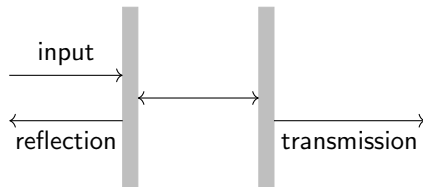
# Example: Fabry-Perot cavity



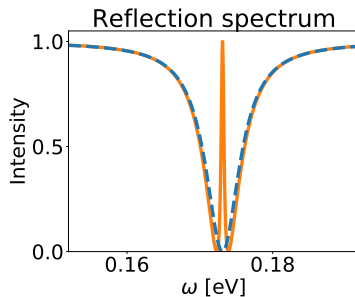
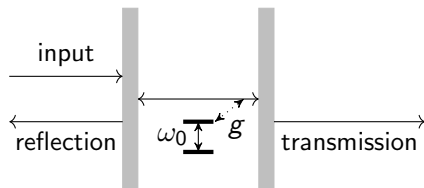
# Example: Fabry-Perot cavity



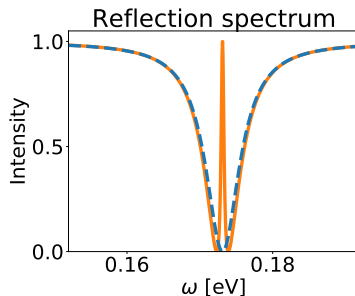
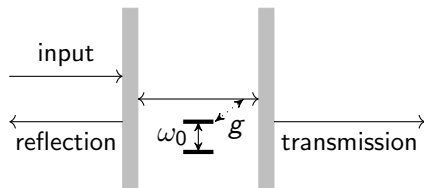
# Example: Fabry-Perot cavity



# Example: Fabry-Perot cavity

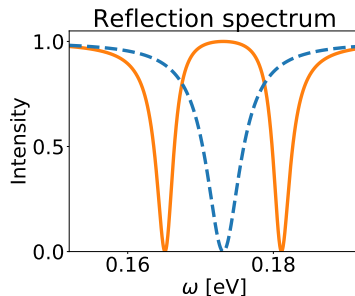
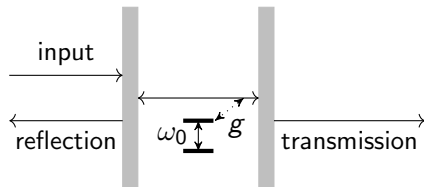


# Example: Fabry-Perot cavity



→ Weak coupling: Purcell effect

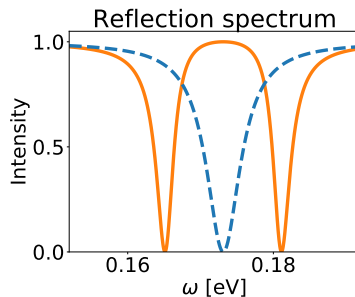
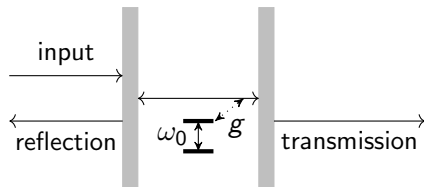
# Example: Fabry-Perot cavity



→ Strong coupling: Vacuum Rabi-splitting



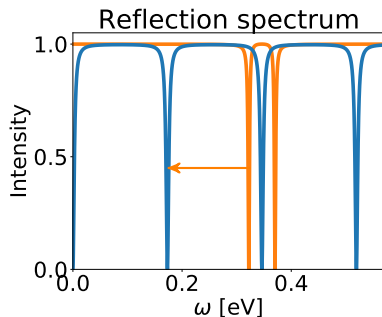
# Example: Fabry-Perot cavity



⇒ Enhance and control light-matter interactions!

# Extreme regimes

- Multi-mode strong coupling



Türeci et al. *Science* **320**, 643 (2008)

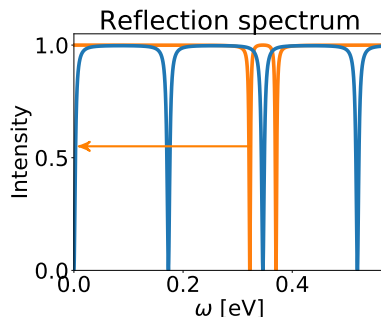
Krimer et al. *Phys. Rev. A* **89**, 033820 (2014)

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)

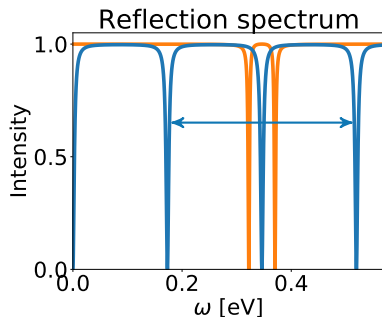
**Experimental:**

Anappara et al. *Phys. Rev. B* **79**, 201303(R) (2009)

... and many more ...

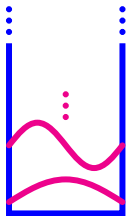
# Extreme regimes

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

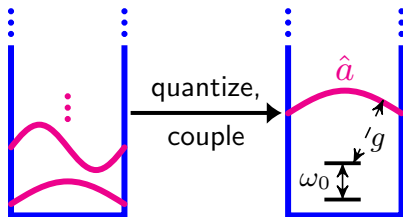


Petermann *IEEE J. Quantum Electron.* **15**, 566 (1979)  
Hackenbroich, Viviescas & Haake *Phys. Rev. Lett.* **89**, 083902 (2002)  
I. Rotter *J. Phys. A: Mathematical and Theoretical* **45**, 15 (2009)  
Heeg et al. *Phys. Rev. Lett.* **114**, 207401 (2015)  
... and many more ...

# From closed to open boxes



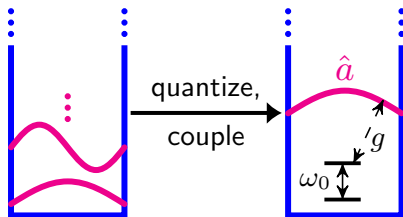
# From closed to open boxes



## Jaynes-Cummings & friends

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

# From closed to open boxes

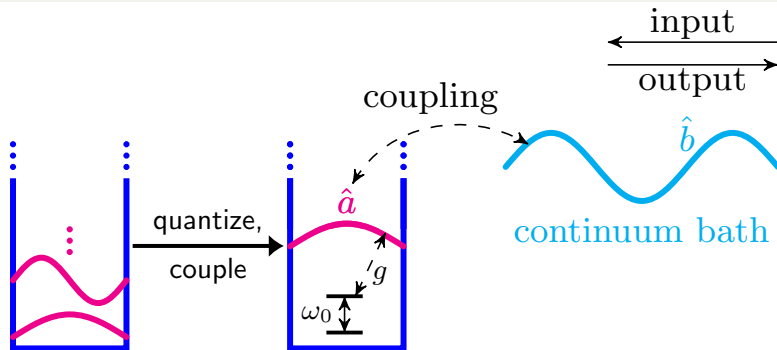


- discrete eigenstates
- closed system
  - × no leakage
  - × no driving
  - × no scattering
  - × no external detection

## Jaynes-Cummings & friends

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

# From closed to open boxes



**Jaynes-Cummings & friends**

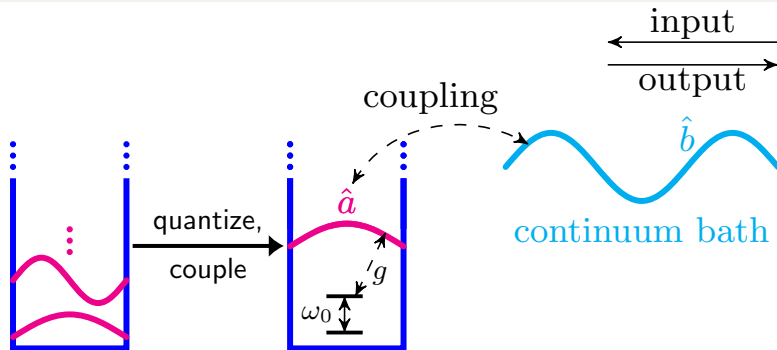
$$H = H_{\text{atom}} + H_{\text{cav}} + g\hat{a}\hat{\sigma}^+ + h.c.$$

**Input-output theory**

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



# From closed to open boxes



**Jaynes-Cummings & friends**  
 $H = H_{\text{atom}} + H_{\text{cav}} + g\hat{a}\hat{\sigma}^+ + h.c.$

→ **few-mode concept**

**Input-output theory**  
 $\hat{b}_{\text{out}} = \hat{b}_{\text{in}} + \kappa\hat{a}$

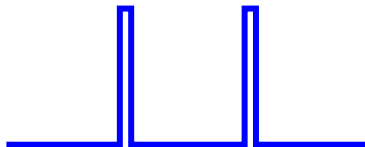
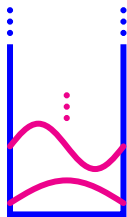
→ **scattering**

⇒ **Big tool box for quantum optics!**

# From closed to open boxes

open system

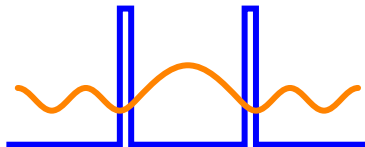
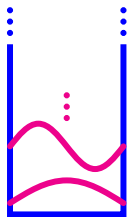
- ✓ leakage
- ✓ driving
- ✓ scattering



# From closed to open boxes

open system

- ✓ leakage
- ✓ driving
- ✓ scattering

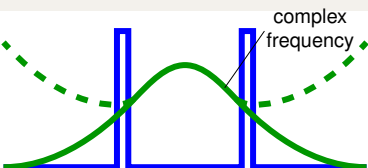


continuum eigenstates

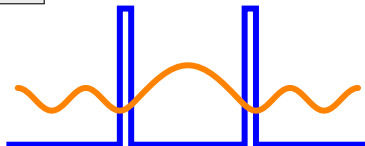


few-mode concept  
is lost

# From closed to open boxes



resonant modes

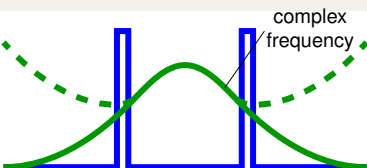


continuum eigenstates

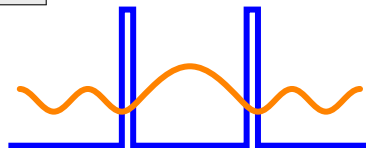


few-mode concept  
is lost

# From closed to open boxes

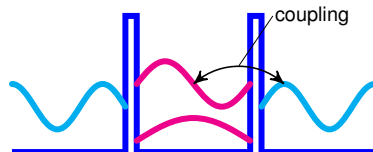


resonant modes



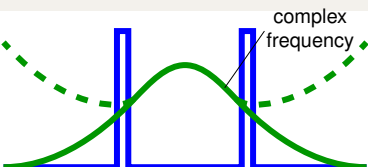
continuum eigenstates

☹️ few-mode concept  
is lost



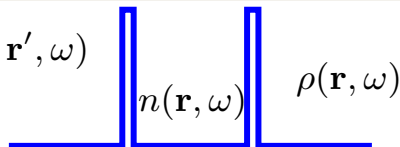
few-mode + bath

# From closed to open boxes

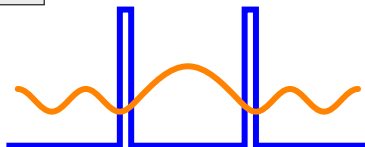


resonant modes

$$\underline{\underline{G}}(\mathbf{r}, \mathbf{r}', \omega)$$



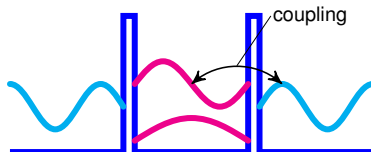
Green fns, LDOS, lin. disp. theory



continuum eigenstates

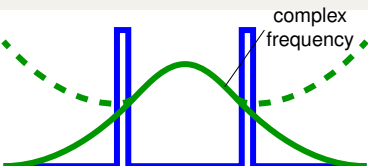


few-mode concept  
is lost



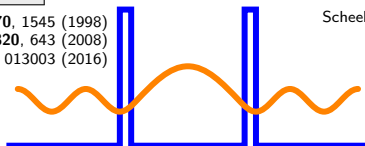
few-mode + bath

# From closed to open boxes



resonant modes

Ching et al. *Rev. Mod. Phys.* **70**, 1545 (1998)  
 Türeci et al. *Science* **320**, 643 (2008)  
 Cerjan & Stone *Phys. Scr.* **91** 013003 (2016)



$$\underline{\underline{G}}(\mathbf{r}, \mathbf{r}', \omega)$$

$$n(\mathbf{r}, \omega) \quad \rho(\mathbf{r}, \omega)$$

Green fns, LDOS, lin. disp. theory

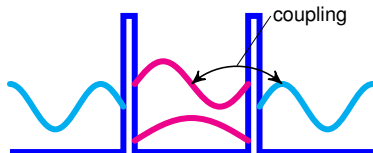
Scheel & Buhmann *Acta Phys. Slov.* **58**, 675 (2008)  
 Krimer et al. *Phys. Rev. A* **89**, 033820 (2014)  
 Zhu et al. *Phys. Rev. Lett.* **64**, 2499 (1990)

continuum eigenstates



few-mode concept  
is lost

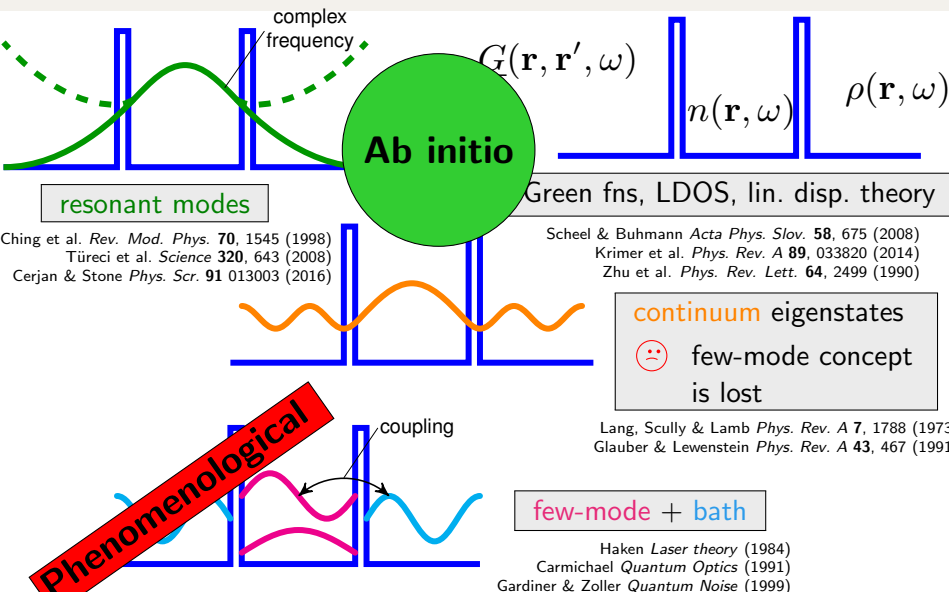
Lang, Scully & Lamb *Phys. Rev. A* **7**, 1788 (1973)  
 Glauber & Lewenstein *Phys. Rev. A* **43**, 467 (1991)



few-mode + bath

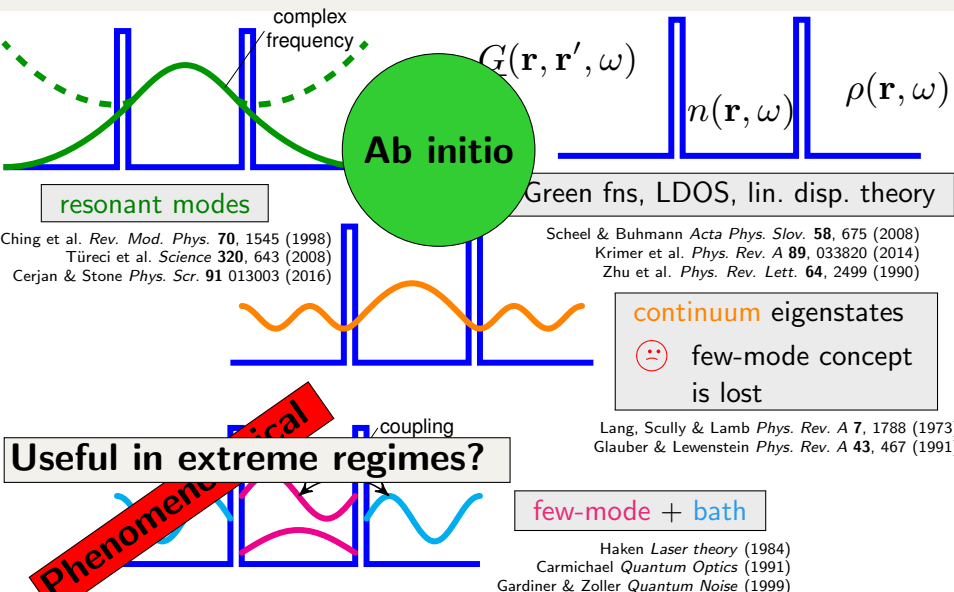
Haken *Laser theory* (1984)  
 Carmichael *Quantum Optics* (1991)  
 Gardiner & Zoller *Quantum Noise* (1999)

# From closed to open boxes

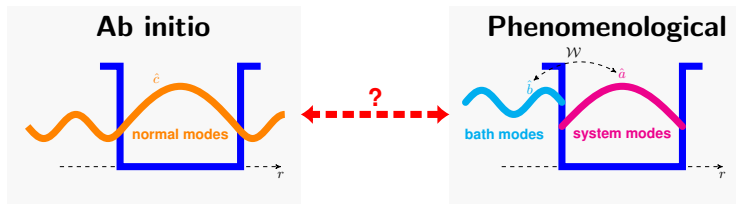




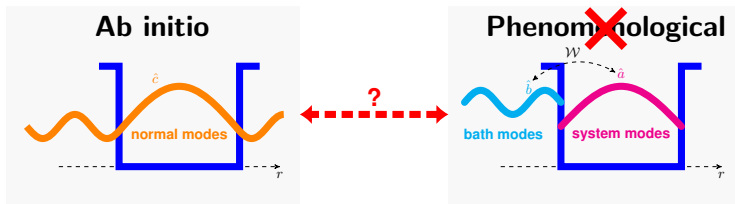
# From closed to open boxes



# The problem



# The problem



How to make

- **few-mode**

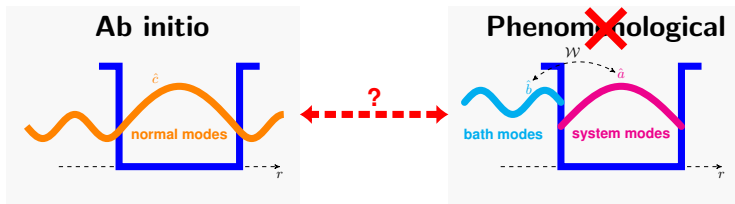
and

- **input-output**

ab initio?

?

# The problem



How to make

- **few-mode**

and

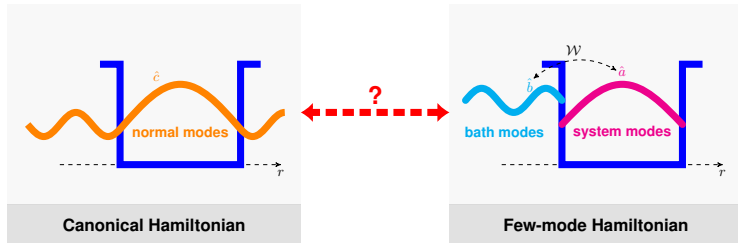
- **input-output**

ab initio?



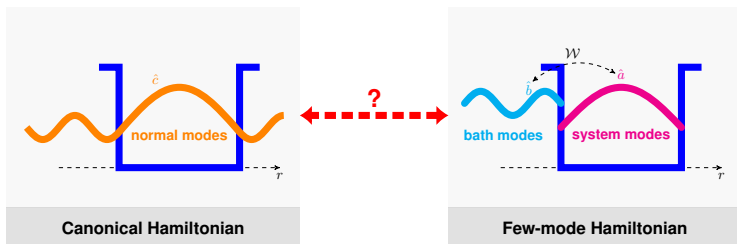
⇒ **Ab initio few-mode theory**

# 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



normal modes

$$\hat{c}(\omega)$$

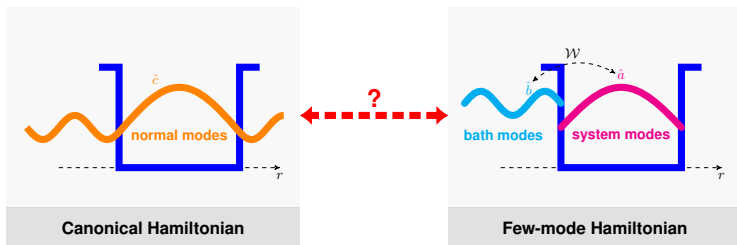
discrete modes

$$= \sum_{\lambda} \alpha_{\lambda}(\omega) \hat{a}_{\lambda}$$

external continuum

$$+ \int d\omega' \beta(\omega, \omega') \hat{b}(\omega')^{1,2}$$

# Ab initio few-mode Hamiltonians



normal modes

$$\hat{c}(\omega)$$

discrete modes

$$= \sum_{\lambda} \alpha_{\lambda}(\omega) \hat{a}_{\lambda}$$

external continuum

$$+ \int d\omega' \beta(\omega, \omega') \hat{b}(\omega')^{1,2}$$

$\Rightarrow$  select resonant states as few-mode basis<sup>3</sup>

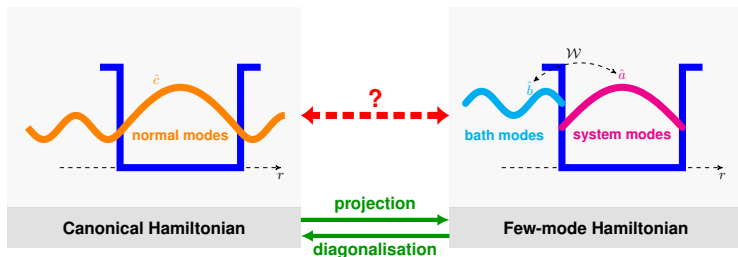
Glauber & Lewenstein, *Phys. Rev. A* **43**, 467 (1991)  
 Gardiner & Collett, *Phys. Rev. A* **31**, 3761 (1985)

<sup>1</sup>Viviescas & Hackenbroich, *Phys. Rev. A* **67**, 013805 (2003)

<sup>2</sup>Domcke, *Phys. Rev. A* **28**, 2777 (1982)

<sup>3</sup>DL & J. Evers, *submitted* arXiv:1812.08556 [quant-ph]

# Ab initio few-mode Hamiltonians



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

⇒ select **resonant states** as few-mode basis<sup>3</sup>

⇒ **ab initio few-mode Hamiltonians** 😊<sup>3</sup>

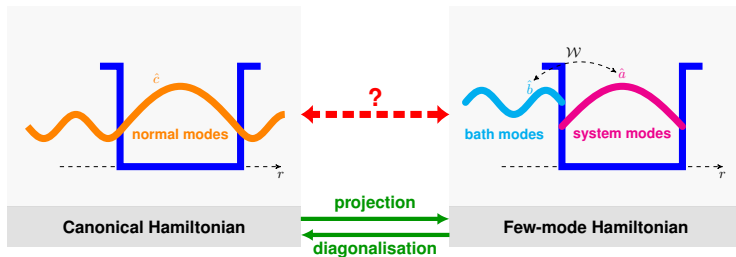
<sup>1</sup>Viviescas & Hackenbroich, *Phys. Rev. A* **67**, 013805 (2003)

<sup>2</sup>Domcke, *Phys. Rev. A* **28**, 2777 (1982)

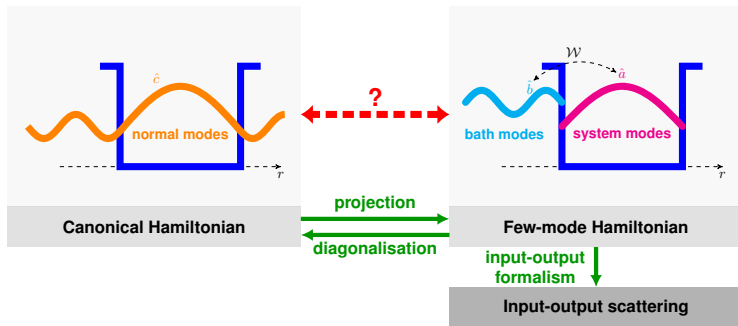
<sup>3</sup>DL & J. Evers, *submitted* arXiv:1812.08556 [quant-ph]



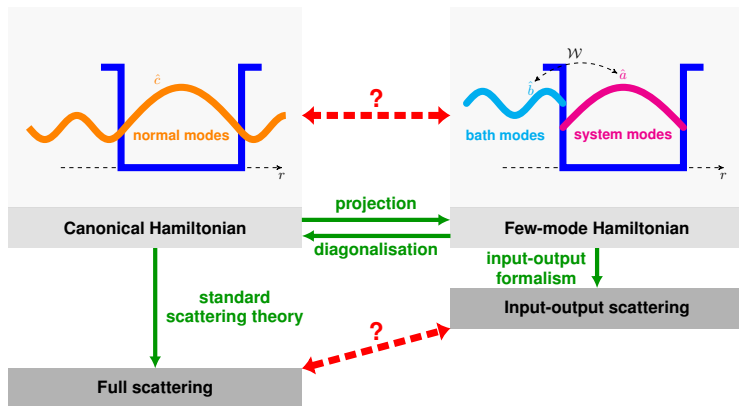
# Few-mode scattering



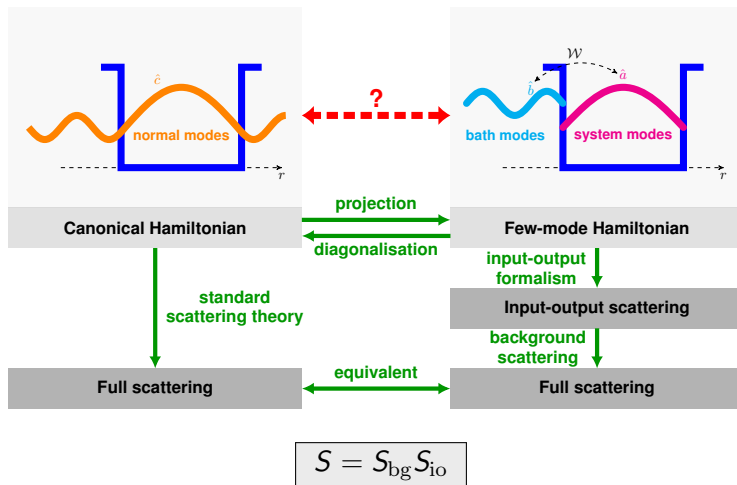
# Few-mode scattering



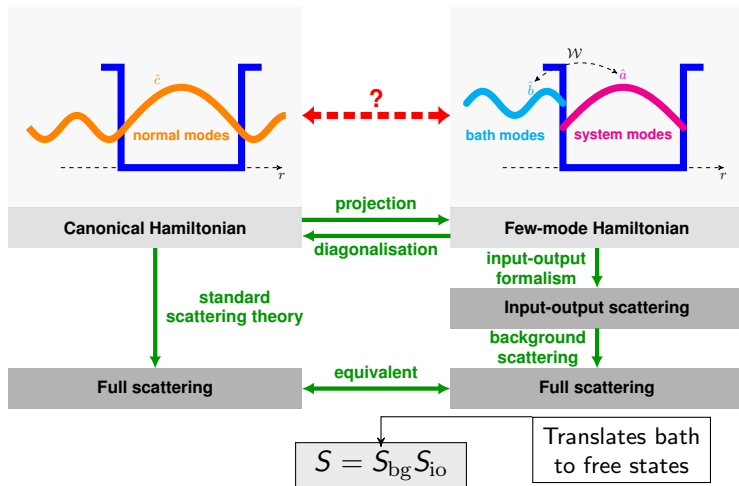
# Few-mode scattering



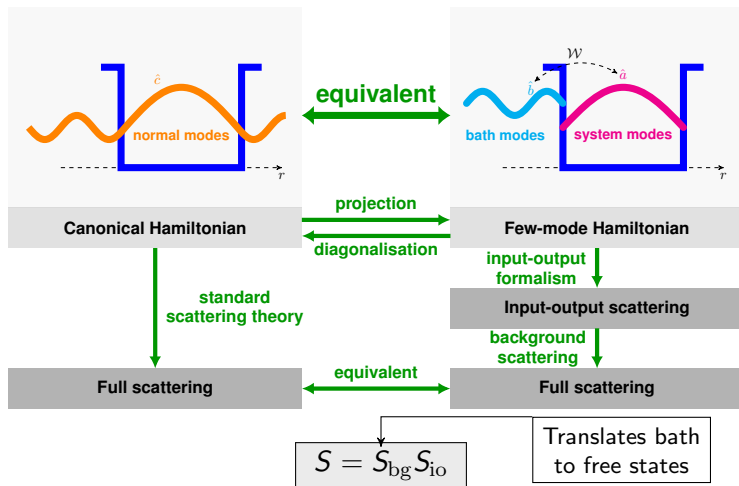
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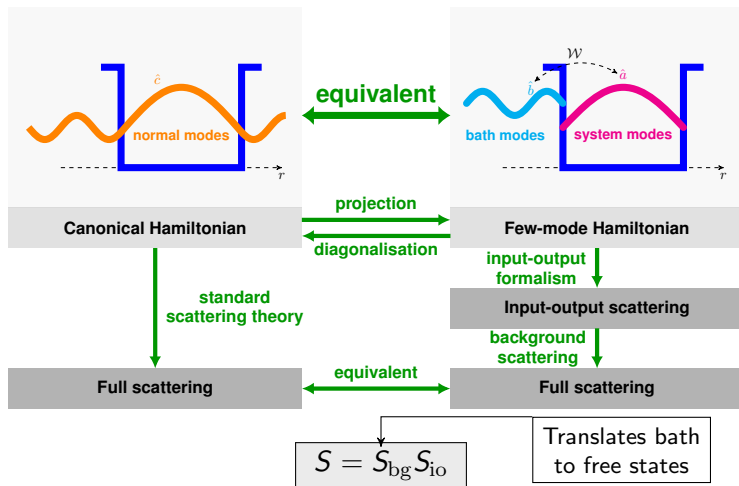
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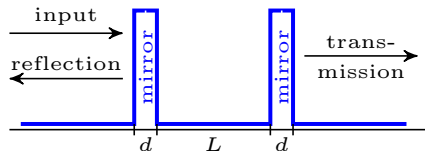


⇒ Few-mode theory is not limited to the good cavity regime!

# Illustrative example

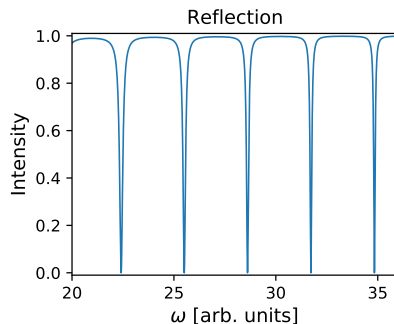
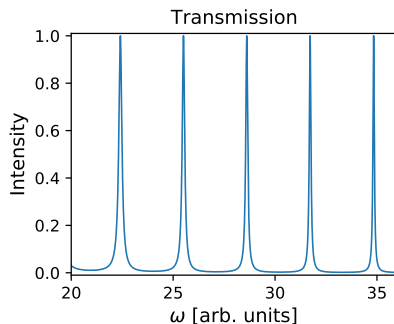
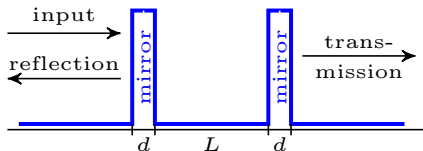


## Example: Two-sided Fabry-Perot cavity

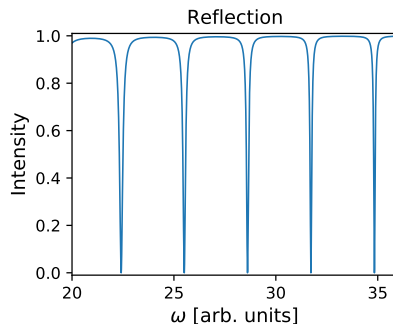
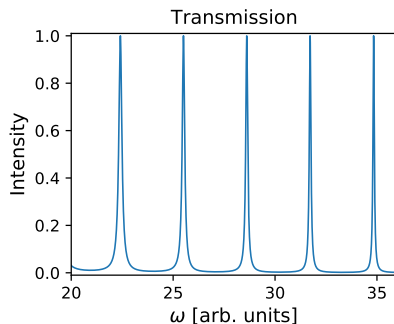
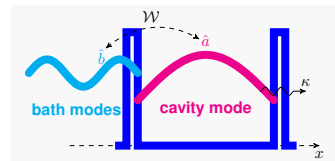
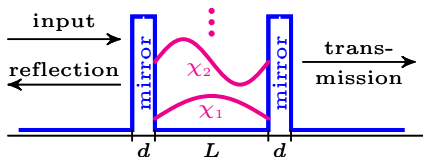


Ley & Loudon *J. Mod. Opt.* **34**, 227-255 (1987)

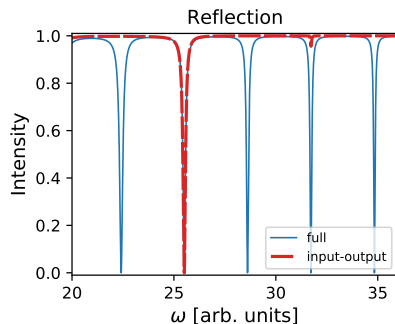
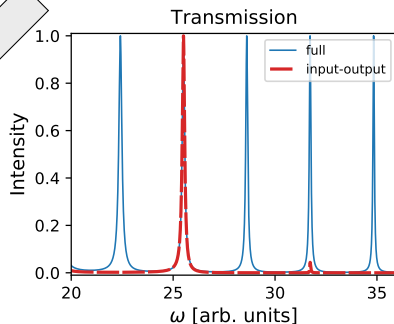
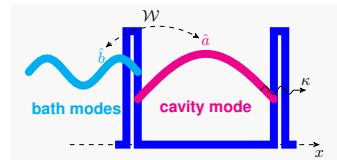
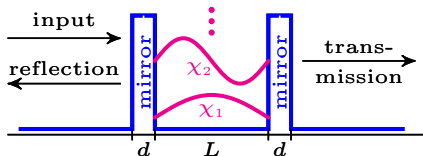
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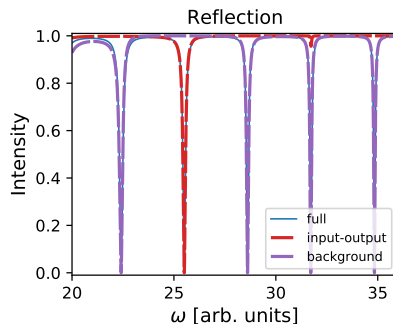
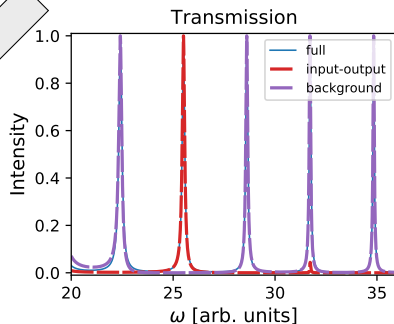
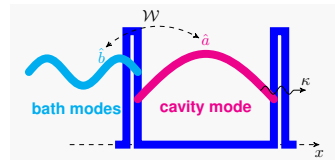
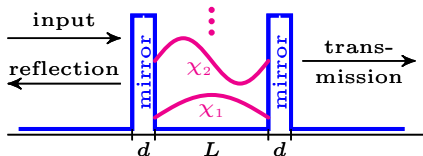


# Example: Two-sided Fabry-Perot cavity



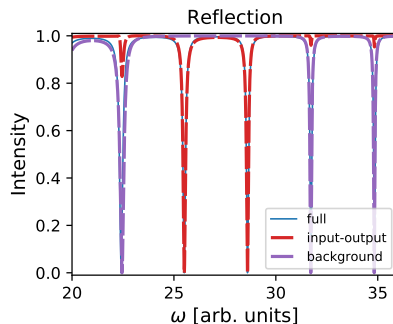
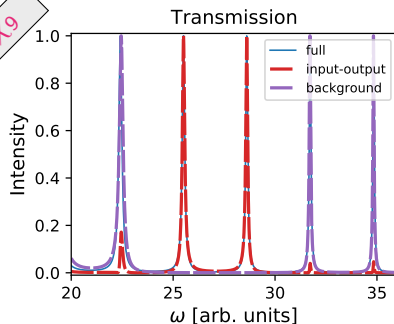
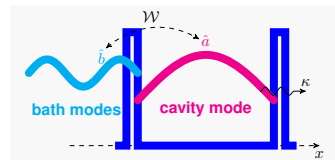
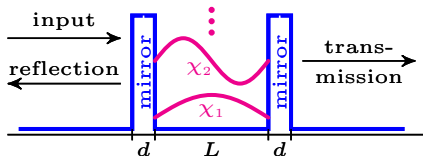
$\Rightarrow$  ab initio, not a fit!

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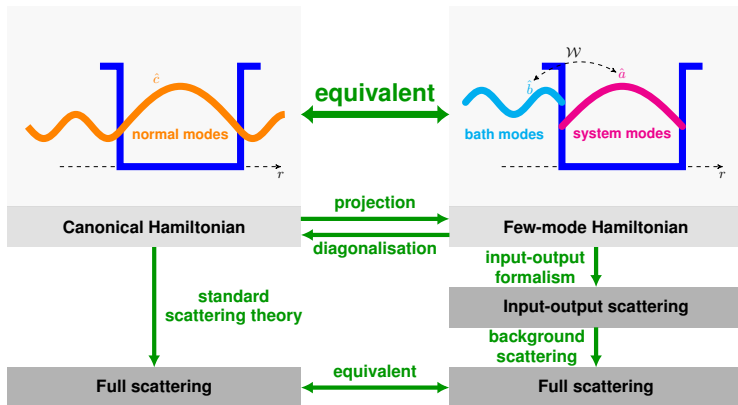
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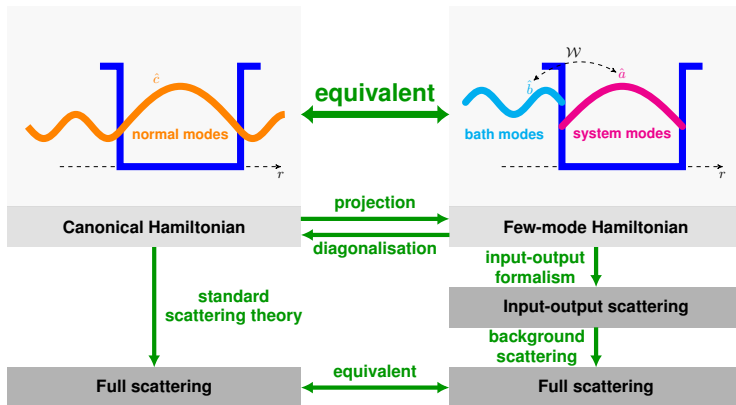
⇒ extract resonant dynamics

# Advantages (so far)



**Exact** few-mode theory for the empty cavity!

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But what about field-matter interactions?

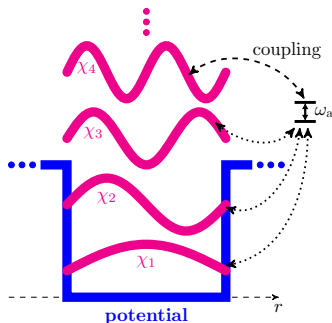


# Effective few-mode expansions

Recipe:

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

⇒ **Expansion scheme!**

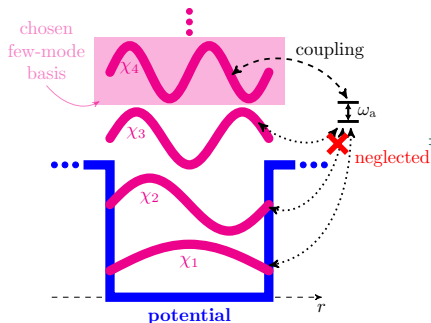


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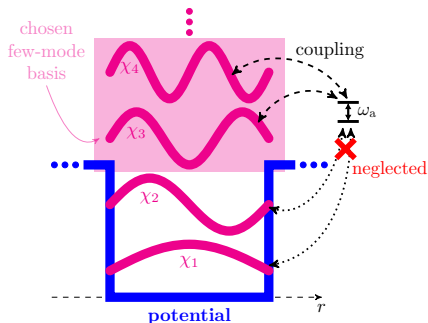


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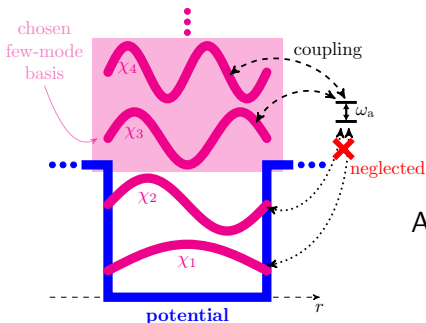
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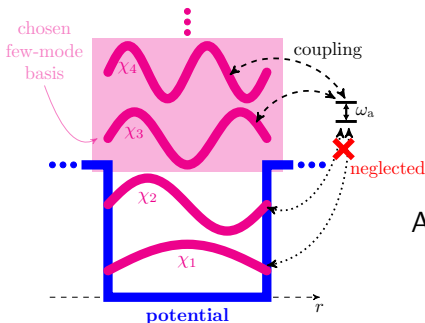
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Advantages of ab initio **few-mode** theory

- **Empty cavity** treated *exactly*
  - ⇒ Approximate interaction only
  - ⇒ Fully include openness, losses
- Connects to existing toolbox

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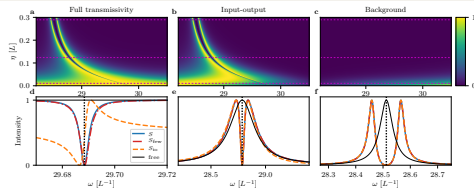
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Advantages of ab initio **few-mode** theory

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  - Connects to existing toolbox
- ⇒ **New regimes accessible!**

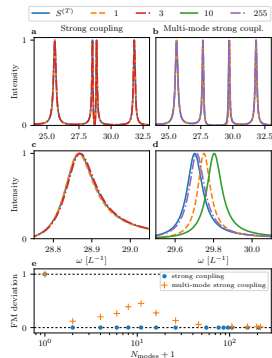
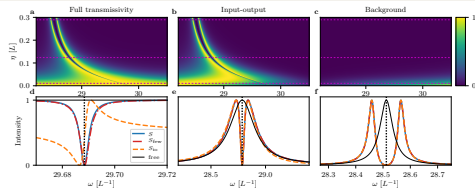
# Practical aspects

- ✓ Benchmarked in linear regime
  - ✓ Highly open systems
- ⇒  $S_{\text{bg}}$  matters!



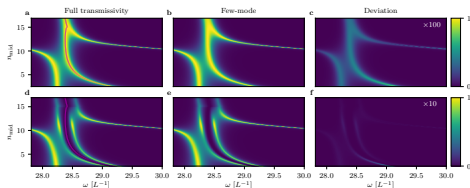
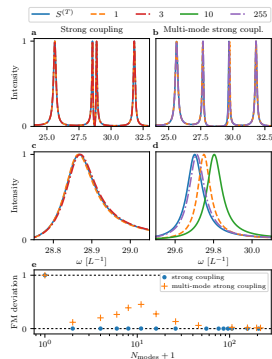
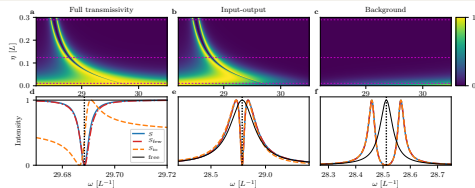
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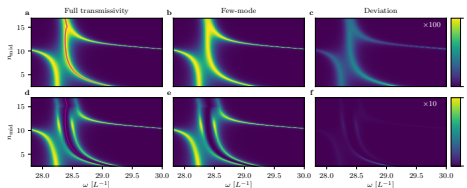
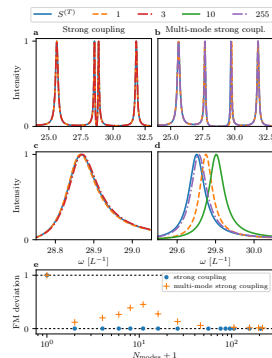
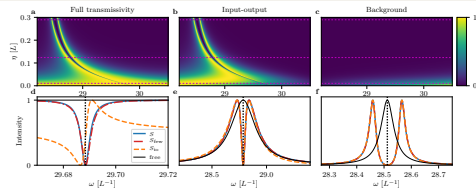
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⇒ Non-trivial bath effects!
- ✓ Ab initio calculation of quantum couplings





# Practical aspects

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⇒ Non-trivial bath effects!
- ✓ Ab initio calculation of quantum couplings
- ? Counter-rotating loss terms<sup>1</sup>, absorption<sup>2</sup>
- ? Optimal few-mode basis?



<sup>1</sup> Ciuti & Carusotto *Phys. Rev. A* **74**, 033811 (2006)

<sup>2</sup> Esteban et al. *Nat. Comm.* **3**, 825 (2012)



# Potential applications

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- Extreme openness, complex environments
  - ▶ Non-Hermitian photonics
  - ▶ Random lasers, complex
  - ▶ Quantum plasmonics
  - ▶ X-ray and nuclear cavity QED
  - ▶ ...
- Extreme light-matter coupling
  - ▶ Open system effects at ultra-strong coupling
  - ▶ Multi-mode strong coupling
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<sup>1</sup>DL, K. P. Heeg, C. H. Keitel, J. Evers *in preparation*

# Conclusion & Outlook

- ✓ Rigorous construction of few-mode Hamiltonians
  - ✓ Scattering theory via input-output formalism
    - ⇒ Empty cavity treated exactly!
  - ✓ Converging expansion scheme for interactions
  - ✓ Linking ab initio theory and models in cavity QED
    - ⇒ Access to new regimes!
- 
- !! Explore quantum effects in X-ray cavities
  - ?! Applications in extreme regimes of light-matter interactions
  - ?? Applications in general quantum scattering and open systems theory?

# Thank you for your attention!



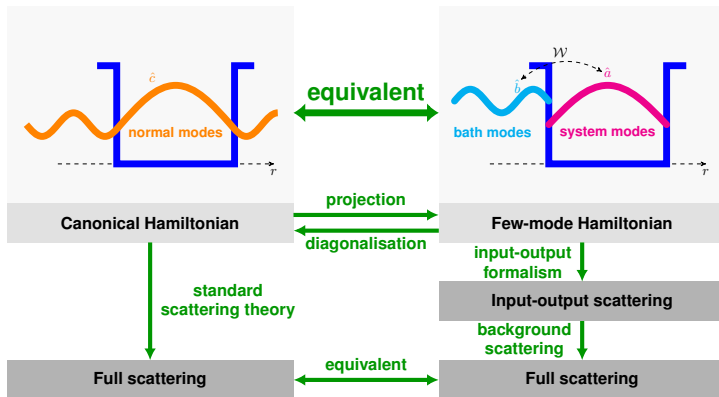
Jörg Evers



Kilian P. Heeg



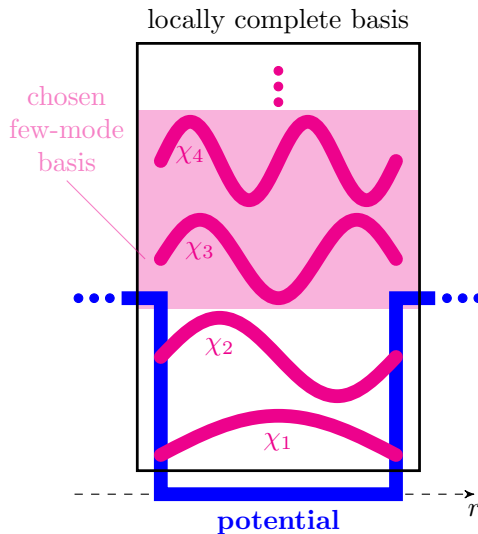
Christoph H. Keitel



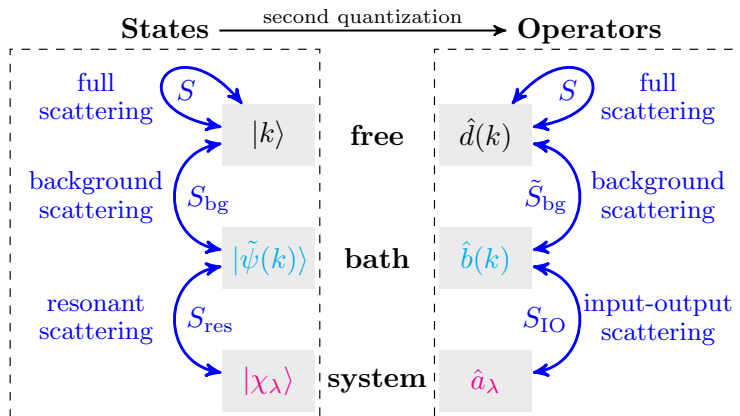


# Bonus slides

# Choosing relevant modes systematically



# Few-mode scattering theory



# Linear dispersion theory

Lorentz-Lorenz formula, Clausius-Mossotti relation and others...

**Summary:** Basic assumption  $\hat{\sigma}^- \approx -1$  (for 2-level system)

$$\begin{aligned} \frac{\partial^2}{\partial r^2} A(r, \omega) = & -\omega^2 \varepsilon(r) A(r, \omega) + c_A \delta(r - r_a) A(r, \omega) \\ & + \frac{4\omega_a^3 |d|^2}{\omega^2 - \omega_a^2} \delta(r - r_a) A(r, \omega) \end{aligned} \quad (1)$$

$$\varepsilon'(r) = \varepsilon(r) - \left( \frac{\omega_a^2}{\omega^2} \frac{4\omega_a^2 |d|^2}{\omega^2 - \omega_a^2} + \frac{c_A}{\omega^2} \right) \delta(r - r_a) \quad (2)$$

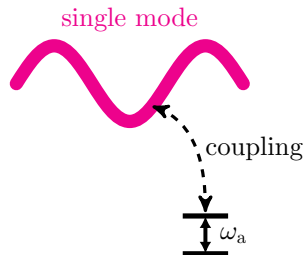
Standard references: Born & Wolf *Principles of optics* (1980)

Zhu et al. *Phys. Rev. Lett.* **64**, 2499 (1990)

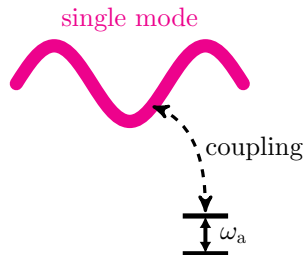
X-ray: Röhlberger *Nuclear condensed matter physics* (2004)

Ultra-strong: Malekakhlagh et al. *Phys. Rev. A* **94**, 063848 (2016)

# Few-mode models in quantum optics



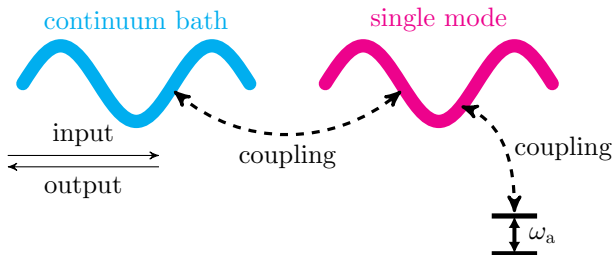
# Few-mode models in quantum optics



## Jaynes-Cummings model

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

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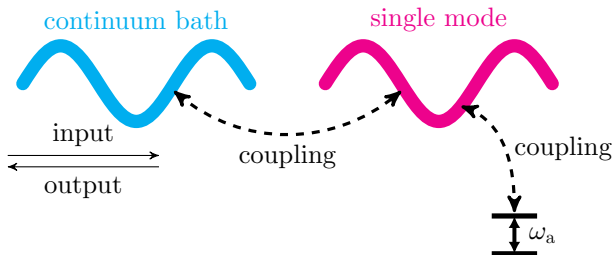
## Input-output formalism

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

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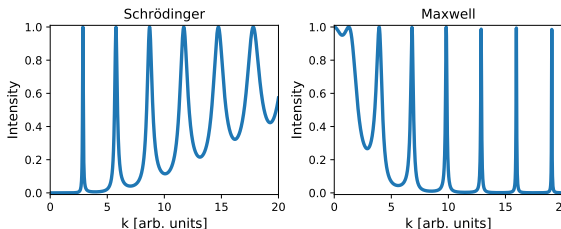
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⇒ **Big tool box!**



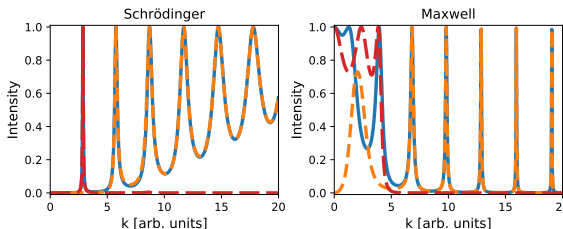
# Input-output methods in general scattering theory?

## Example: Schrödinger vs Maxwell Fabry-Perot



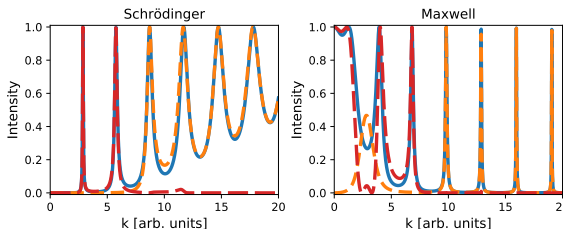
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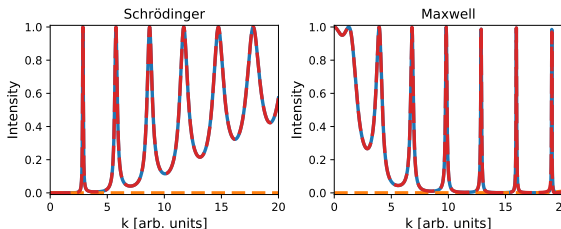
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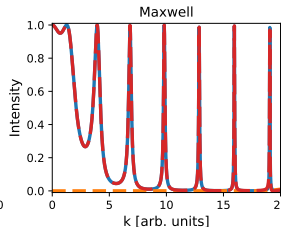
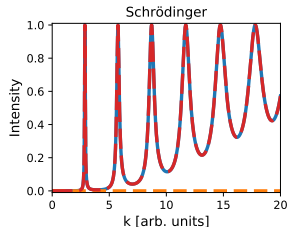


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## Example: Schrödinger vs Maxwell Fabry-Perot

$$S(E) = \mathbb{I} - 2\pi i \mathcal{W}^\dagger \frac{1}{E - H_{\text{eff}}} \mathcal{W}$$

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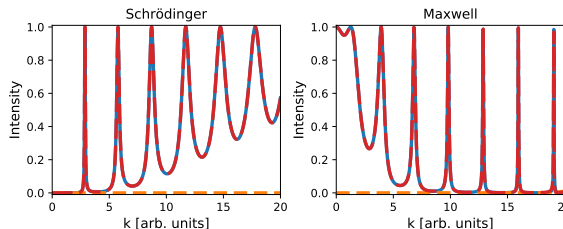


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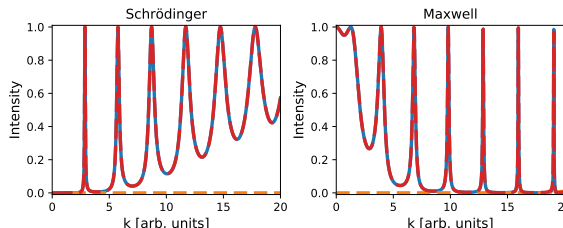
Generalized to second quantized level with interactions!

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Generalized to second quantized level with interactions!

**Potential applications:** quantum chemistry<sup>1</sup>, electronic transport<sup>2</sup>, chaotic scattering<sup>3,4</sup>, tunneling<sup>5</sup>, random lasers<sup>6</sup>...

<sup>1</sup>Domcke, *Phys. Rev. A* **28**, 2777 (1982)

<sup>2</sup>Datta, *Electronic Transport in Mesoscopic Systems* (1995)

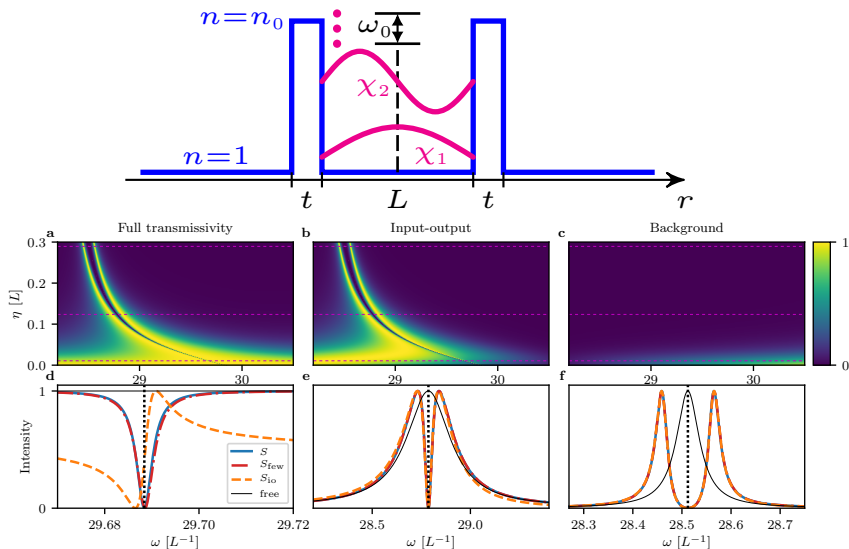
<sup>3</sup>Stöckmann, *Quantum Chaos* (1999)

<sup>4</sup>Weidenmüller&Mitchell, *Rev. Mod. Phys.* **81**, 539 (2009)

<sup>5</sup>Prange, *Phys. Rev.* **131**, 1083 (1963)

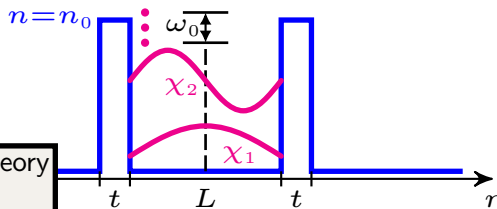
<sup>6</sup>Türeci et al, *Science* **320**, 643 (2008)

# From strong coupling to free space

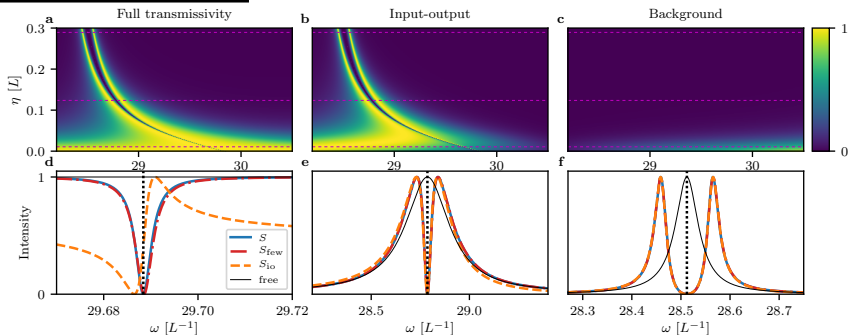




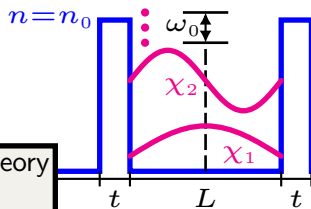
# From strong coupling to free space



Linear dispersion theory  
as benchmark!

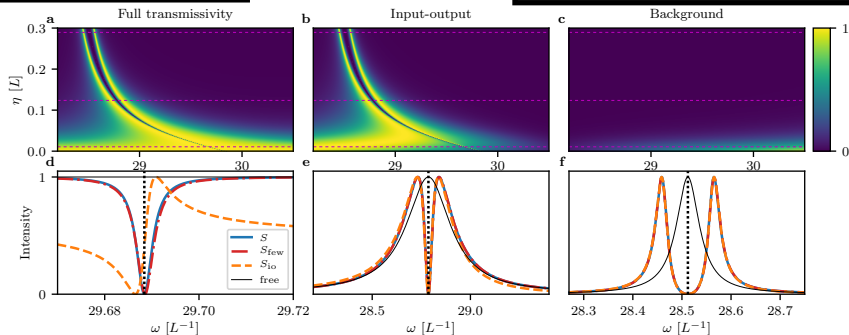


# From strong coupling to free space

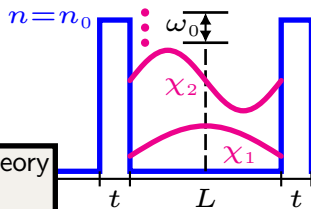


Linear dispersion theory  
as benchmark!

Ab initio few-mode theory  
captures the full range!

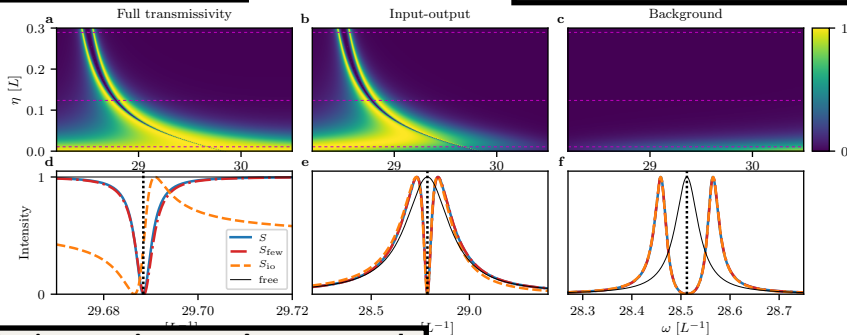


# From strong coupling to free space



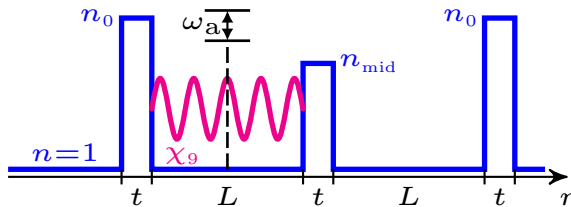
Linear dispersion theory  
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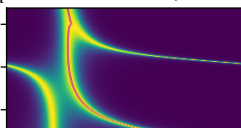
Background scattering matters!

# Quantum optical properties with overlapping modes

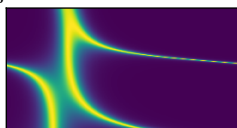


empty cavity

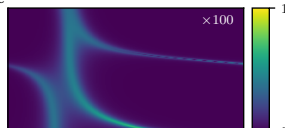
a Full transmissivity



b Few-mode

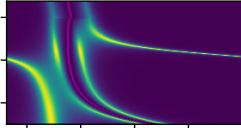


c Deviation  $\times 100$

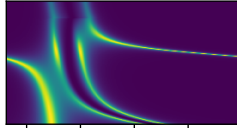


with atom

d Full transmissivity



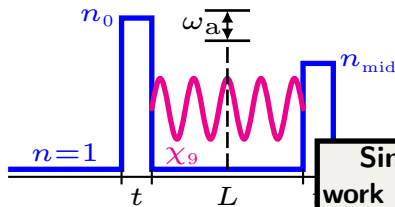
e Few-mode



f Deviation  $\times 10$



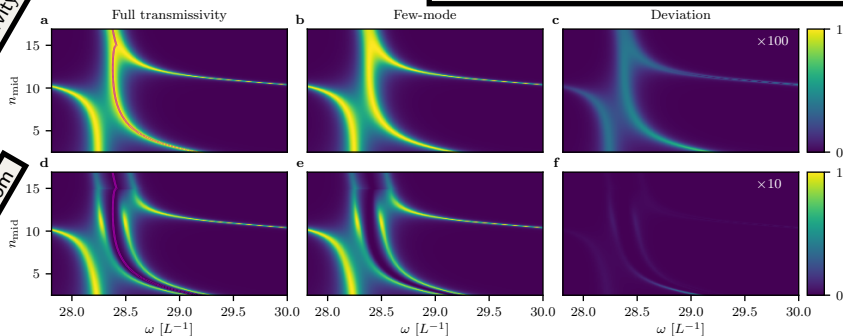
# Quantum optical properties with overlapping modes



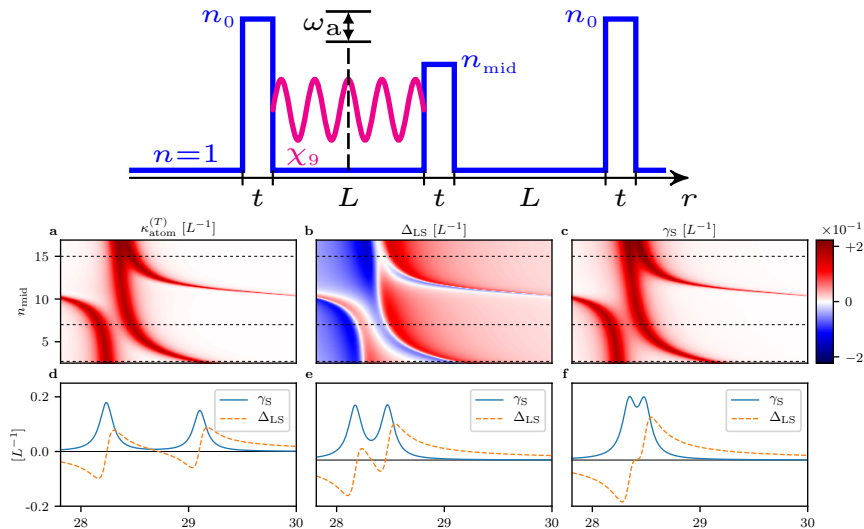
**Single mode description can work even for overlapping modes!**

empty cavity

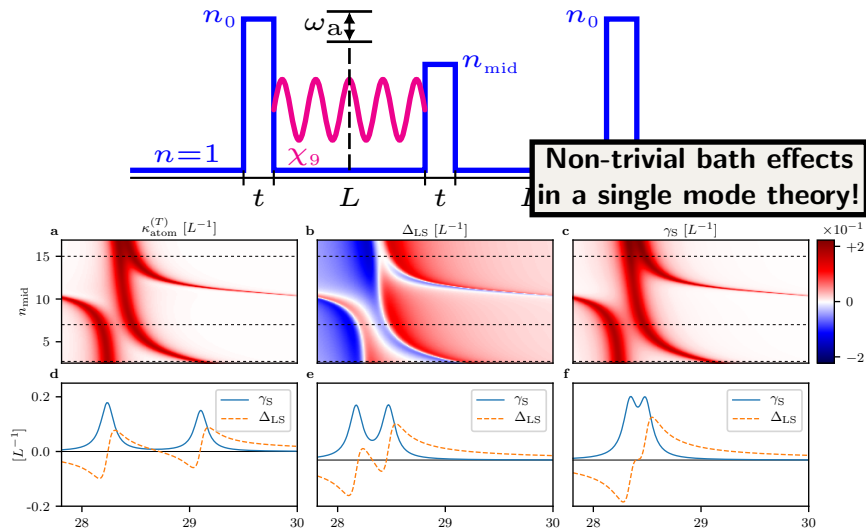
with atom



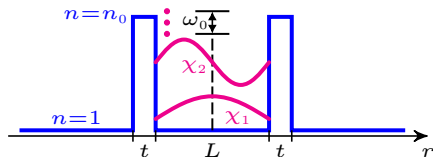
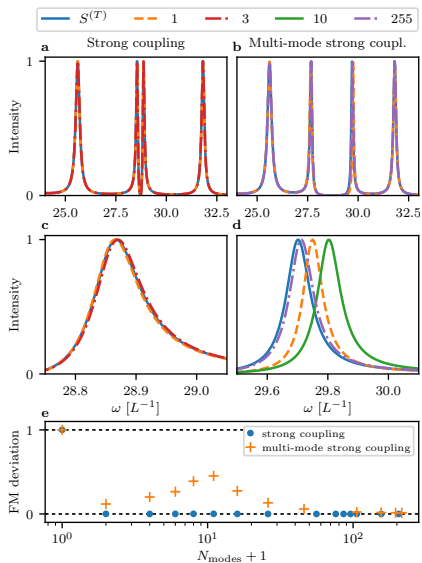
# Quantum optical properties with overlapping modes



# Quantum optical properties with overlapping modes

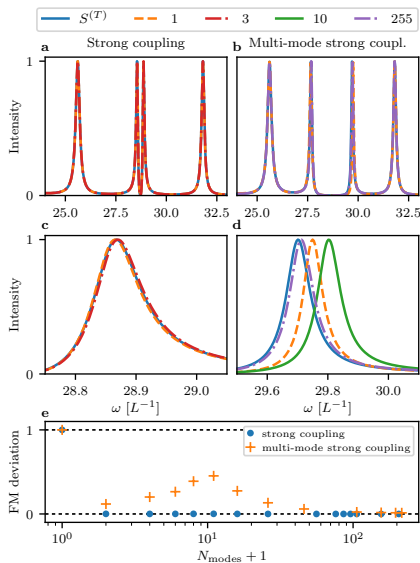


# Convergence and extreme regimes

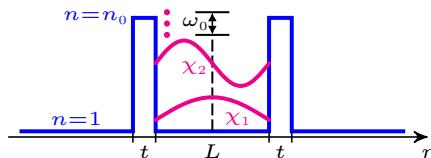




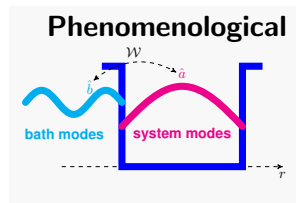
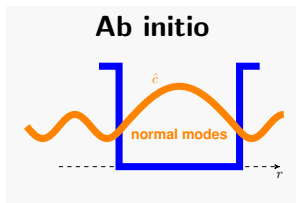
# Convergence and extreme regimes



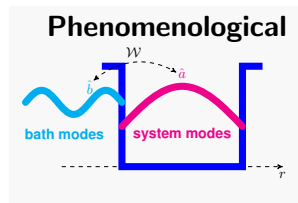
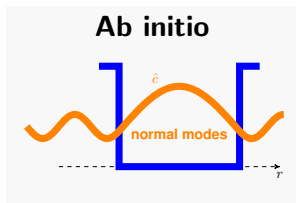
**Convergence can also be shown analytically!**



# Few-mode models in cavity QED



# Few-mode models in cavity QED



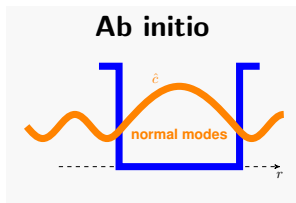
e.g. Canonical Hamiltonian

$$H_{\text{cav}} = \int d\omega \hbar \omega \hat{c}^\dagger(\omega) \hat{c}(\omega)$$

→ **Ab initio quantization**<sup>1</sup>

<sup>1</sup>Glauber & Lewenstein, *Phys. Rev. A* **43**, 467 (1991)

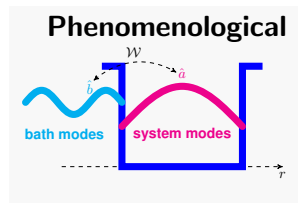
# Few-mode models in cavity QED



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Few-mode **system-bath** Hamiltonian

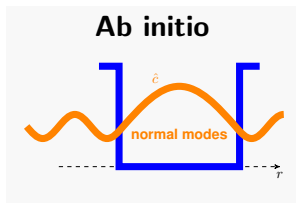
$$H_{\text{cav}} = H_{\text{syst}} + H_{\text{bath}} + \mathcal{W} \hat{a} \hat{b}^\dagger + h.c.$$

→ **Input-output model**<sup>2</sup>

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<sup>2</sup>Gardiner & Collett, *Phys. Rev. A* **31**, 3761 (1985)

# Few-mode models in cavity QED



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Continuum modes



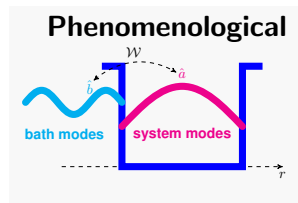
Often hard to solve



Ab initio



Limitations clear



Few-mode **system-bath** Hamiltonian

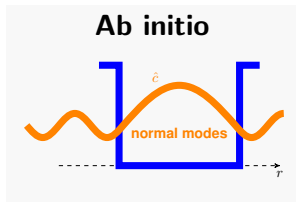
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# Few-mode models in cavity QED

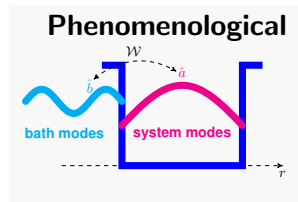


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- ☹ Continuum modes
- ☹ Often hard to solve
- 😊 Ab initio
- 😊 Limitations clear



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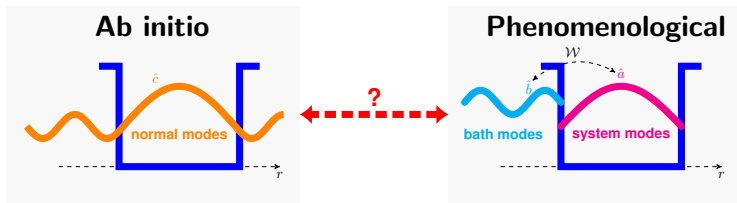
→ **Input-output model**<sup>2</sup>

- 😊 Few-mode
- 😊 Huge toolbox available
- ☹ Phenomenological
- ☹ Limitations unknown
- ?! Useful in extreme regimes?

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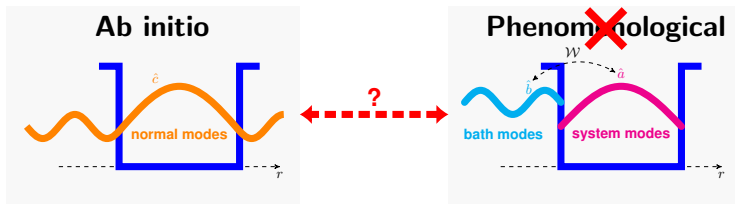
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# Few-mode models in cavity QED



How to make

- **few-mode**

and

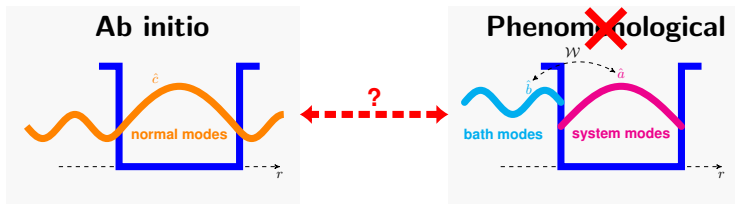
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ab initio?





# Few-mode models in cavity QED



How to make

- **few-mode**

and

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ab initio?



⇒ **Ab initio few-mode theory**