Ab initio few-mode theory

for quantum potential scattering problems

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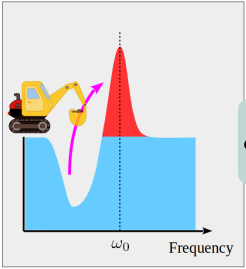
Christoph H. Keitel and Jörg Evers

Max-Planck-Institut für Kernphysik, Heidelberg

https://xkcd.com/1070/

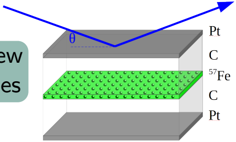
Group of Jörg Evers at MPIK in Heidelberg



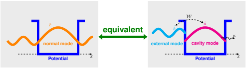
Coherent control of x-rays and nuclei

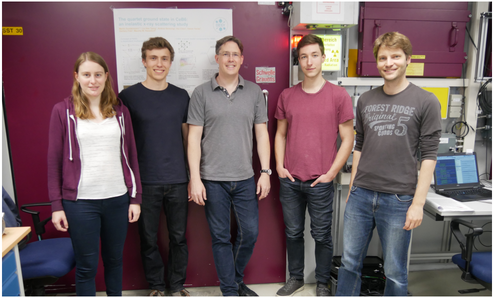
Nuclear quantum optics

X-rays excite new quantum regimes



Understand fundamentals





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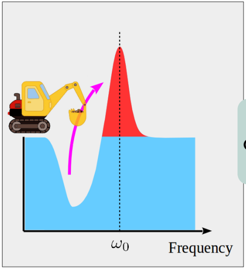

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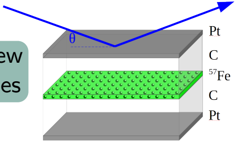
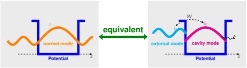
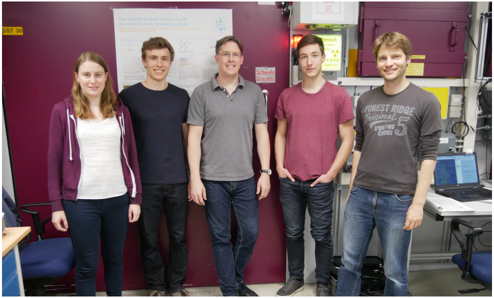


today

Understand fundamentals





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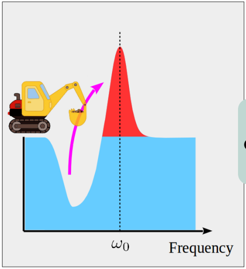

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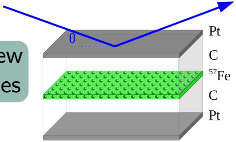

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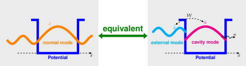

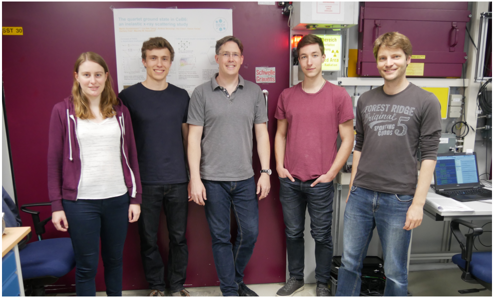

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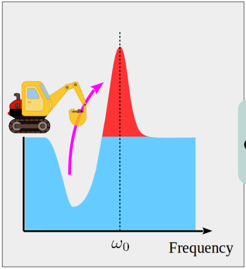

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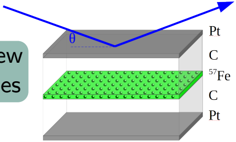

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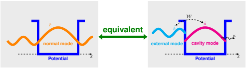
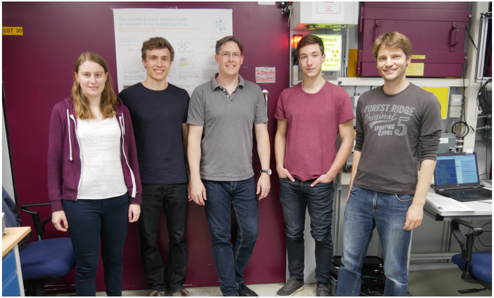




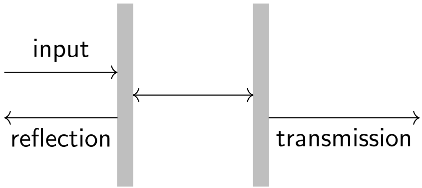
Light-matter interactions

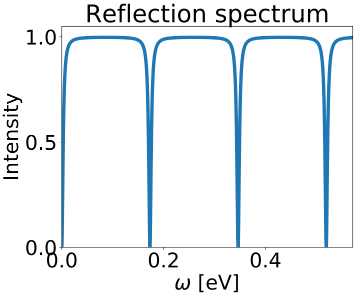
Cavity QED, Circuit QED

...

Transport theory

Example: Fabry-Perot cavity





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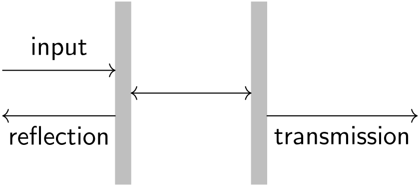

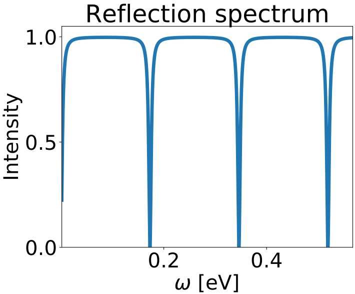

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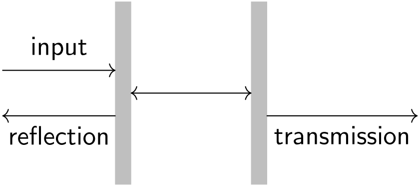

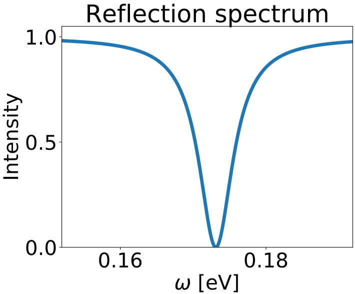

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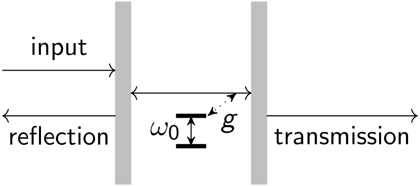

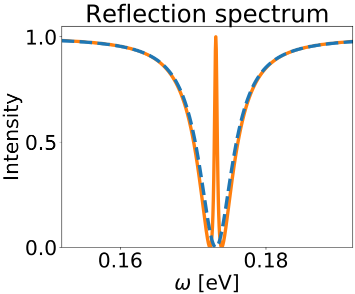

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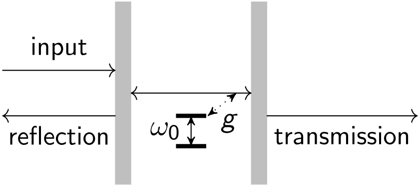
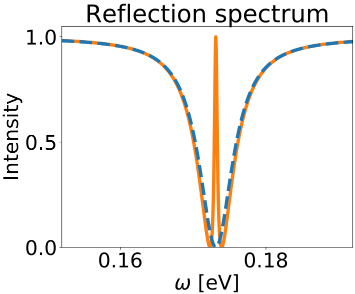
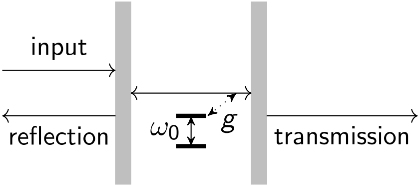
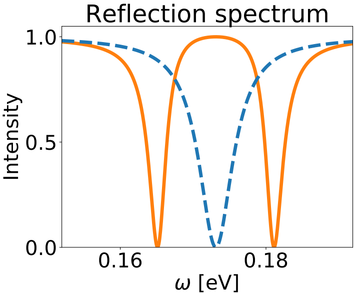




$\rightarrow$ Weak coupling: Purcell effect

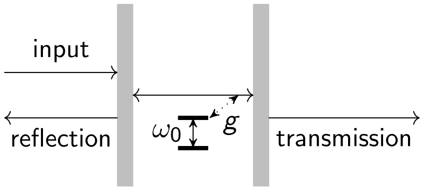
Example: Fabry-Perot cavity

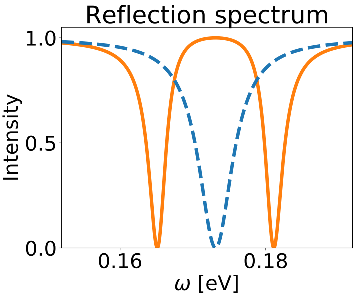




$\rightarrow$ Strong coupling: Vacuum Rabi-splitting

Example: Fabry-Perot cavity

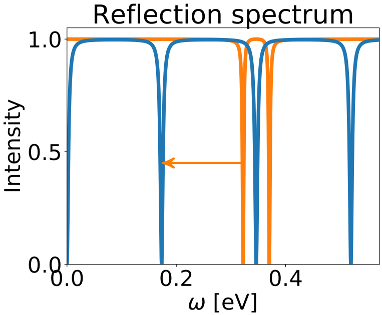




$\Rightarrow$ Enhance and control light-matter interactions!

Extreme regimes

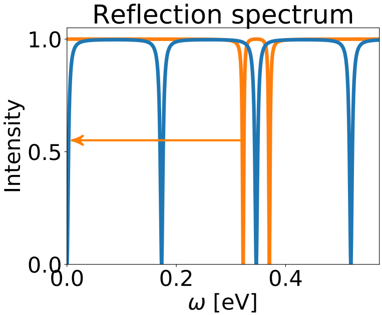
- Multi-mode strong coupling



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

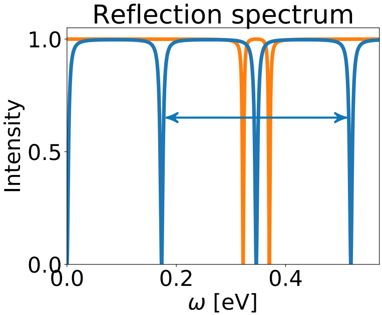
- Multi-mode strong coupling
- Ultra-strong coupling
- Deep-strong coupling



Recent reviews:
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)
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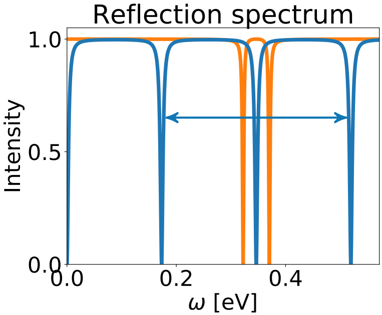
I. Rotter *J. Phys. A: Mathematical and Theoretical* **45**, 15 (2009)
Heeg et al. *Phys. Rev. Lett.* **114**, 207401 (2015)
. . . and many more . . .

Extreme regimes

- Multi-mode strong coupling
- Ultra-strong coupling
- Deep-strong coupling
- **Overlapping modes**
  - Exceptional points
  - Petermann factor
  - Photonic Fano interference
  - ...



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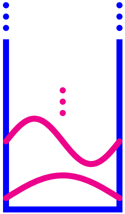
From closed to open boxes



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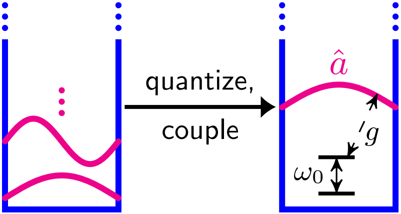

Jaynes-Cummings model

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

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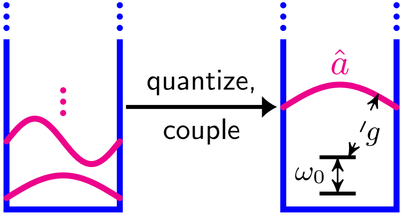

- discrete eigenstates
- closed system
  - × no leakage
  - × no driving
  - × no scattering
  - × no external detection

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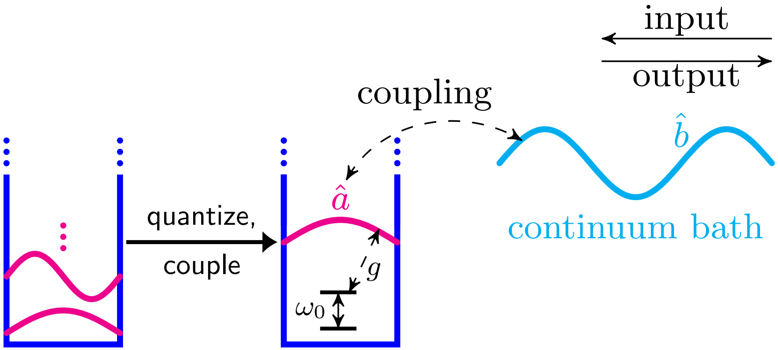

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Input-output theory

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

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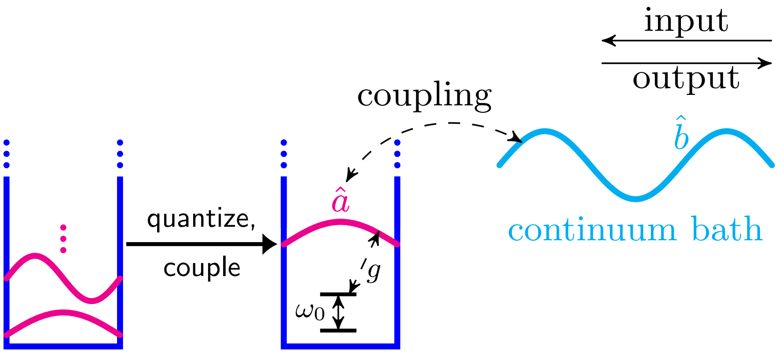

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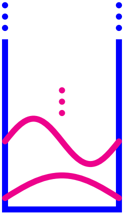
$\rightarrow$ **few-mode concept**

$\rightarrow$ **scattering**

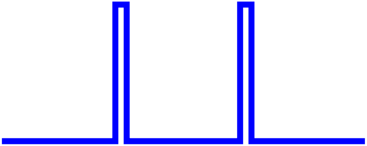
$\Rightarrow$ **Big tool box for quantum optics!**

From closed to open boxes



open system

- ✓ leakage
- ✓ driving
- ✓ scattering



From closed to open boxes

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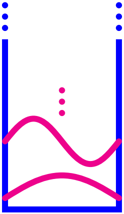
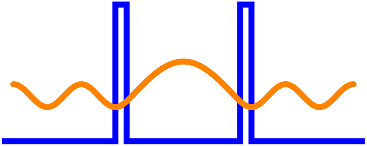
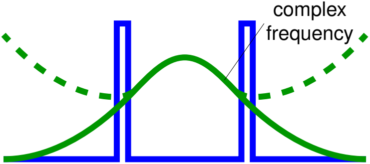




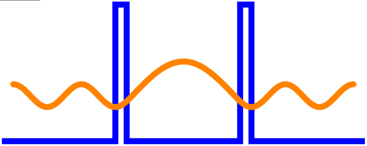
continuum eigenstates

☹ few-mode concept is lost

From closed to open boxes



resonant modes



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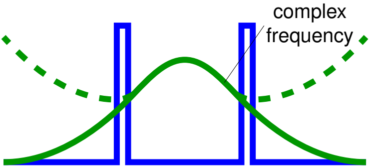

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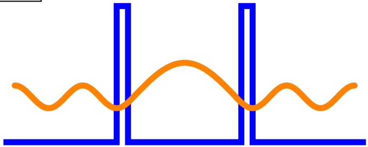

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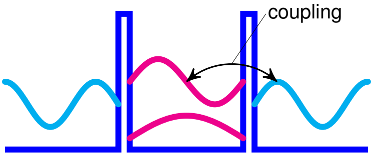

few-mode + bath

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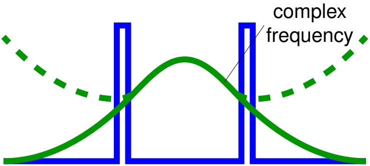

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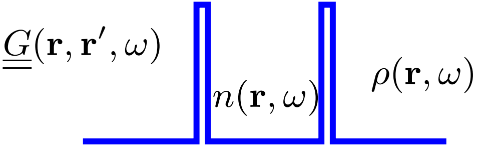
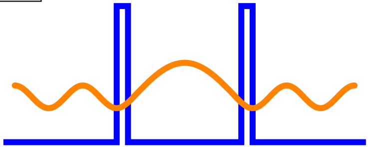


Green fns, LDOS, lin. disp. theory



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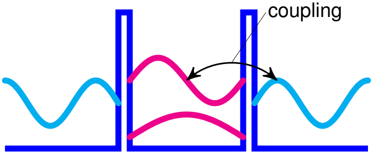

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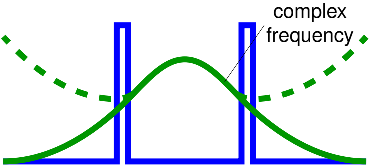

resonant modes

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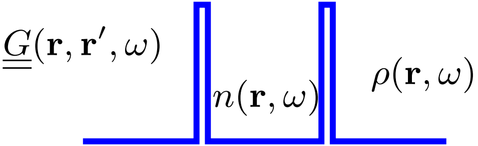

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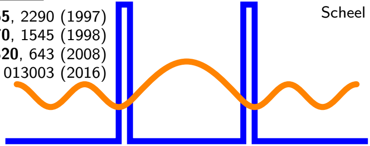

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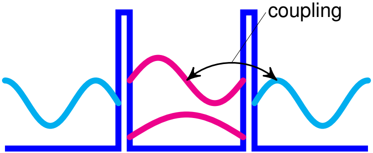

few-mode + bath

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

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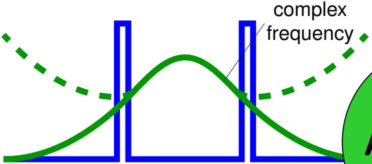

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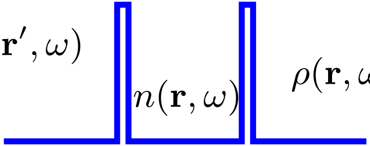
Ab initio

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



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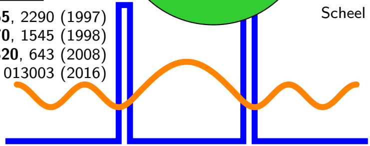

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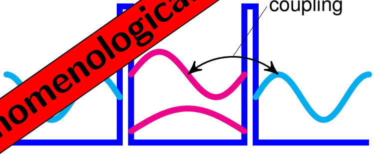
Glauber & Lewenstein *Phys. Rev. A* **43**, 467 (1991)

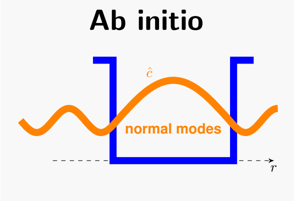
Phenomenological

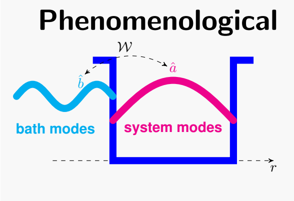


few-mode + bath

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

Few-mode models in cavity QED





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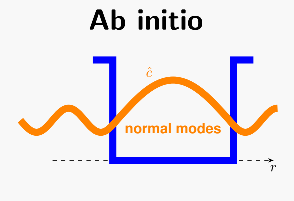
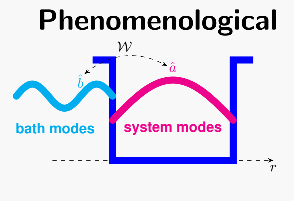




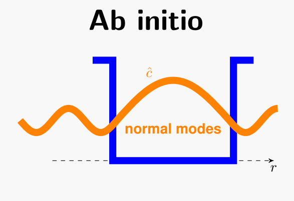
e.g. Canonical Hamiltonian

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

$\rightarrow$ **Ab initio quantization**[1]

[1] Glauber & Lewenstein, *Phys. Rev. A* **43**, 467 (1991)

Few-mode models in cavity QED



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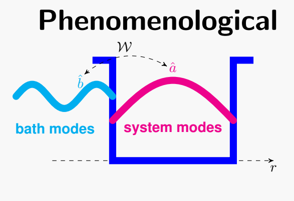


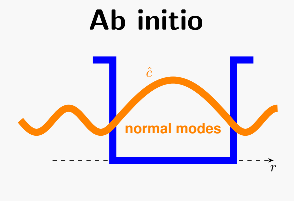
Few-mode system-bath Hamiltonian

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

$\rightarrow$ **Input-output model**[2]

[1] Glauber & Lewenstein, *Phys. Rev. A* **43**, 467 (1991)
[2] 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
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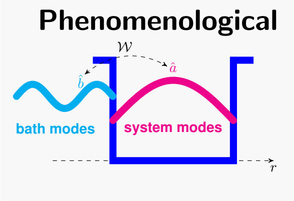

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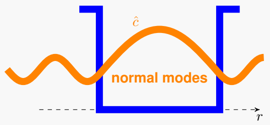
Few-mode models in cavity QED

Ab initio



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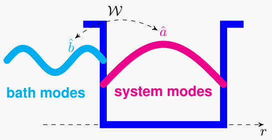

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- ☺ Huge toolbox available
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- ?! Useful in extreme regimes?

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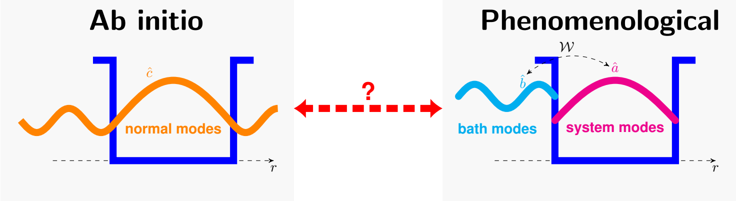
Few-mode models in cavity QED



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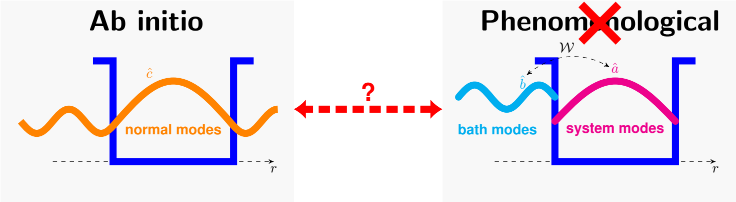
Few-mode models in cavity QED



How to make

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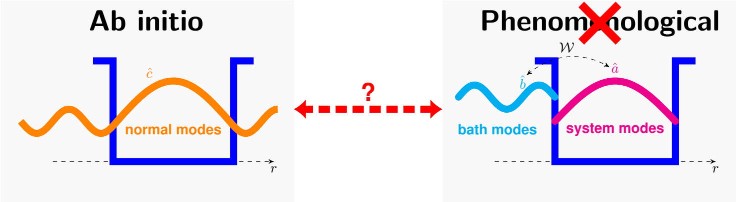
and

- **input-output**

ab initio?

?

Few-mode models in cavity QED



How to make

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and

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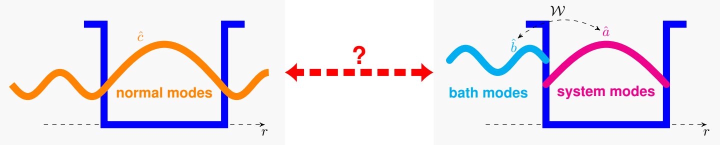
?

⇒ Ab initio few-mode theory

Ab initio few-mode Hamiltonians



Canonical Hamiltonian

Few-mode Hamiltonian

[1] Viviescas & Hackenbroich, *Phys. Rev. A* **67**, 013805 (2003)
Dalton, Barnett, Garraway *Phys. Rev. A* **64**, 053813 (2001)

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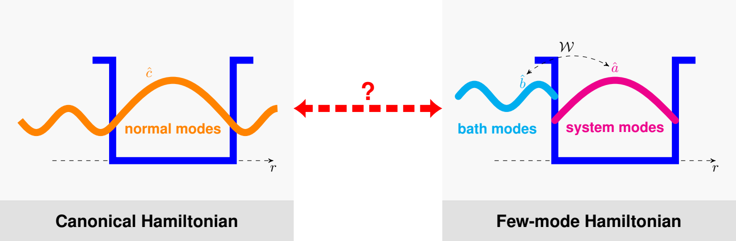
[3] DL & J. Evers, *submitted* arXiv:1812.08556 [quant-ph]

Ab initio few-mode Hamiltonians



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

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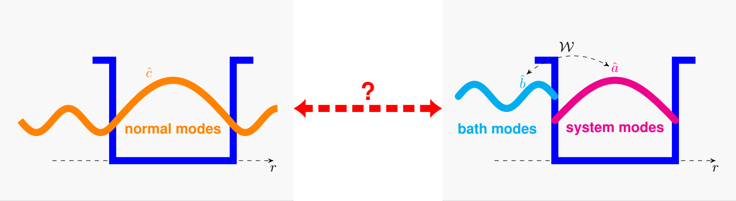
Ab initio few-mode Hamiltonians



Canonical Hamiltonian | **Few-mode Hamiltonian**

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

$\Rightarrow$ select resonant states[2] as few-mode basis[3]

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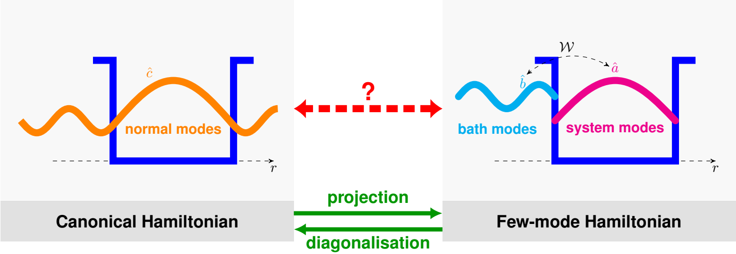
Ab initio few-mode Hamiltonians



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

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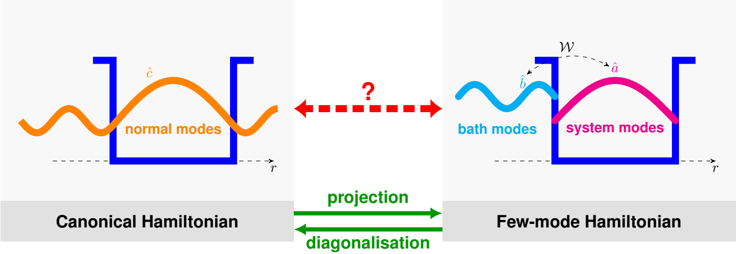
Few-mode scattering



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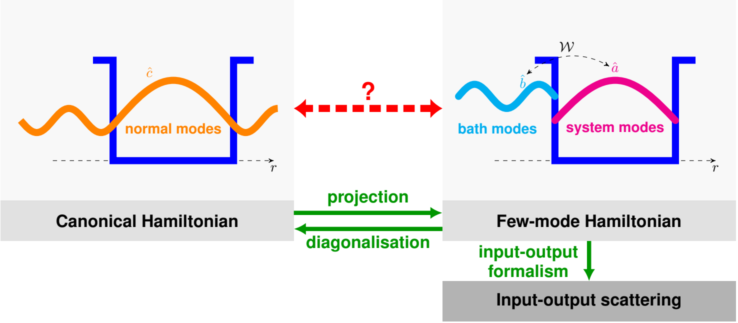

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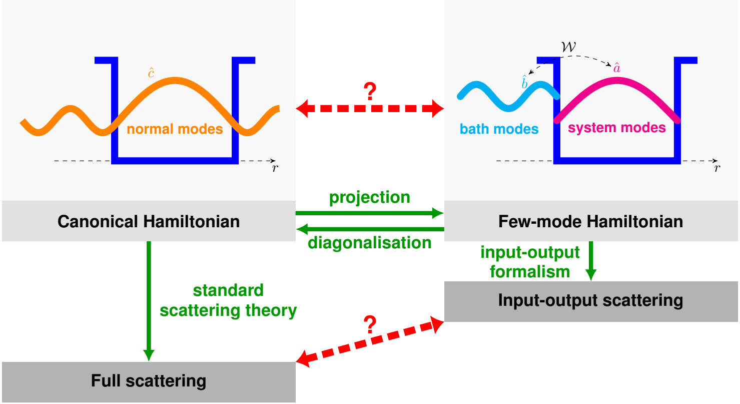

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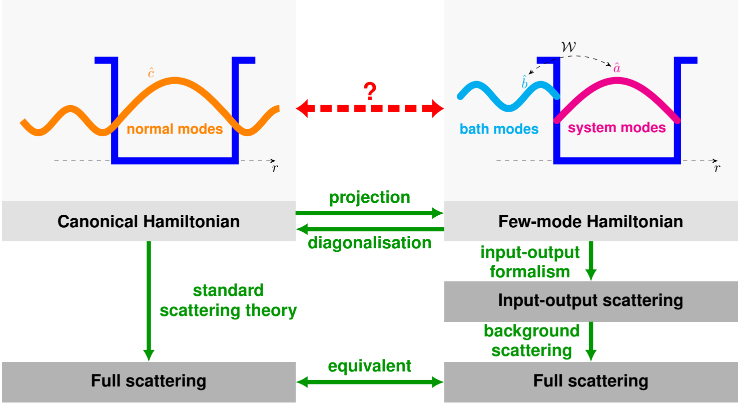
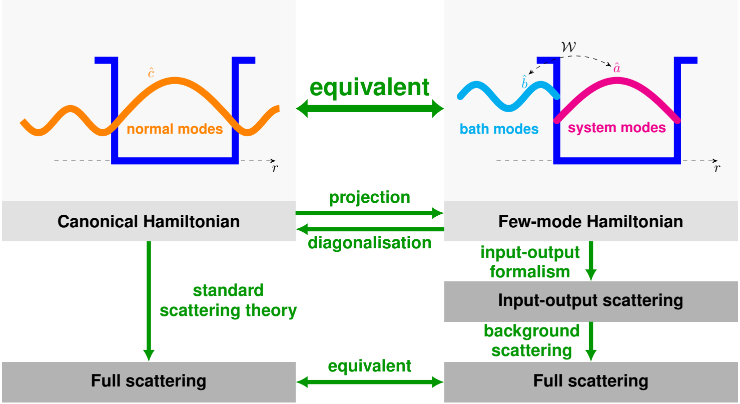


$$\boxed{S = S_{\mathrm{bg}} S_{\mathrm{io}}}$$

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

Few-mode scattering



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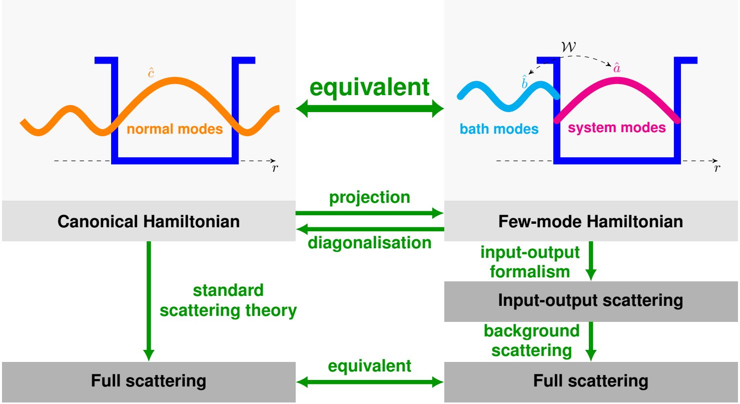

$$\boxed{S = S_{\mathrm{bg}} S_{\mathrm{io}}}$$

$\Rightarrow$ Few-mode theory is not limited to the good cavity regime!

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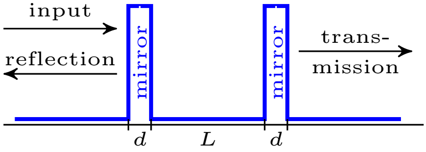
Illustrative example

Example: Two-sided Fabry-Perot cavity



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

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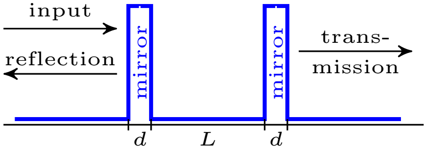

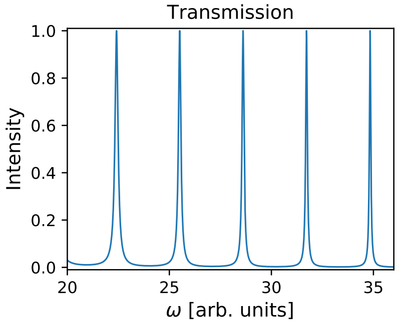

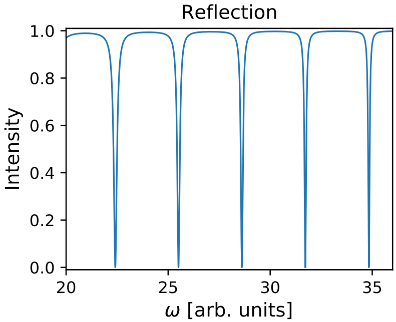

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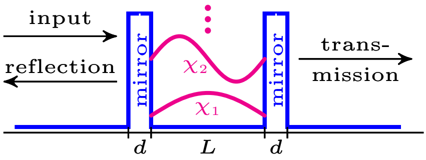

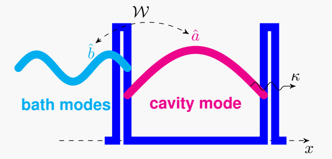

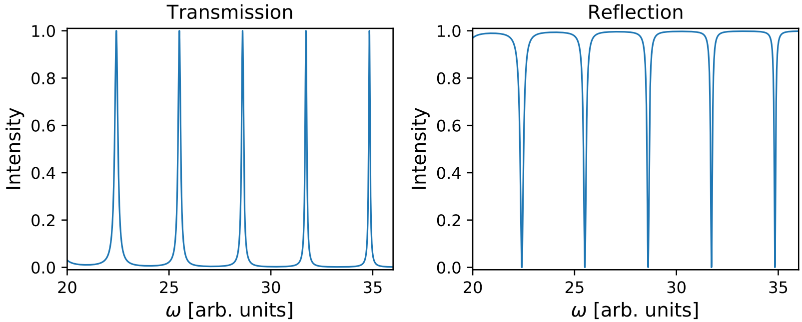

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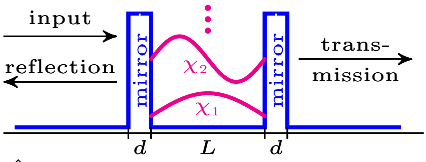

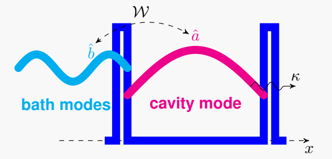

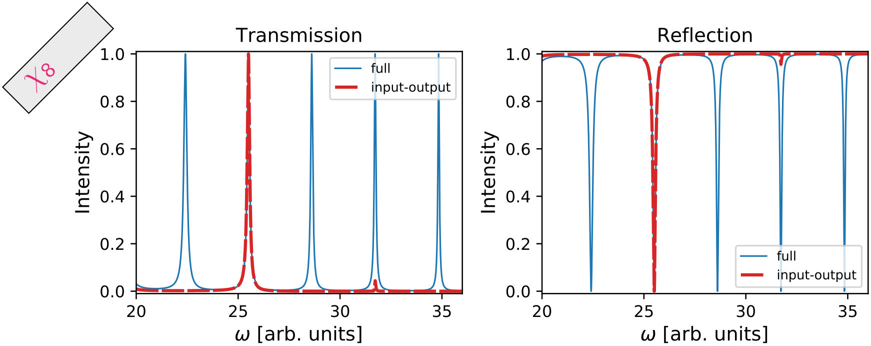

$\Rightarrow$ ab initio, not a fit!

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

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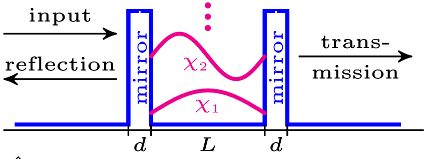
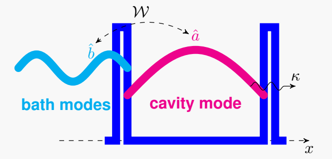
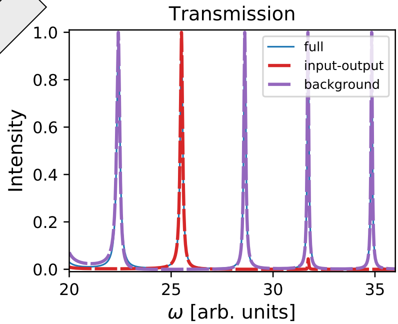
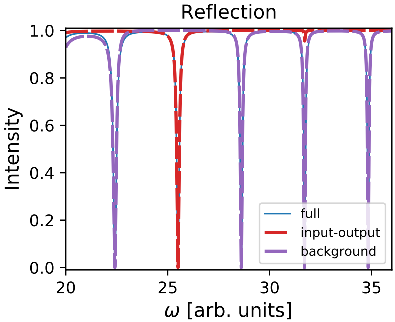




χ_8





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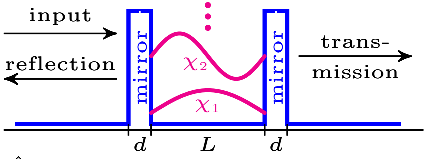
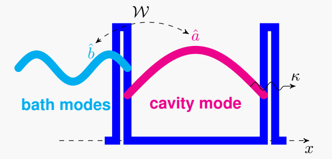
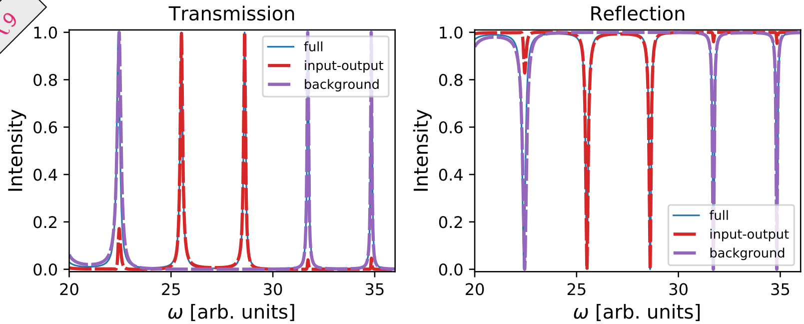




χ_8, χ_9



$\Rightarrow$ extract resonant dynamics

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

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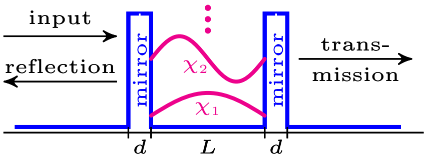

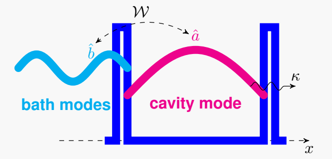

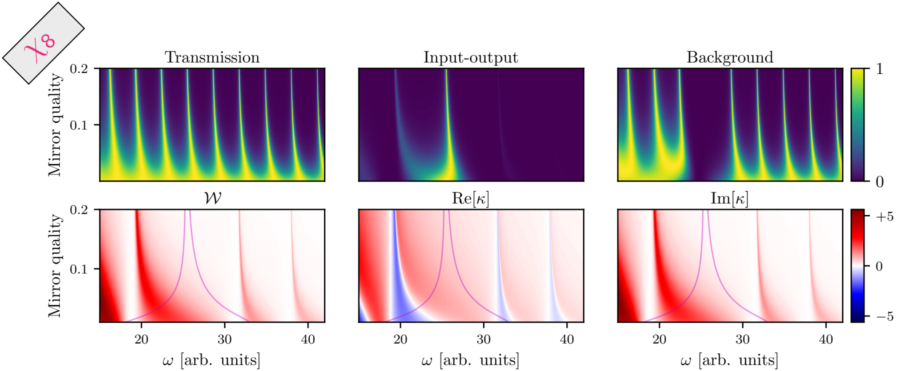

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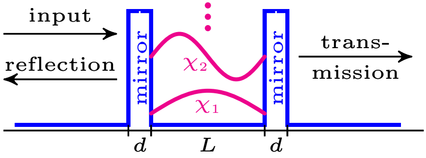
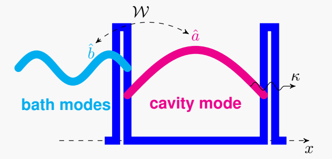
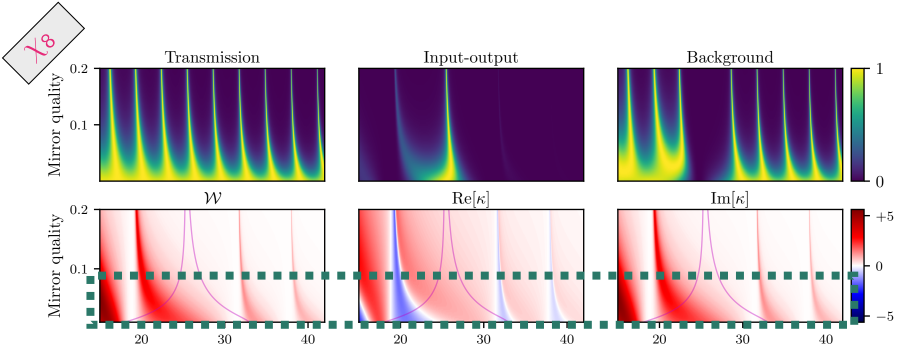


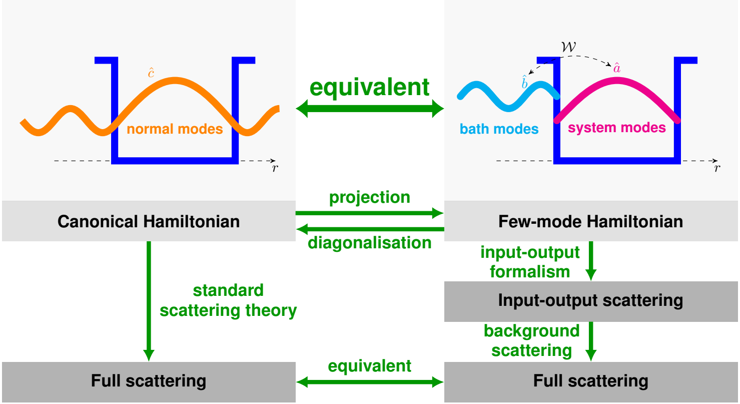




Strong frequency dependence!

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

Advantages (so far)



Exact few-mode theory for the empty cavity!

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

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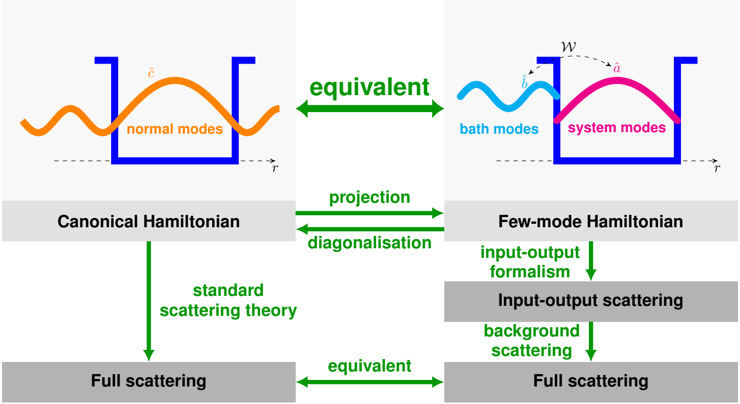
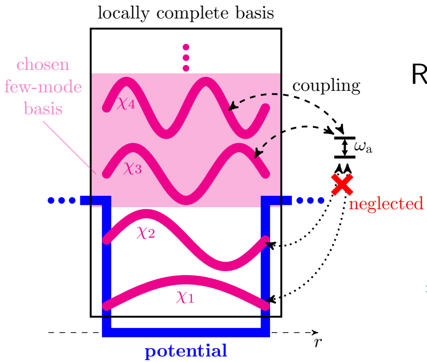


Exact few-mode theory for the empty cavity!

But what about field-matter interactions?

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

Effective few-mode expansions



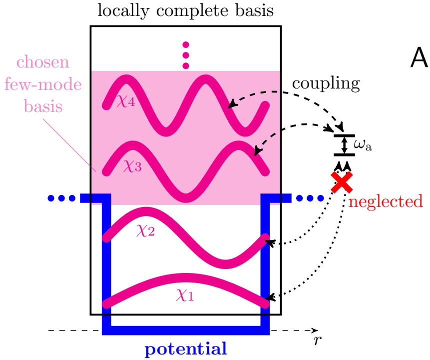
Recipe:

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

$\Rightarrow$ **Expansion scheme!**

DL & J. Evers, *submitted*

Effective few-mode expansions

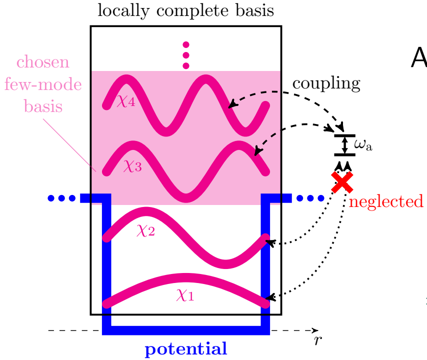


Advantages of ab initio few-mode theory

- Empty cavity treated *exactly*
  - ⇒ Approximate interaction only
  - ⇒ Disentangle approximations
- Connects to existing toolbox
- New extreme regimes accessible

DL & J. Evers, *submitted*

Effective few-mode expansions



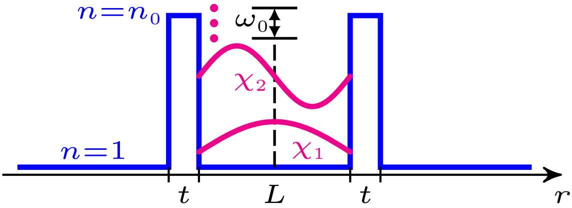
Advantages of ab initio few-mode theory

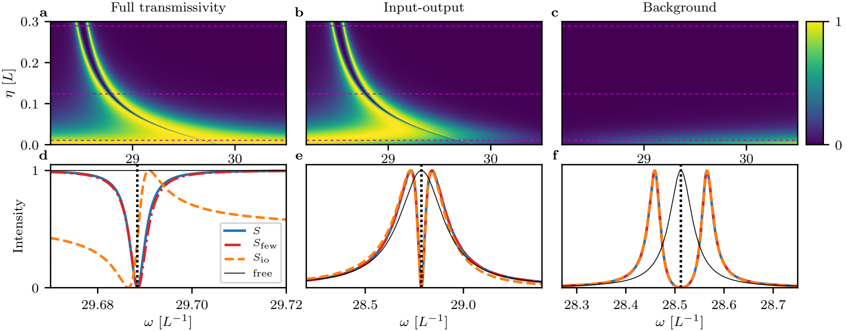
- Empty cavity treated *exactly*
  - ⇒ Approximate interaction only
  - ⇒ Disentangle approximations
- Connects to existing toolbox
- New extreme regimes accessible

⇒ **Many potential applications!**

DL & J. Evers, *submitted*

From strong coupling to free space





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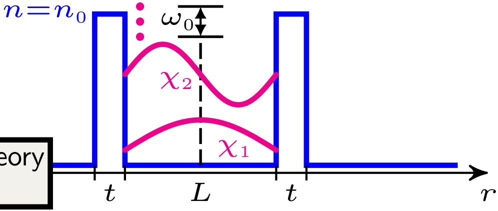
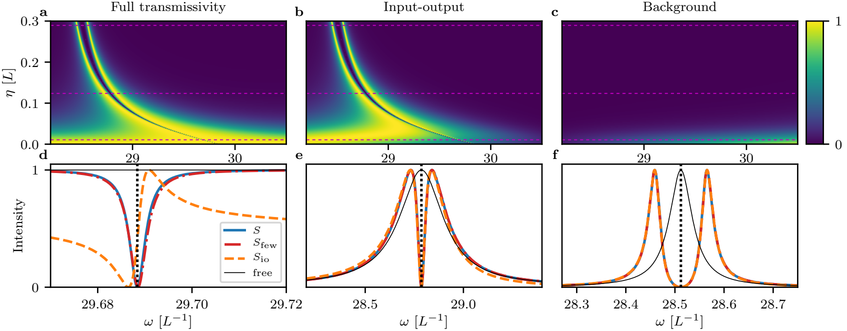


Linear dispersion theory
as benchmark!



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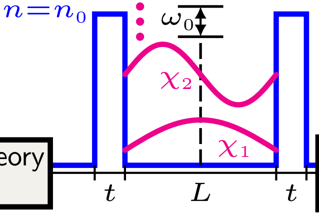
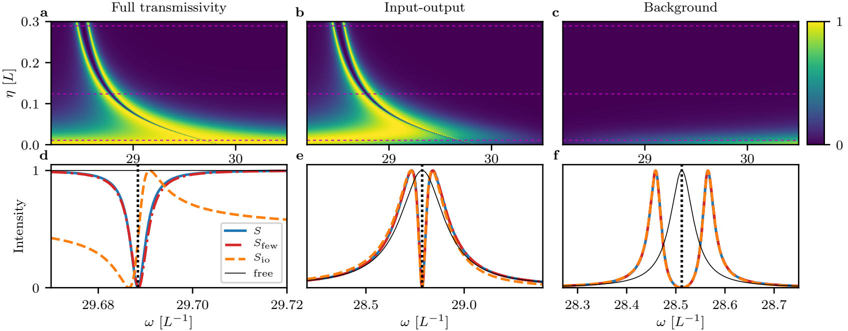


Linear dispersion theory as benchmark!

Ab initio few-mode theory captures the full range!



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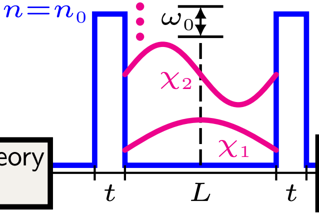

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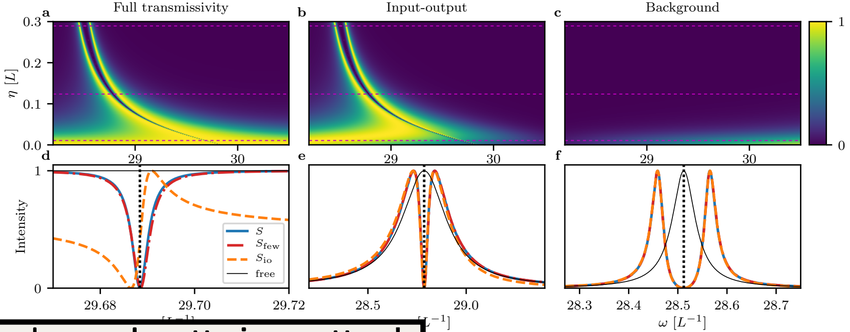
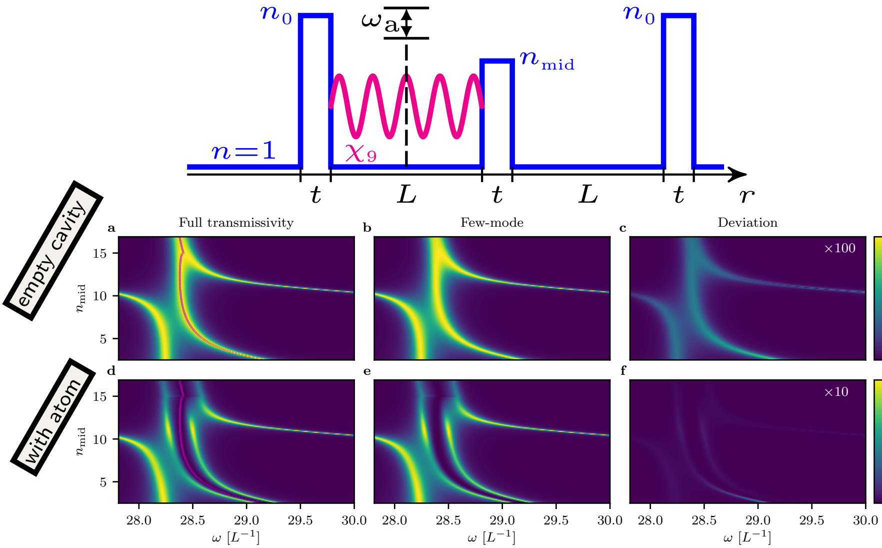


Background scattering matters!

DL & J. Evers, *submitted*

Quantum optical properties with overlapping modes



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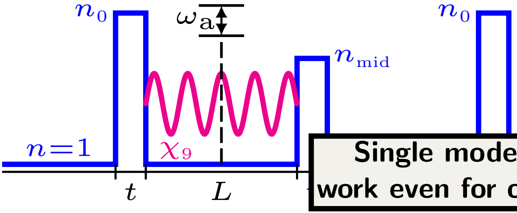
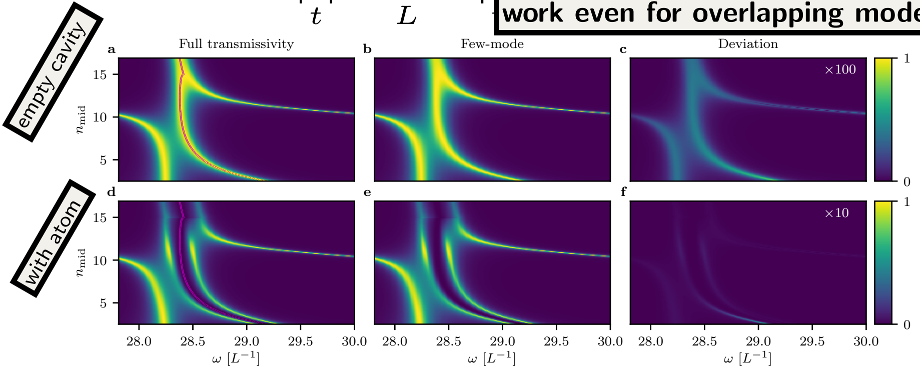


Single mode description can work even for overlapping modes!



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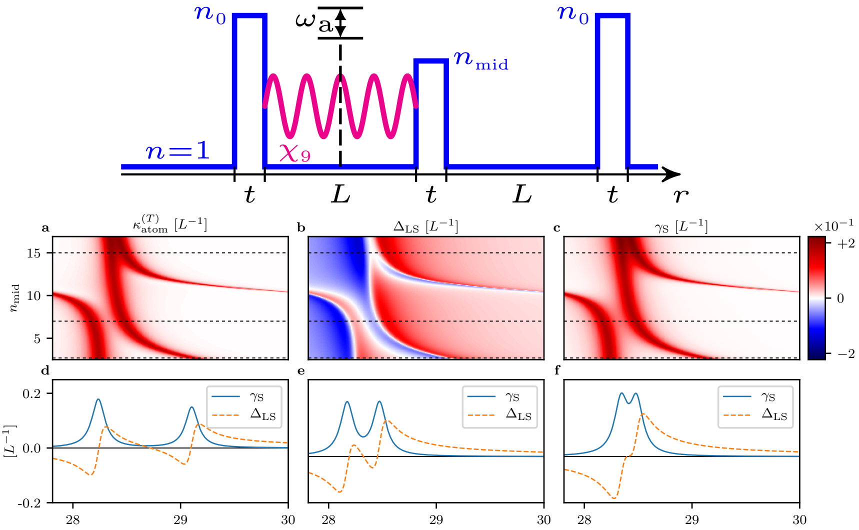

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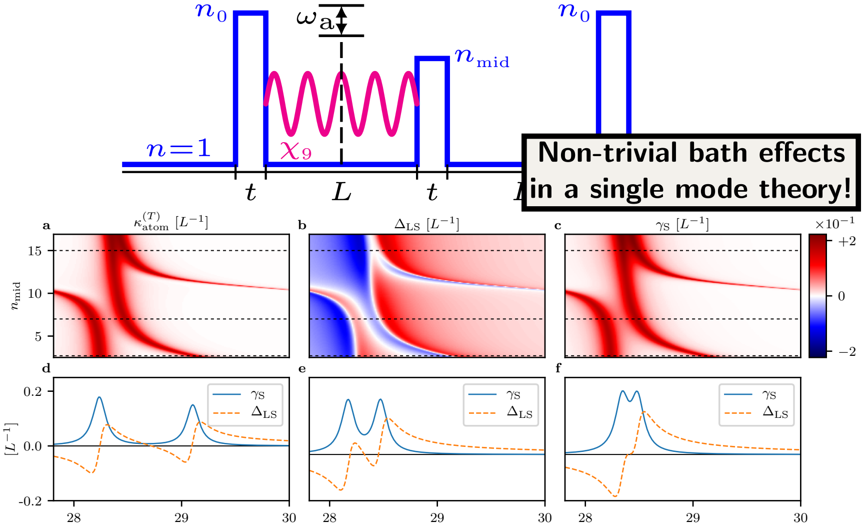

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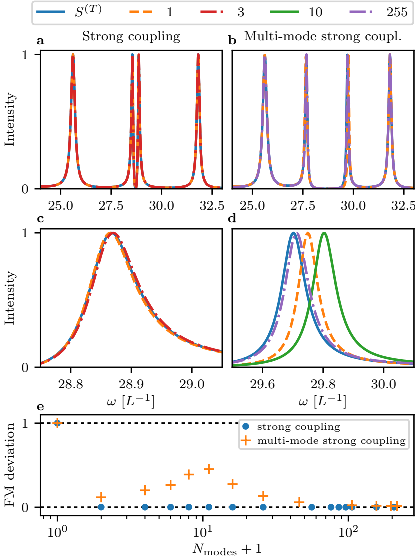
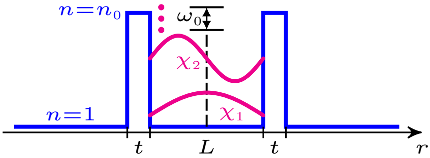
Convergence and extreme regimes





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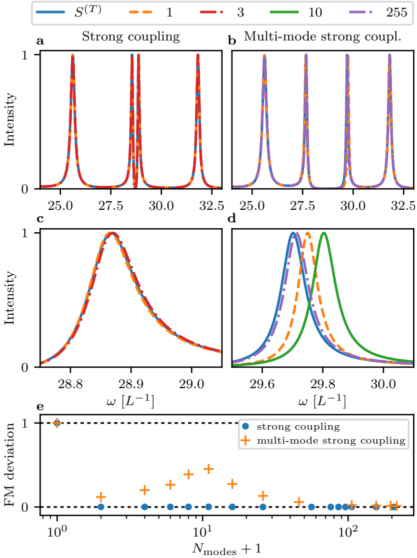
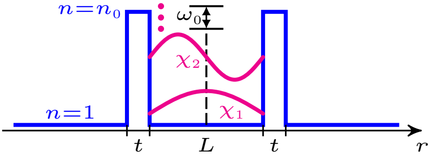


Convergence can also be shown analytically!



DL & J. Evers, *submitted*

Potential applications

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- Extreme openness, complex environments
  - Non-Hermitian photonics
  - Random lasers, complex lasers
  - Quantum plasmonics
  - X-ray and nuclear cavity QED
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- Extreme light-matter coupling
  - Open system effects in ultra-strong coupling
  - Multi-mode strong coupling
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Conclusion & Outlook

✓ Rigorous construction of few-mode Hamiltonians

✓ Scattering theory via input-output formalism

$\Rightarrow$ Empty cavity treated exactly!

✓ Converging 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 light-matter interactions

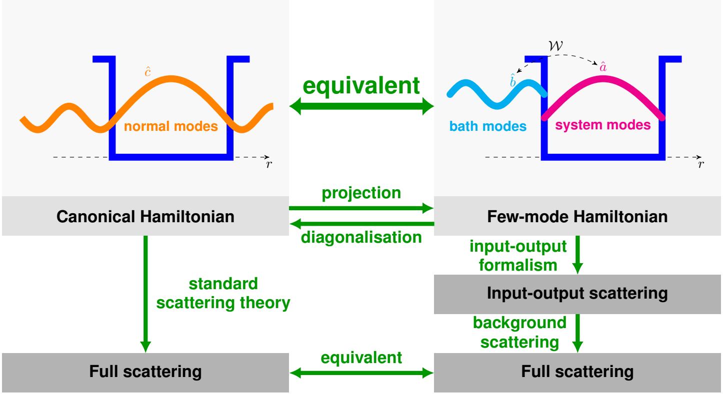
?? Applications in general quantum scattering and open systems theory?

Thank you for your attention!

Jörg Evers

Kilian P. Heeg

Christoph H. Keitel



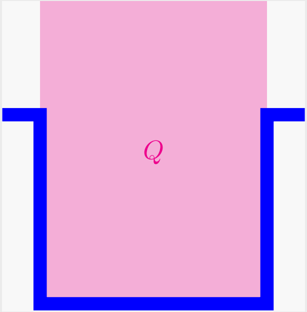
DL & J. Evers, *submitted* arXiv:1812.08556 [quant-ph]

Bonus slides

History: Relation to Viviescas & Hackenbroich

Feshbach projection operators[2,3]: P for bath, Q for system

Viviescas & Hackenbroich[1]:



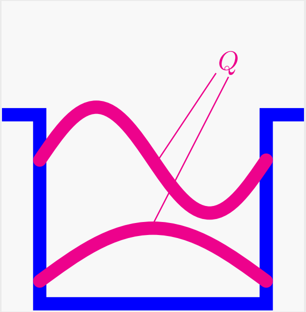
⇒ space projection

⇒ infinitely many modes

⇒ infinities for scattering

⇒ how to use as a tool?

Our approach[4]:



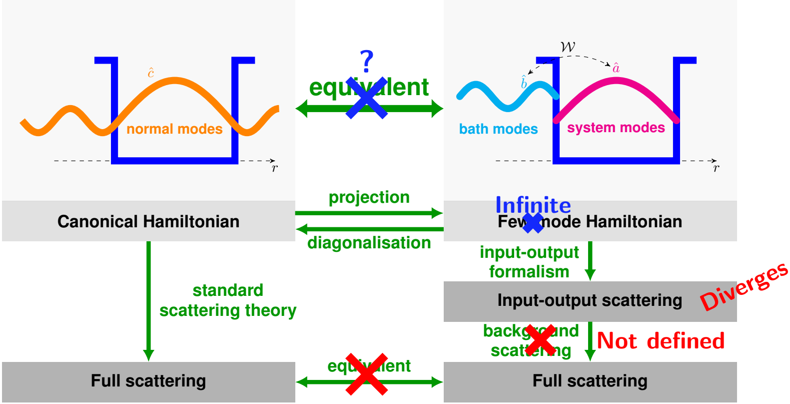
⇒ state projection

⇒ choice of modes

⇒ few-mode Hamiltonian ☺

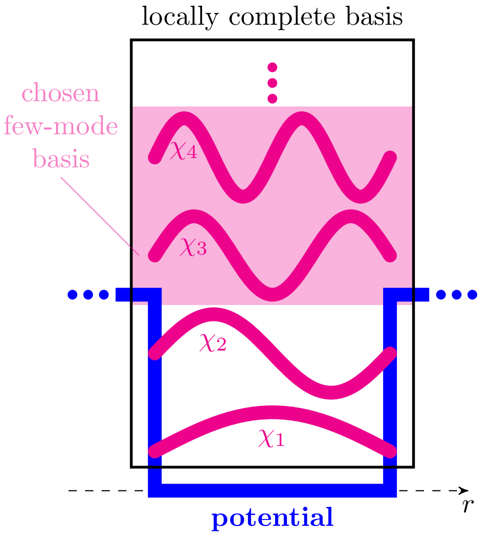
⇒ no infinities, no cutoffs ☺

Scattering in Viviescas & Hackenbroich2003

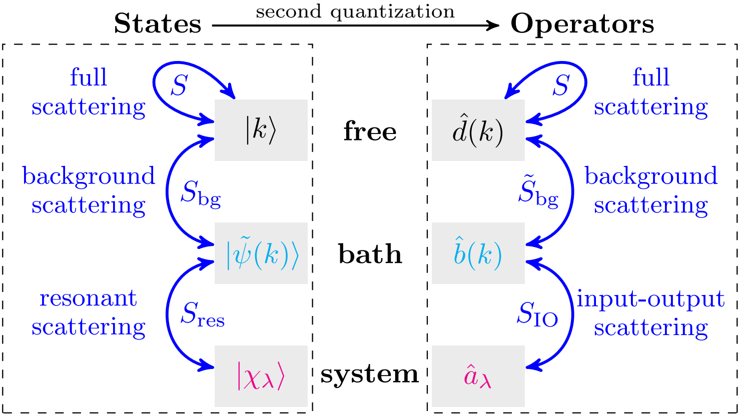


$\Rightarrow$ Get a system-bath Hamiltonian, but how to calculate scattering properties? How to extract relevant modes?

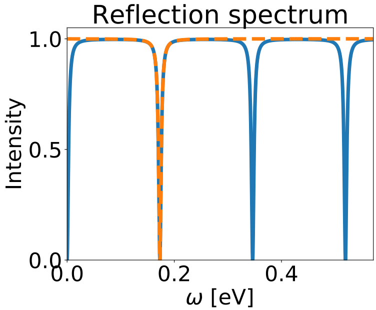
Choosing relevant modes systematically

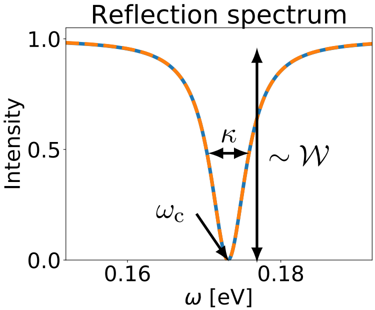


Few-mode scattering theory



Parameters in phenomenological models





$\rightarrow$ Fit Lorentzian to spectrum

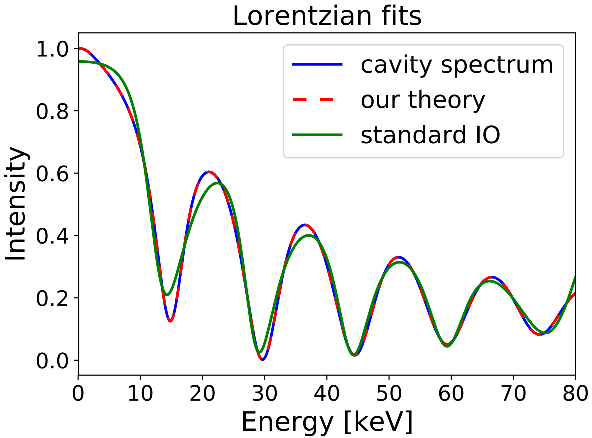
$\rightarrow$ Extract resonance parameters

$\rightarrow$ Model Hamiltonian?

Gardiner & Zoller *Quantum Noise* (1999)

Carmichael, *Statistical Methods in Quantum Optics 1* (1999)

Beyond input-output with X-ray cavities



$\Rightarrow$ no Lorentzians

$\Rightarrow$ beyond input-output models

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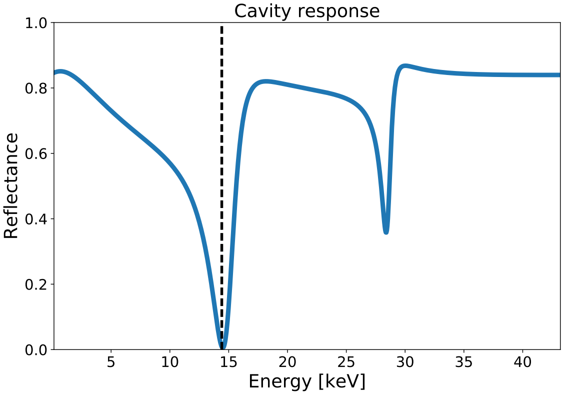

$\Rightarrow$ no Lorentzians

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Linear dispersion theory

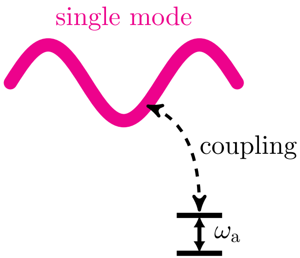
Lorentz-Lorenz formula, Clausius-Mossotti relation and others...
Summary: Basic assumption $\hat{\sigma}^- \approx -1$ (for 2-level system)

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

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

Standard references: Born & Wolf *Principles of optics* (1980)
Zhu et al. *Phys. Rev. Lett.* **64**, 2499 (1990)
X-ray: Röhlsberger *Nuclear condensed matter physics*(2004)
Ultra-strong: Malekakhlagh et al. *Phys. Rev. A* **94**, 063848 (2016)

Few-mode models in quantum optics



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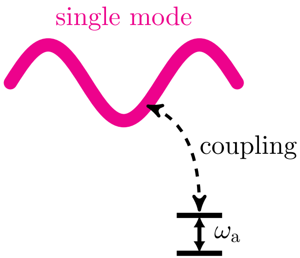

Jaynes-Cummings model

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

Jaynes & Cummings, *Proc. IEEE* **51**, 89 (1963)

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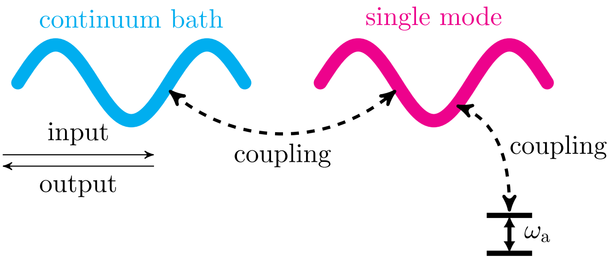

Input-output formalism

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

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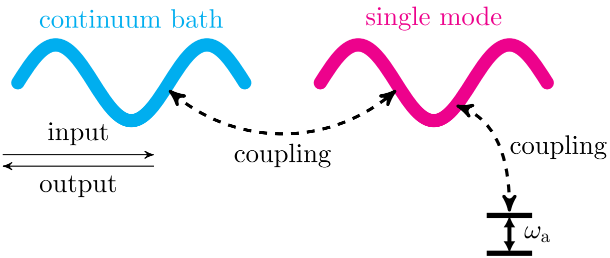

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$\Rightarrow$ **Big tool box!**

Gardiner & Collett, *Phys. Rev. A* **31**, 3761 (1985)

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Input-output methods in general scattering theory?

$$\boxed{\text{Cavity QED: } -\nabla \times \nabla \times \mathbf{A} = \frac{\varepsilon(r)}{c^2}\ddot{\mathbf{A}}}$$

$$\downarrow$$

$$\boxed{\text{Schrödinger equation: } -\frac{1}{2}\nabla^2\psi + V(r)\psi = i\dot{\psi}}$$

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Example: *s*-wave scattering from tunnelling barrier[1]

[1] Domcke, *Phys. Rev. A* **28**, 2777 (1982)

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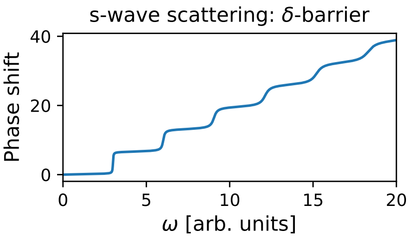

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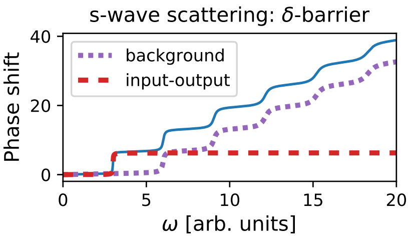

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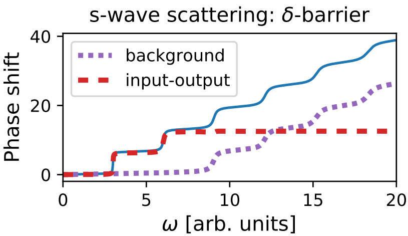

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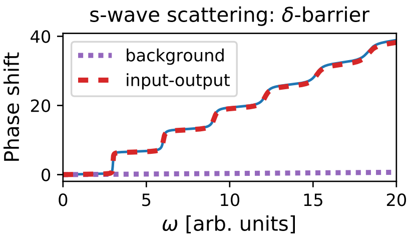

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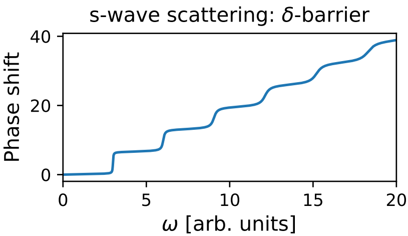

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↓

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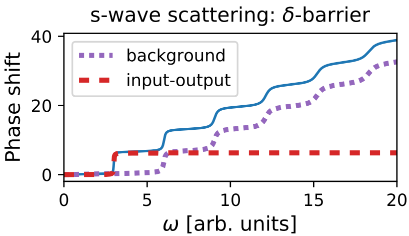
Example: *s*-wave scattering from tunnelling barrier[1]



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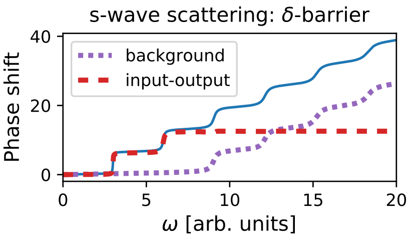

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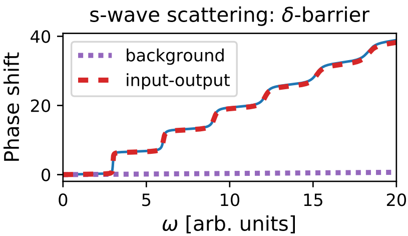

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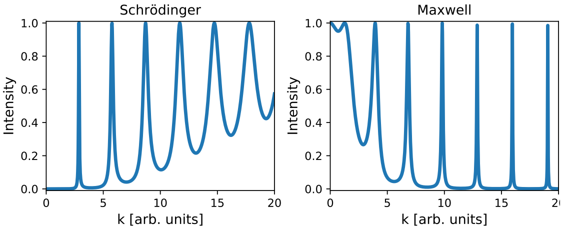

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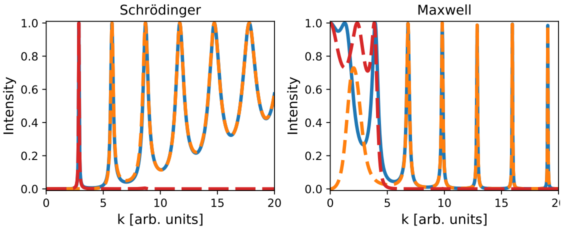

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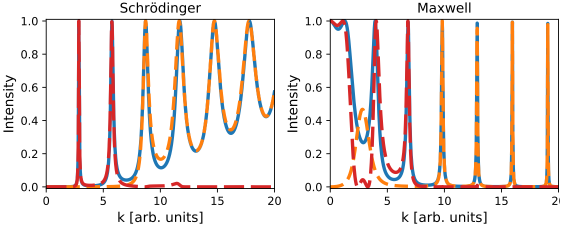

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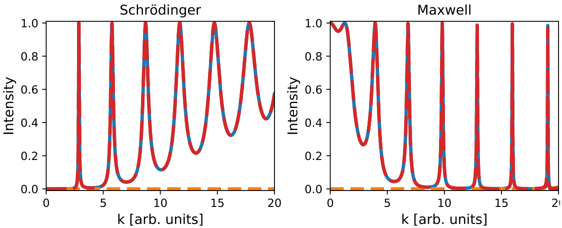

Input-output methods in general scattering theory?

Example: Schrödinger vs Maxwell Fabry-Perot

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

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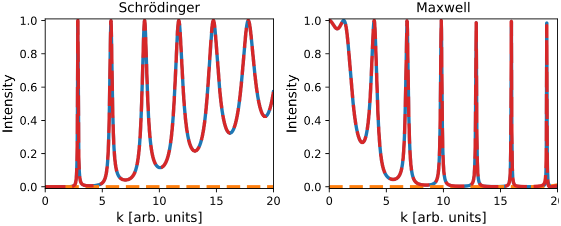

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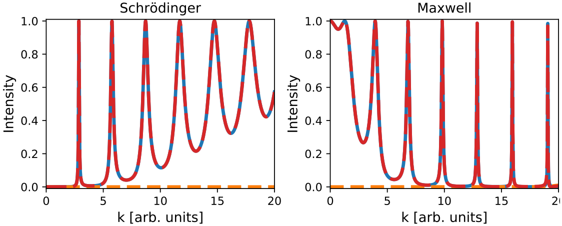

Generalized to second quantized level with interactions!

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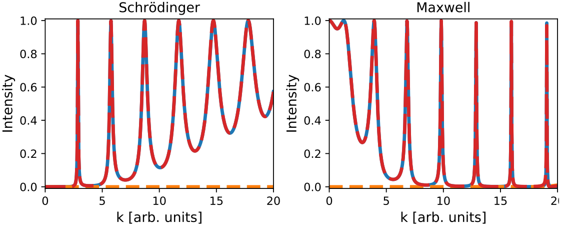

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Potential applications: quantum chemistry[1], electronic transport[2], chaotic scattering[3,4], tunneling[5], random lasers[6]...

[1] Domcke, *Phys. Rev. A* **28**, 2777 (1982)
[2] Datta, *Electronic Transport in Mesoscopic Systems* (1995)
[3] Stöckmann, *Quantum Chaos* (1999)
[4] Weidenmüller&Mitchell, *Rev. Mod. Phys.* **81**, 539 (2009)
[5] Prange, *Phys. Rev.* **131**, 1083 (1963)
[6] Türeci et al, *Science* **320**, 643 (2008)