

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



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FÜR KERNPHYSIK



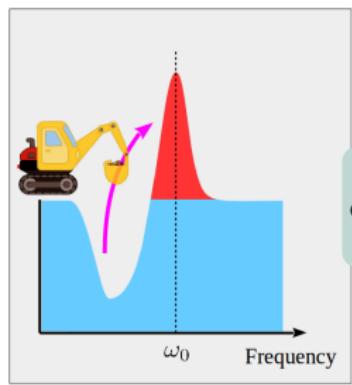
JUST TO CLEAR THINGS UP:

A FEW	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)

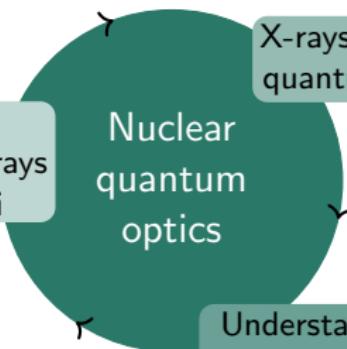
<https://xkcd.com/1070/>



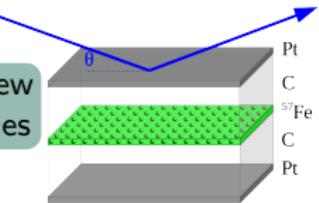
Background & Motivation



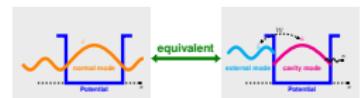
Coherent control of x-rays and nuclei



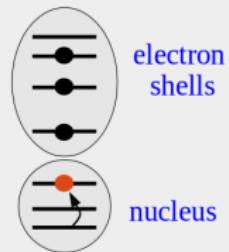
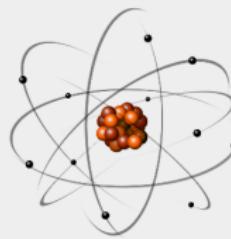
X-rays excite new quantum regimes



Understand fundamentals



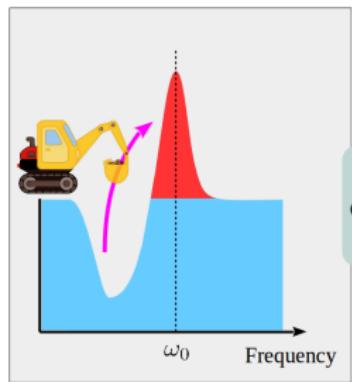
“Nuclear” quantum optics



electron shells

nucleus

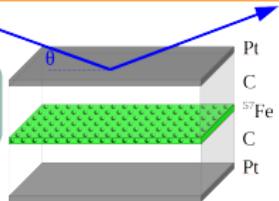
Background & Motivation



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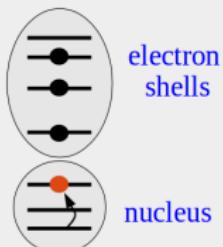
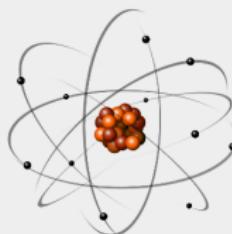


Mössbauer transitions as extreme qubits

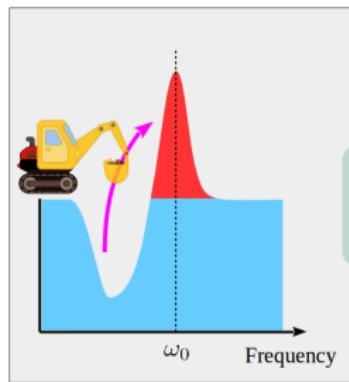
- Tiny decoherence ($Q = 10^{12}$ to 10^{24})
- Room temperature
- Solid state (no vacuum necessary)
- Large coherently interacting ensembles

Motivations: metrology, spectroscopy, . . .

“Nuclear” quantum optics



Background & Motivation

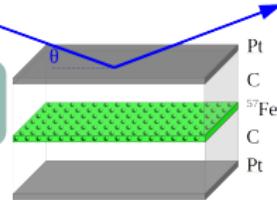


Coherent control of x-rays and nuclei

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Understand fundamentals



Mössbauer transitions as extreme qubits

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Röhlsberger et. al. *Science* **328** 5983 (2010)

Röhlsberger et. al. *Nature* **482** 7384 (2012)

Heeg & Evers *Phys. Rev. A* **88**, 043828 (2013)

Heeg et. al. *Phys. Rev. Lett.* **111** 073601 (2013)

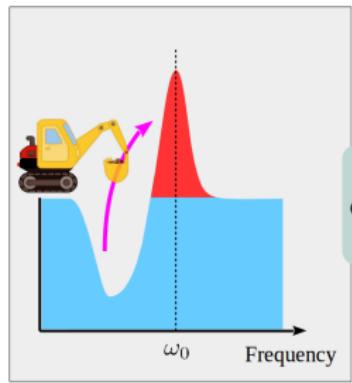
Heeg et. al. *Phys. Rev. Lett.* **114** 203601 (2015)

Heeg et. al. *Phys. Rev. Lett.* **114**, 207401 (2015)

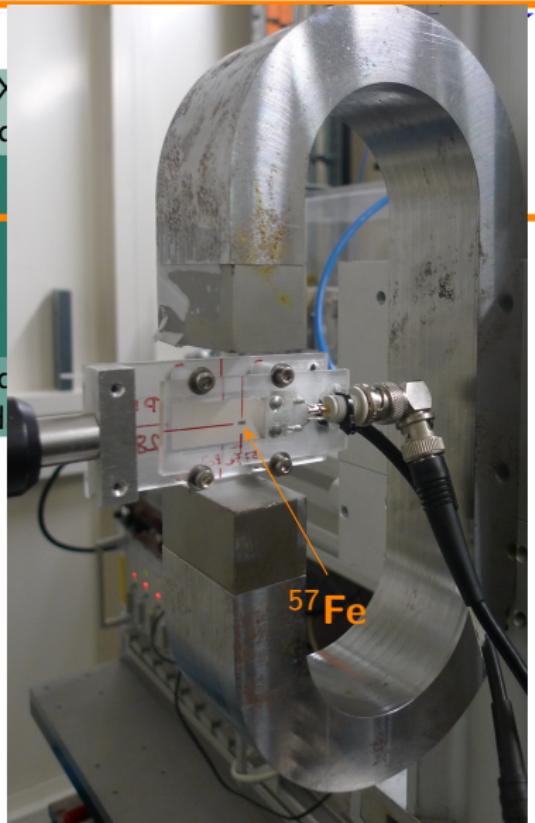
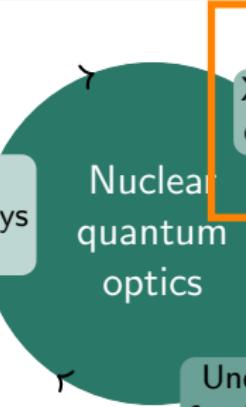
Haber et. al. *Nature Photonics* **10** 445 (2016)

Haber et. al. *Nature Photonics* **11** 720 (2017)

Background & Motivation



Coherent
control of x-rays
and nuclei

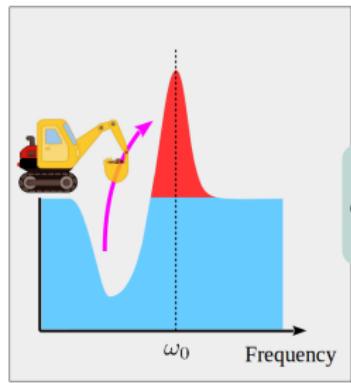


Mössbauer transitions as extreme qubits

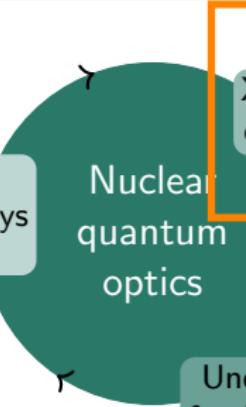
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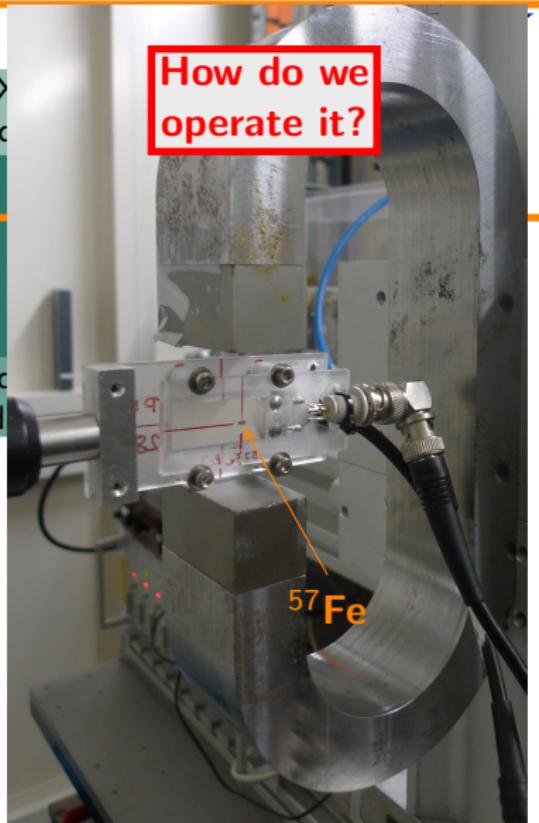
Background & Motivation



Coherent control of x-rays and nuclei



How do we operate it?

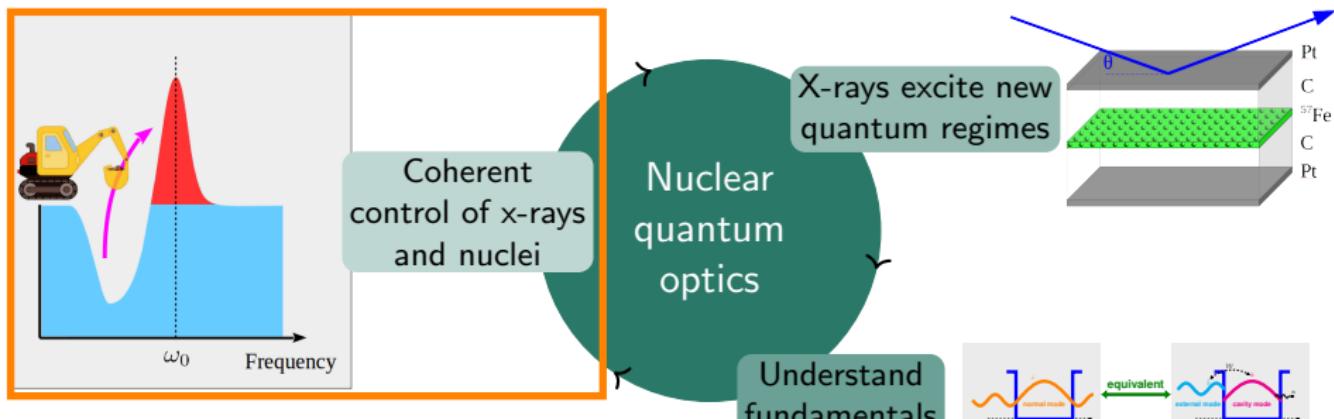


Mössbauer transitions as extreme qubits

- Tiny decoherence ($Q = 10^{12}$ to 10^{24})
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Background & Motivation



New X-ray sources

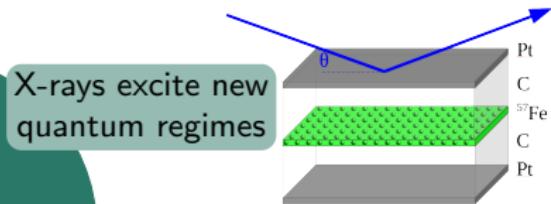
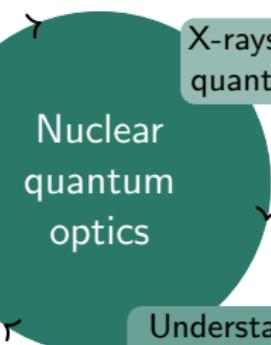
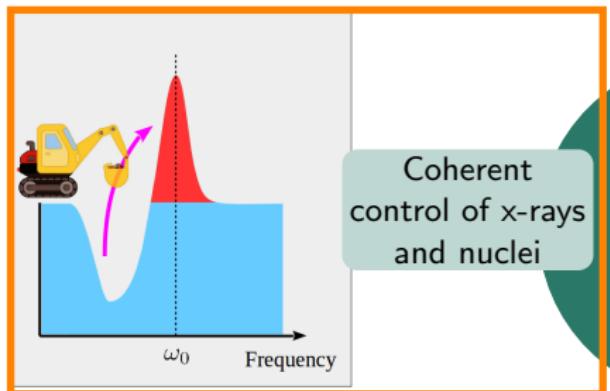
- 4th generation synchrotron
- X-ray free electron lasers
- Lab-based X-ray sources

Control techniques

- Pulse shaping
- Coherent excitation control

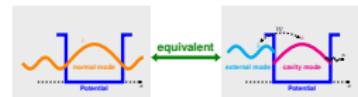
Shvyd'ko et. al. *Phys. Rev. Lett.* **77**, 3232 (1996)
 Bürenich, Evers, Keitel *Phys. Rev. Lett.* **96** 142 (2006)
 Pálffy et. al. *Phys. Rev. Lett.* **103** 017401 (2009)
 Adams et. al. *J. Mod. Opt.* **60** 2 (2013)
 Vagizov et. al. *Nature* **508**, 80 (2014)
 Heeg et. al. *Science* **357** 6349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

Background & Motivation



X-rays excite new quantum regimes

Understand fundamentals

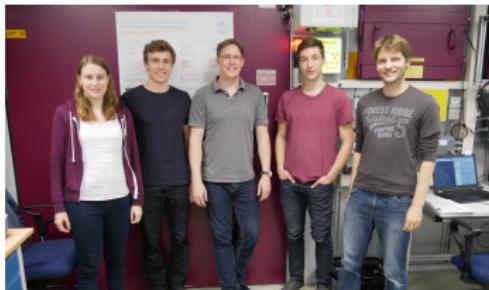


New X-ray sources

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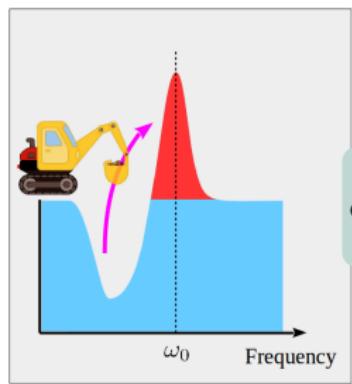
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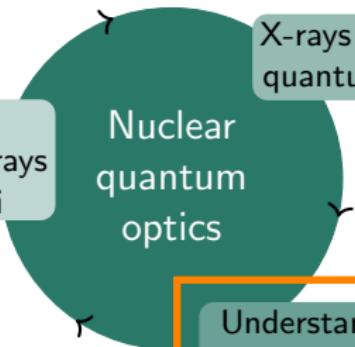


Heeg, Kaldun, Strohm, Reiser, Ott, Subramanian, DL, Haber, Wille, Goerttler, Rüffer, Keitel, Röhlsberger, Pfeifer, Evers, *Science* **357**, 375 (2017) + submitted

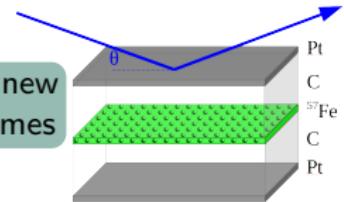
Background & Motivation



Coherent control of x-rays and nuclei



X-rays excite new quantum regimes

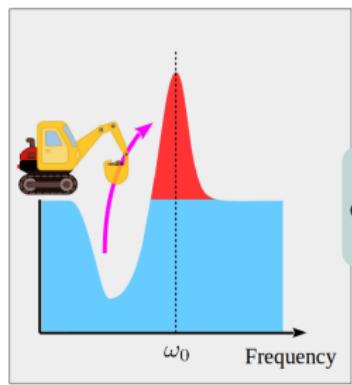


Understand fundamentals

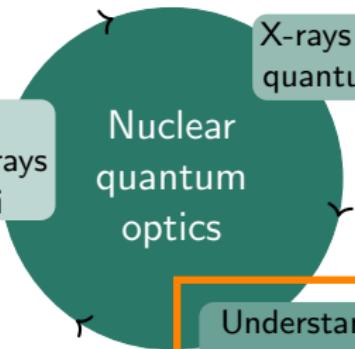


today

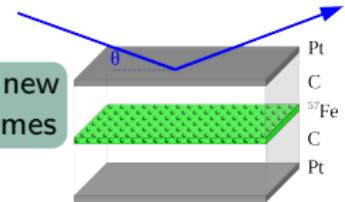
Background & Motivation



Coherent control of x-rays and nuclei



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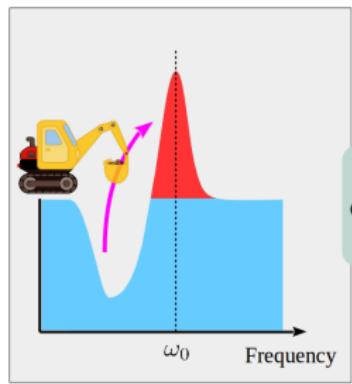
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Understand fundamentals



Extreme regimes
⇒ New theoretical challenges

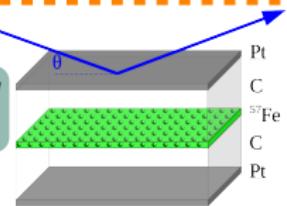
Background & Motivation



Coherent control of x-rays and nuclei

Nuclear quantum optics

X-rays excite new quantum regimes



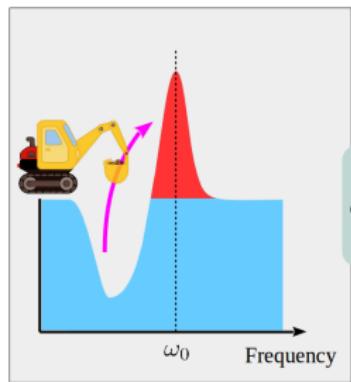
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Understand fundamentals



Extreme regimes
⇒ New theoretical challenges

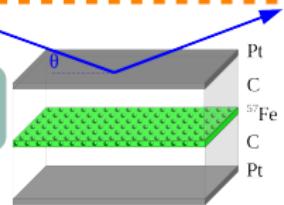
Background & Motivation



Coherent control of x-rays and nuclei

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X-rays excite new quantum regimes

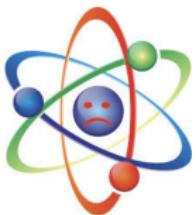


today

Understand fundamentals



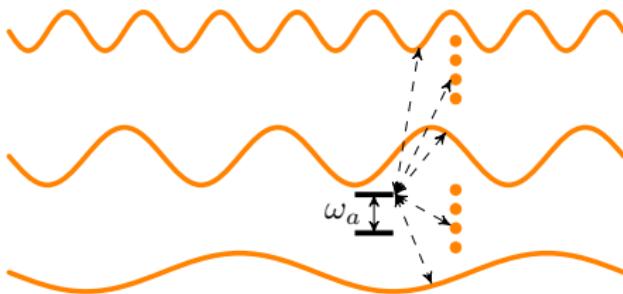
Extreme regimes
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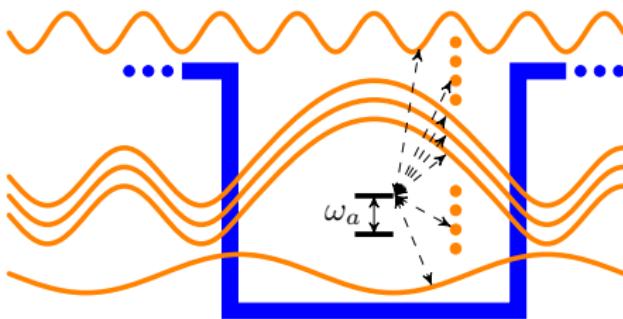
Extreme **atomic** systems

Overview

Continuum
coupling

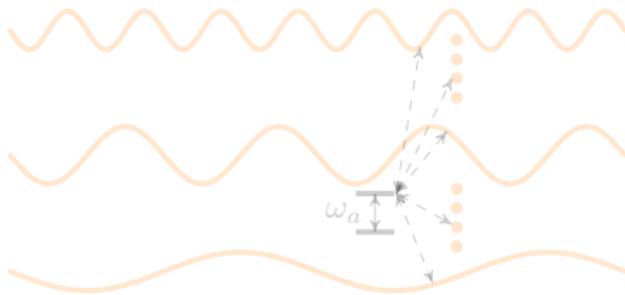


Structured continuum
featuring resonances



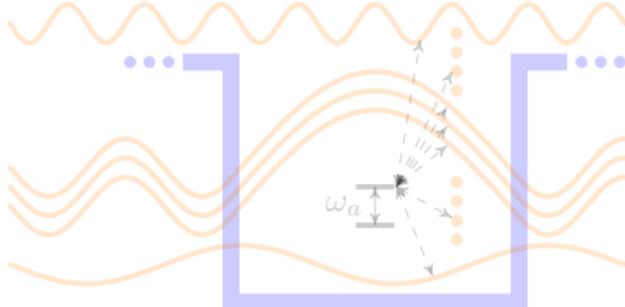
Overview

Continuum
coupling

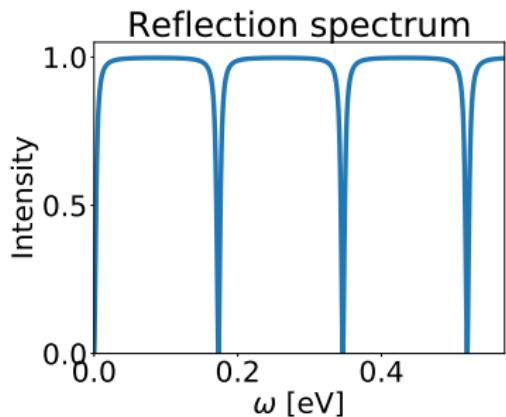
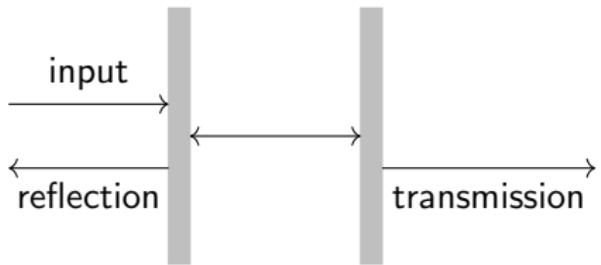


Can we extract **relevant** degrees of freedom from a continuum?

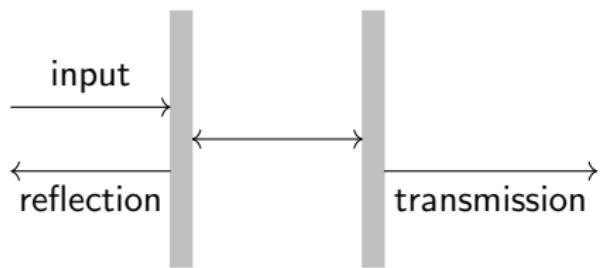
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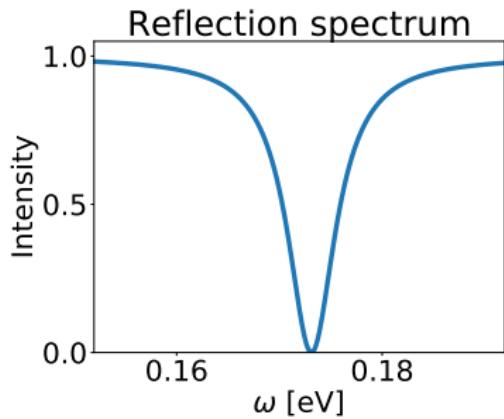
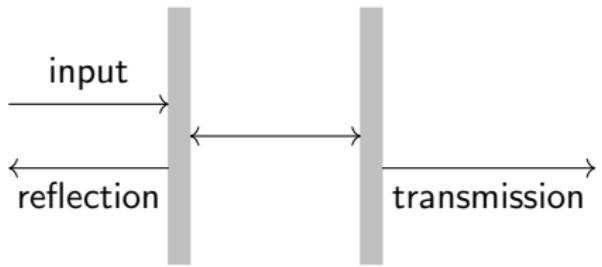
Example: Fabry-Perot cavity



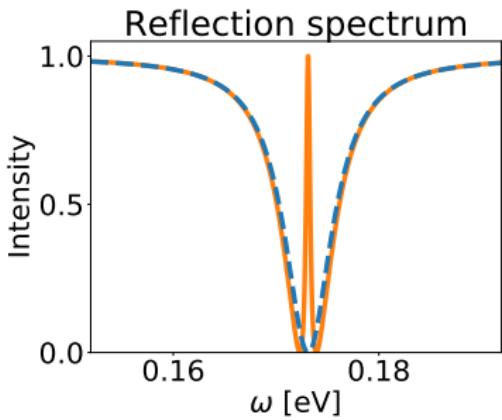
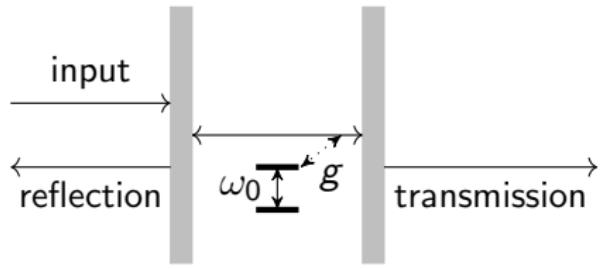
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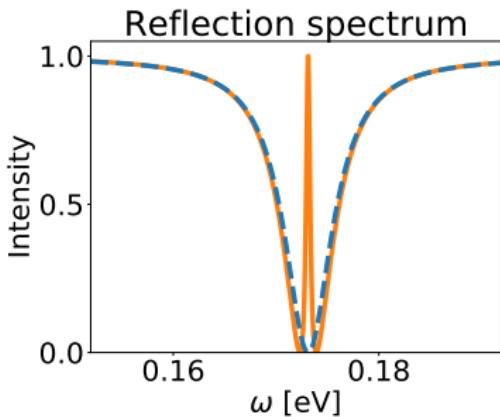
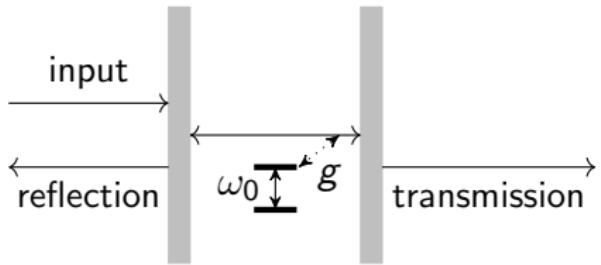
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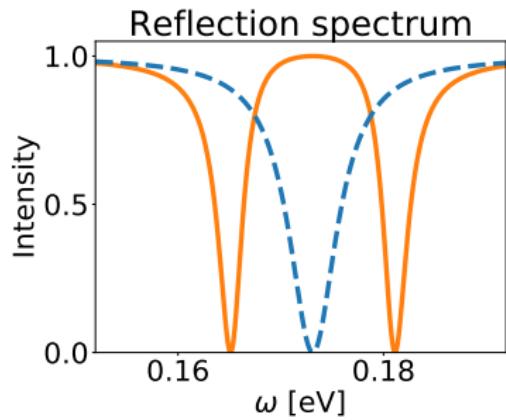
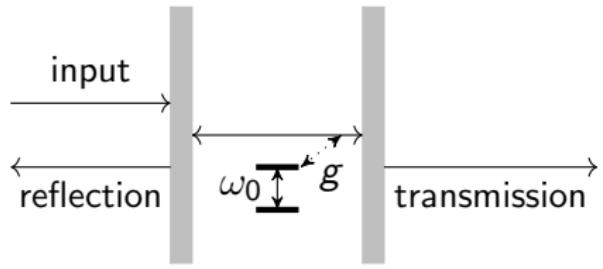


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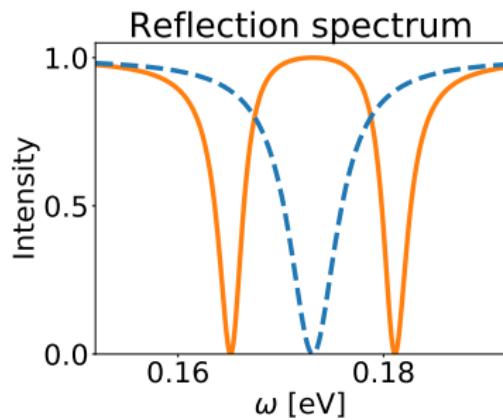
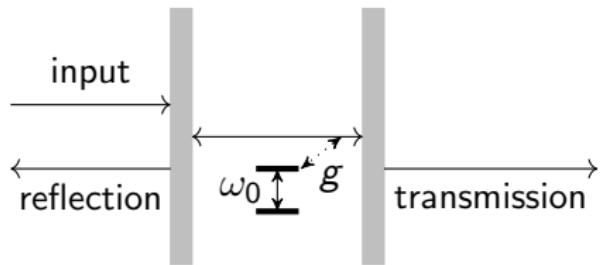
→ Weak coupling: Purcell effect

Example: Fabry-Perot cavity



→ Strong coupling: Vacuum Rabi-splitting

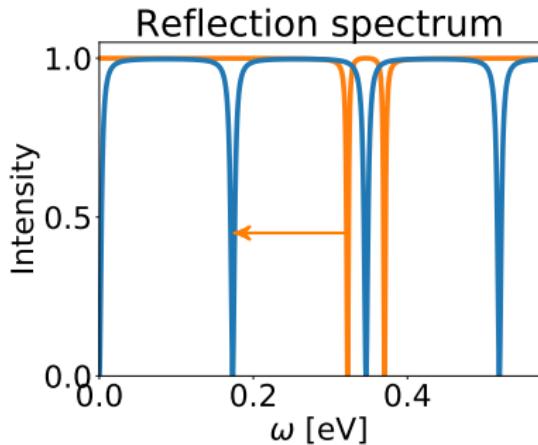
Example: Fabry-Perot cavity



⇒ Quantum effects via strong light-matter interactions!

Extreme regimes

- Multi-mode strong coupling



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

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

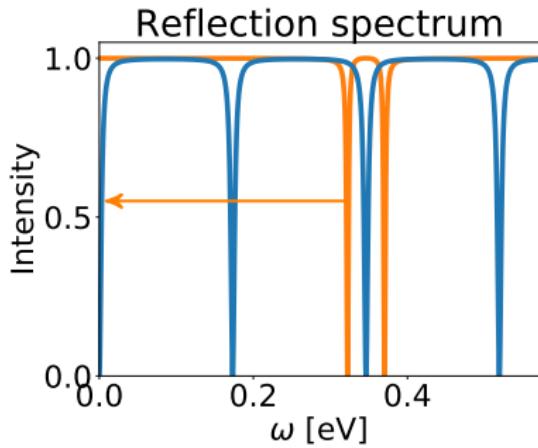
Sundaresan et al. *Phys. Rev. X* **5**, 021035 (2015)

... and many more ...



Extreme regimes

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



Recent reviews:

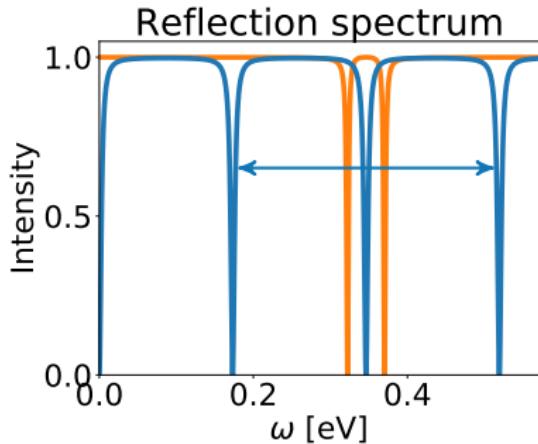
Carusotto & Ciuti *Rev. Mod. Phys.* **85**, 299 (2013)
Frisk Kockum et al. *Nat. Rev. Phys.* **1**, 19 (2019)
Forn-Díaz et al. *Rev. Mod. Phys.* **91**, 025005 (2019)

Experimental:

Niemczyk et al. *Nat. Phys.* **6**, 772 (2010)
... and many more ...

Extreme regimes

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

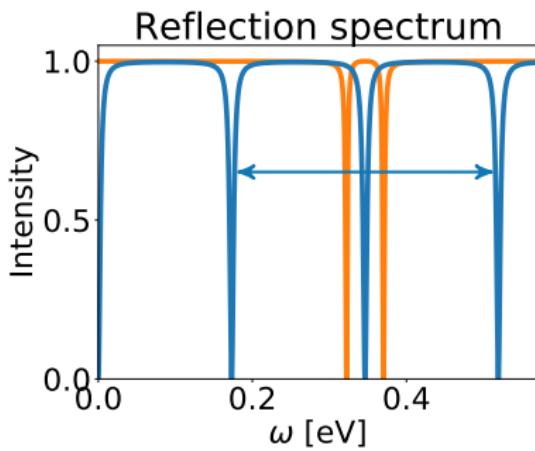


Petermann *IEEE J. Quantum Electron.* **15**, 566 (1979)
Hackenbroich, Viviescas & Haake *Phys. Rev. Lett.* **89**, 083902 (2002);
I. Rotter *J. Phys. A: Mathematical and Theoretical* **45**, 15 (2009)
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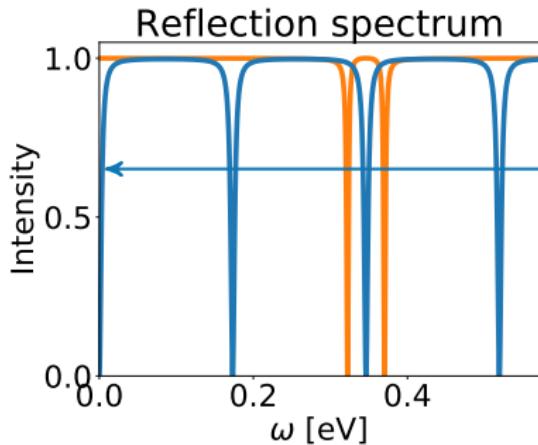
e.g. non-Hermitian
photonics



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 ...

Extreme regimes

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



Experimentally relevant:

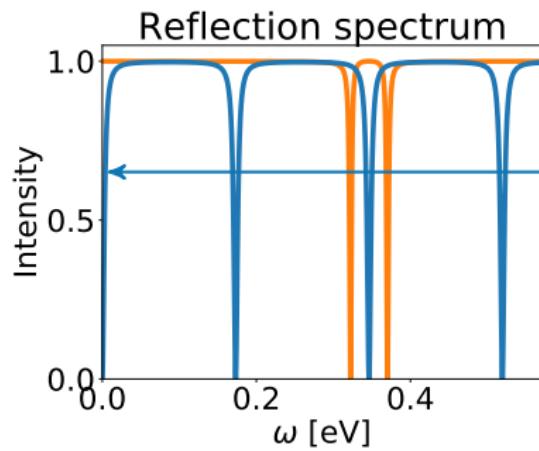
Altewischer et al. *Nature* **418**, 304306 (2002)
Savage et al. *Nature* **491**, 574577 (2012)
Esteban et al. *Nat. Comm.* **3**, 825 (2012)
Tame et al. *Nat. Phys.* **9**, 329340 (2013)
... and many more ...



Extreme regimes

Extreme coupling

- Multi-mode strong coupling
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- Large leakage



Extreme openness

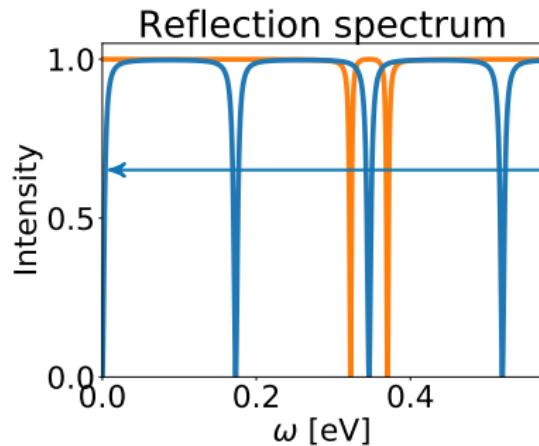
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Extreme regimes

Extreme coupling

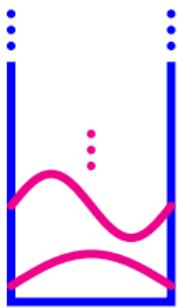
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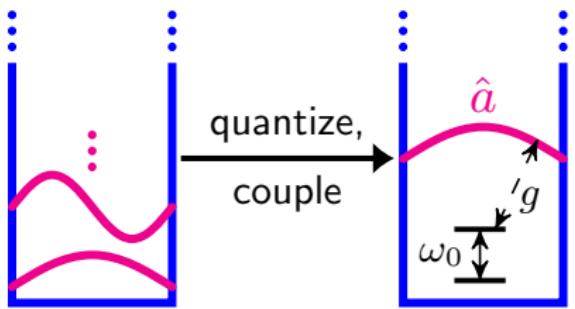
Extreme openness

Extreme complexity
(e.g. many-body)

From closed to open boxes



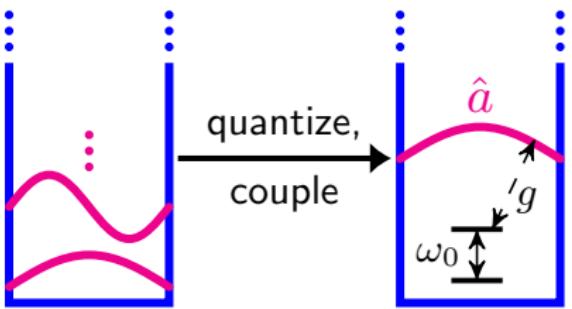
From closed to open boxes



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

→ **few-mode concept**

From closed to open boxes



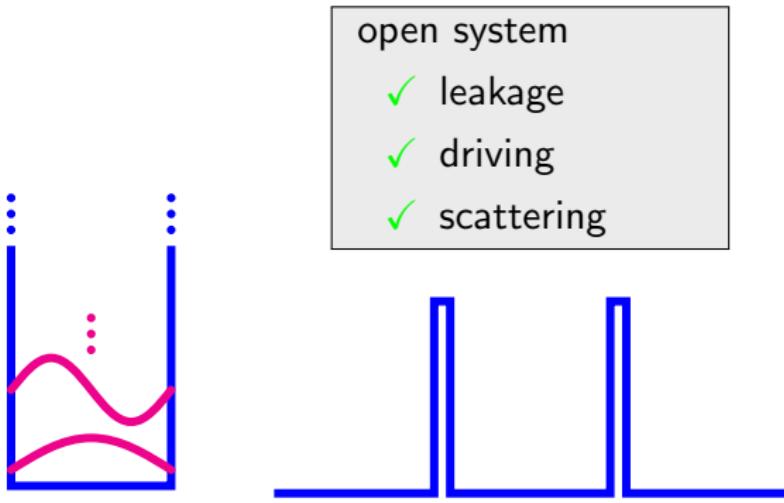
- discrete eigenstates
- closed system
 - ✗ no leakage
 - ✗ no driving
 - ✗ no scattering
 - ✗ no external detection

Jaynes-Cummings & friends

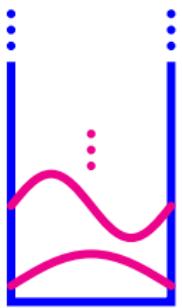
$$H = H_{\text{atom}} + H_{\text{cav}} + g \hat{a} \hat{\sigma}^+ + h.c.$$

→ **few-mode concept**

From closed to open boxes

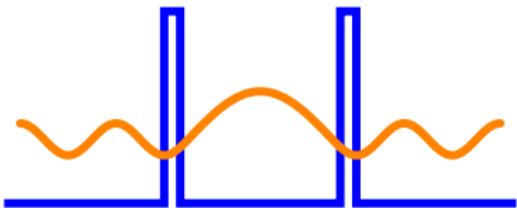


From closed to open boxes



open system

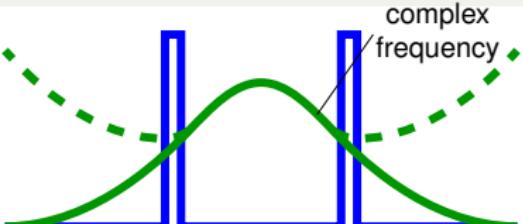
- ✓ leakage
- ✓ driving
- ✓ scattering



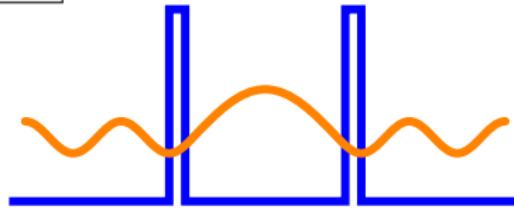
continuum eigenstates

(😢) few-mode concept
is lost

From closed to open boxes

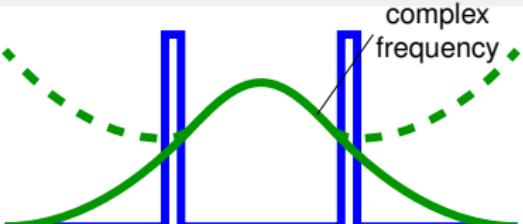


resonant modes

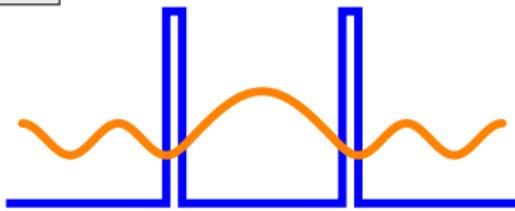


continuum eigenstates
😢 few-mode concept
is lost

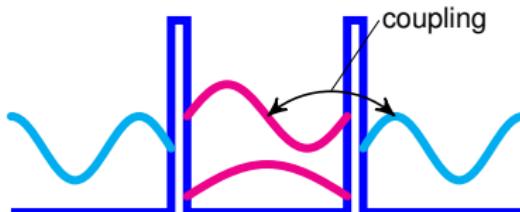
From closed to open boxes



resonant modes

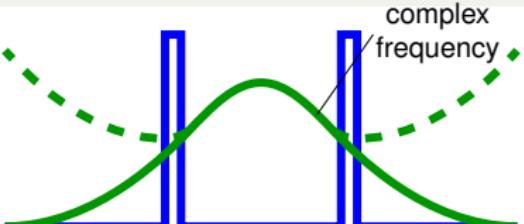


continuum eigenstates
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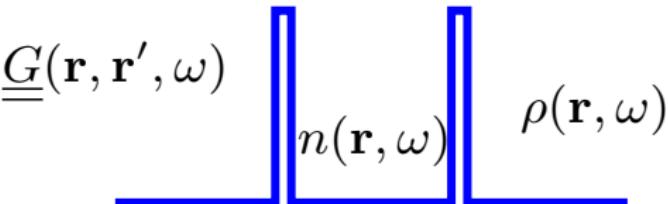


few-mode + input-output

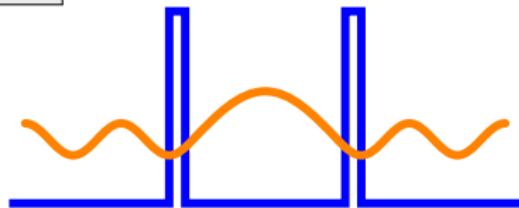
From closed to open boxes



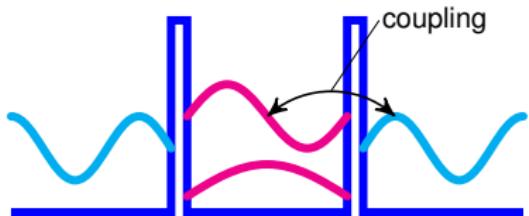
resonant modes



Green fns, LDOS, Master eqs.

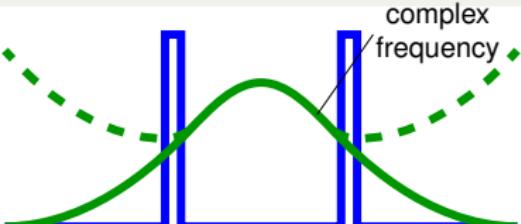


continuum eigenstates
:(few-mode concept
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few-mode + input-output

From closed to open boxes



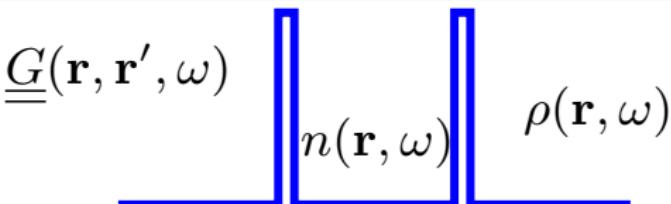
resonant modes

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

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

Cerjan & Stone *Phys. Scr.* **91** 013003 (2016)

Franke et al. *PRL* **122**, 213901 (2019)

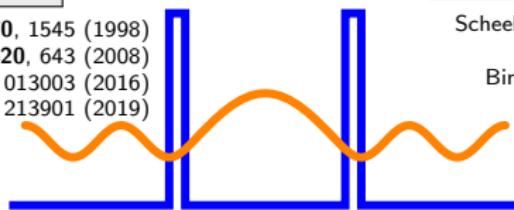


Green fns, LDOS, Master eqs.

Scheel & Buhmann *Acta Phys. Slov.* **58**, 675 (2008)

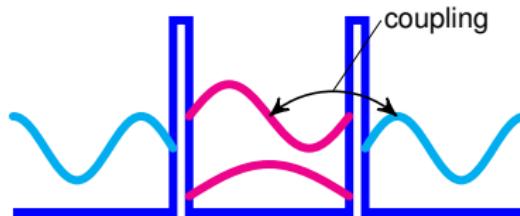
Krimer et al. *Phys. Rev. A* **89**, 033820 (2014)

Binninger et al. *Phys. Rev. A* **100**, 033816 (2019)



continuum eigenstates

few-mode concept
is lost



few-mode + input-output

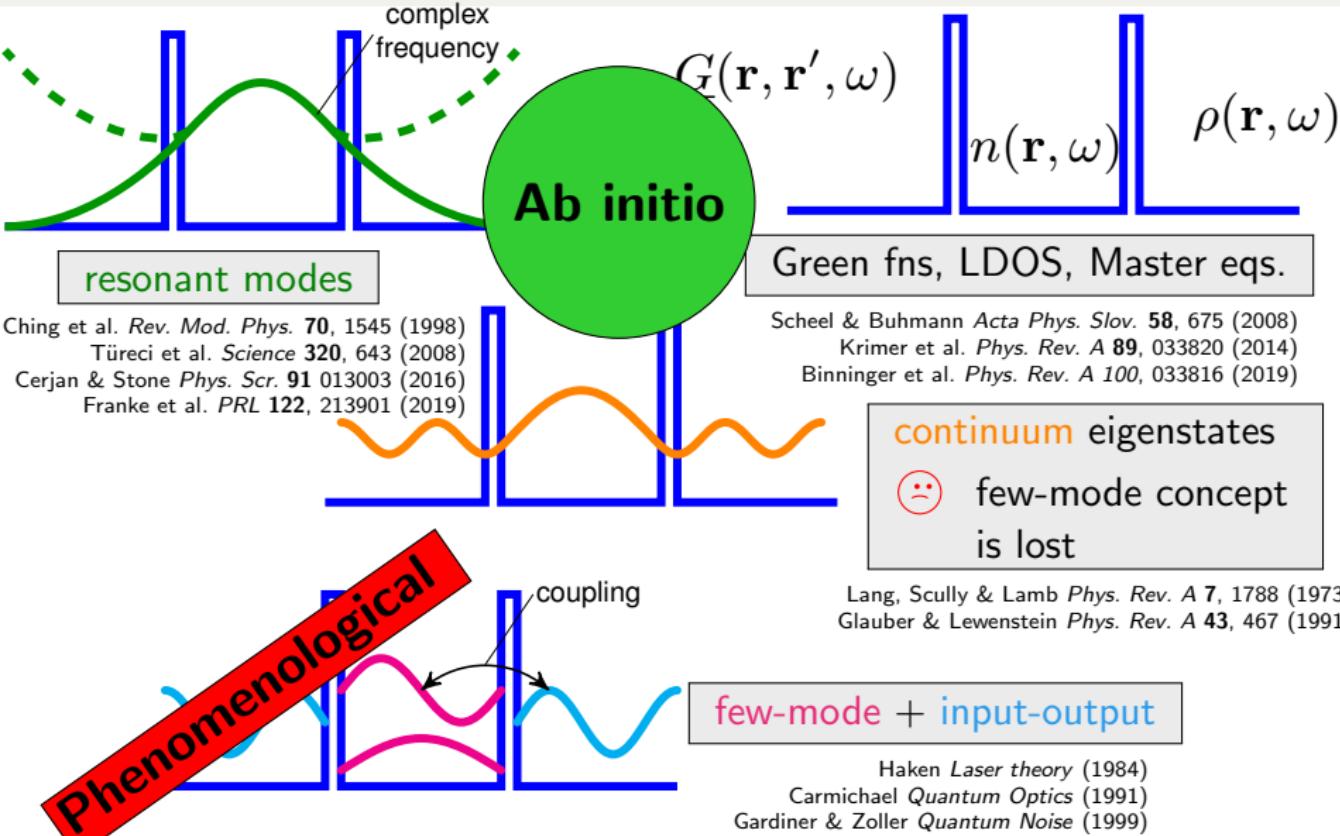
Haken *Laser theory* (1984)

Carmichael *Quantum Optics* (1991)

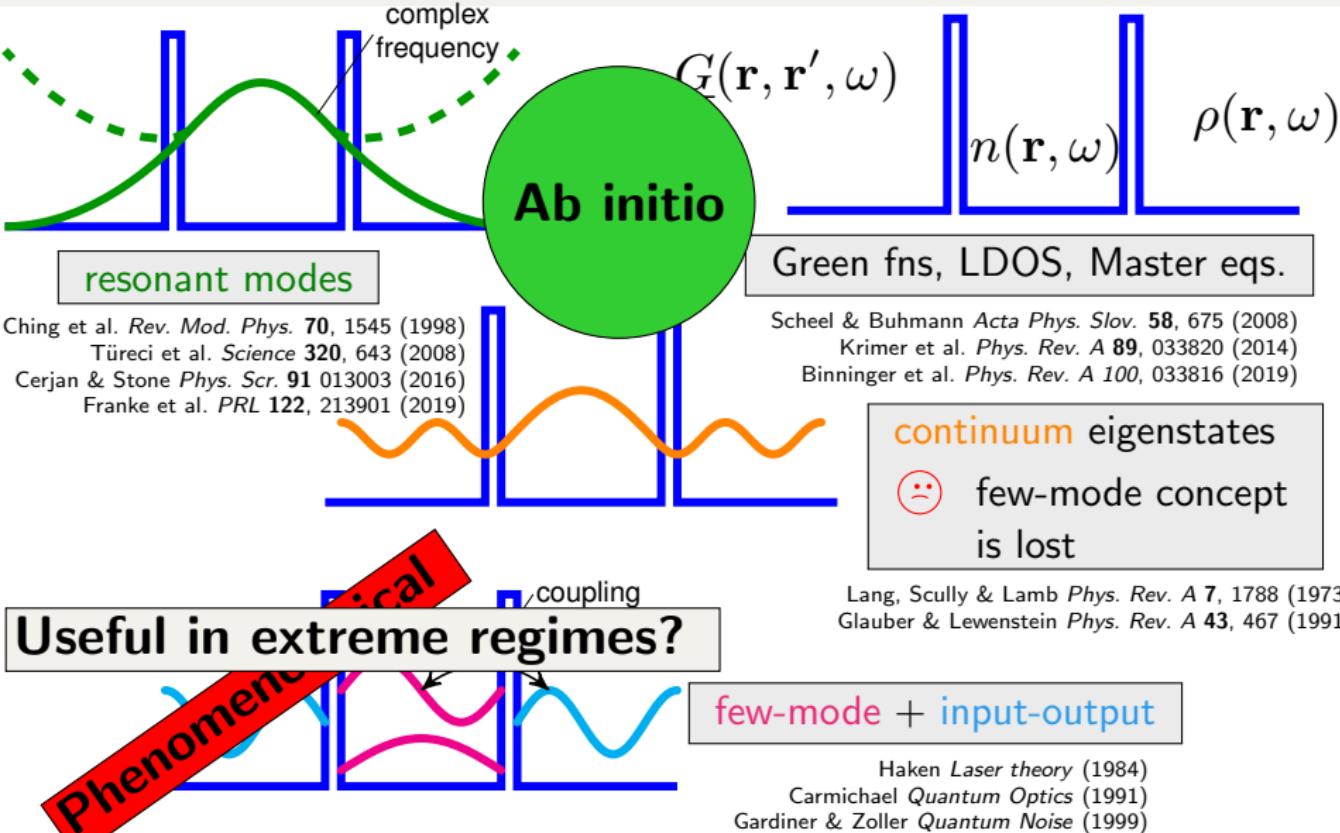
Gardiner & Zoller *Quantum Noise* (1999)

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

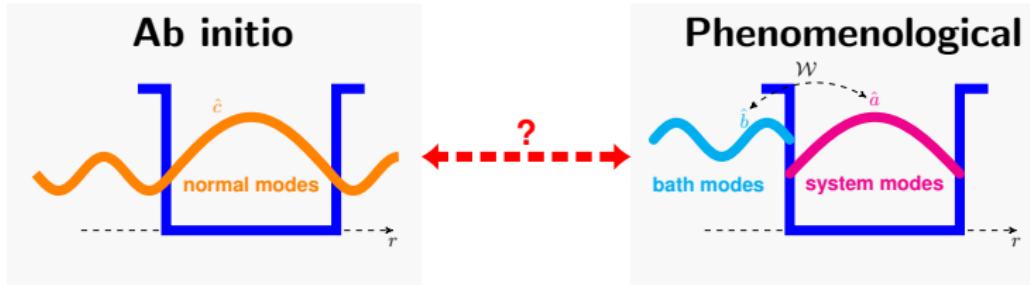
From closed to open boxes



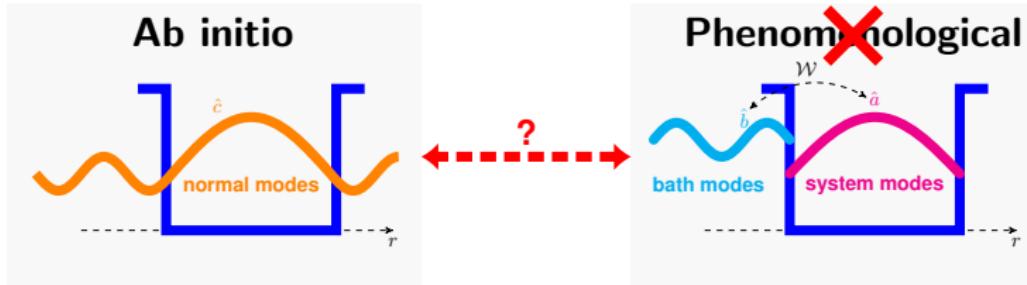
From closed to open boxes



The problem



The problem



How to make

- **few-mode**

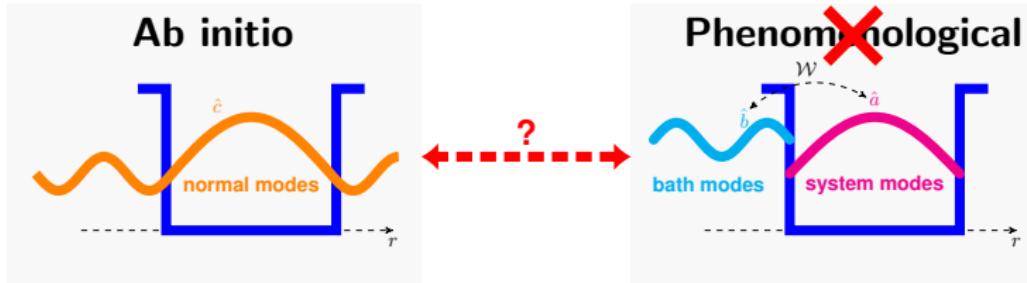
and

- **input-output**

ab initio?



The problem



How to make

- **few-mode**

and

- **input-output**

ab initio?

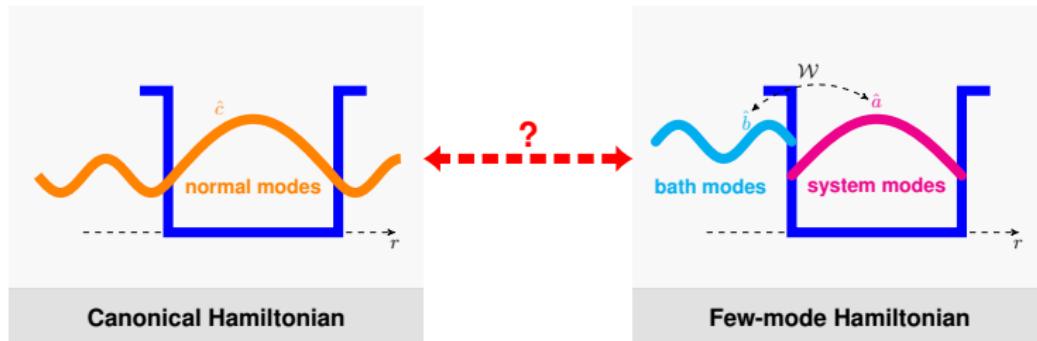


⇒ **Ab initio few-mode theory**

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



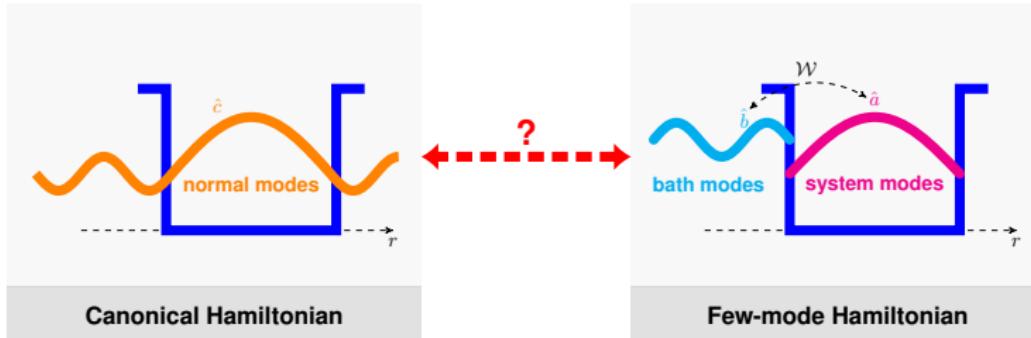
Ab initio few-mode Hamiltonians



Canonical Hamiltonian

Few-mode Hamiltonian

Ab initio few-mode Hamiltonians



normal modes

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

discrete modes

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

external continuum

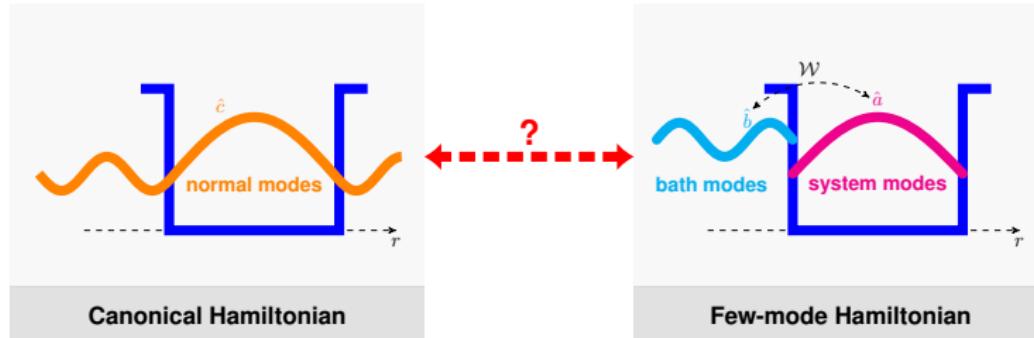
$$+ \int d\omega' \beta(\omega, \omega') \hat{b}(\omega')$$
1,2

¹Viviescas & Hackenbroich, *Phys. Rev. A* **67**, 013805 (2003)

²Domcke, *Phys. Rev. A* **28**, 2777 (1982)

³DL & J. Evers, *Phys. Rev. X* **10**, 011008 (2020)

Ab initio few-mode Hamiltonians



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

^{1,2}

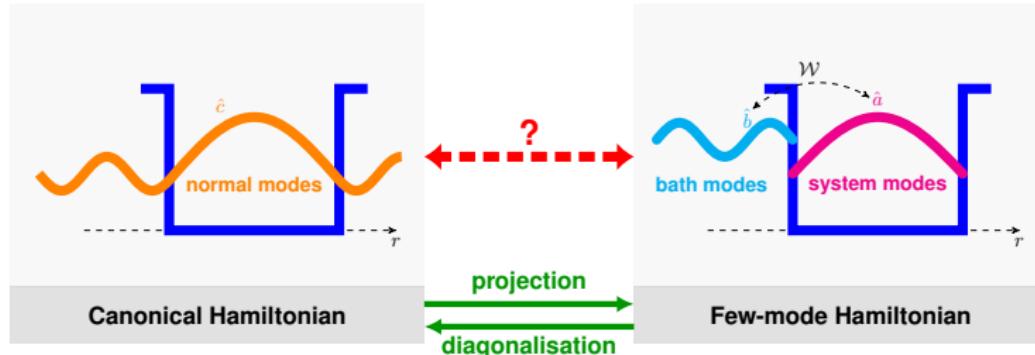
⇒ select **resonant states** as few-mode basis³

¹Viviescas & Hackenbroich, *Phys. Rev. A* **67**, 013805 (2003)

²Domcke, *Phys. Rev. A* **28**, 2777 (1982)

³DL & J. Evers, *Phys. Rev. X* **10**, 011008 (2020)

Ab initio few-mode Hamiltonians



$$\hat{c}(\omega) = \sum_{\lambda} \alpha_{\lambda}(\omega) \hat{a}_{\lambda} + \int d\omega' \beta(\omega, \omega') \hat{b}(\omega')$$

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⇒ select **resonant states** as few-mode basis³

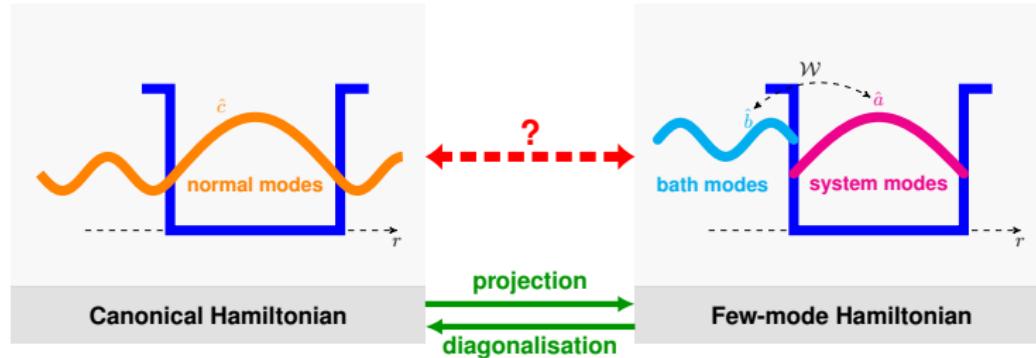
⇒ **ab initio few-mode Hamiltonians** ☺³

¹Viviescas & Hackenbroich, *Phys. Rev. A* **67**, 013805 (2003)

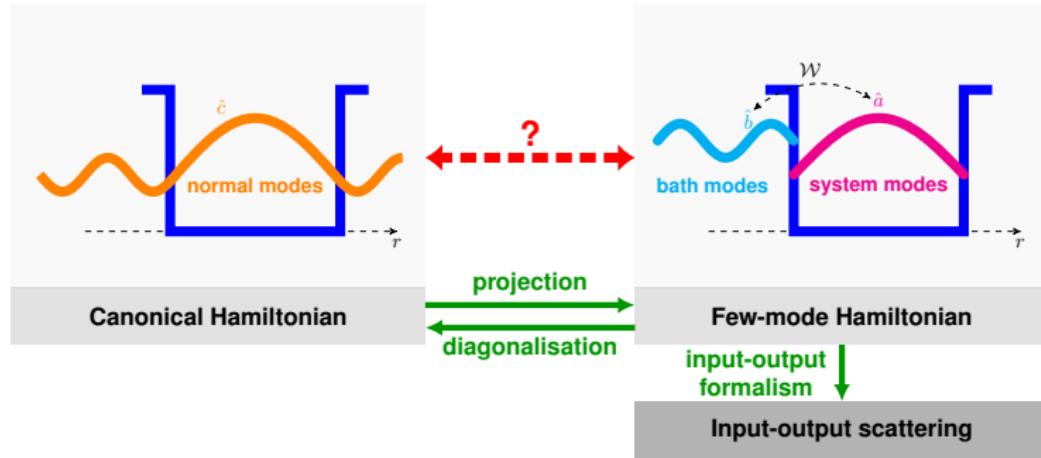
²Domcke, *Phys. Rev. A* **28**, 2777 (1982)

³DL & J. Evers, *Phys. Rev. X* **10**, 011008 (2020)

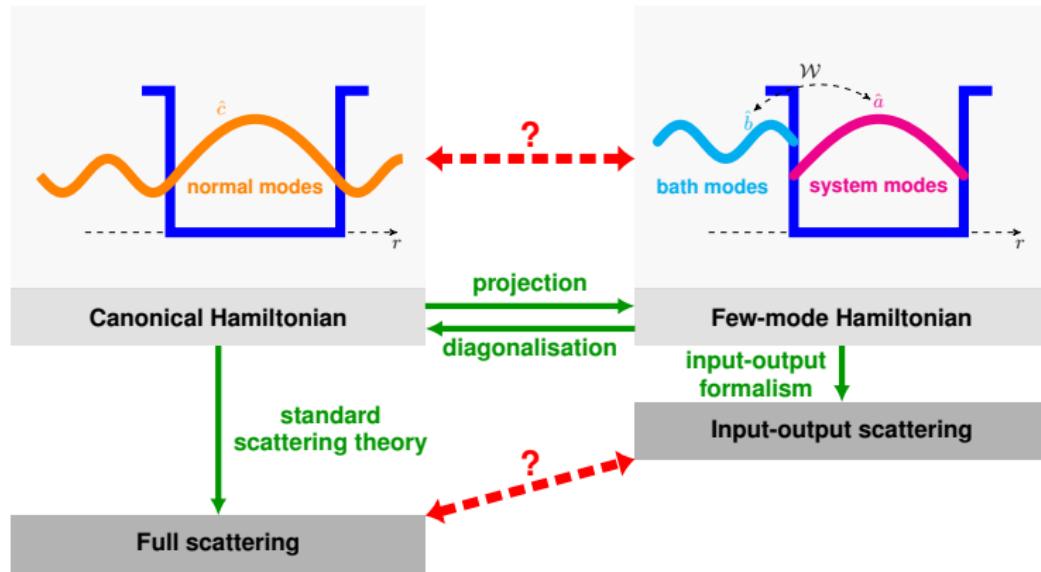
Few-mode scattering



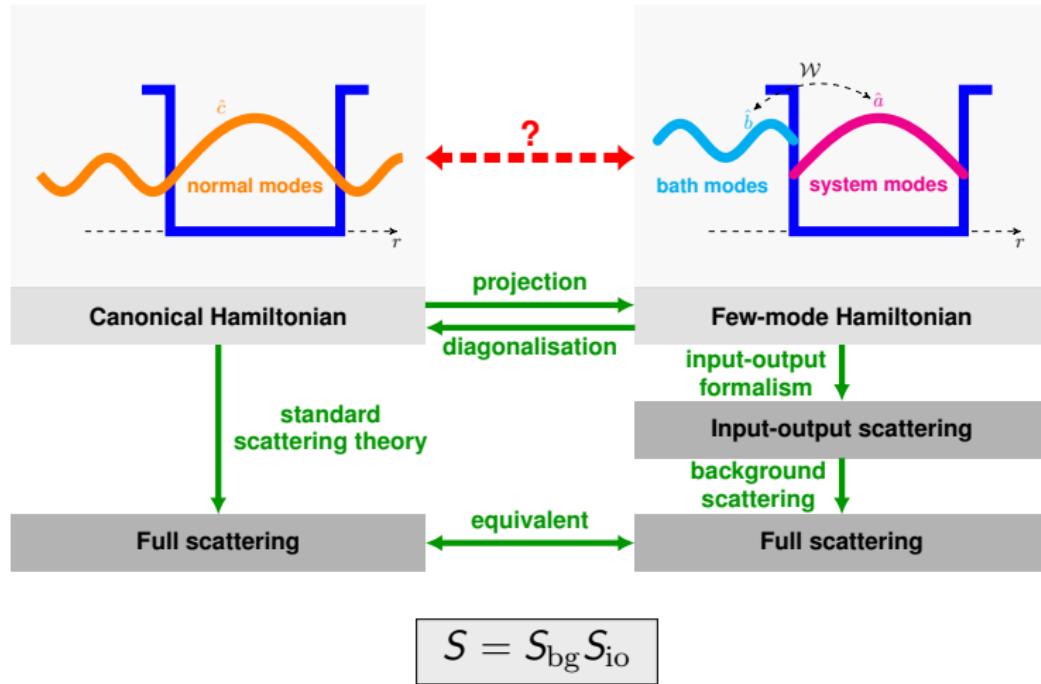
Few-mode scattering



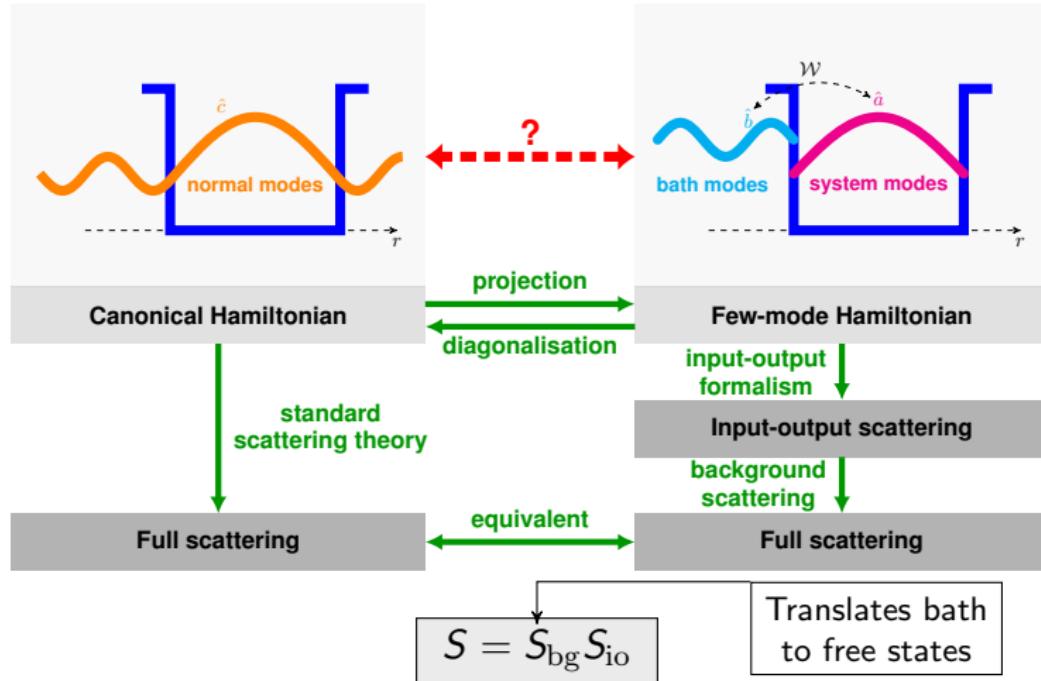
Few-mode scattering



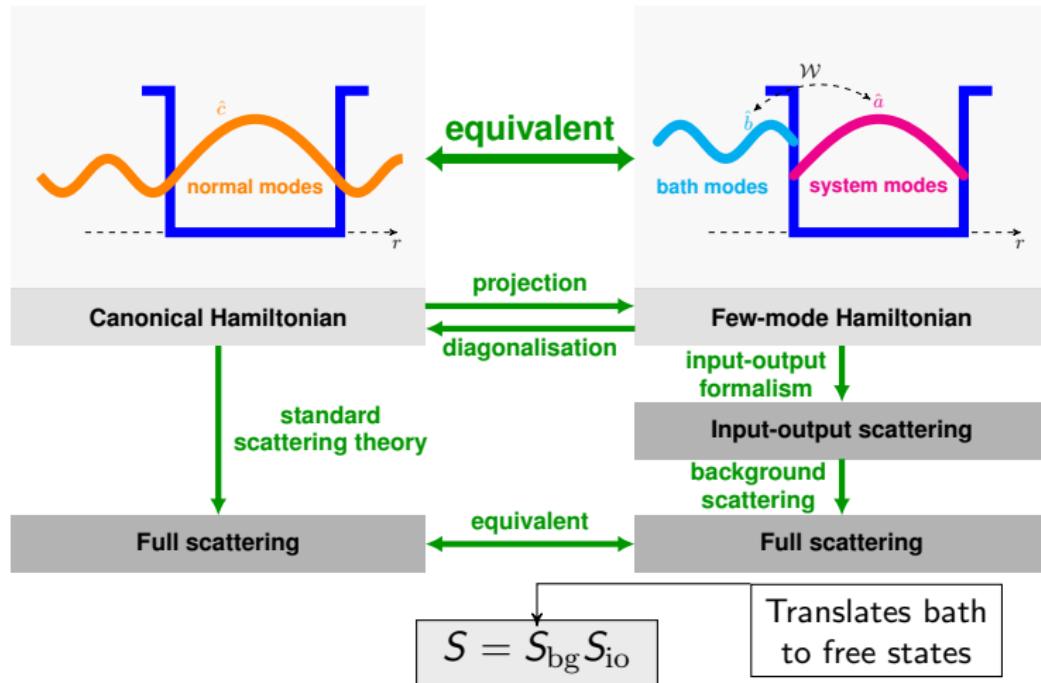
Few-mode scattering



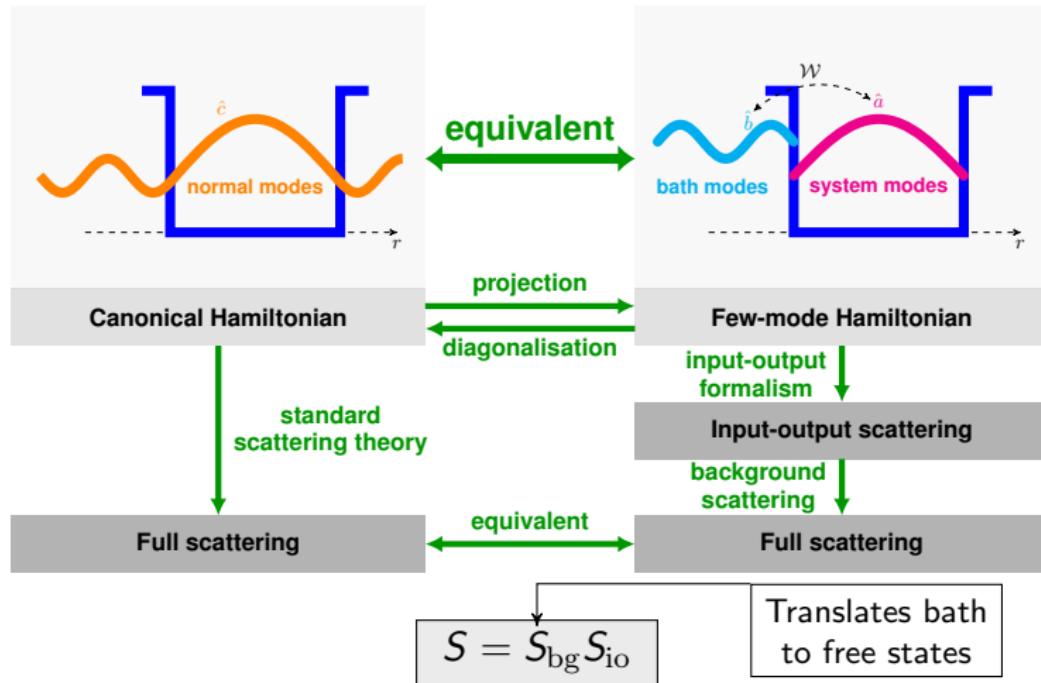
Few-mode scattering



Few-mode scattering



Few-mode scattering

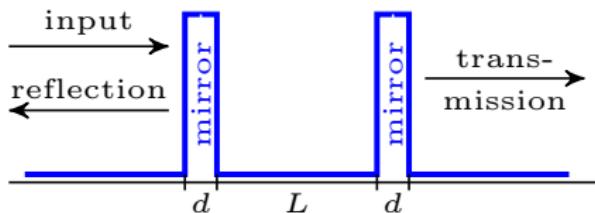


⇒ Few-mode theory can apply in extreme regimes!



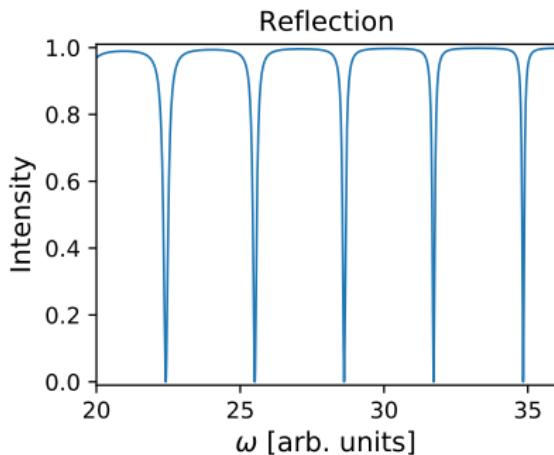
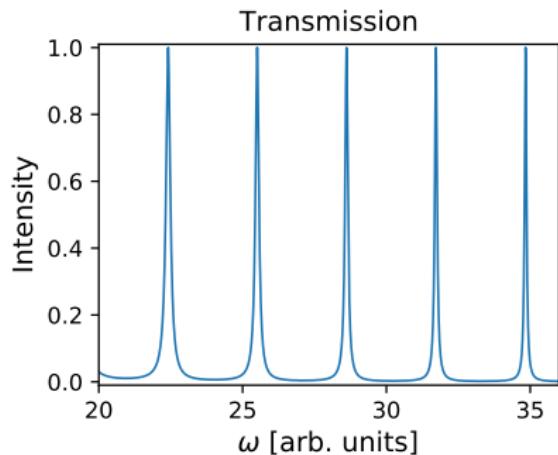
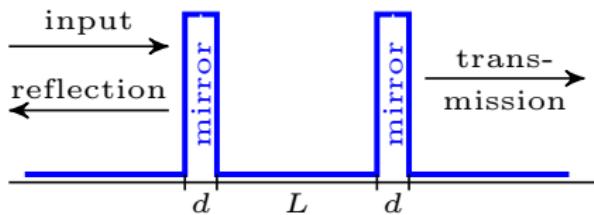
Illustrative example

Example: Two-sided Fabry-Perot cavity

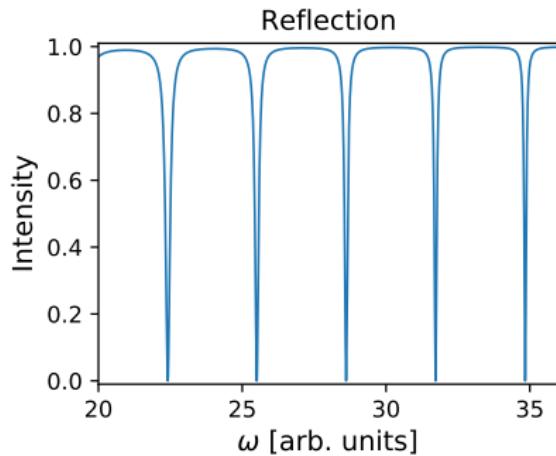
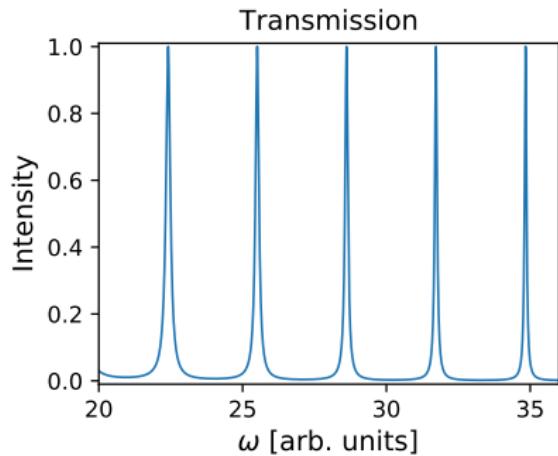
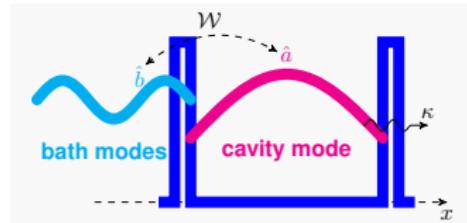
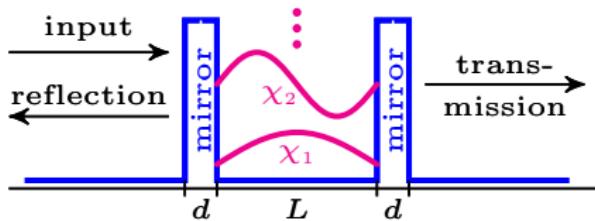


Ley & Loudon *J. Mod. Opt.* **34**, 227-255 (1987)

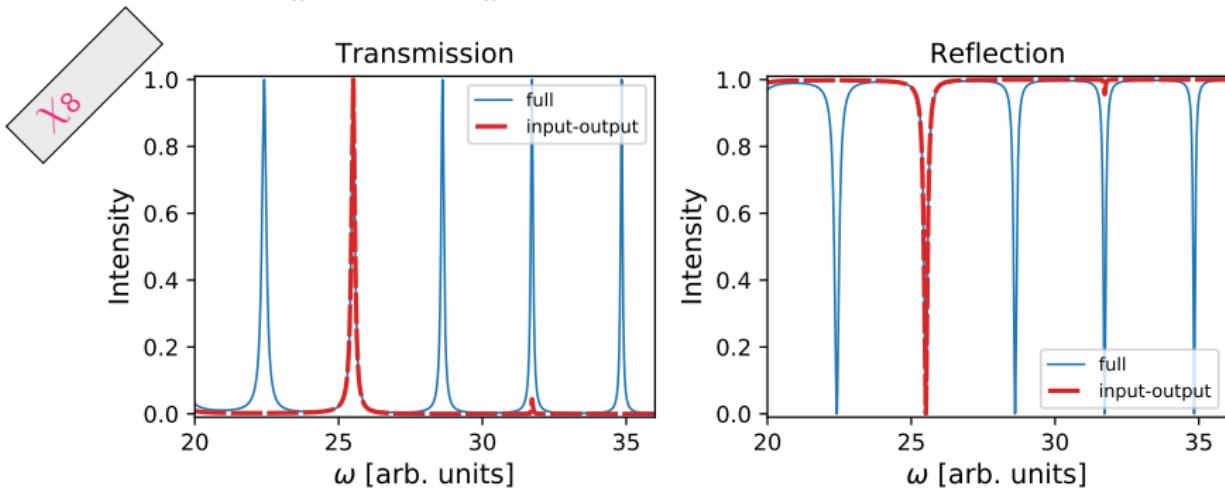
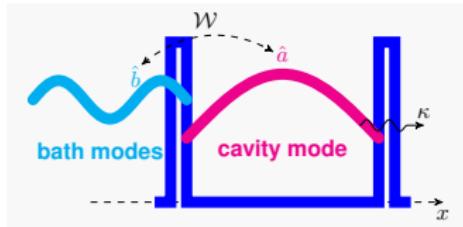
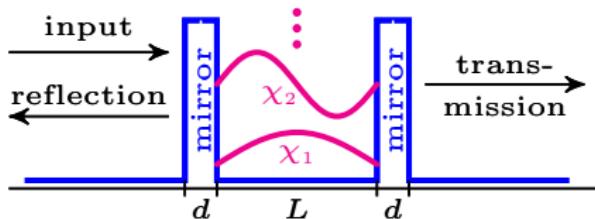
Example: Two-sided Fabry-Perot cavity



Example: Two-sided Fabry-Perot cavity

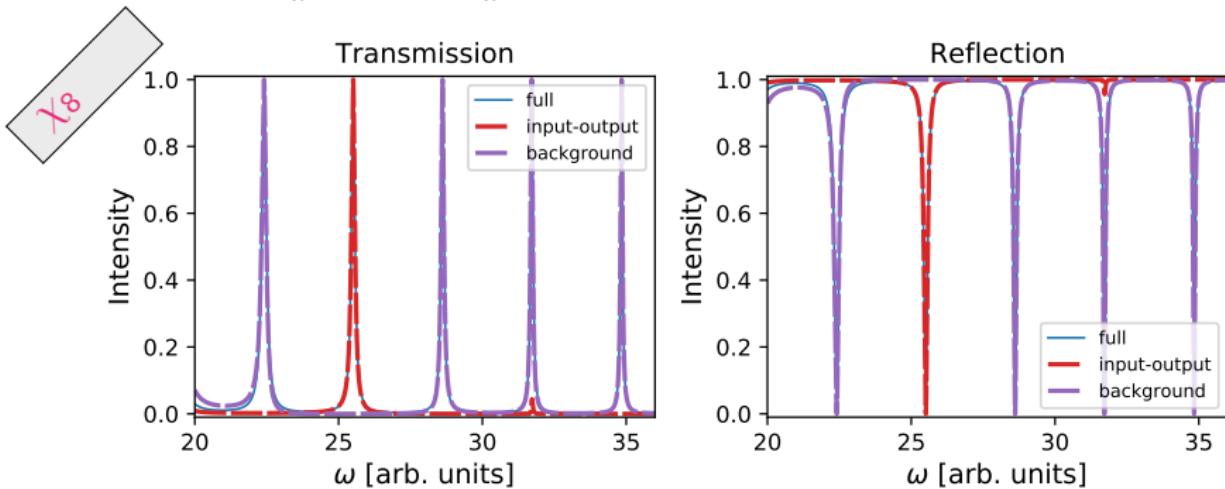
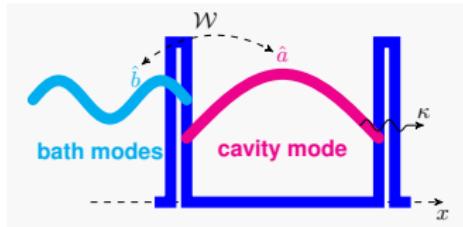
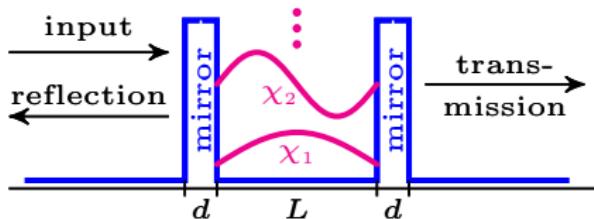


Example: Two-sided Fabry-Perot cavity



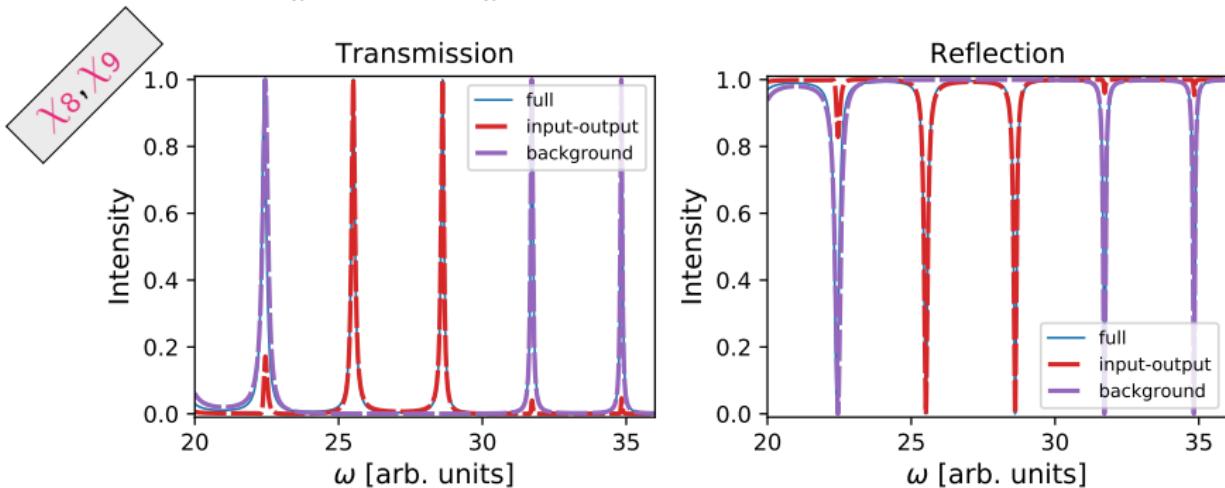
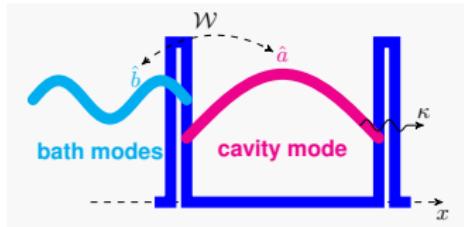
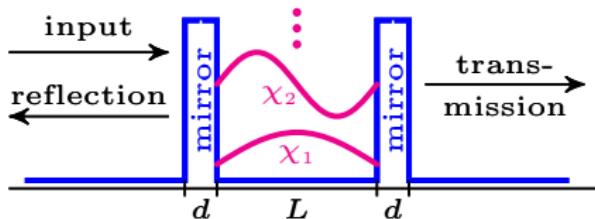
⇒ ab initio, not a fit!

Example: Two-sided Fabry-Perot cavity



⇒ ab initio, not a fit!

Example: Two-sided Fabry-Perot cavity



⇒ extract resonant dynamics

Interacting systems



Interacting systems



- Many degrees of freedom
- Often difficult!

Interacting systems



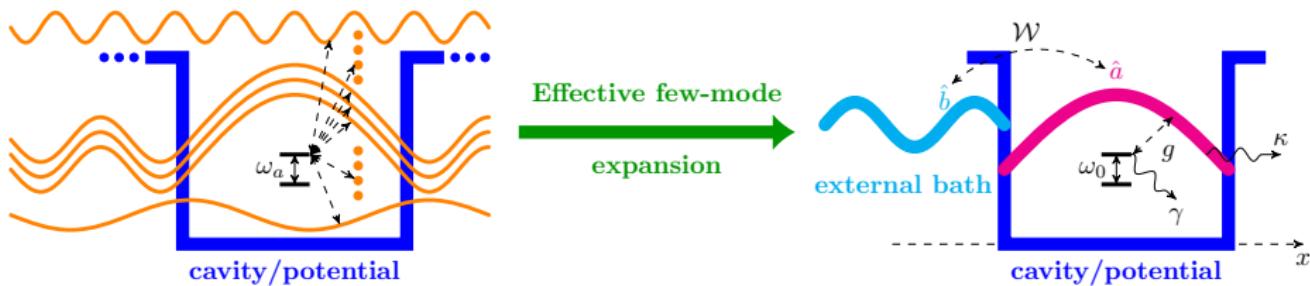
- Many degrees of freedom
- Often difficult!
- Much easier to solve!
- Many methods already exist!^{1,2,3}
- Advantages to model version
- ⇒ Non-interacting system exact!

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

² Gardiner & Zoller *Quantum Noise* (1999)

³ Kirton et al. *Adv. Quantum Technol.* **2**, 1800043 (2019)

Interacting systems



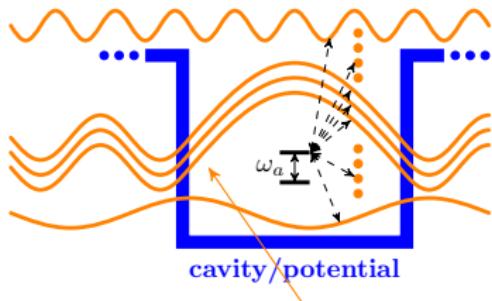
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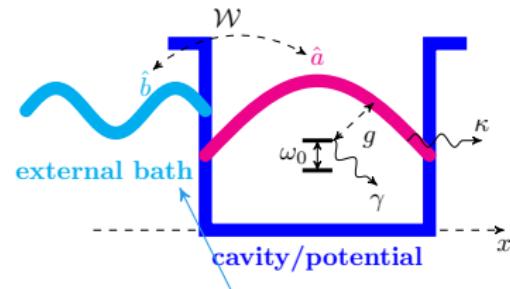
³ Kirton et al. *Adv. Quantum Technol.* **2**, 1800043 (2019)

Interacting systems



non-perturbative/non-Markovian

- Many degrees of freedom
- Often difficult!



perturbative/Markovian

- Much easier to solve!
 - Many methods already exist!^{1,2,3}
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¹ Carmichael, *Statistical Methods in Quantum Optics 1*(1999)

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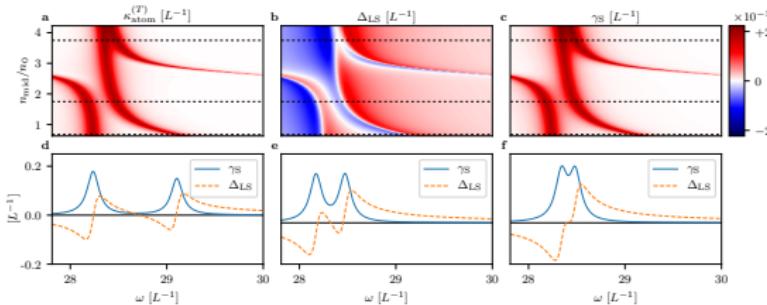
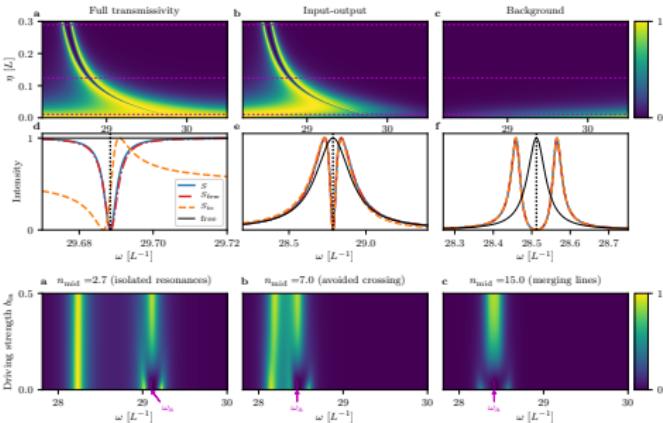
³ Kirton et al. *Adv. Quantum Technol.* **2**, 1800043 (2019)

Benchmarks and advantages

- ✓ Benchmarked in linear regime
- ✓ Highly open systems

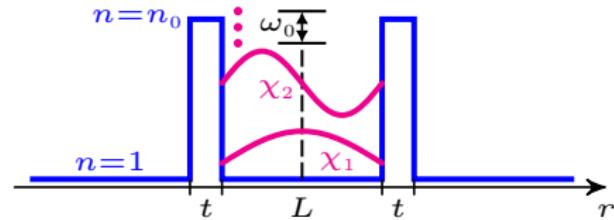
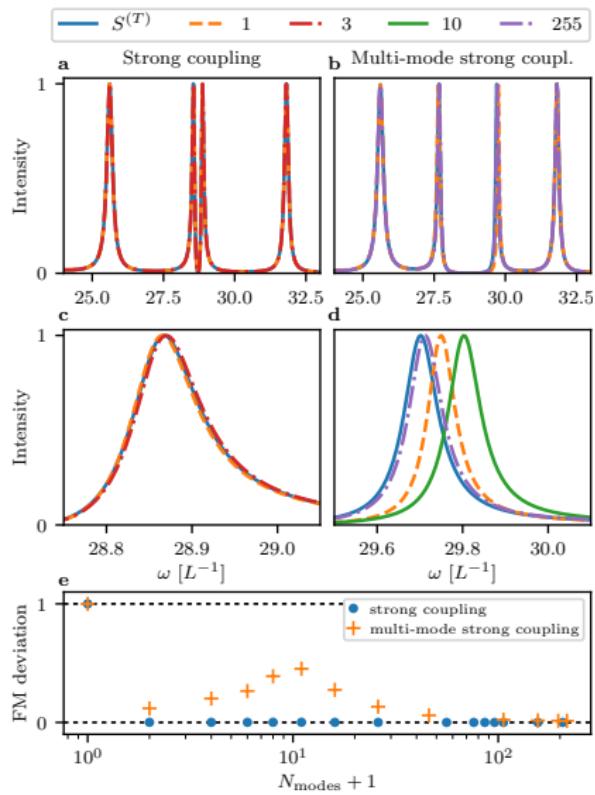
- ✓ Non-linear effects

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

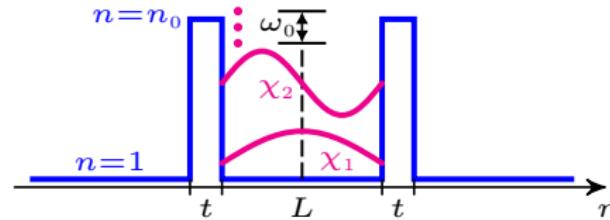
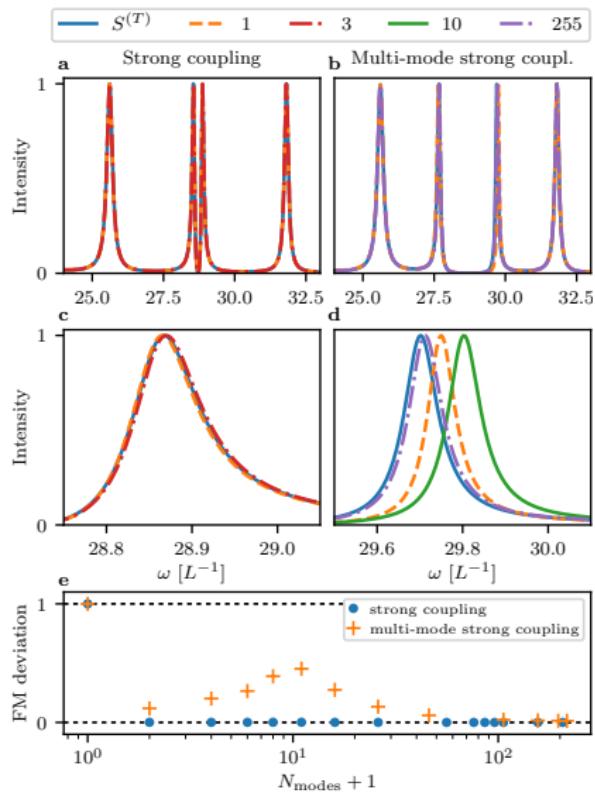


DL & J. Evers, Phys. Rev. X 10, 011008 (2020)

Convergence and extreme regimes



Convergence and extreme regimes

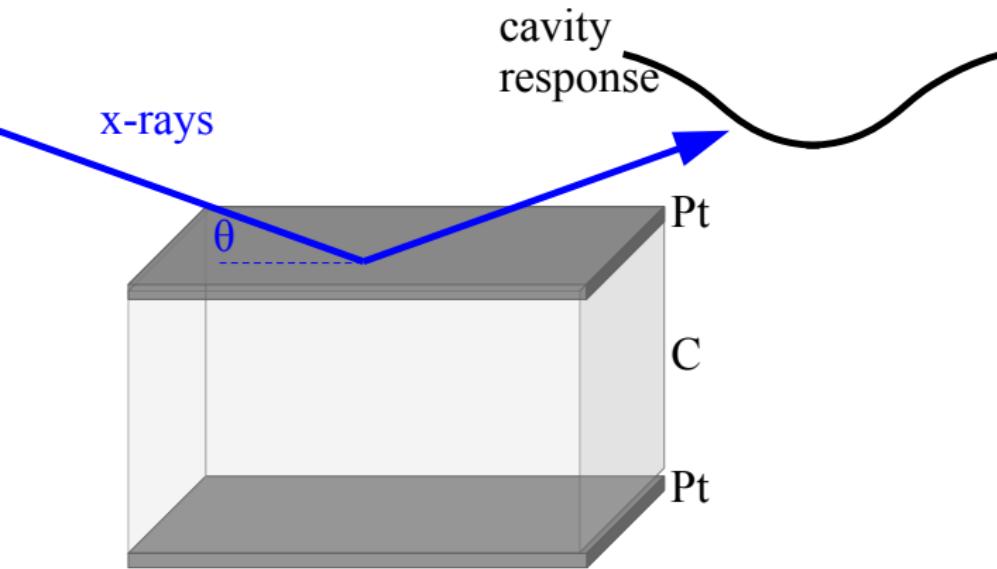


Convergence of light-matter coupling models is non-trivial!¹

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

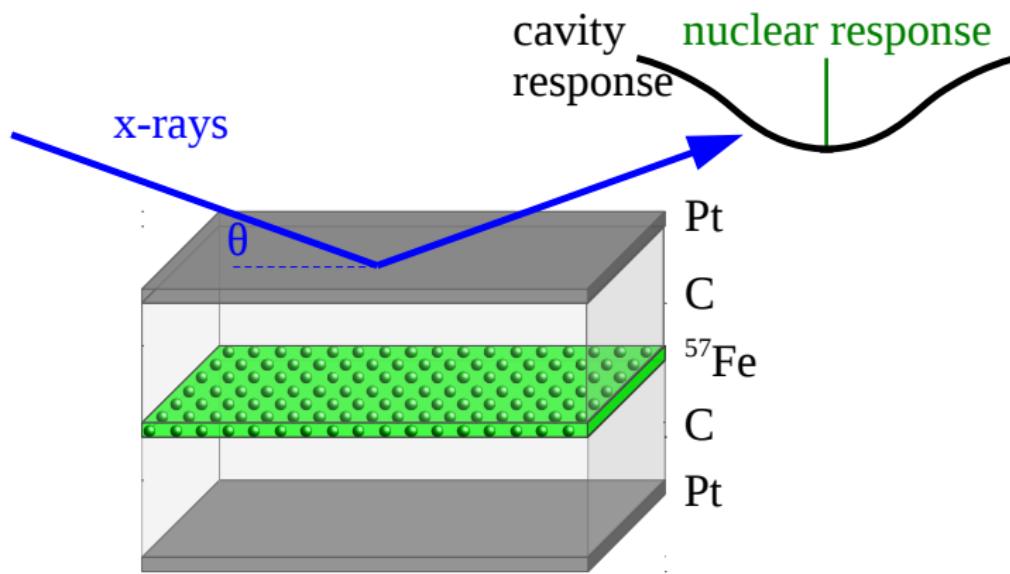
X-ray cavity QED

New experimental platform:



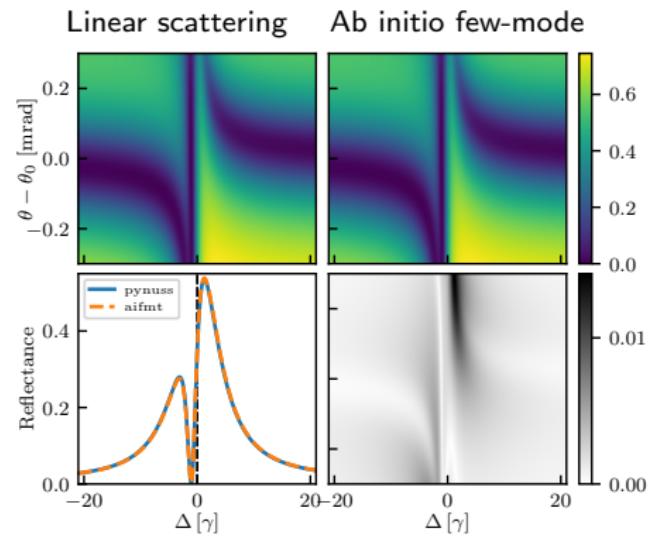
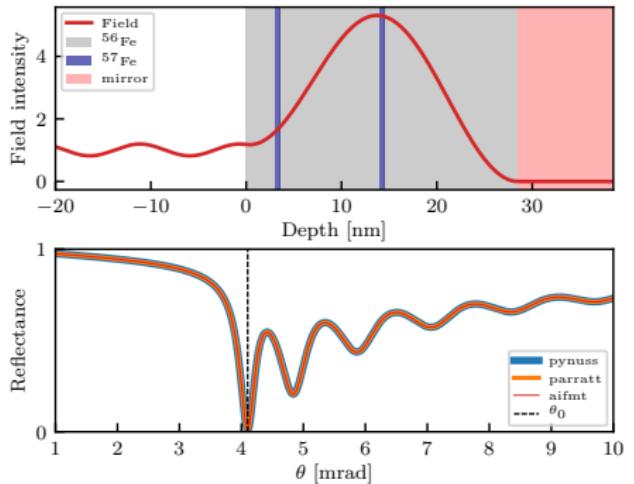
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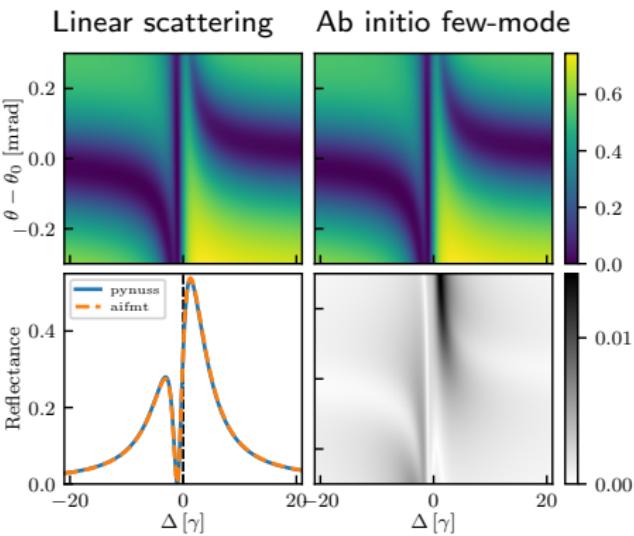
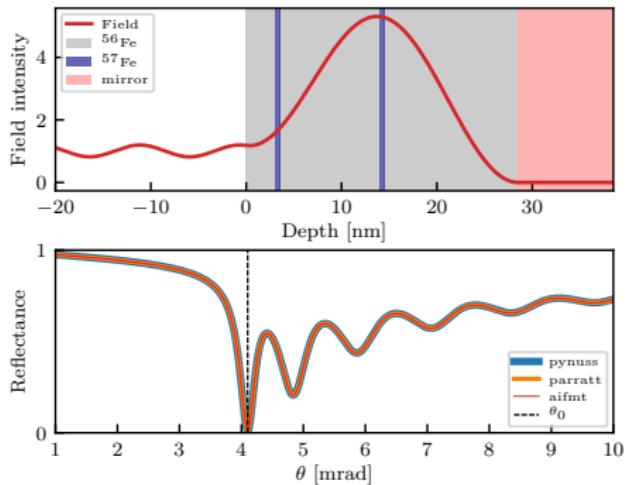
Fabry-Perot + Many-body ensemble

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



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

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



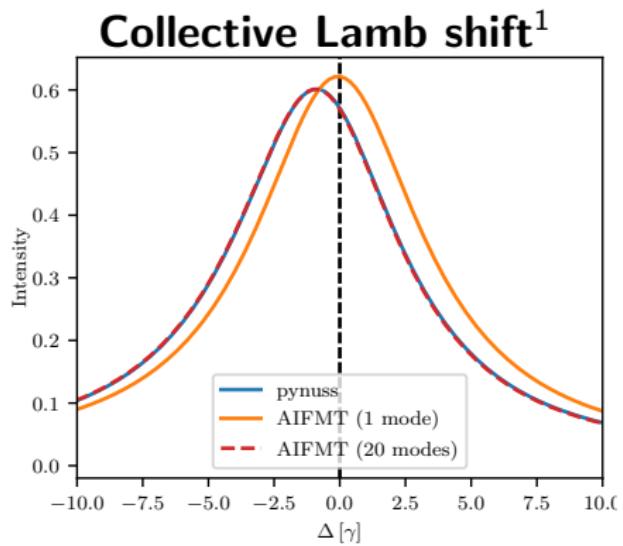
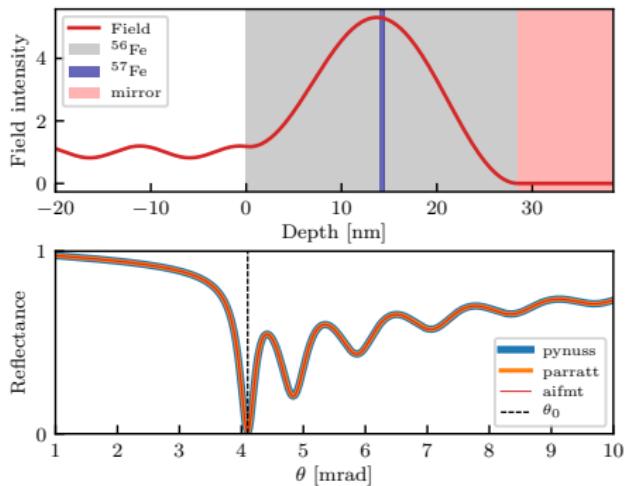
DL, Heeg, Keitel & Evers, *to be submitted*

⇒ improves successful phenomenological model^{1,2}

¹Heeg & Evers *PRA* (2013)

²Heeg & Evers *PRA* (2015)

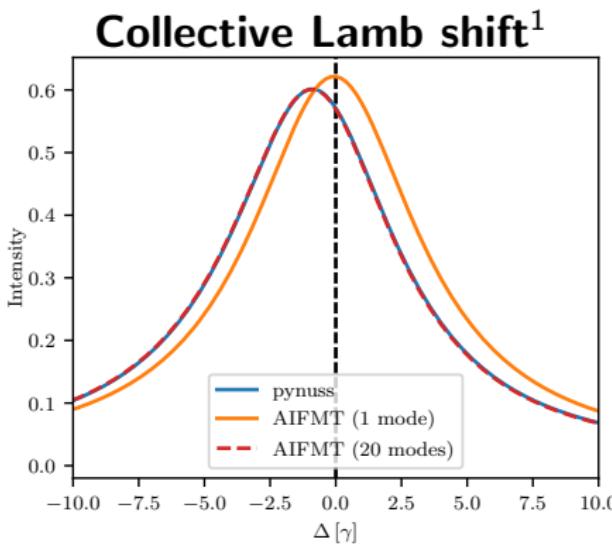
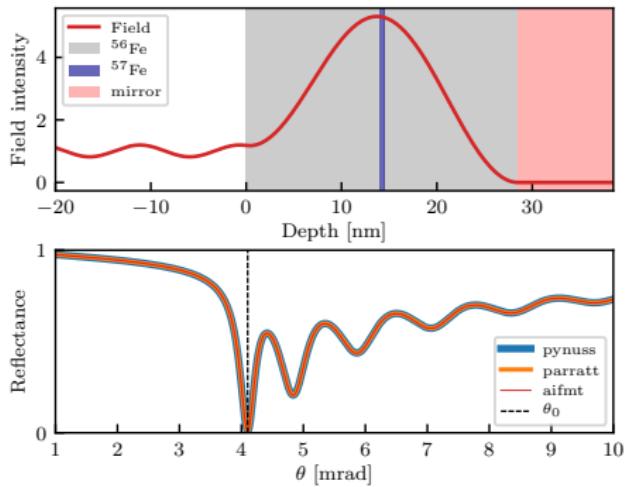
Overlapping modes effects beyond input-output models



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



Overlapping modes effects beyond input-output models

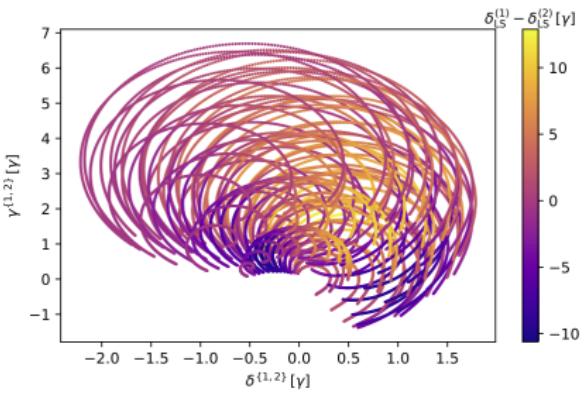
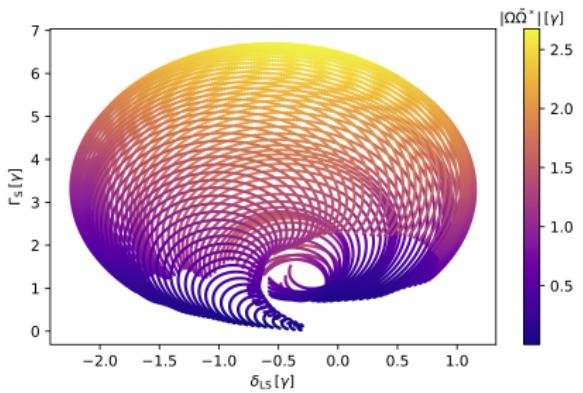
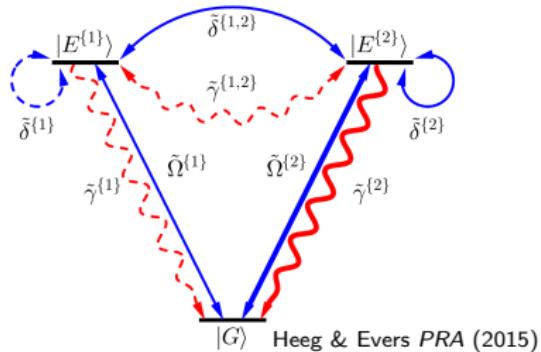
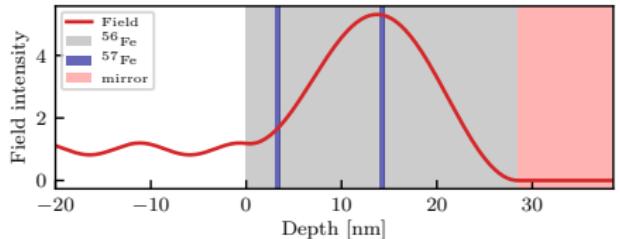


¹Röhlsberger et. al. *Science* **328** 5983 (2010)

⇒ overlapping modes effect



Towards designing nuclear level schemes



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

EAS41, Riezlern, 29.01.2020



Conclusion

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

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

Thank you for your attention!



Jörg Evers



Kilian P. Heeg



Christoph H. Keitel

