Non-equilibrium Statistical Physics of Small Quantum Systems: Transport, Fluctuations, Engineered devices

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UNIVERSITY OF TORONTO

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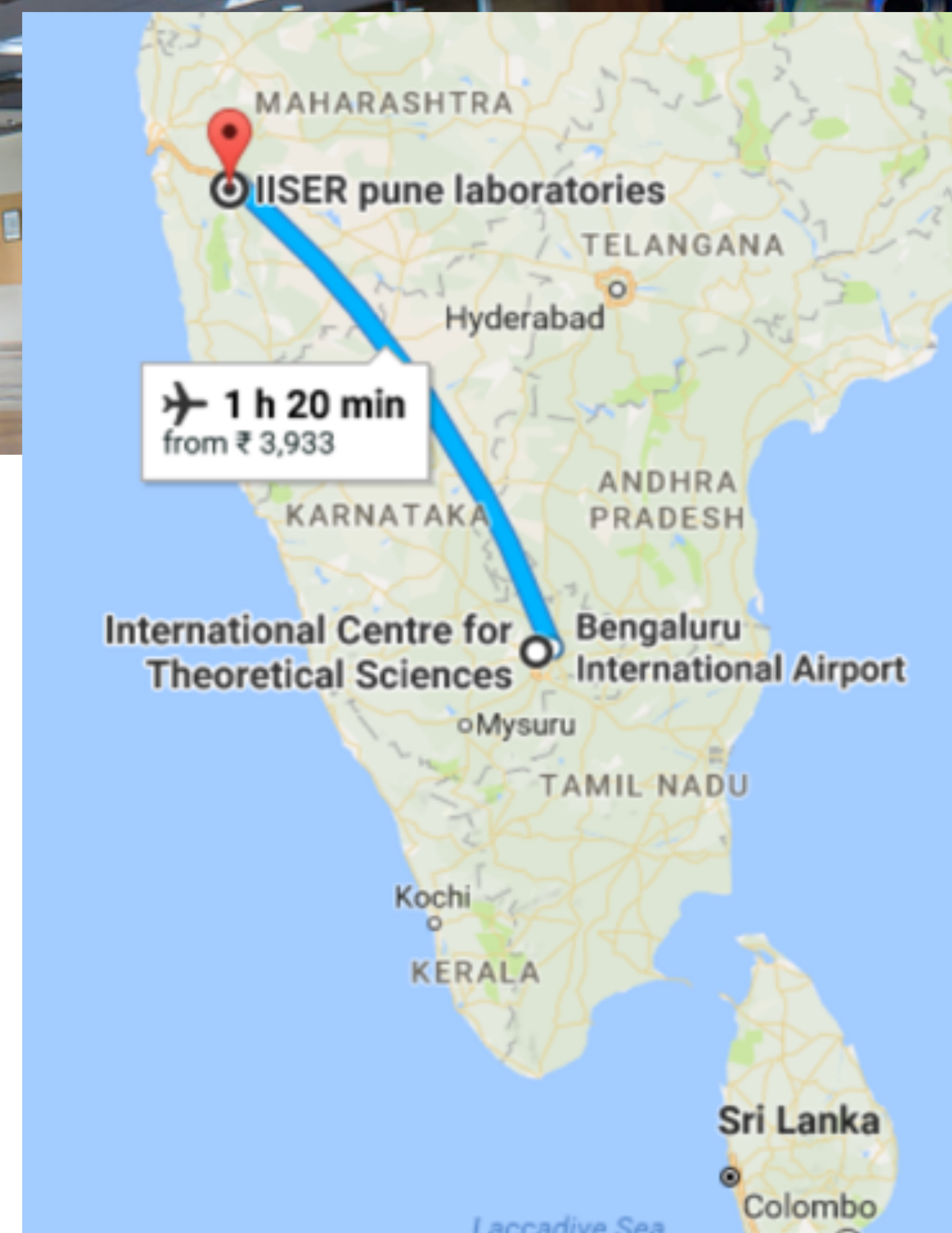
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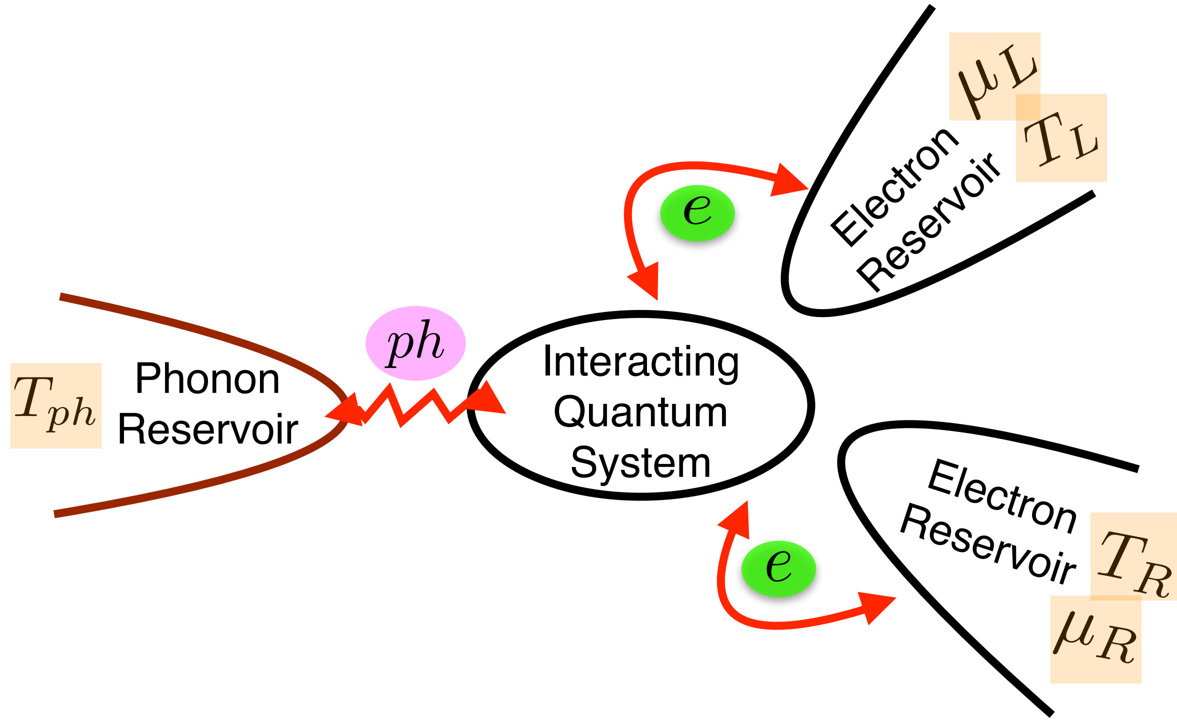
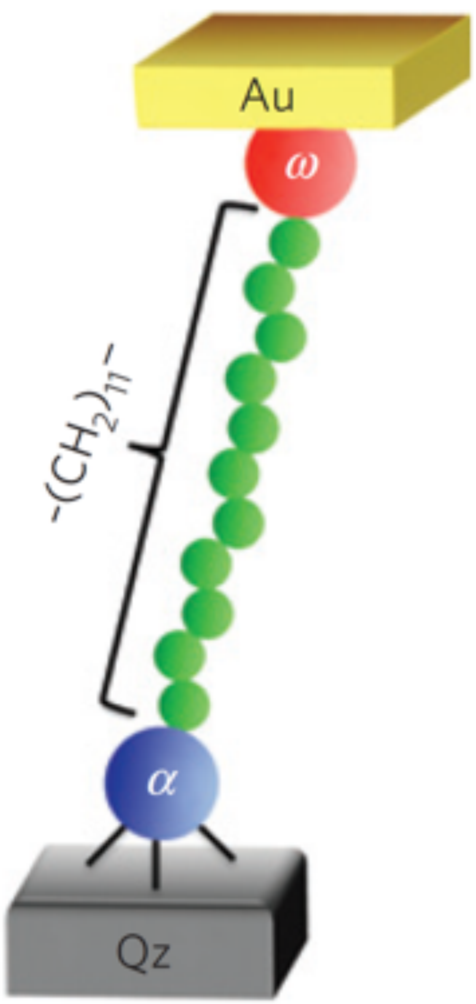
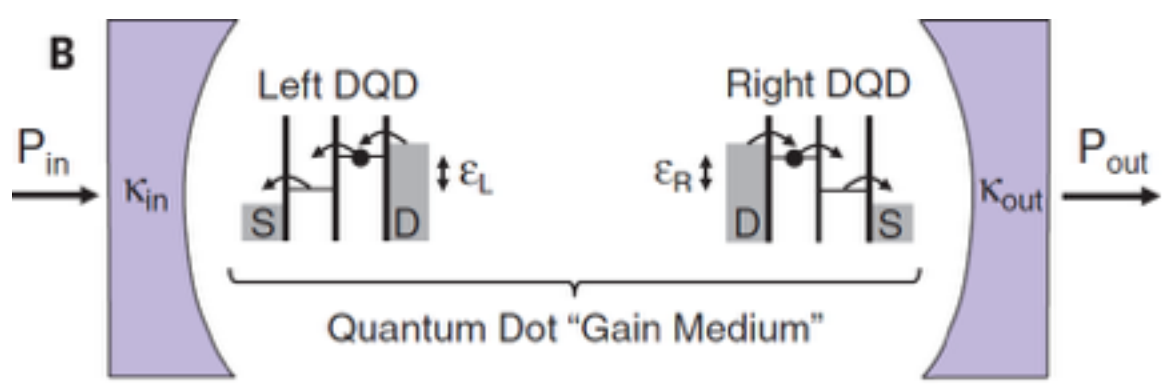


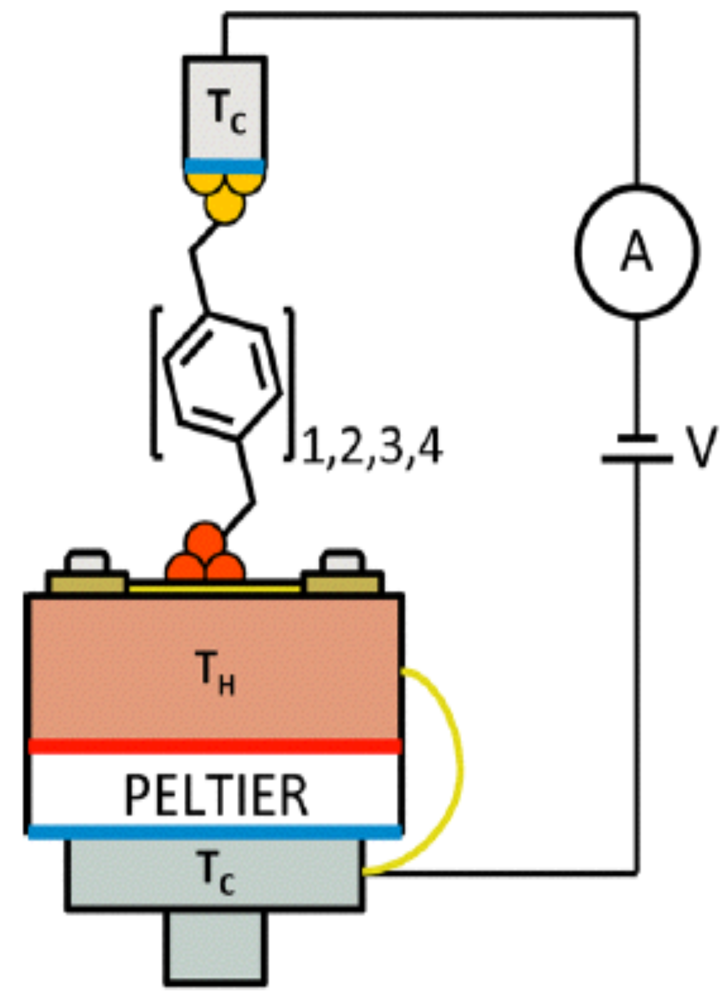


… D. Cahill, Nature Mat. 11 502 (2012)

Micromaser (optoelectronic)

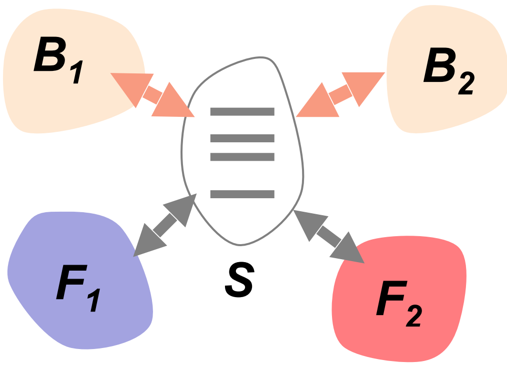


…petta, Science 347, 285 (2015)



…, L. Venkataraman, Nano Lett 13 2889 (2013)

Non-Equilibrium Quantum Systems: Questions and Challenges



Non-Eq. Quantum Systems
Open + Many-body interactions + Non-eq Conditions

$\rho_s(t)$

$I_e(t), I_Q(t)$

$J_Q(t)$

$\langle I(t)I(\tau)\rangle$

$\eta = W/Q$

Fundamental

- **Quantum Dynamics** (Transient, Steady state, relaxation)
- **Quantum Thermodynamics** Thermodynamic phenomena from quantum dynamical laws?
- **Large Fluctuations**: **Average behaviour contained limited information:** Probabilistic theory of measurable quantities

Challenge

Theoretical and computational methods to incorporate

1. non-equilibrium conditions,
2. many-body interactions,
3. finite system-environment coupling (dissipation)
4. non-Markovian dynamics (finite memory)

Practical

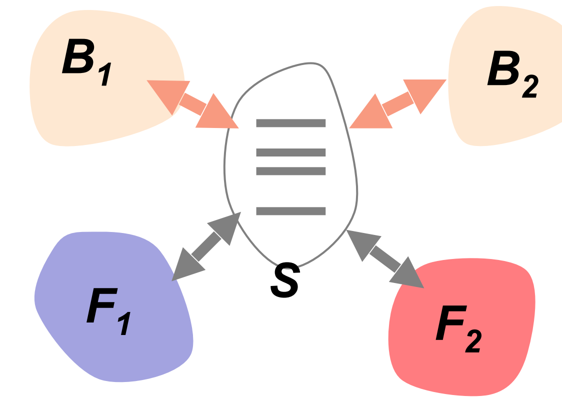
Quantum Devices

(Diode, Thermoelectric, Optoelectronics, Optomechanics)

- How do we engineer the system to obtain a **specific functionality**,
- How do **we maximize the efficiency** of non-equilibrium quantum devices

Theoretical Methods:

Method Developments: Open Quantum Systems



Theoretical Tools :

- **Non-Equilibrium Green's function** $G = G_0 + G_0 \Sigma G$
- **Quantum Langevin equations**
- **Quantum Master Equation (Rate equations, NIBA)** $\frac{dp}{dt} = Mp$
- **Mean-field, hybrid QME-NEGF**

Review Articles:

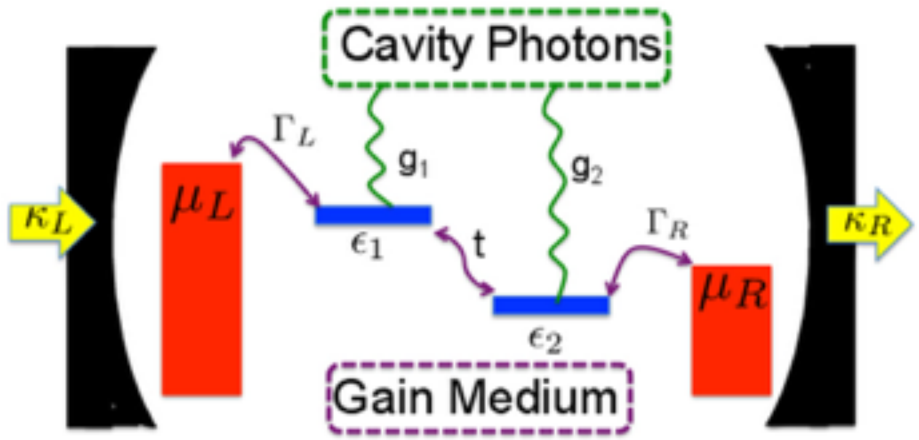
Nonequilibrium Green's function method for quantum thermal transport",
J.-S. Wang, Bijay. K. Agarwalla, Huanan Li, and J. Thingna **Front. Physics 9, 673 (2014)**

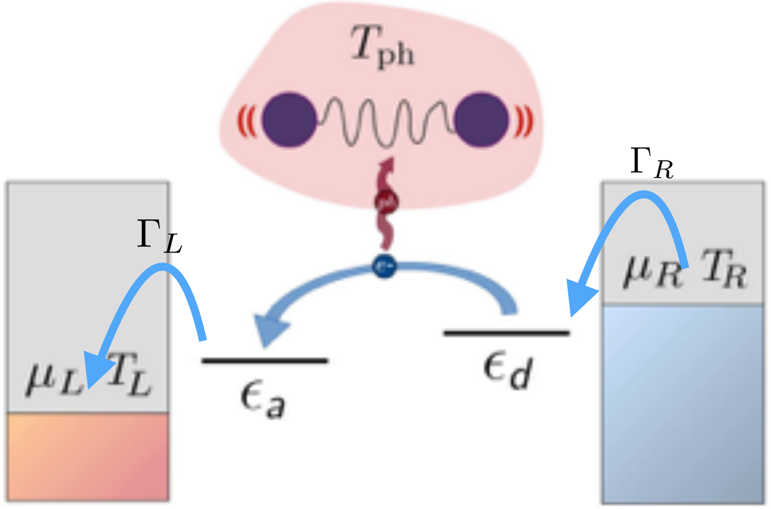
Vibrational heat transport in molecular junctions,
D. Segal, Bijay, K, Agarwalla , **Ann. Rev. Phys. Chem 67, 185 (2016)**.

Computational Tools: (Exact)

Iterative Influence Functional Path-Integral Approach (**Ongoing**),
HEOM, QMC

Plan of the talk



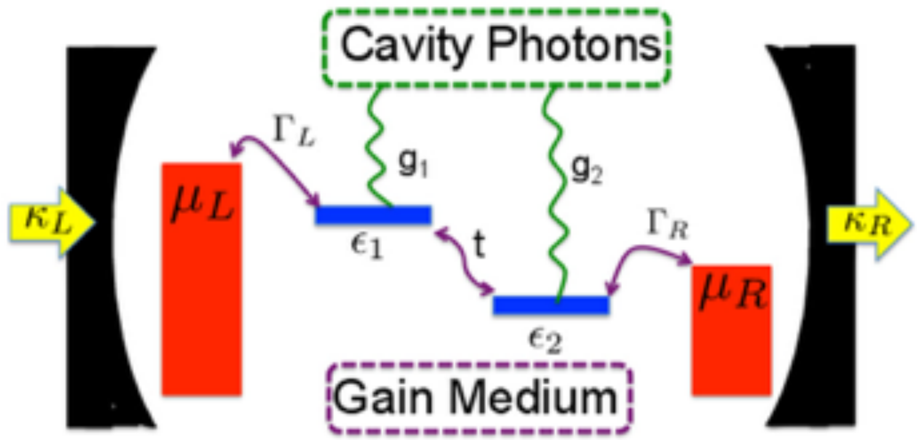


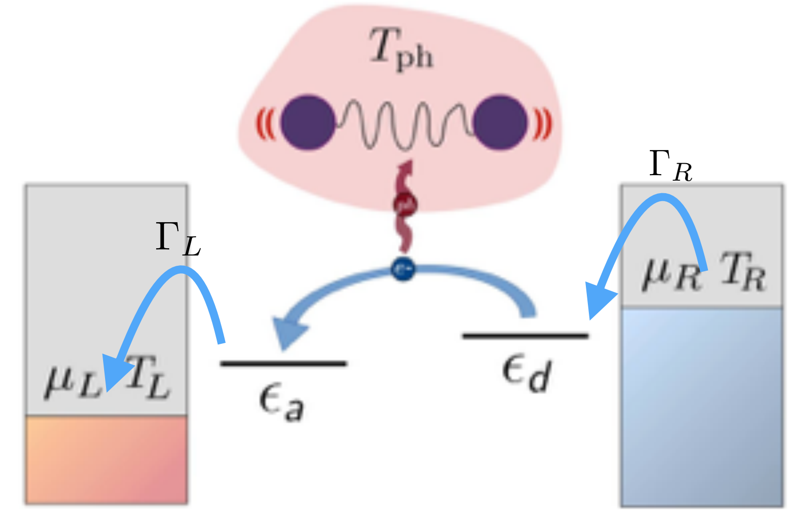
- Hybrid (light + matter) Quantum systems: Photon Amplifier
  CIRCUIT QUANTUM ELECTRODYNAMICS

- Quantum Transport :
  1. Fluctuation relations
  2. Vibrationally assisted charge transport
  3. Numerically exact path integral approach

- Conclusion

Plan of the talk





- Hybrid (light + matter) Quantum systems: Photon Amplifier

  CIRCUIT QUANTUM ELECTRODYNAMICS

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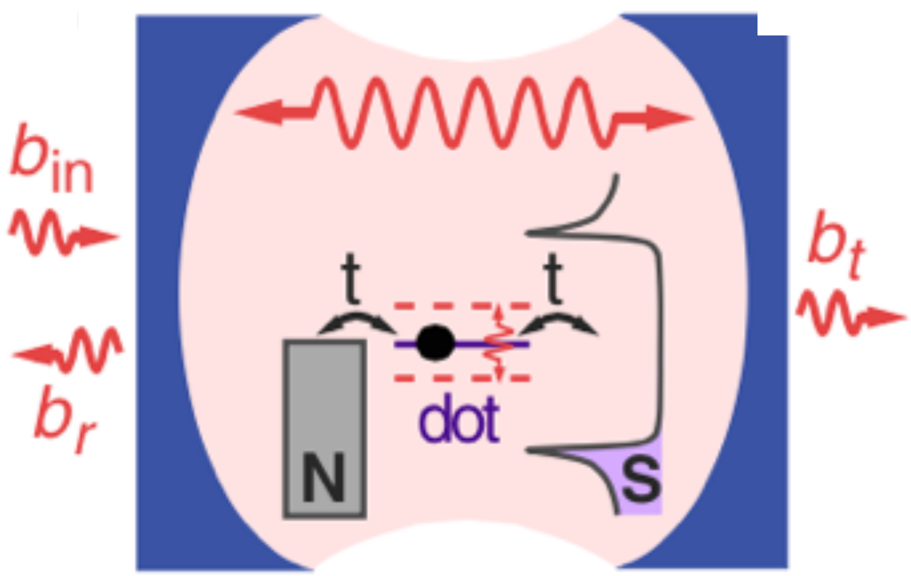
Circuit Quantum Electrodynamics Experiments

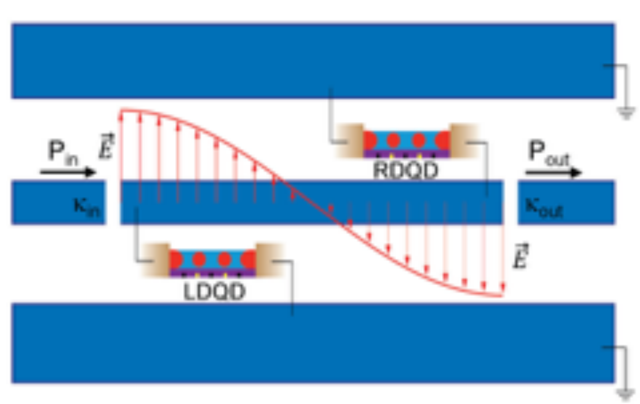
- Experiments are widely tunable: Access to new parameter regimes



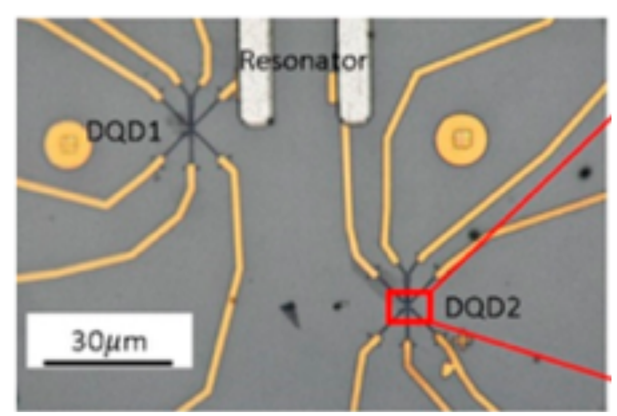
…Cottet et al Phys. Rev. X **6**, 021014 (2016)

Excellent test bed to answer fundamental questions in quantum optics and quantum impurity systems

- Different circuit geometries : Versatile nano fabrication techniques



.. Petta et al. Science **347**, 285 (2015)



Deng et al. Nano Lett. 15, 6620 (**2015**),

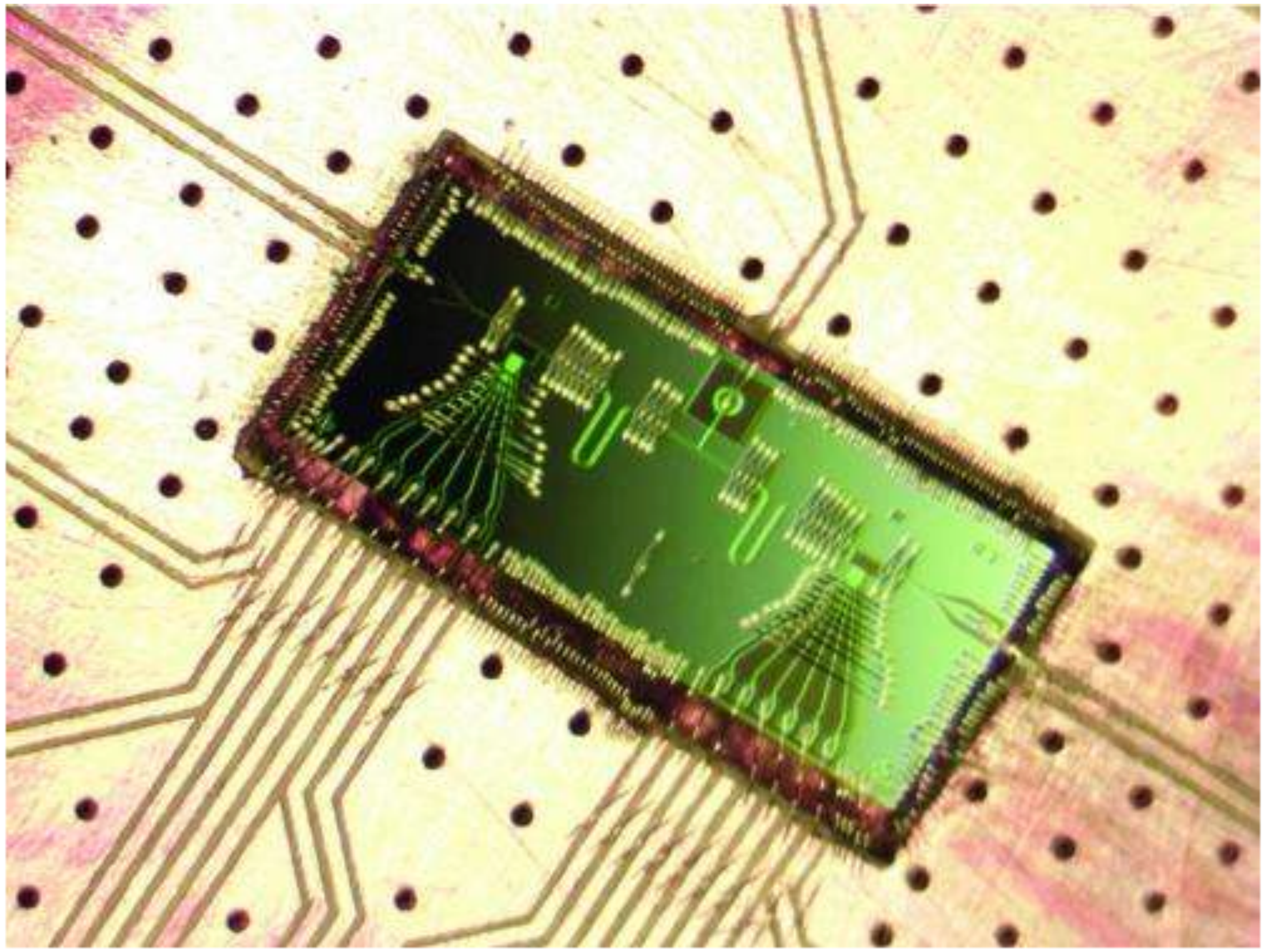
photon mediated coupling between two distant quantum dots

- Various types of Fermionic contacts: *Normal, Superconducting, Ferromagnetic*

NEWS

Rice-sized laser, powered one electron at a time, bodes well for quantum computing

January 15, 2015



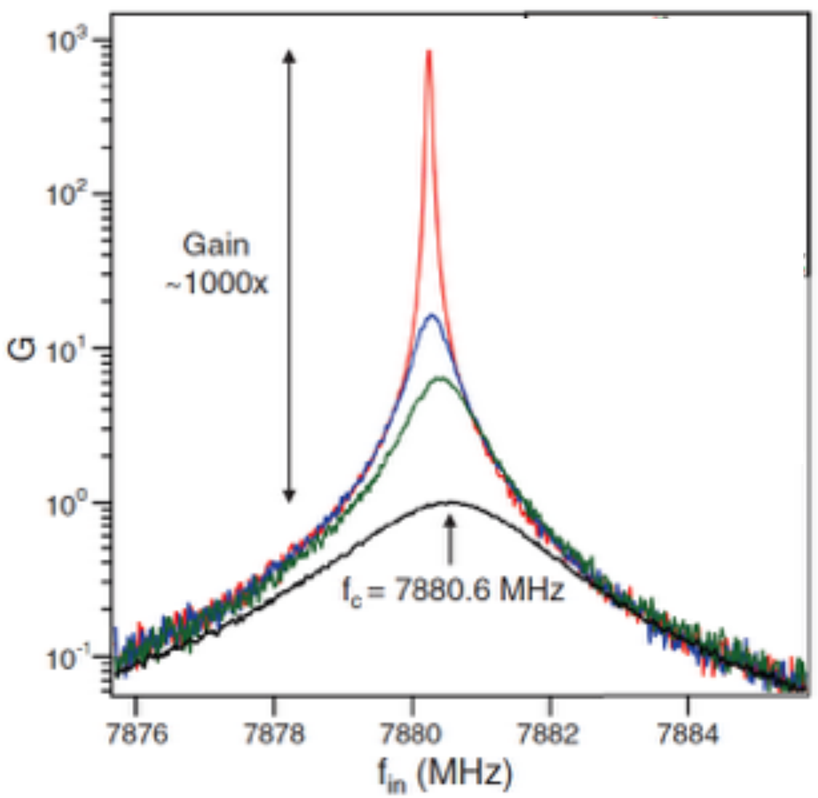
Princeton University researchers have built a rice grain-sized microwave laser. Credit: Jason Petta, Princeton University

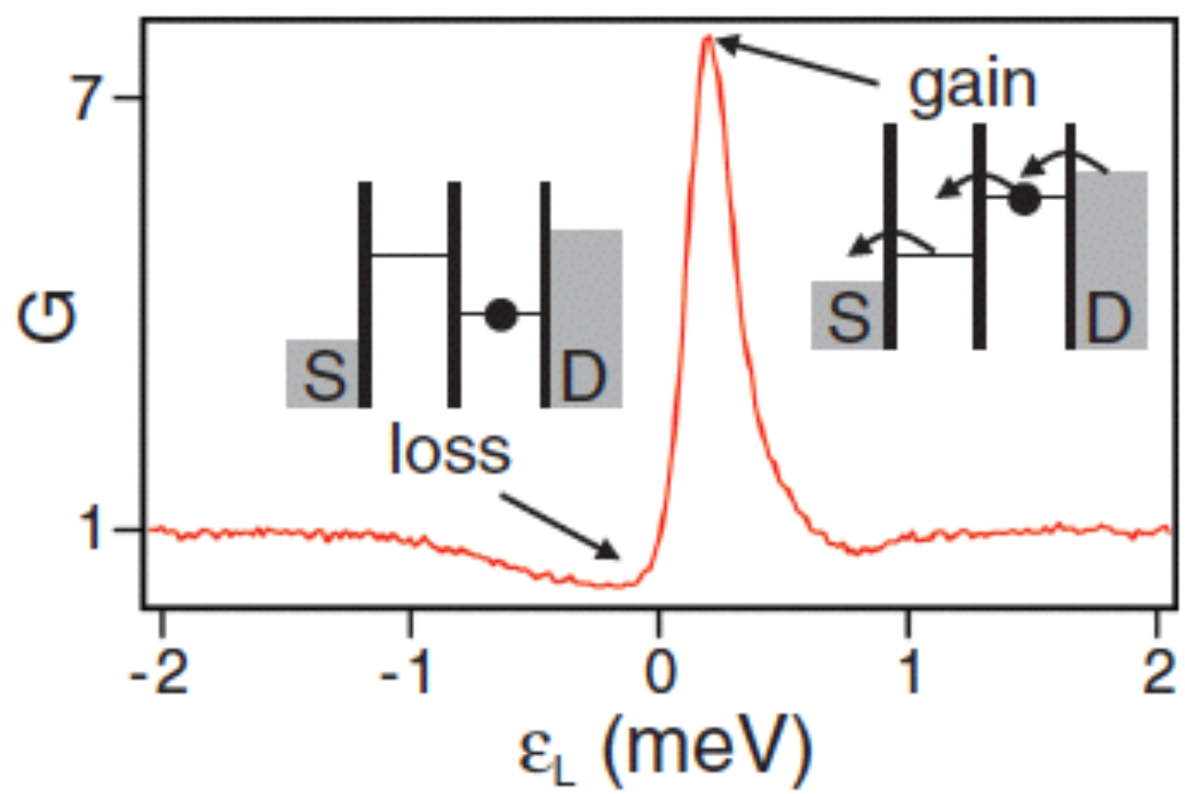
Science **347**, 285 (2015)

Petta's lab Princeton

Photonic Measurements:

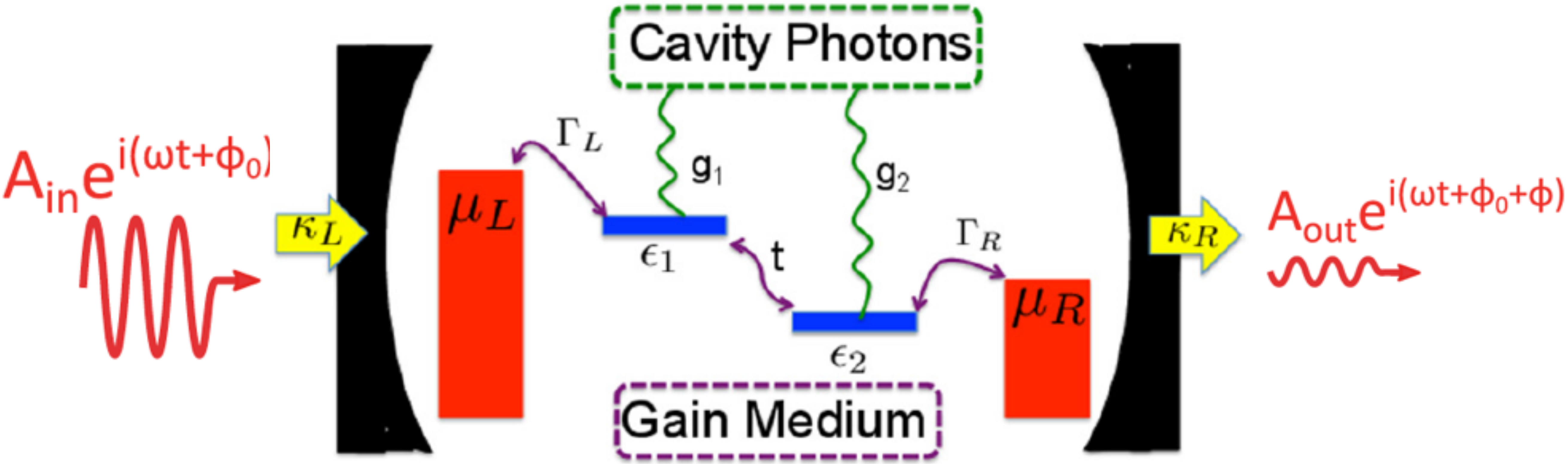
- **Photon Transmission (Gain)**
- Emission Spectrum
- Phase Response (**information about electronic charge susceptibility**)
- Photon Statistics





Liu et. al. Science **347**, 285 (2015)

DQD circuit-QED setup

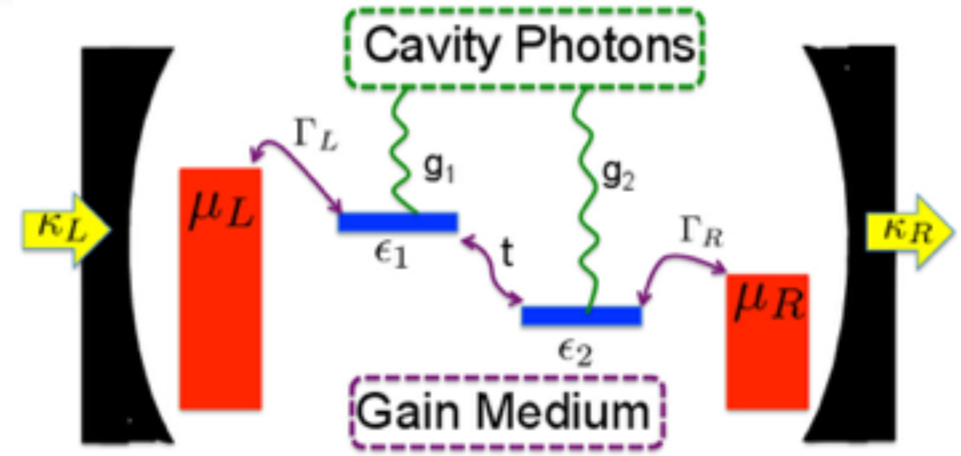


Double Quantum Dot c-QED setup

Agarwalla, Kulkarni, Mukamel, Segal
Phys. Rev. B, **94**, 035434 (2016)

Model Hamiltonian

$$\hat{H}_T = \hat{H}_{el} + \hat{H}_{ph} + \hat{H}_{el-ph}$$



Electronic part:

$$\hat{H}_{el} = \underbrace{\epsilon_1 \hat{c}_1^\dagger \hat{c}_1 + \hat{c}_2^\dagger \hat{c}_2 + t(\hat{c}_1^\dagger \hat{c}_2 + h.c)}_{\text{Double quantum dot}} + \underbrace{\hat{H}_B}_{\text{Fermionic baths}} + \underbrace{\hat{H}_{SB}}_{\text{system-bath coupling}}$$

Photonic part:

$$\hat{H}_{ph} = \underbrace{\omega_0 \hat{a}^\dagger \hat{a}}_{\text{Cavity mode}} + \sum_{j \in K} \underbrace{\omega_{jK} \hat{a}_{jK}^\dagger \hat{a}_{jK}}_{\text{Transmission line}} + \sum_{j \in K} \nu_j \underbrace{\hat{a}_{jK}^\dagger \hat{a} + \text{H.c.}}_{\text{Coupling}}$$

Light-Matter coupling: (Dipole-coupled)

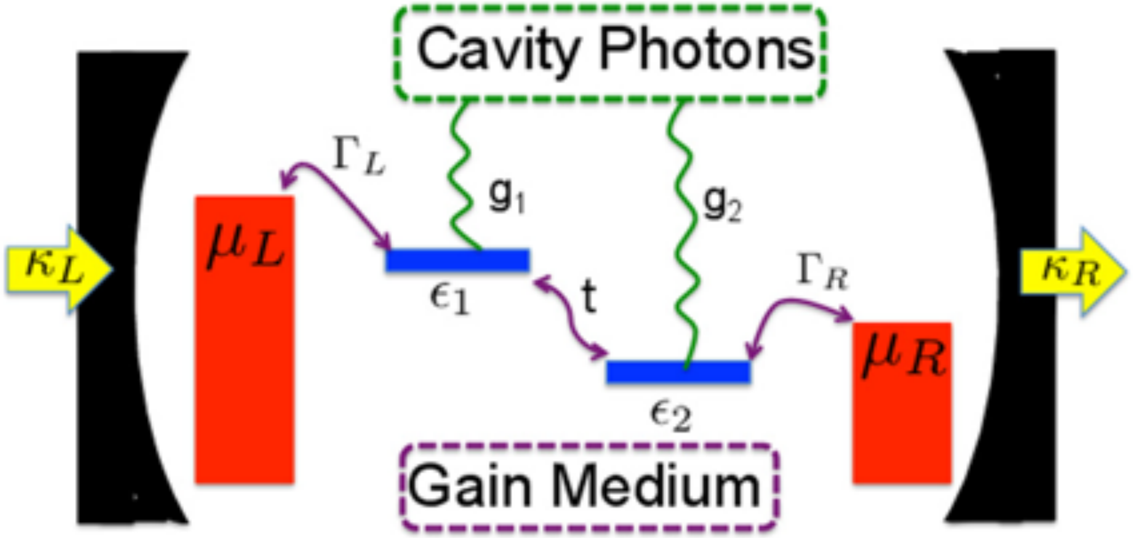
$$\hat{H}_{el-ph} = g(\hat{c}_1^\dagger \hat{c}_1 - \hat{c}_2^\dagger \hat{c}_2)(\hat{a}^\dagger + \hat{a})$$

$\boxed{\text{Experiments: Coupling strength is typically weak}}$

Quantities of Interest

Photon Green's function (contour-ordered) :

$$\boxed{D(\tau,\tau') \equiv -i\langle T_c \hat{a}(\tau)\hat{a}^{\dagger}(\tau')\rangle}$$



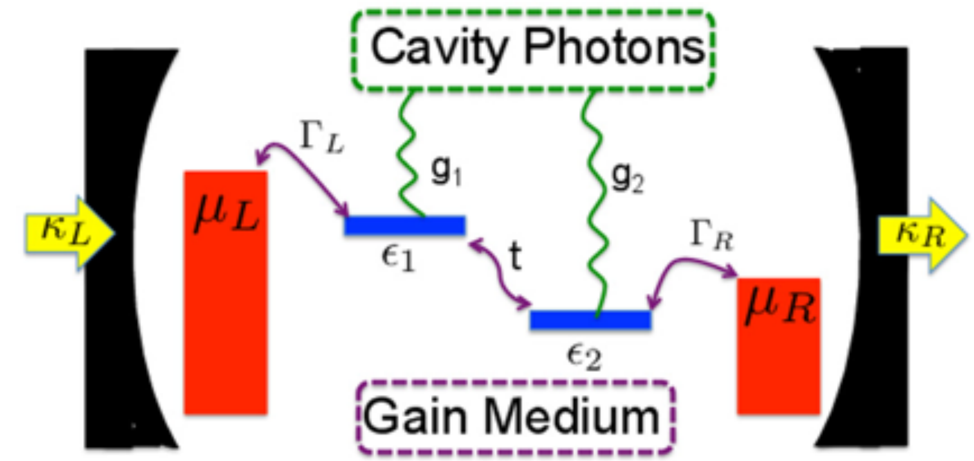
Photon Number: $\langle \hat{n}_c\rangle \equiv i\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}D^{<}(\omega)$

Power Spectrum: $S(\omega) = \int_{-\infty}^{\infty} dt\,\langle \hat{a}^{\dagger}(0)\hat{a}(t)\rangle e^{i\omega t} = i\,D^{<}(\omega)$

Transmission and phase Response: $t(\omega) = i\kappa\, D^{r}(\omega) = |t(\omega)|\, e^{i\phi(\omega)}$

Gain in photon $\Rightarrow$ $|t(\omega)| > 1$

Keldysh NEGF Diagrammatic approach



Dyson Equation for Photon Green's functions:

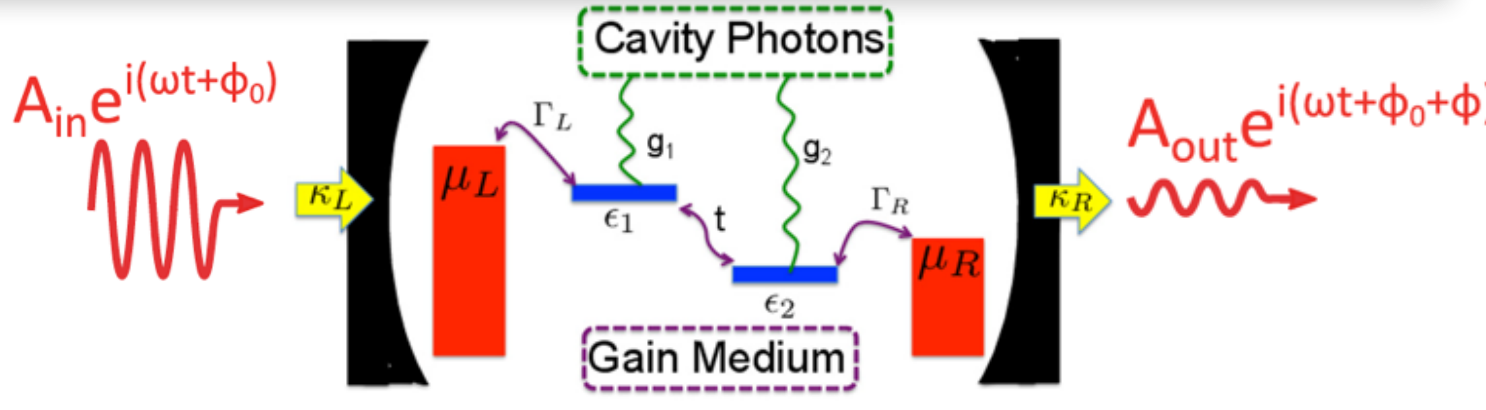
$$D(\tau,\tau') = D_0(\tau,\tau') + \int d\tau_1 \int d\tau_2 D_0(\tau,\tau_1) F_{el}(\tau_1,\tau_2) D(\tau_2,\tau')$$

$$F_{el}(\tau_1,\tau_2) = -i\langle T_c n(\tau_1) n(\tau_2)\rangle$$

density-density correlation function

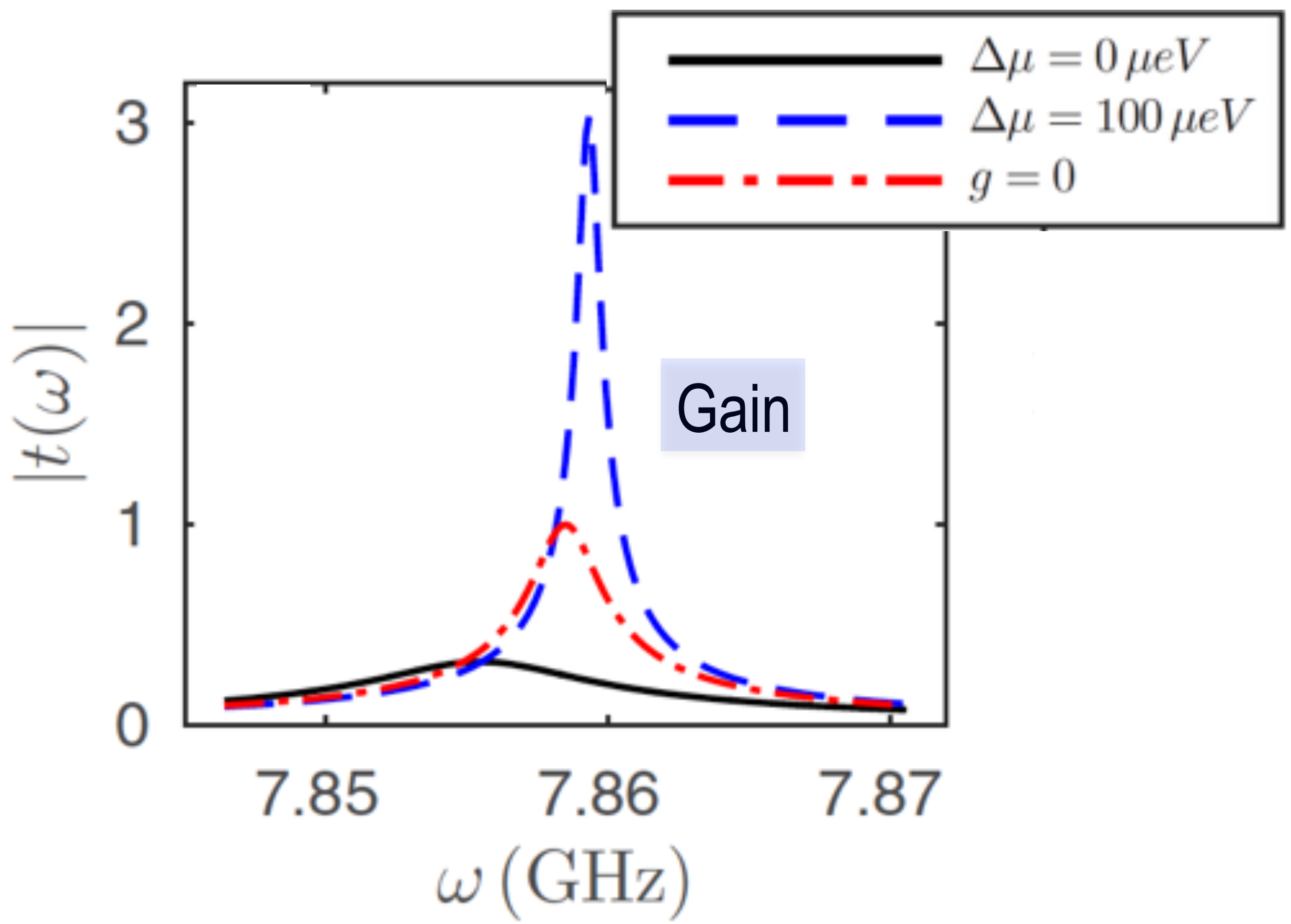
$$F^r_{el}(t-t') \propto -i\theta(t-t')\langle [n(t), n(t')]\rangle_{el}$$

- Retarded Component: **Non-equilibrium charge susceptibility**



- **Transmission (GAIN)**

$$t(\omega) \equiv i\kappa D^r(\omega) = \frac{i\kappa}{(\omega - \omega_0 - F'_{el}(\omega)) + i(\kappa - F''_{el}(\omega))} \qquad (\kappa > F''_{el}(\omega))$$



- **Exact Result (NEGF):**

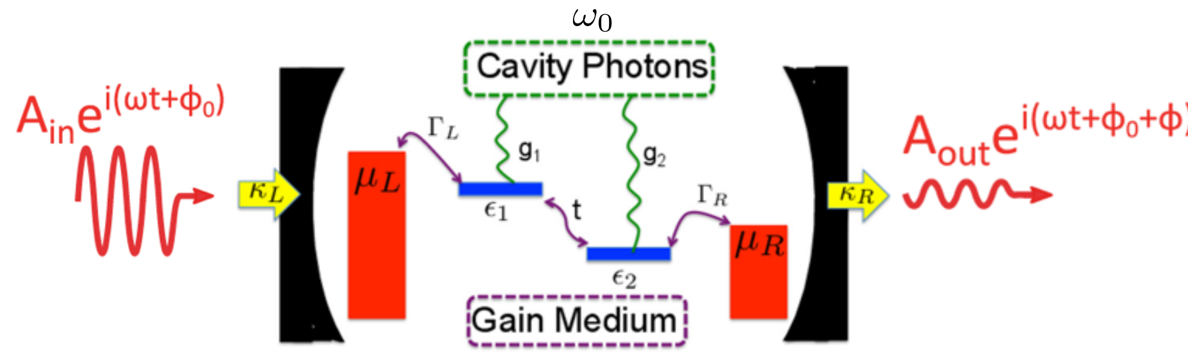
Sum Rule for Transmission

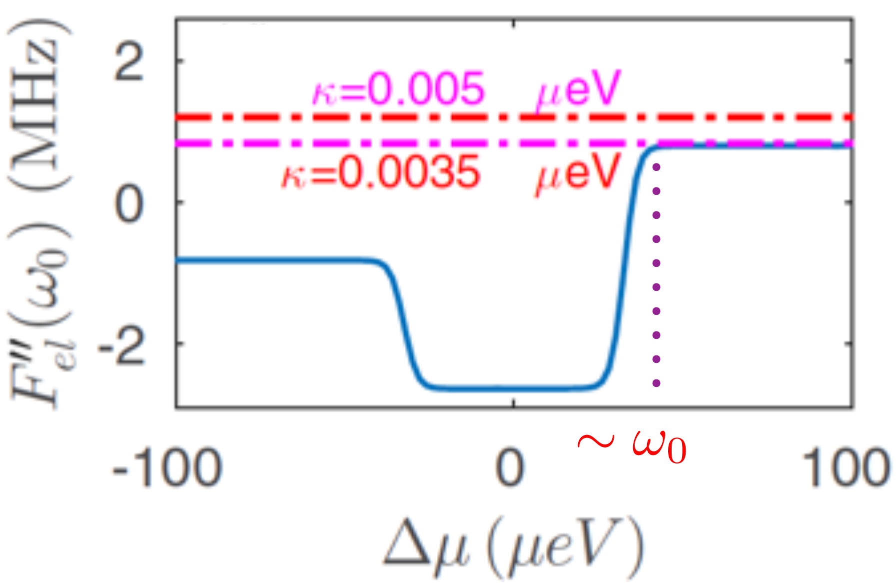
$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, t(\omega) = \frac{\kappa}{2}$$

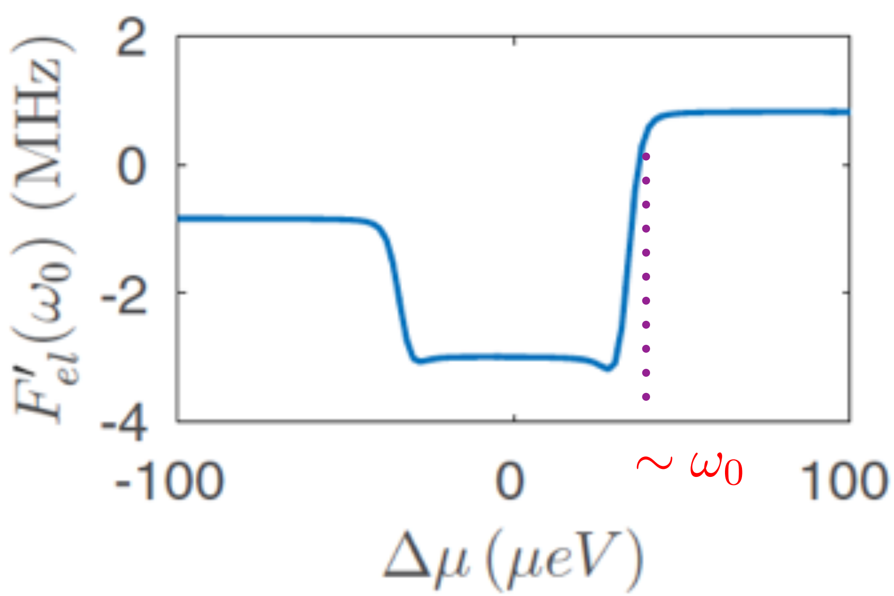
B. K. Agarwalla, M. Kulkarni, S. Mukamel, D. Segal, Phys. Rev. B, **94**, 035434 (2016)
B. K. Agarwalla, M. Kulkarni, S. Mukamel, D. Segal, Phys. Rev. B, **94**, 121305 **(R)** (2016)

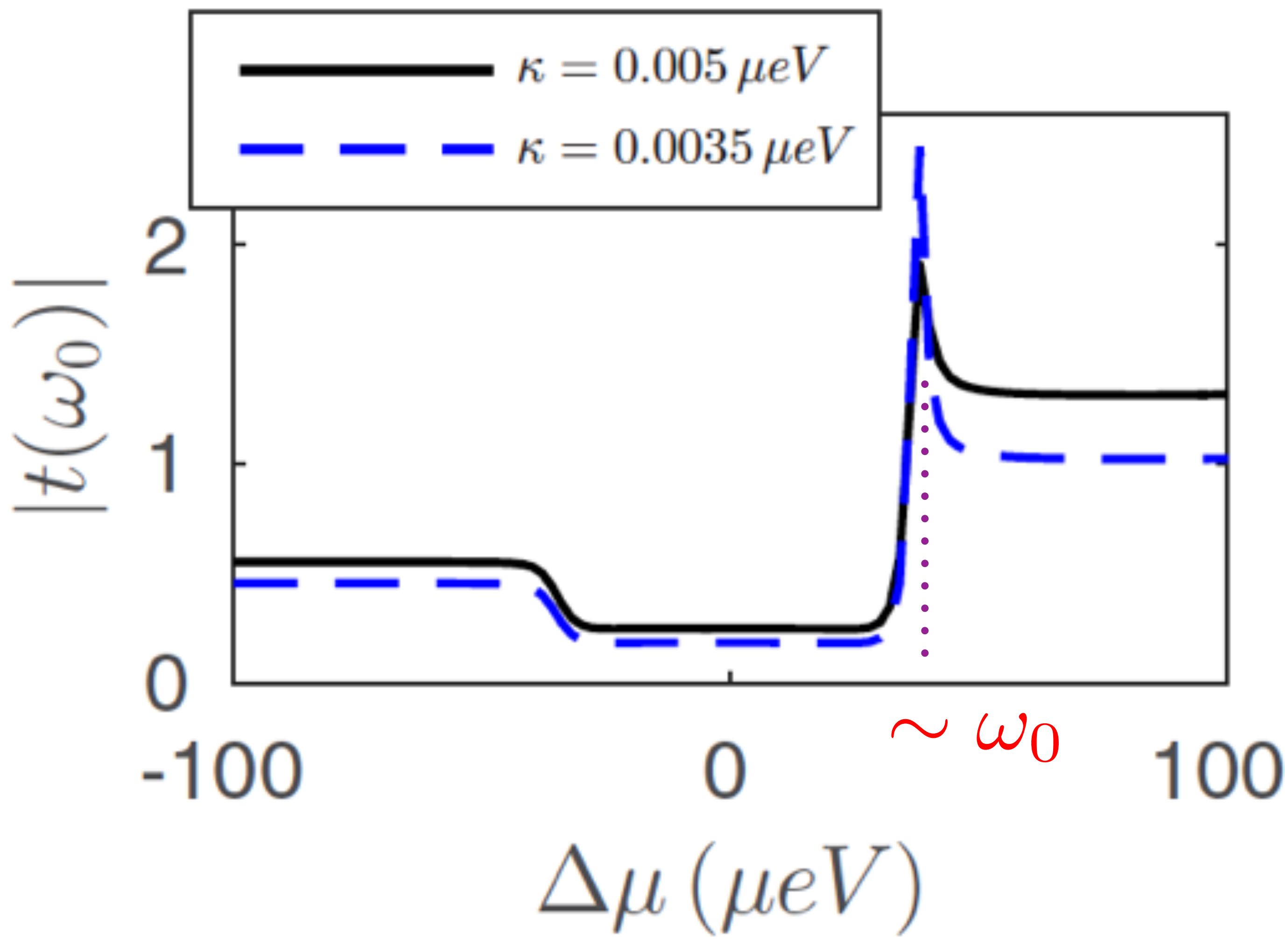
Photon Transmission

$$|t(\omega_0)| = \frac{\kappa}{\{[F'_{el}(\omega_0)]^2 + [F''_{el}(\omega_0) - \kappa]^2\}^{1/2}}$$

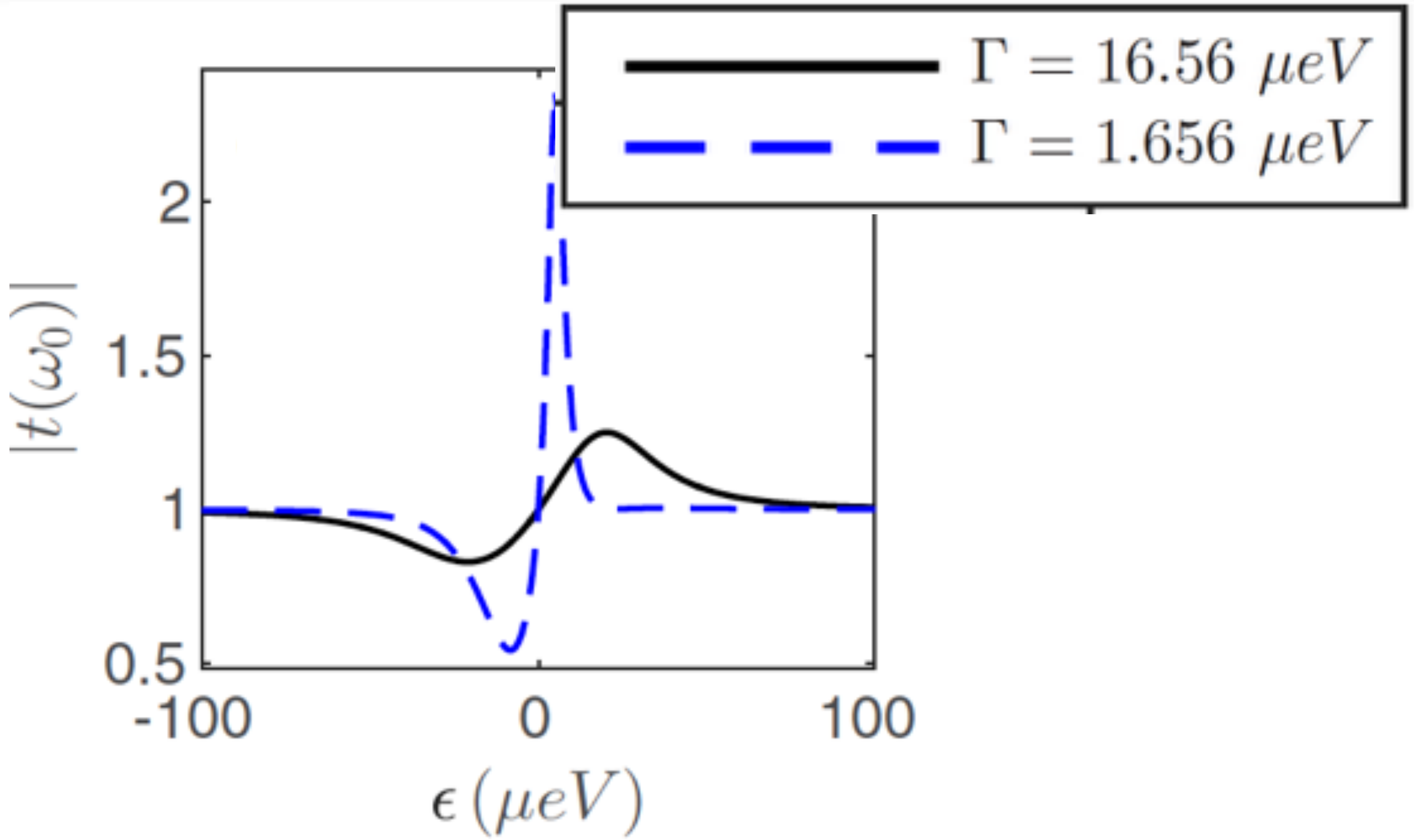


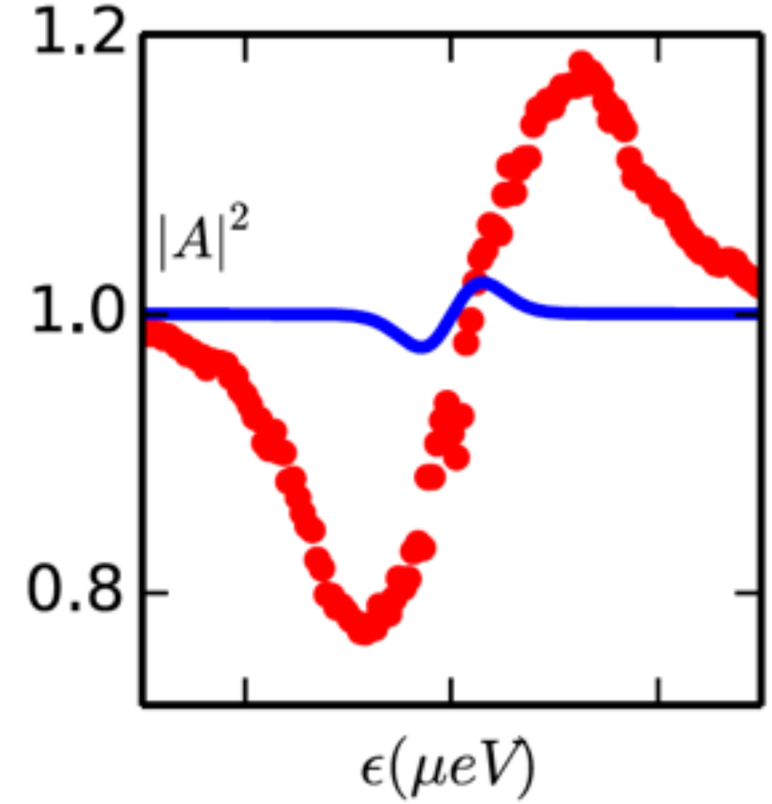






Photon Transmission

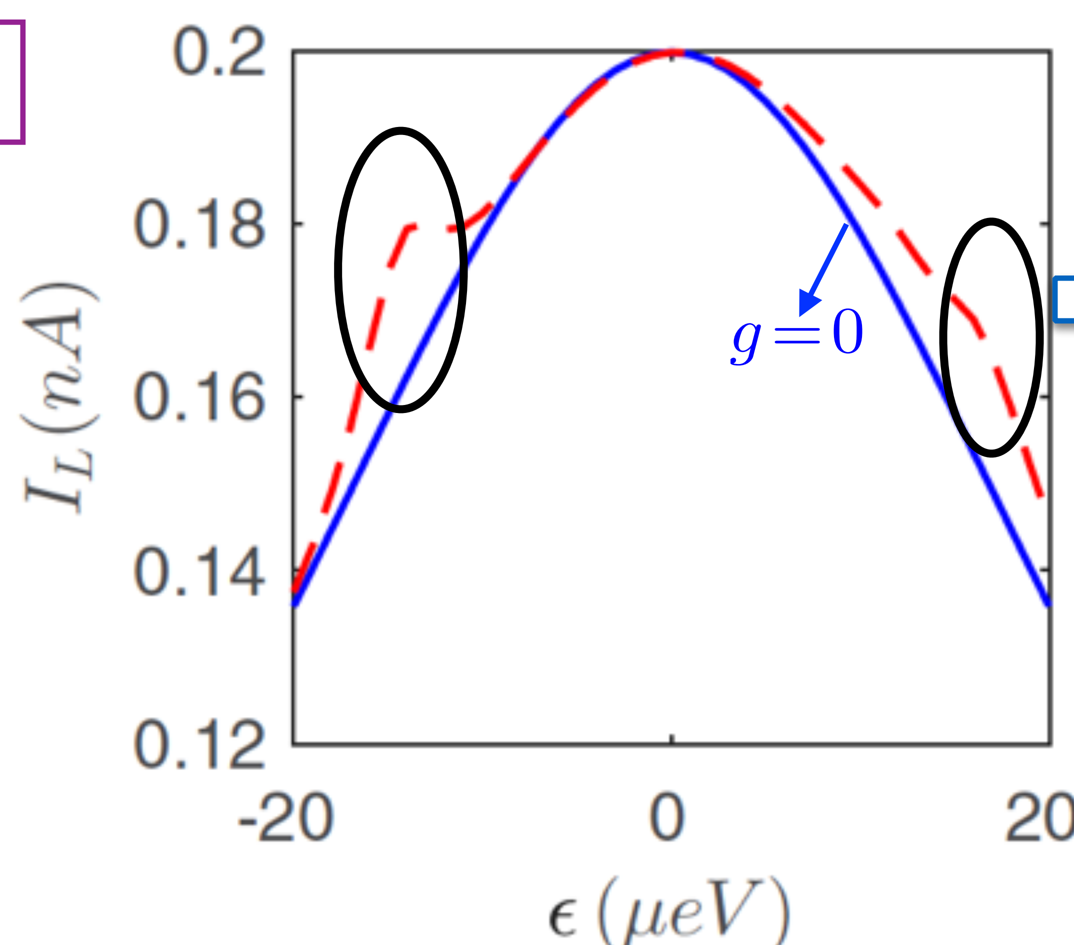




Princeton Experiment (Red)

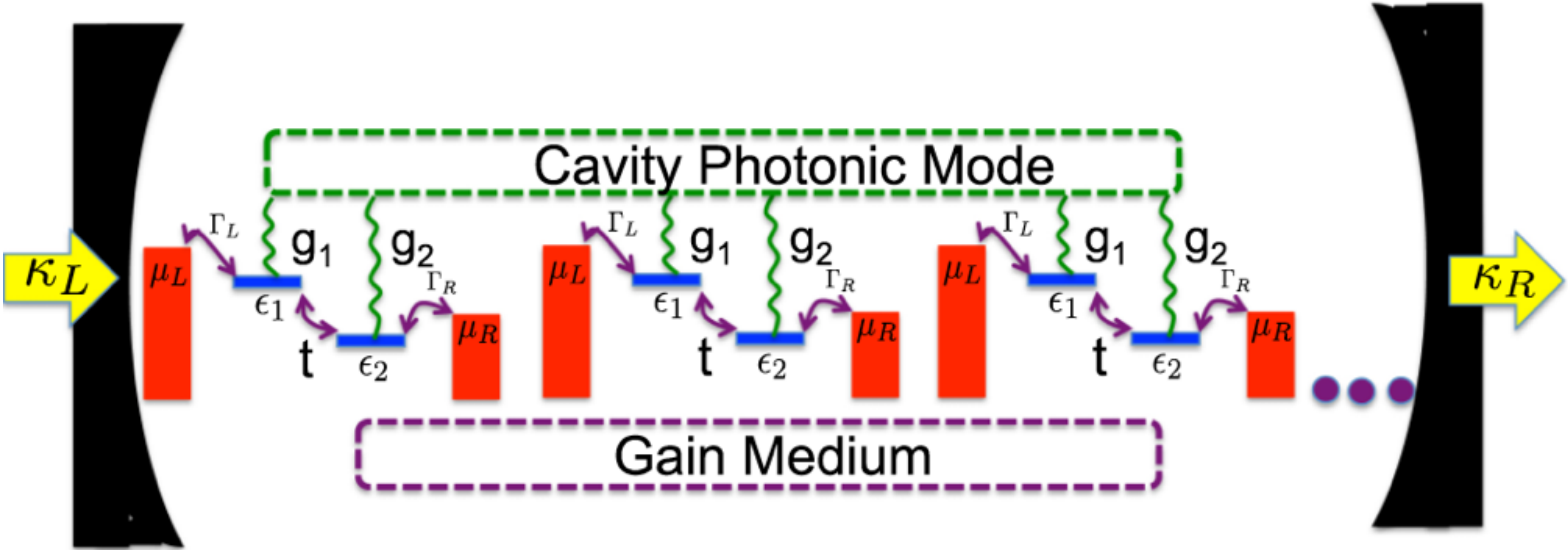
Kulkarni et al PRB (2014)

Electronic Current:



Photon assisted transport

N-DQD Circuit-QED



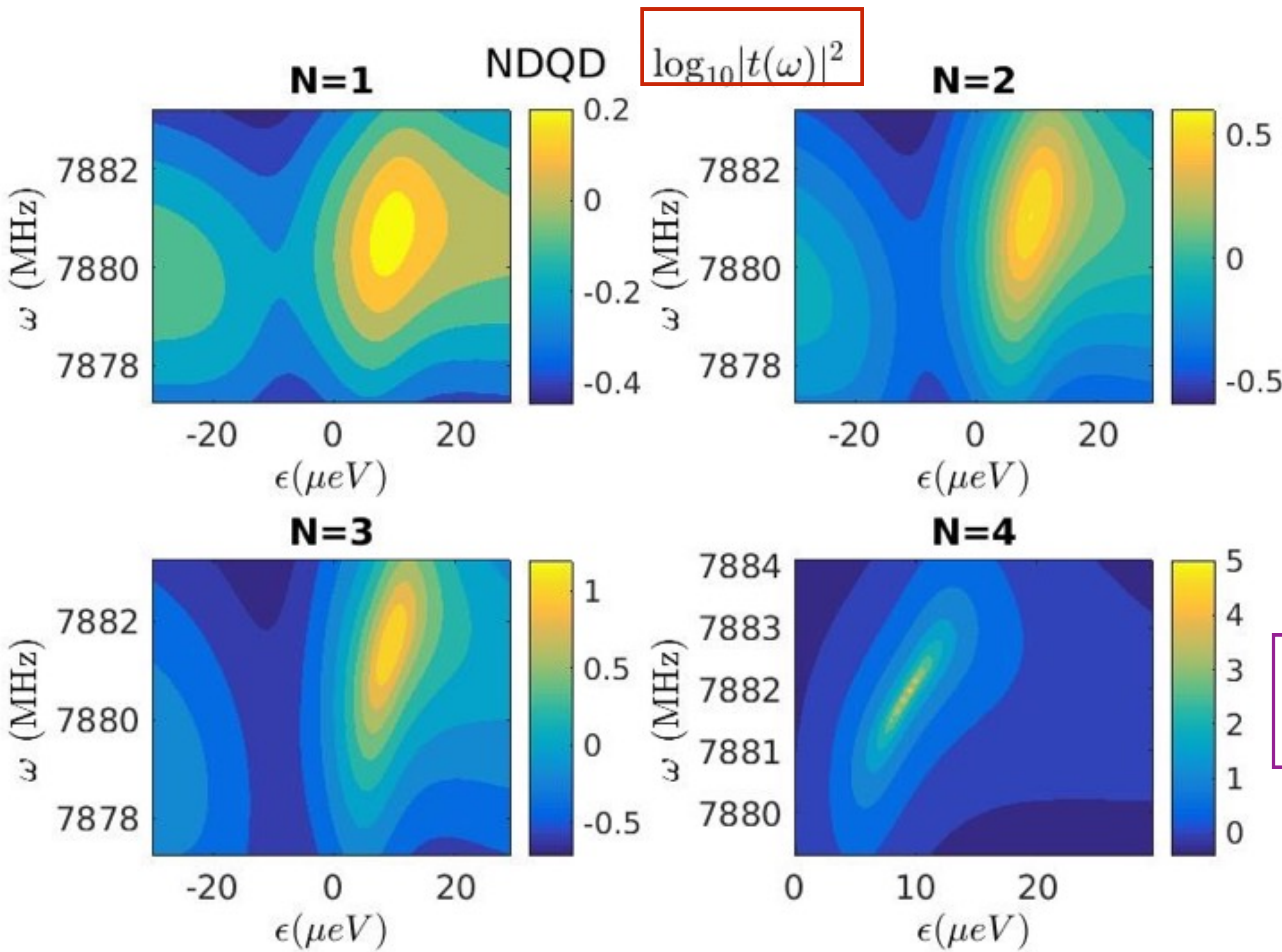
N- Double Quantum Dot Circuit-QED setup

Agarwalla et. al Phys. Rev. B, **94**, 121305 **(R)** (2016)

Principle for Giant Photon Gain

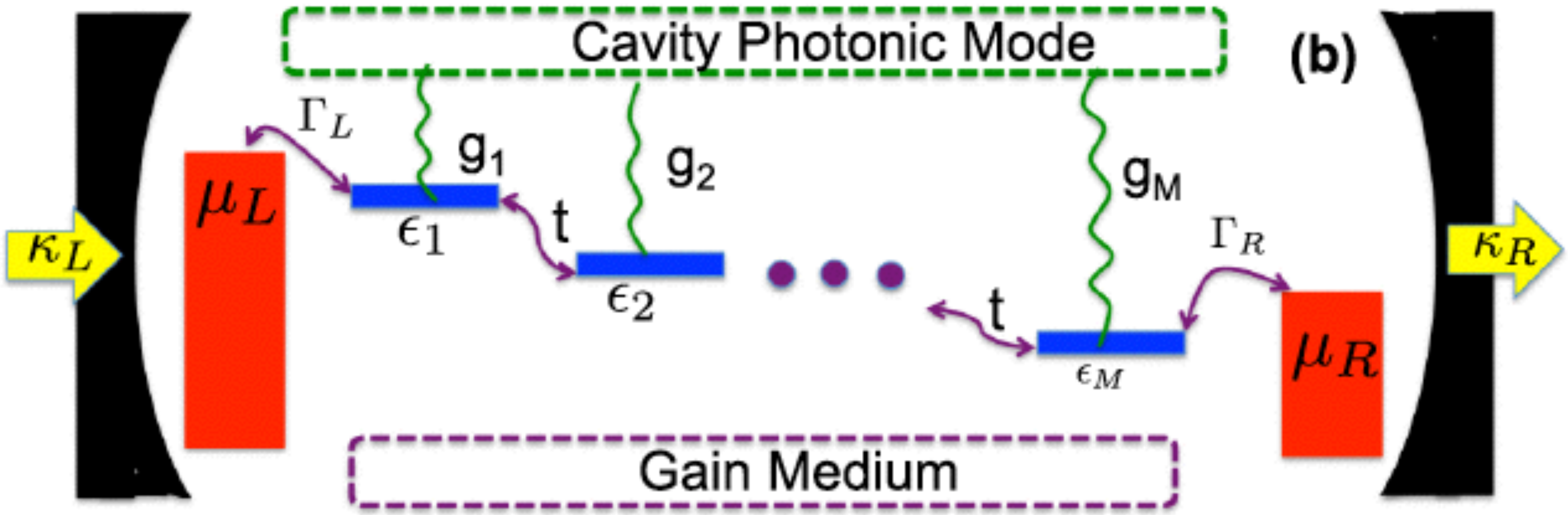
$$t(\omega) = \frac{i\kappa}{(\omega - \omega_0 - N F'_{el}(\omega)) + i(\kappa - N F''_{el}(\omega))}$$

Extensive Scaling

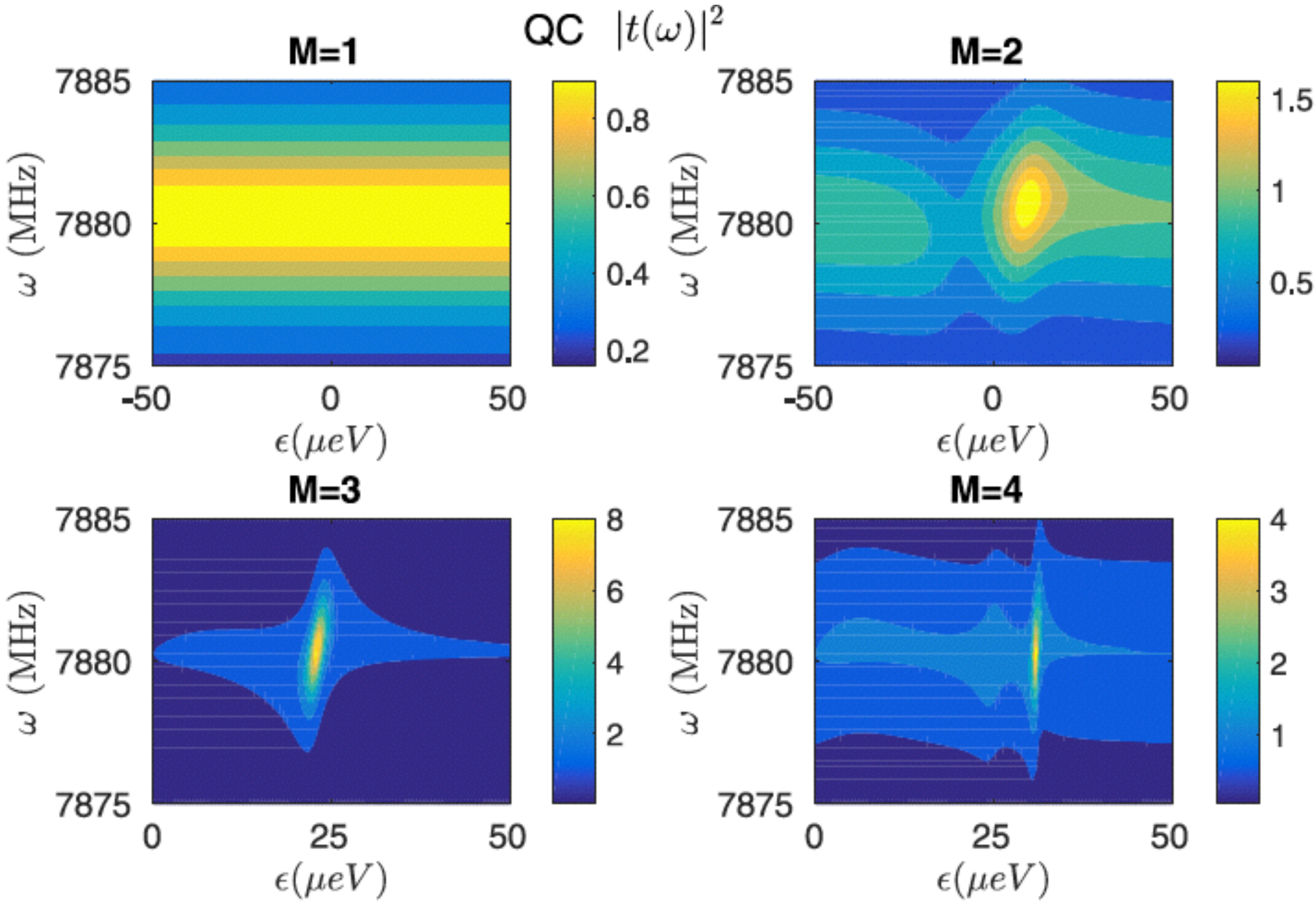


Agarwalla, Kulkarni, Mukamel, Segal, PRB, **94**, 121305 **(R)** (2016)

Quantum Cascade Laser



Agarwalla et. al Phys. Rev. B, **94**, 121305 **(R)** (2016)


QC $|t(\omega)|^2$
M=1
M=2
M=3
M=4
7885
7880
7875
ω (MHz)
-50
0
50
25
$\epsilon(\mu eV)$
0.8
0.6
0.4
0.2
1.5
1
0.5
8
6
4
2
3

Summary I:

- DQD electronic system can serve as a gain medium for the cavity photons
- **Principle for Gain**: Imaginary component of charge density response should counteract the cavity decay rate $F''_{el}(\omega) \Rightarrow \kappa$
- **Emission Spectrum**

$$S(\omega) = i\frac{N\, F^{<}_{el}(\omega)}{\left[\omega - \omega_c - N\, F'_{el}(\omega)\right]^2 + \left[\kappa - N\, F''_{el}(\omega)\right]^2}$$

- **Mean photon number**

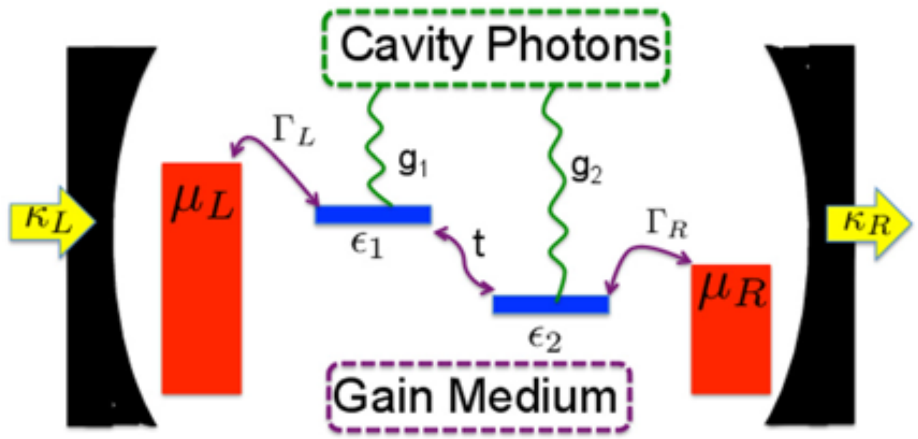
$$\langle \hat{n}_c \rangle = \frac{i\, N\, F^{<}_{el}(\omega_c)}{2\left[\kappa - N\, F''_{el}(\omega_c)\right]}$$

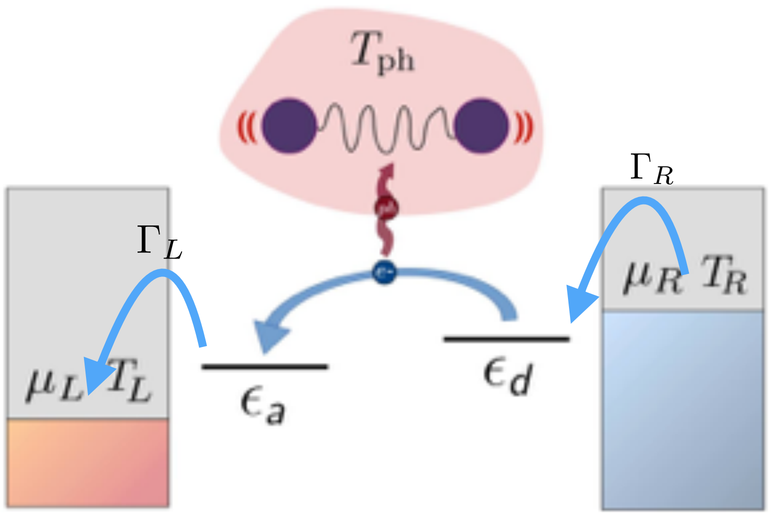
Future prospects:

Going beyond the threshold— masing regime

Effect of electron-phonon coupling

Plan of the talk





- Hybrid (light + matter) Quantum systems: Photon Amplifier
  CIRCUIT QUANTUM ELECTRODYNAMICS

- Quantum Transport :
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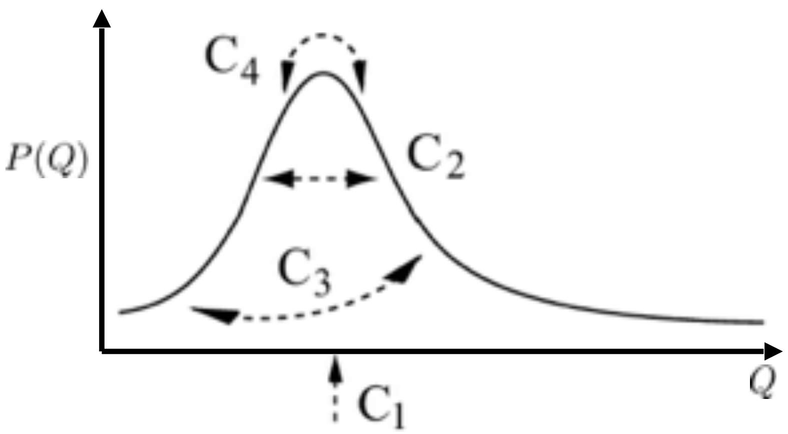
- Conclusion

What is Full-Counting Statistics (FCS)?

- **Full probability distribution** of transferred charge, heat, in a given time interval
- Origin of FCS - Quantum optics (Photon counting)



Cumulants

- 1st cumulant – mean: $C_1 = \langle Q \rangle$.
- 2nd cumulant – Variance : $C_2 \equiv \langle\langle Q^2 \rangle\rangle = \langle (Q - \langle Q \rangle)^2 \rangle$.
- 3rd cumulant – Skewness: $C_3 = \langle\langle Q^3 \rangle\rangle = \langle (Q - \langle Q \rangle)^3 \rangle$.

- Instead of the distribution we often look at the characteristic function

$$\mathcal{Z}(\lambda) = \int dQ\, P(Q)\, e^{i\lambda Q}$$

$$\langle\langle Q^m \rangle\rangle = \frac{\partial^m \ln \mathcal{Z}(\lambda)}{\partial (i\lambda)^m}\Big|_{\lambda=0}$$

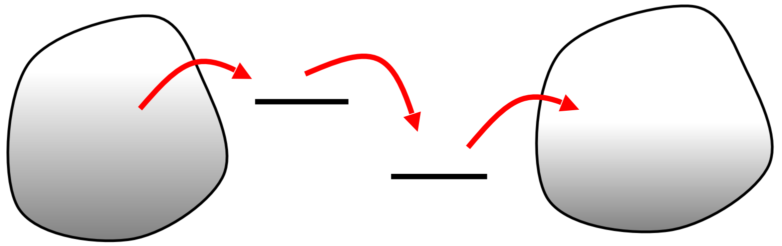
Cumulant generating function

Fluctuation Relations: Microscopic statement of second law

- Charge transport

$$n = \int I_{el}(\tau)d\tau \quad \text{stochastic variable}$$

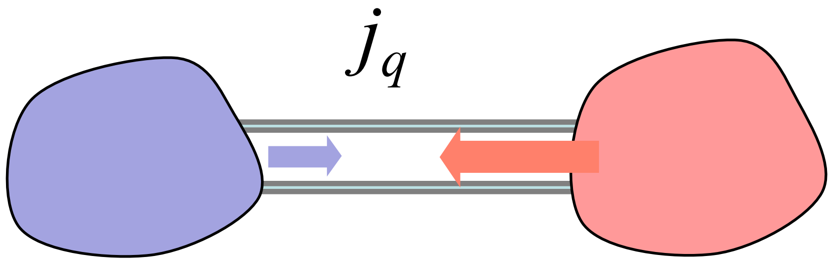
$$\ln\left[\frac{P_t(+n)}{P_t(-n)}\right] = \beta(\mu_L - \mu_R)n$$



- Heat transport

$$Q = \int I_Q(\tau)d\tau \quad \text{stochastic variable}$$

$$\ln\left[\frac{P_t(+Q)}{P_t(-Q)}\right] = (\beta_R - \beta_L)Q$$



- General results: $$\ln\left[\frac{P_t(+S)}{P_t(-S)}\right] = S$$ total entropy production

Proof of fluctuation relations

- Microscopic reversibility of the underlying Hamiltonian dynamics
- Initial condition, typically taken in canonical form

Fluctuation Relations: Microscopic statement of second law

$$\ln\left[\frac{P_t(+S)}{P_t(-S)}\right] = S \quad \Longrightarrow \quad \mathcal{Z}(\lambda) = \int dS e^{i\lambda S} P(S)$$

Characteristic function

$$P(S) = e^S P(-S) \;\leftrightarrow\; \mathcal{Z}(\lambda) = \mathcal{Z}(-\lambda + i)$$

$\mathrm{Gallavotti-Cohen\ fluctuation\ symmetry}$

$$1 = \langle e^{-S} \rangle \xrightarrow{e^{\langle x \rangle} \leq \langle e^x \rangle} \langle S \rangle \geq 0$$

$\mathrm{Second\ law\ of\ thermodynamics!}$

- Familiar inequalities of macroscopic thermodynamics are now equalities!
- Thermodynamic laws are recovered at the level of the ensemble average

M. Esposito, U. Harbola, S. Mukamel, Rev. Mod. Phys. 81, 1665 (2009).
M. Campisi, P. Hanggi, P. Talkner, Rev. Mod. Phys. 83, 771 (2011).

Thermoelectric Efficiency and Universal Statistics

Steady State Fluctuation symmetry

$$\mathcal{G}(\lambda_e, \lambda_p) = \mathcal{G}(-\lambda_e + i(\beta_L - \beta_R), -\lambda_p + i(\beta_R\mu_R - \beta_L\mu_L))$$

Affinity for Energy flux

Affinity for Particle flux

- **Fluctuations in charge and energy currents translates to fluctuations in efficiency**

$$\eta \propto \frac{\text{charge current}}{\text{heat current}} \Rightarrow$$ **stochastic quantity**

Thermoelectric device:

$$\boxed{\mathcal{G}(\lambda_w, \lambda_q) = \mathcal{G}(-\lambda_w + i\beta_L, -\lambda_q + i(\beta_L - \beta_R))}$$

B. K. Agarwalla, J.-H. Jiang, and D. Segal, PRB 92, 245418 (2015)

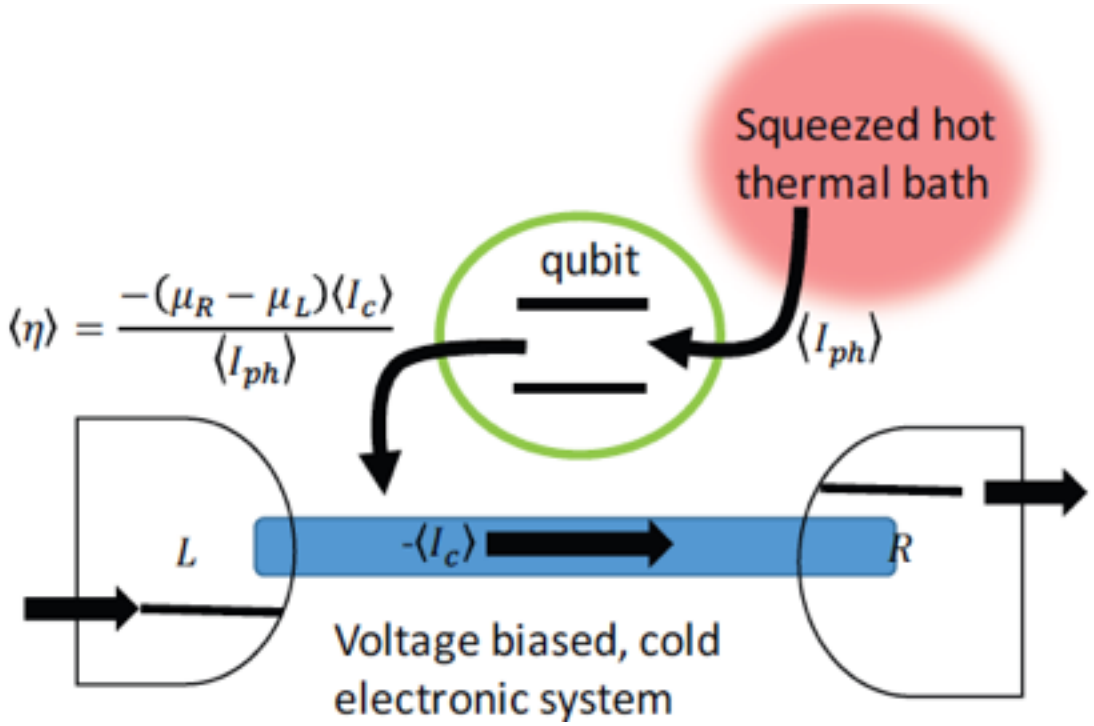
$$\lambda_w = \lambda_q = 0 \Rightarrow \boxed{\Big\langle \exp\Big[-\frac{w}{T_L} - \Big(\frac{1}{T_L} - \frac{1}{T_R}\Big)q\Big]\Big\rangle = 1}$$

Following Jensen's inequality $\langle \eta \rangle = -\langle w \rangle / \langle q \rangle \leq \eta_c$ **Upper bound of efficiency**

Thermoelectric Efficiency and Universal Statistics

- Quantum efficiency bound for heat engines for non-canonical reservoir

Agarwalla, Jiang, Segal ArXiv: 1706.06206.

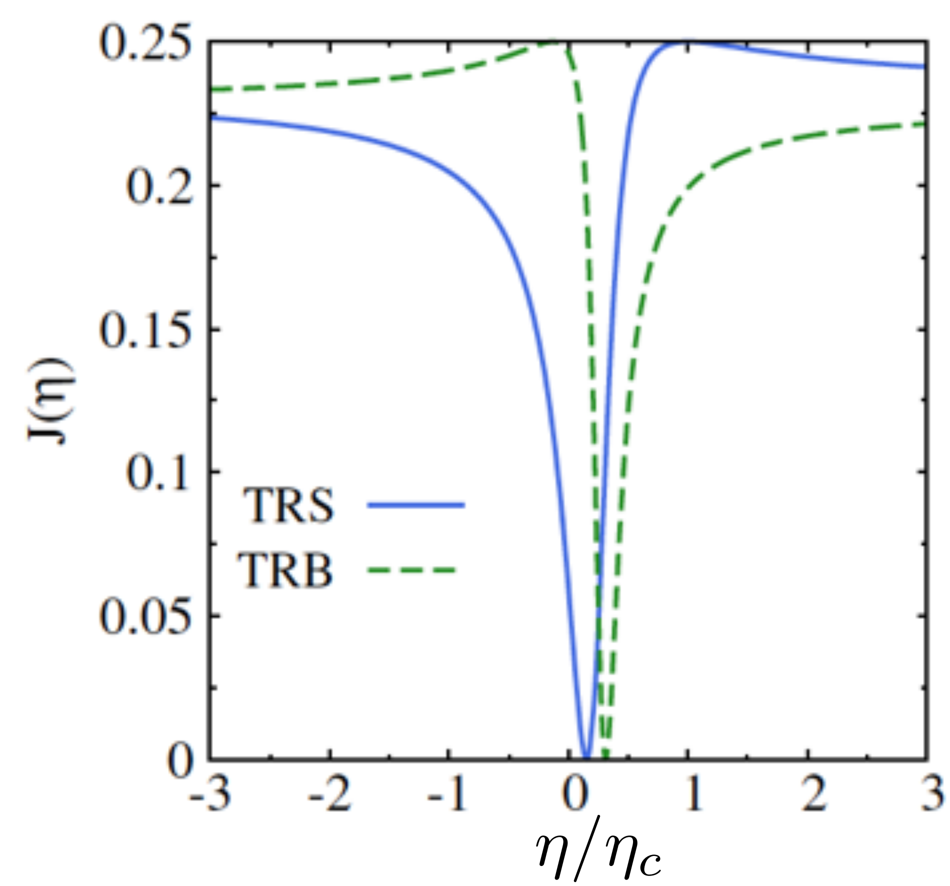


$$\langle \eta \rangle \leq 1 - \frac{\beta_{eff}}{\beta_{el}}$$

- Universality in Efficiency statistics

Verley et al. Nat. Commun. 5, 4721 (2014)

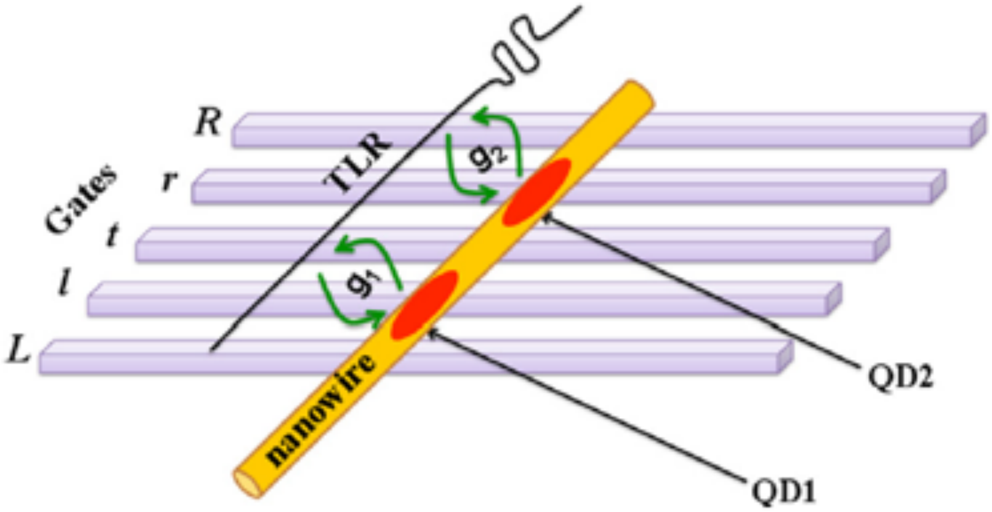
Jiang, Agarwalla, Segal Phys. Rev. Lett 115, 040601 (2015)

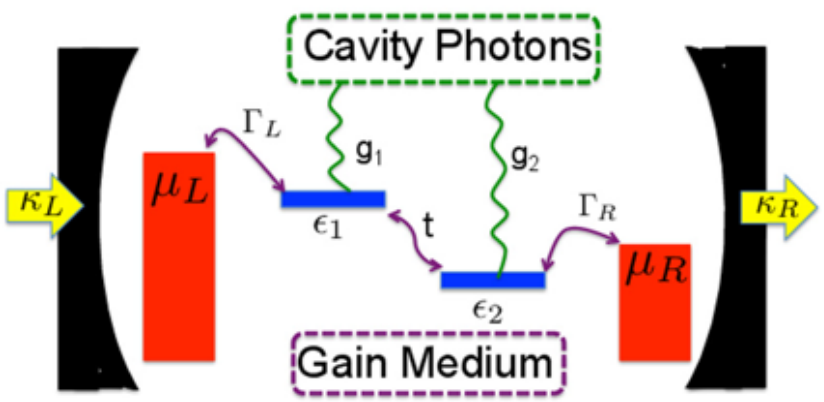


Model Variants:

Electron-Photon interaction:

Circuit-Quantum Electrodynamics

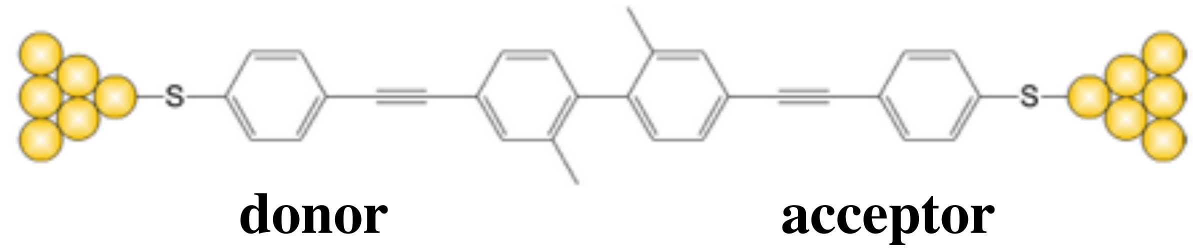




DC transport of electrons lead to photon emission: micromasers

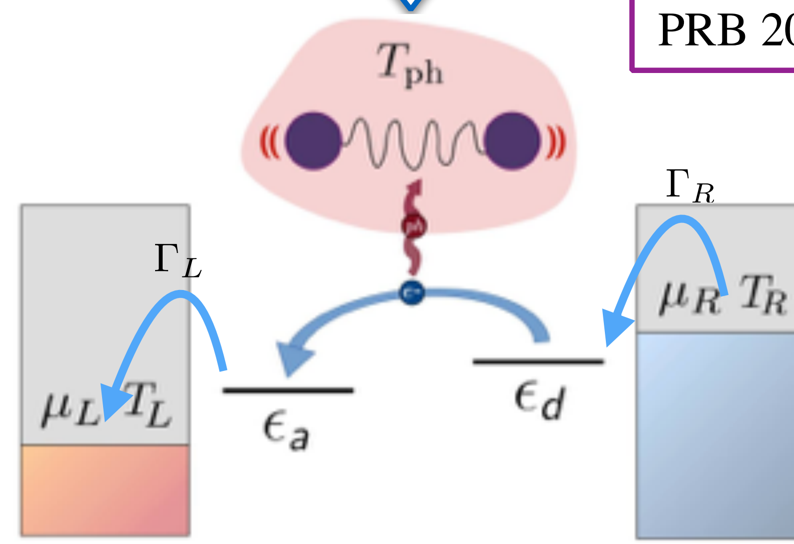
Electron-vibration interaction:

(Nano-Electromechanical system)



Ballman et al., Phys. Rev. Lett. 109, 056801 (2012)

Agarwalla et al.
PRB 2015, JCP 2016



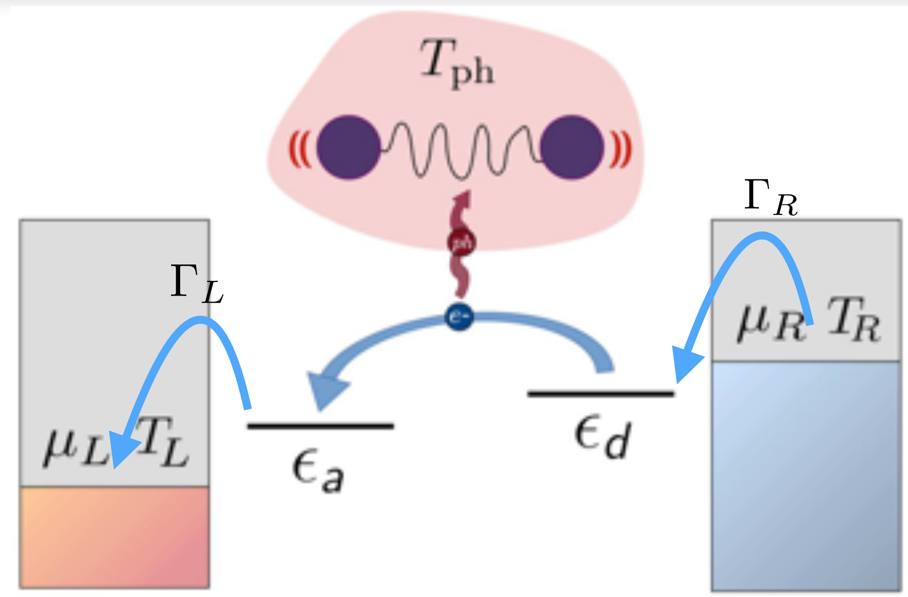
Donor-Acceptor model

Questions:

- Current statistics and fluctuation relations.
- Signature of different types vibrational modes (harmonic, anharmonic)
- **Operational questions** (diode, heating/cooling effects, thermoelectricity)

Vibrationally assisted Charge Transfer

$$\hat{H}_T = \hat{H}_{\mathrm{el}} + \hat{H}_{\mathrm{vib}} + \hat{H}_{\mathrm{el-vib}}$$



$$\hat{H}_{\mathrm{el}} = \epsilon_d \hat{c}_d^\dagger \hat{c}_d + \epsilon_a \hat{c}_a^\dagger \hat{c}_a + \sum_{l\in L} \epsilon_l \hat{c}_l^\dagger \hat{c}_l + \sum_{r\in R} \epsilon_r \hat{c}_r^\dagger \hat{c}_r$$

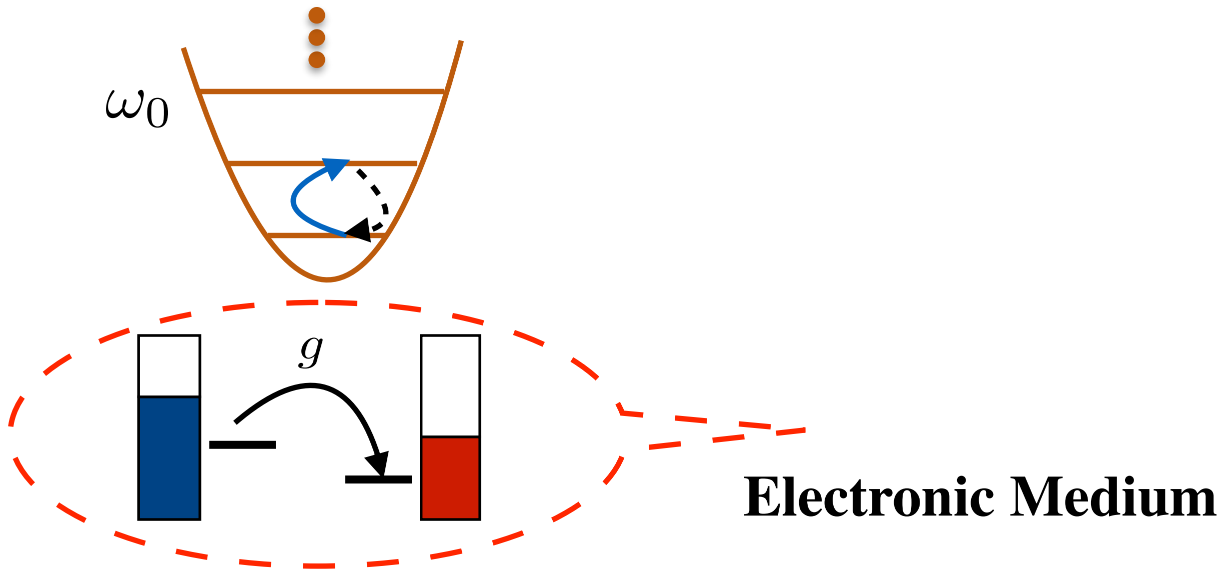
$$+ \sum_{l\in L} v_l(\hat{c}_l^\dagger \hat{c}_d + \hat{c}_d^\dagger \hat{c}_l) + \sum_{r\in R} v_r(\hat{c}_r^\dagger \hat{c}_a + \hat{c}_a^\dagger \hat{c}_r) \qquad \cancel{+t\left(\hat{c}_a^\dagger \hat{c}_d + \hat{c}_d^\dagger \hat{c}_a\right)}$$

$$\hat{H}_{\mathrm{vib}} = \omega_0 \hat{b}_0^\dagger \hat{b}_0 + \sum_j \omega_j \hat{b}_j^\dagger \hat{b}_j + (\hat{b}_0^\dagger + \hat{b}_0) \sum_j v_j(\hat{b}_j^\dagger + \hat{b}_j)$$

$$\hat{H}_{\mathrm{el-vib}} = g[\hat{c}_d^\dagger \hat{c}_a + \hat{c}_a^\dagger \hat{c}_d](\hat{b}_0^\dagger + \hat{b}_0)$$

Vibrationally assisted charge transport

- **Weak el-ph interaction** $g/\omega_0 \ll 1$



- **Electron flow excites/de-excites the vibrational mode— heating and cooling of the vibrational mode**

$$[k_u^{\lambda}]^{L\to R} = \int \frac{d\epsilon}{2\pi}\Big[J_L(\epsilon)f_L(\epsilon)\, J_R(\epsilon-\omega_0)(1-f_R(\epsilon-\omega_0))e^{-i(\lambda_p+(\epsilon-\omega_0)\lambda_e)}\Big]$$

$$[k_d^{\lambda}]^{L\to R} = [k_u^{\lambda}]^{L\to R}[\omega_0 \to -\omega_0]$$

$$\frac{k_d^{L\to R}}{k_u^{R\to L}} = e^{\beta\Delta\mu}\, e^{\beta\omega_0}$$

$$\frac{k_d^{R\to L}}{k_u^{L\to R}} = e^{-\beta\Delta\mu}\, e^{\beta\omega_0}$$

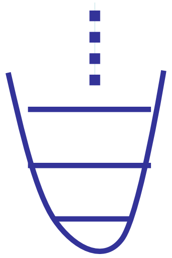
B. K. Agarwalla, J.-H. Jiang, and D. Segal, PRB 92, 245418 (2015)
B. K. Agarwalla and D. Segal, JCP 144, 074102 (2016)

CGF for Vibrationally assisted charge transport

$$\mathcal{Z}(\lambda_e,\lambda_p) = \left\langle e^{i\lambda_e H_R + i\lambda_p N_R}\, e^{-i\lambda_e H_R^H(t) - i\lambda_p N_R^H(t)} \right\rangle$$

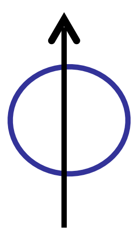
$$\mathcal{G}(\lambda) = \lim_{t\to\infty} \frac{1}{t} \ln \mathcal{Z}(\lambda)$$

Harmonic (HO) mode (Keldysh Non-equilibrium Green's function approach)



$$\boxed{\mathcal{G}_{HO}(\lambda_e,\lambda_p) = \frac{1}{2}(k_d - k_u) - \frac{1}{2}\sqrt{(k_u + k_d)^2 - 4k_u^\lambda k_d^\lambda}}$$

2-state impurity mode (Quantum master equation approach)



$$\boxed{\mathcal{G}_{AH}(\lambda_e,\lambda_p) = -\frac{1}{2}(k_u + k_d) + \frac{1}{2}\sqrt{(k_u - k_d)^2 + 4\, k_u^\lambda k_d^\lambda}}$$

Steady State Fluctuation Symmetry

$$\mathcal{G}(\lambda_e,\lambda_p) = \mathcal{G}(-\lambda_e + i(\beta_L - \beta_R), -\lambda_p + i(\beta_R\mu_R - \beta_L\mu_L))$$

Affinity for Energy flux **Affinity for Particle flux**

B. K. Agarwalla, J.-H. Jiang, and D. Segal, PRB 92, 245418 (2015)
B. K. Agarwalla and D. Segal, JCP 144, 074102 (2016)

Comparison of currents for harmonic and 2-state vibrational mode

$$\langle I_p \rangle = \frac{\partial \mathcal{G}(\lambda_e, \lambda_p)}{\partial (i\lambda_p)}\Big|_{\lambda_e=\lambda_p=0} \quad \Bigg| \quad \langle I_e \rangle = \frac{\partial G(\lambda_e, \lambda_p)}{\partial (i\lambda_p)}\Big|_{\lambda_e=\lambda_p=0}$$

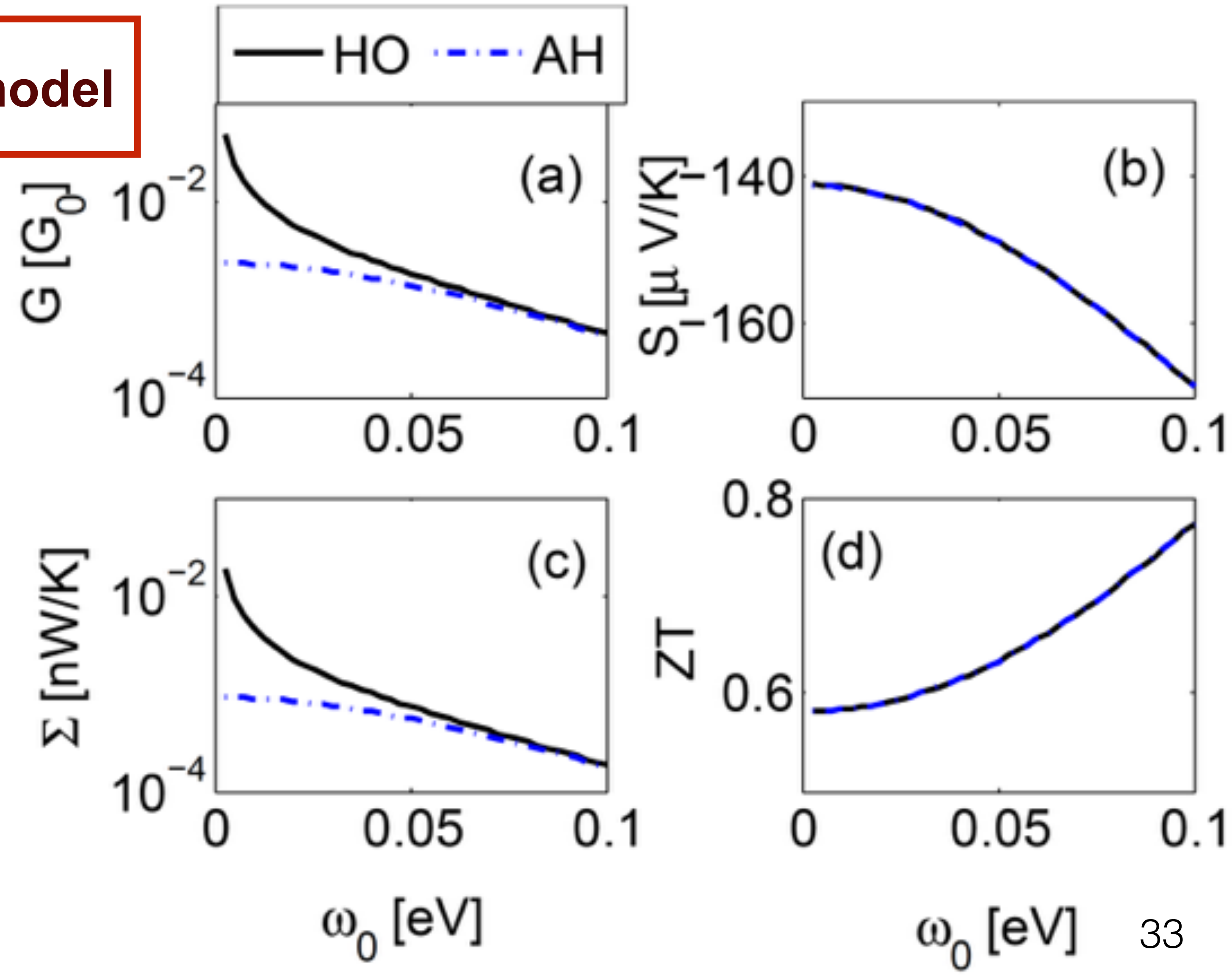
$$\langle I_p^{AH/HO} \rangle = 2\,\frac{k_d^{R\to L} k_u^{R\to L} - k_d^{L\to R} k_u^{L\to R}}{k_d + s k_u},$$

$$\langle I_e^{AH/HO} \rangle = \frac{k_d\left[\partial_{(i\lambda_e)} k_u^{\lambda}|_{\lambda_e=0}\right] + k_u\left[\partial_{(i\lambda_e)} k_d^{\lambda}|_{\lambda_e=0}\right]}{k_d + s\, k_u}$$

s = +1 for AH model and s = -1 for HO model

identical for low bias and low temperature

$$k_u \ll k_d$$



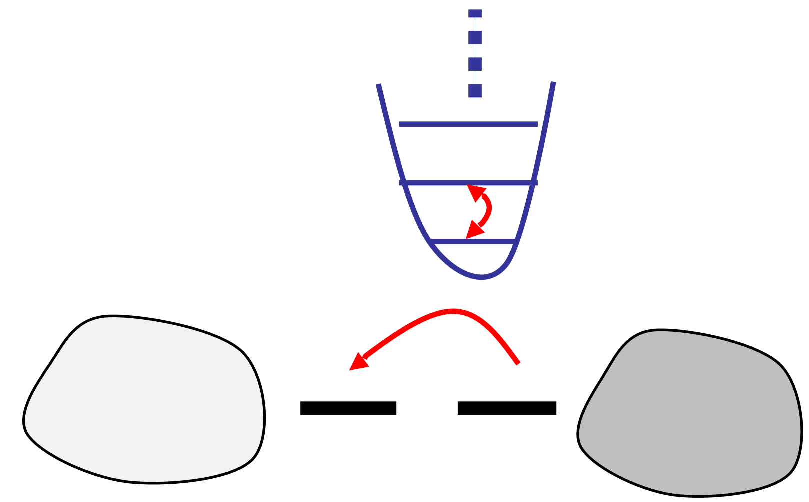
Nonlinear Transport Regime

- high bias, large hybridization, low T

$$\langle I_p^{HO} \rangle = \frac{\bar{g}^2 \omega_0}{\Gamma_L \Gamma_R} \left(\frac{\Delta\mu^2}{\omega_0^2} - 1 \right)$$

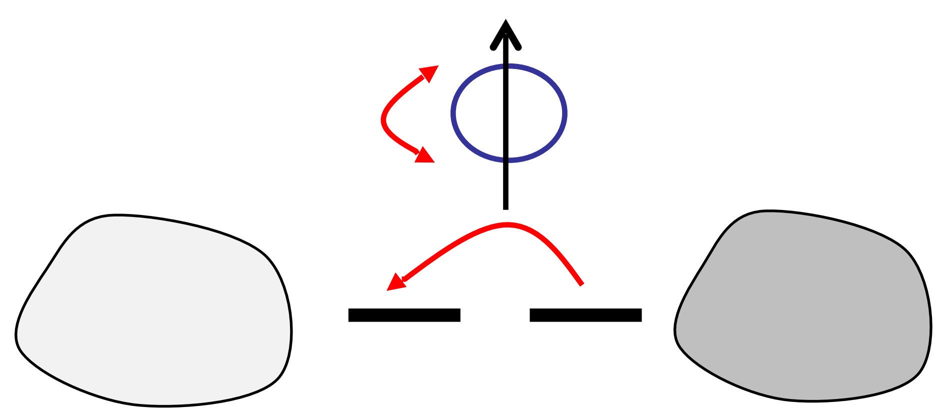
$$\langle S_p^{HO} \rangle = \frac{\bar{g}^2 \omega_0}{\Gamma_L \Gamma_R} \left(\frac{\Delta\mu^4}{\omega_0^4} - 1 \right)$$

$F^{HO} \sim \Delta\mu^2$



$$\langle I_p^{AH} \rangle = \frac{\bar{g}^2 \Delta\mu}{\Gamma_L \Gamma_R} \left(1 - \frac{\omega_0^2}{\Delta\mu^2} \right)$$

$F^{AH} \sim 1$

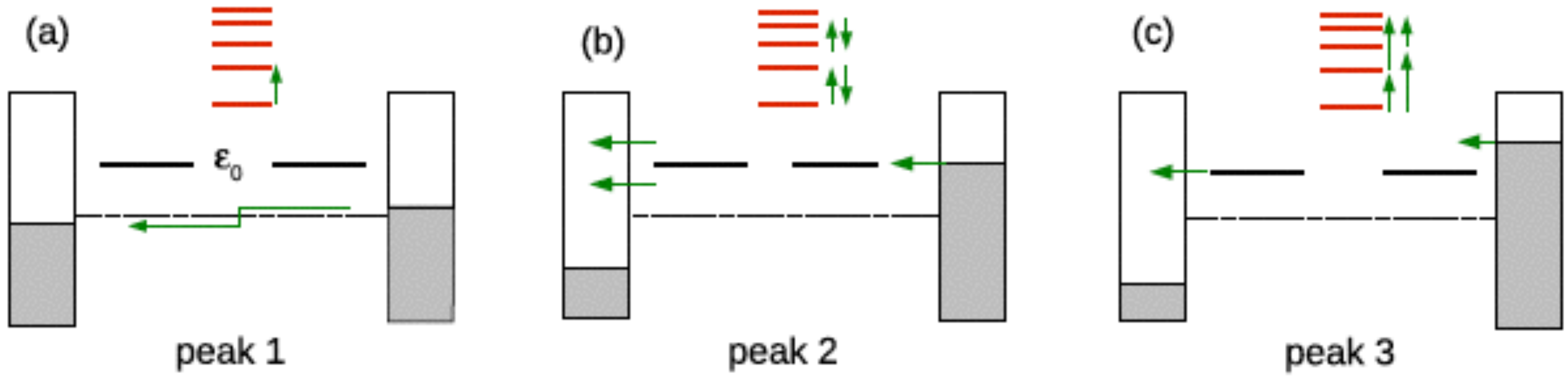


$$\langle S_p^{AH} \rangle = \frac{\bar{g}^2 \Delta\mu}{\Gamma_L \Gamma_R} \left(1 - \frac{\omega_0^4}{\Delta\mu^4} \right)$$

- **Noise characteristics can expose the nature of the vibrational mode**

B. K. Agarwalla, J.-H. Jiang, and D. Segal, PRB 92, 245418 (2015)

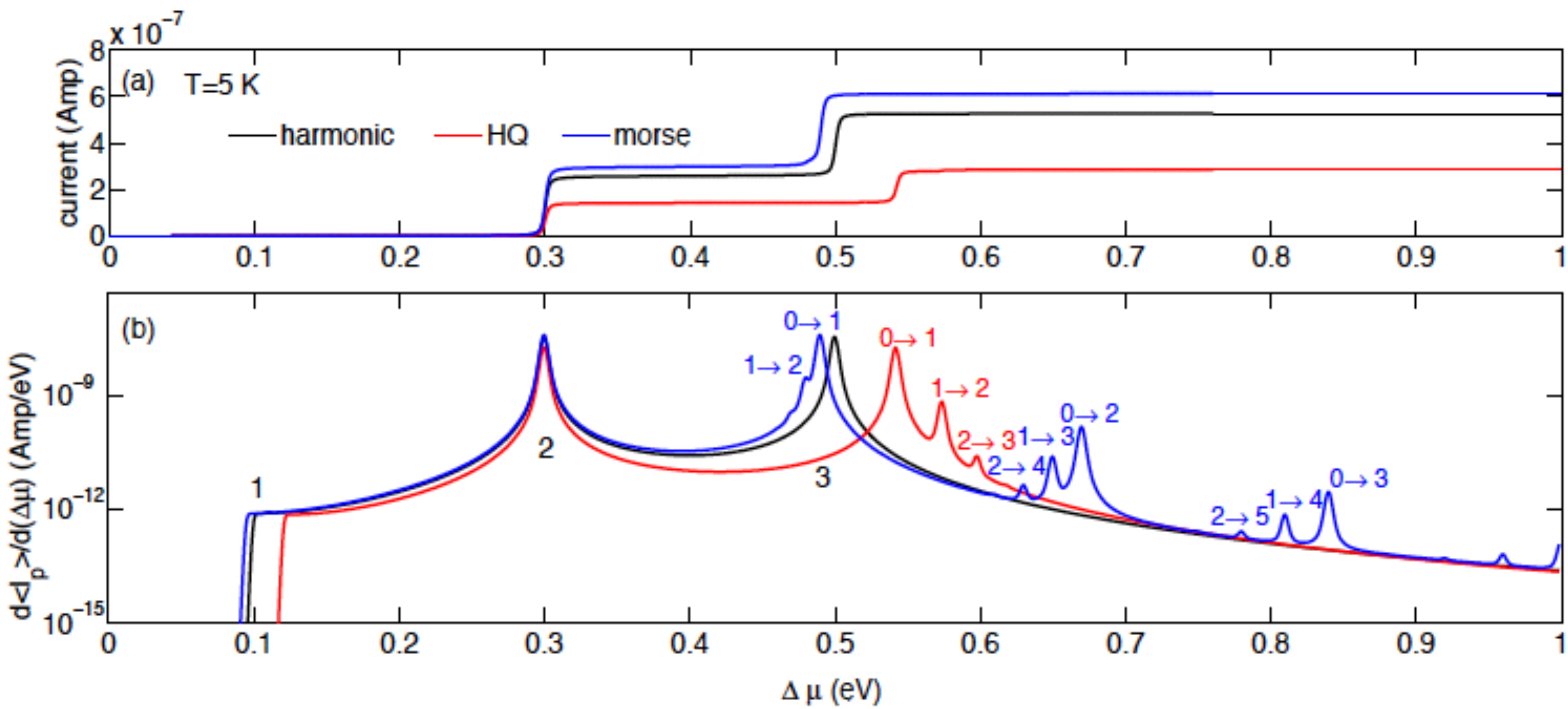
I-V for other vibrational modes



Low-bias excitation
$\Delta\mu = E_1 - E_0$

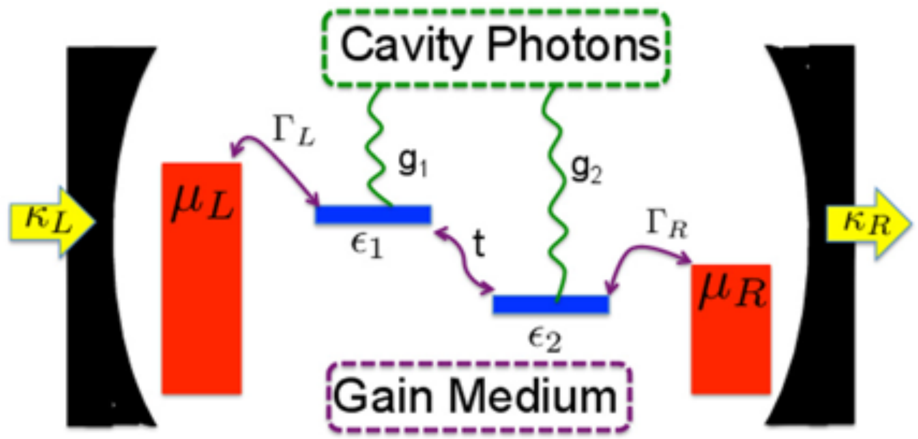
Resonant condition
$\Delta\mu = 2\epsilon_0$

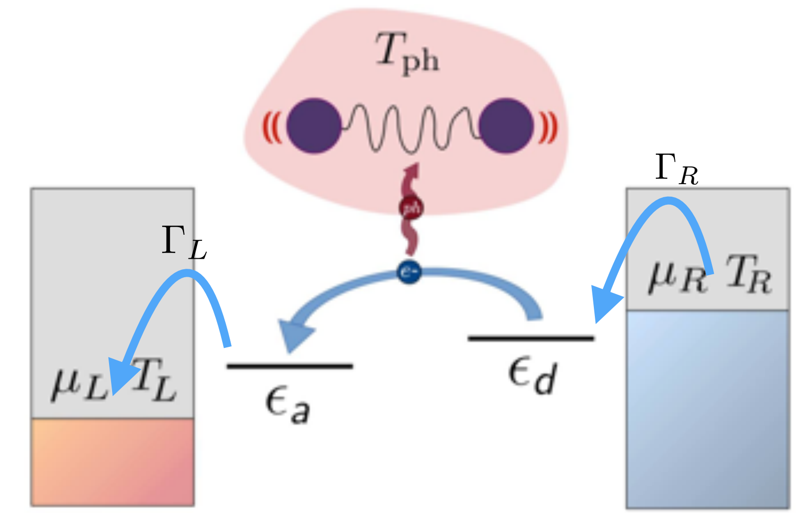
Mode heating
$\Delta\mu = 2(\epsilon_0 + E_n - E_m)$



H. Friedman, B. K. Agarwalla, D Segal, JCP, 2017

Plan of the talk





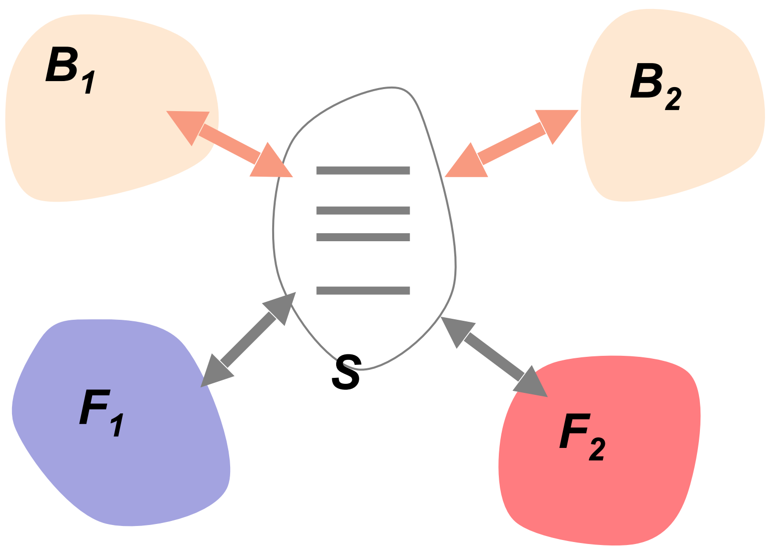
- Hybrid (light + matter) Quantum systems: Photon Amplifier
  CIRCUIT QUANTUM ELECTRODYNAMICS

- Quantum Transport :
  1. Fluctuation relations
  2. Vibrationally assisted charge transport
  3. Numerically exact path integral approach

- Conclusion

- **Iterative Influence functional Path-Integral approach**

D. Segal, A. J. Mills, D. R. Reichmann, Phys. Rev. B **82**, 205303 (2010).
L. Simine, D. Segal, J. Chem. Phys. **138**, 214111 (2013).



$$\rho_S(s'',s';t) = \mathrm{Tr}_B \langle s''| e^{-iHt}\, \rho(0)\, e^{iHt} | s' \rangle$$

$$e^{iHt} = (e^{iH\delta t})^N$$

Trotter decomposition

$$e^{-iH\delta t} = e^{-i(H_B+V_{SB})\delta t/2}\, e^{-iH_S\delta t}\, e^{-i(H_B+V_{SB})\delta t/2}$$

$$\begin{aligned}\rho_S(s'',s',t) &= \int ds_0^+ \int ds_1^+ \cdots \int ds_{N-1}^+ \\ &\times \int ds_0^- \int ds_1^- \cdots \int ds_{N-1}^- \, \mathrm{Tr_B}\{\langle s''|\mathcal{G}^\dagger|s_{N-1}^+\rangle \\ &\times \langle s_{N-1}^+|\mathcal{G}^\dagger|s_{N-2}^+\rangle \cdots \langle s_0^+|\rho(0)|s_0^-\rangle \cdots \langle s_{N-2}^-|\mathcal{G}|s_{N-1}^-\rangle \\ &\times \langle s_{N-1}^-|\mathcal{G}|s'\rangle\},\end{aligned}$$

Feynman-Vernon Influence Functional

Harmonic bath, linear coupling

$$I^{har}(s_0^{\pm} \cdots s_N^{\pm}) = \exp\left[-\sum_{k=0}^{N} \sum_{k'=0}^{k} (s_k^+ - s_k^-)(\eta_{k,k'} s_{k'}^+ - \eta_{k,k'}^* s_{k'}^-) \right]$$

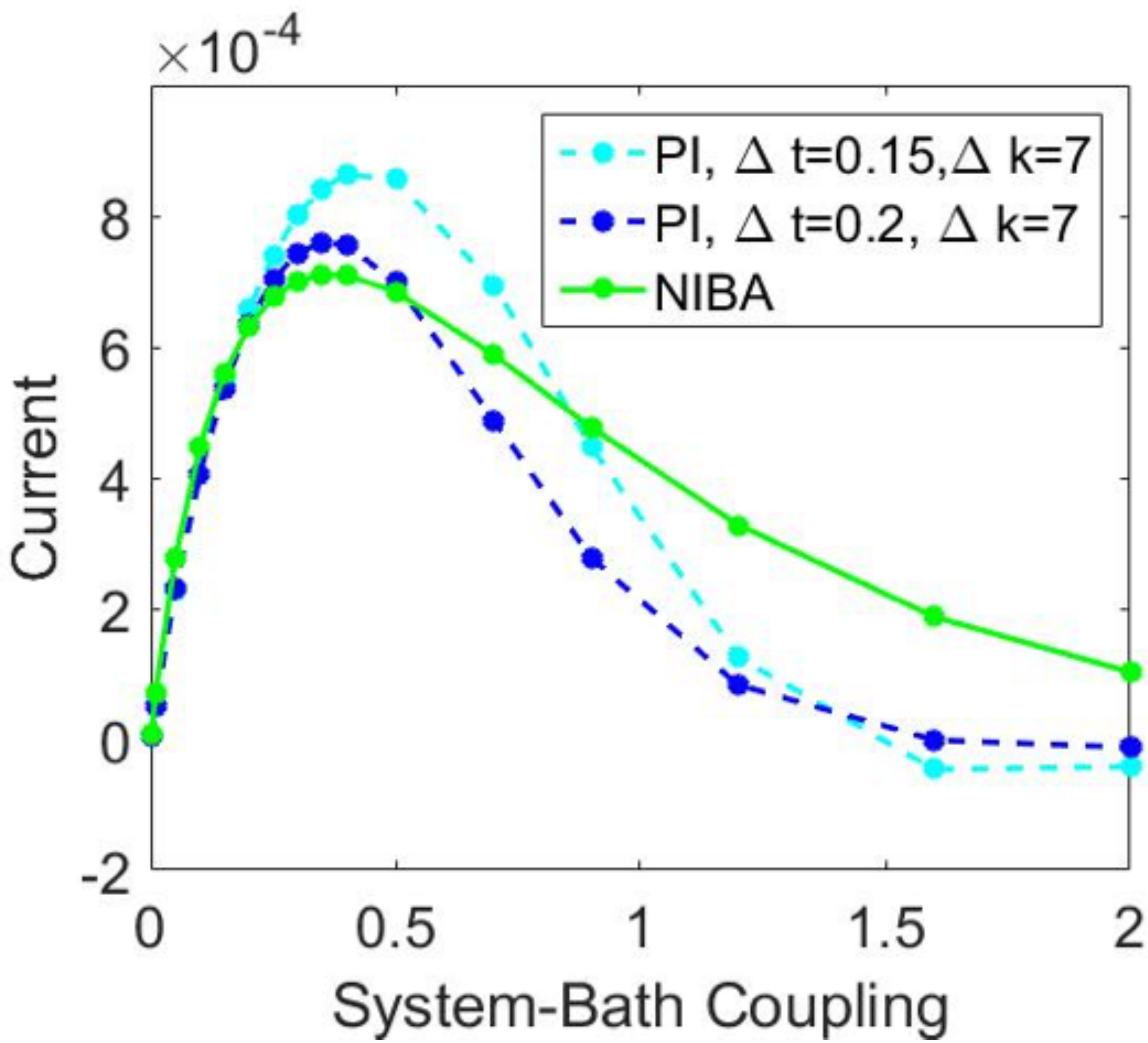
IF can be truncated beyond a memory time

$$\tau_c = N_s \delta t \approx 1/max(\Delta\mu, T)$$

$$I(s_0^{\pm}, s_1^{\pm} \cdots s_N^{\pm}) \approx I(s_0^{\pm}, s_1^{\pm} \cdots s_{N_s}^{\pm}) \frac{I(s_1^{\pm}, s_2^{\pm} \cdots s_{N_{s+1}}^{\pm})}{I(s_1^{\pm}, s_2^{\pm} \cdots s_{N_s}^{\pm})} \cdots$$

Results: Non-equilibrium spin-boson model

$$\mathcal{Z}(\xi) = \mathrm{Tr}\left[U_{-\xi/2}(t,0)\,\rho(0)\,U^{\dagger}_{\xi/2}(t,0)\right]$$



M. Kilgour, B. K. Agarwalla, D. Segal (under preparation)

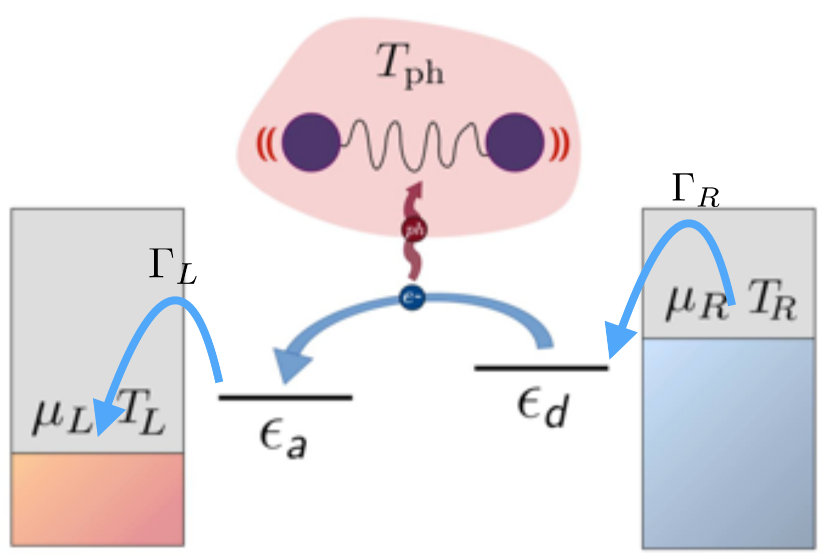
Summary 2:

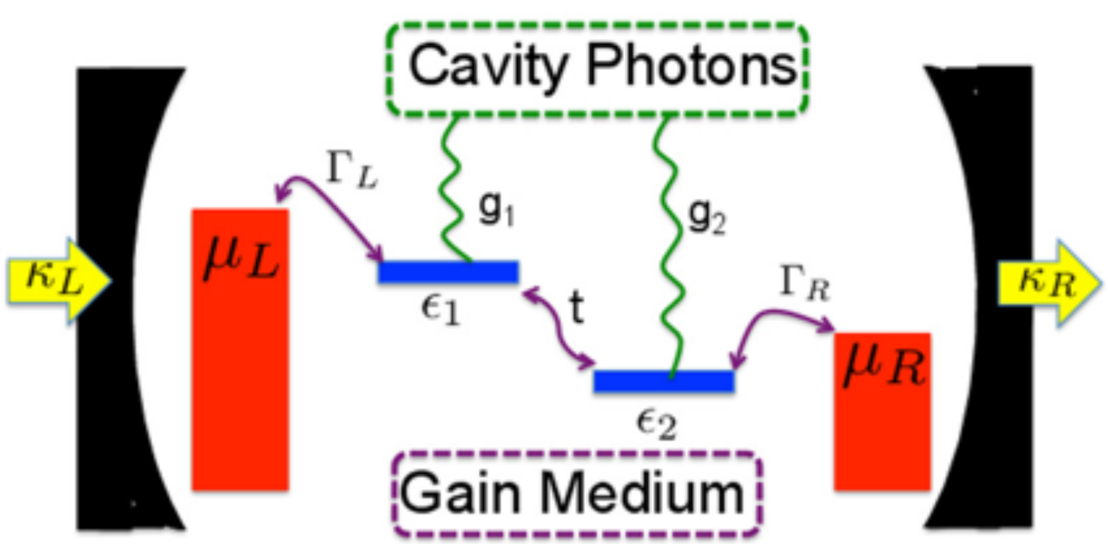
$$\ln\left[\frac{P_t(+S)}{P_t(-S)}\right] = S$$

- Small systems require statistical description: Important information beyond typical mean or average.

- Extend open quantum systems methodologies to study quantum transport

Full Counting Statistics: fluctuation theorem, cumulants , scaling laws
Method Development: numerically exact technique
Functions: thermoelectricity, optical gain





Thank you!

NSERC
CRSNG

People. Discovery. Innovation.

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