Quantum Simulation of Open-System Chemical Dynamics with Trapped Ions

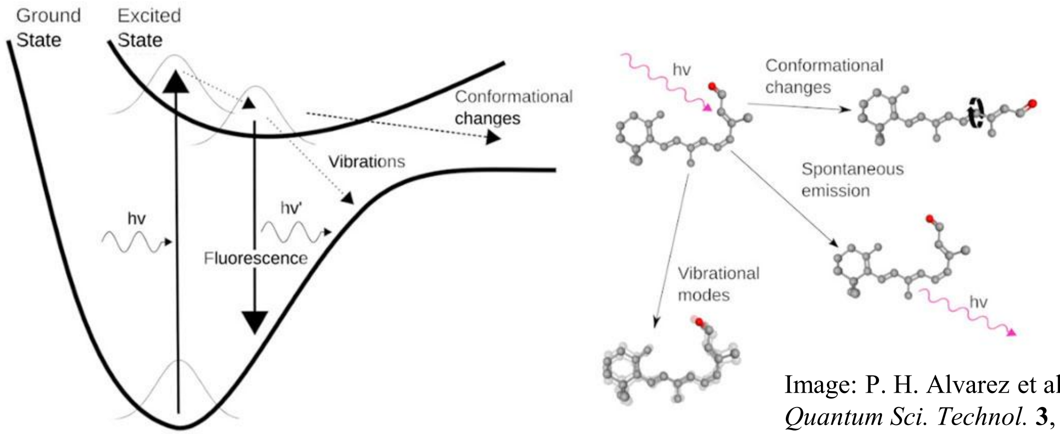

Image: P. H. Alvarez et al., Front. *Quantum Sci. Technol.* **3**, 1466906 (2024)

Quantum Talents Symposium Munich 2025

Visal So

Pagano Quantum Simulation Lab, Physics and Astronomy Department

24 November 2025

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Outline

- Motivation
- Linear vibronic coupling model (LVCM)
- Open-system analog quantum simulation of LVCMs with trapped ions
- Experimental implementation
- Single-mode electron (charge) transfer [**VS** et al., *Sci. Adv.* **10**, eads8011 (2024)]
- Multi-mode excitation transfer [**VS** et al., arXiv: 2505.22729 (2025), to appear in *Nat Commun*]
- Thermal effects in excitation transfer [**VS** et al., arXiv: 2511.08689 (2025)]
- Summary
- Outlook

Motivation

- Excitation and energy transfer are fundamental processes in physical, chemical, and biological reactions
- To better understand nature, to develop efficient and clean technologies, and to guide material design
- Requires simultaneous quantum treatment of both electronic and vibrational degrees of freedom
  - ➢ Breakdown of Born-Oppenheimer approximation
- Systems interact with environment → dissipation or decoherence → Open-system modeling
- Challenging to study the quantum effects of the dynamics with classical methods and traditional experiments

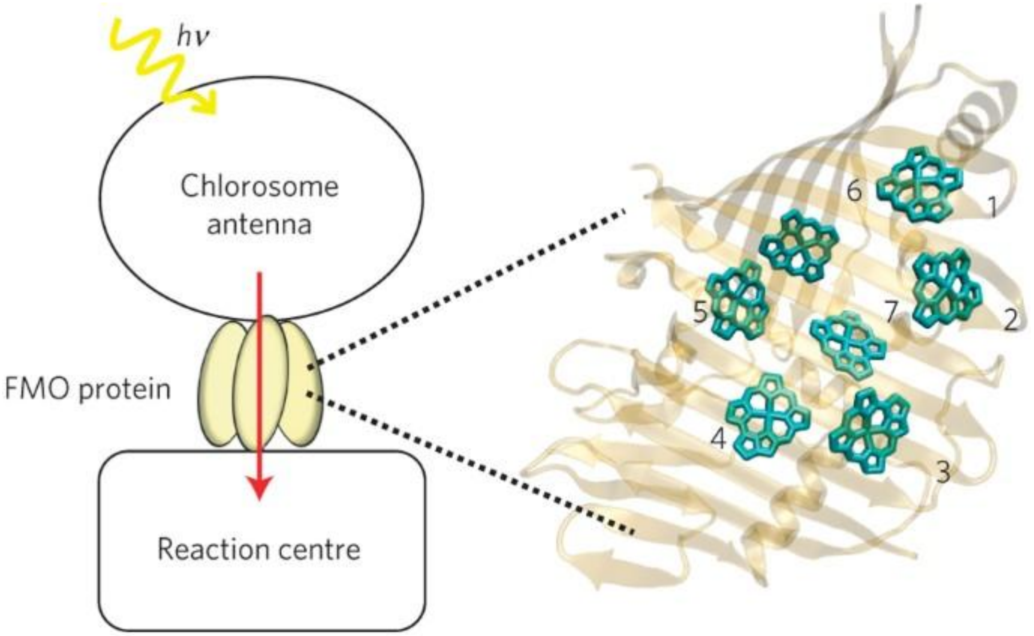


Image: M. Sarovar et al., *Nat. Phys.* **6**, 462-467 (2010)

Linear Vibronic Coupling Model (LVCM)

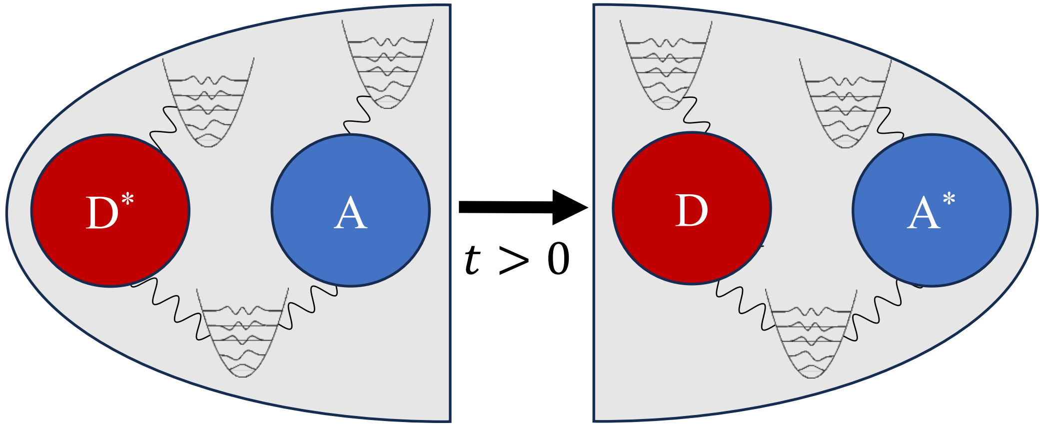
$$H_{\mathrm{LVCM}} = \boxed{\sum_{n} \epsilon_n |n\rangle\langle n|} + \boxed{\sum_{n\neq m} V_{nm} |n\rangle\langle m|} + \boxed{\sum_{i\in(t\cup c)} \omega_i a_i^{\dagger} a_i} + \boxed{\sum_{n}\sum_{i\in t} g_n |n\rangle\langle n| \left(a_i + a_i^{\dagger}\right) + \sum_{n\neq m}\sum_{i\in c} \Delta_{nm} |n\rangle\langle m| \left(a_i + a_i^{\dagger}\right).}$$

Electronic levels

Electronic couplings

Vibrational modes

Vibrational-electronic (vibronic) couplings



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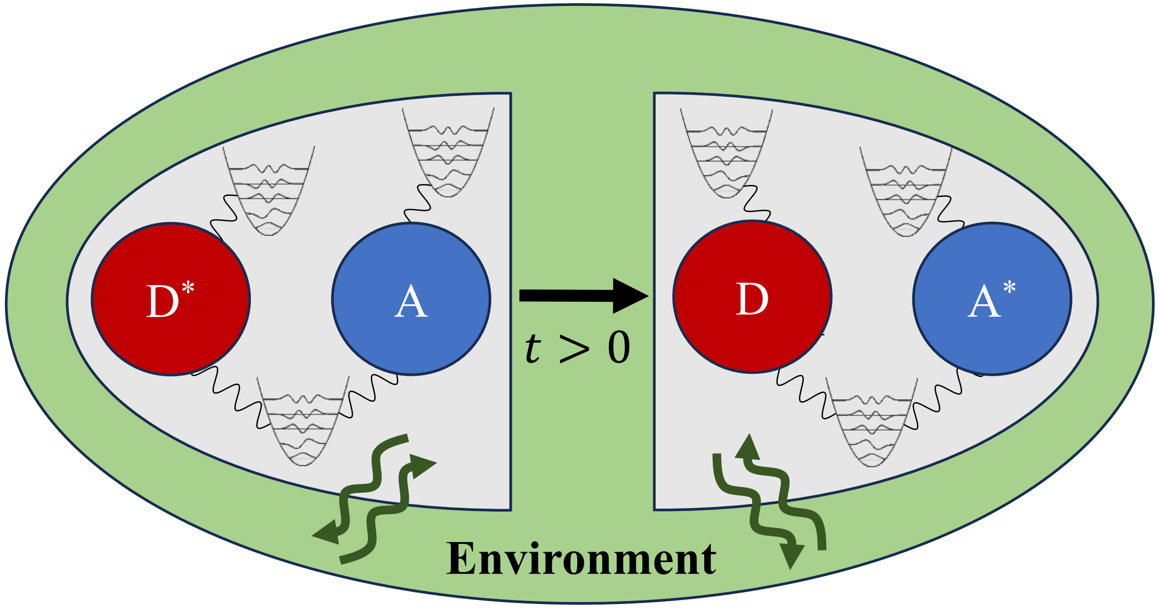
Electronic levels | Electronic couplings | Vibrational modes | Vibrational-electronic (vibronic) couplings



- Environment ≈ Continuous harmonic oscillators ~ $J(\omega)$

$$H_{\text{total}} = H_{\text{LVCM}} + H_{\text{Bath}} + H_{\text{System-Bath}}.$$

- $\gamma_i \ll \omega_i$ and $k_B T_i$, where $k_B T_i = \omega_i / \log(1 + 1/\bar{n}_i)$: Ohmic bath ($J(\omega_i) \sim \omega_i$) ≈ Damped spin-boson model

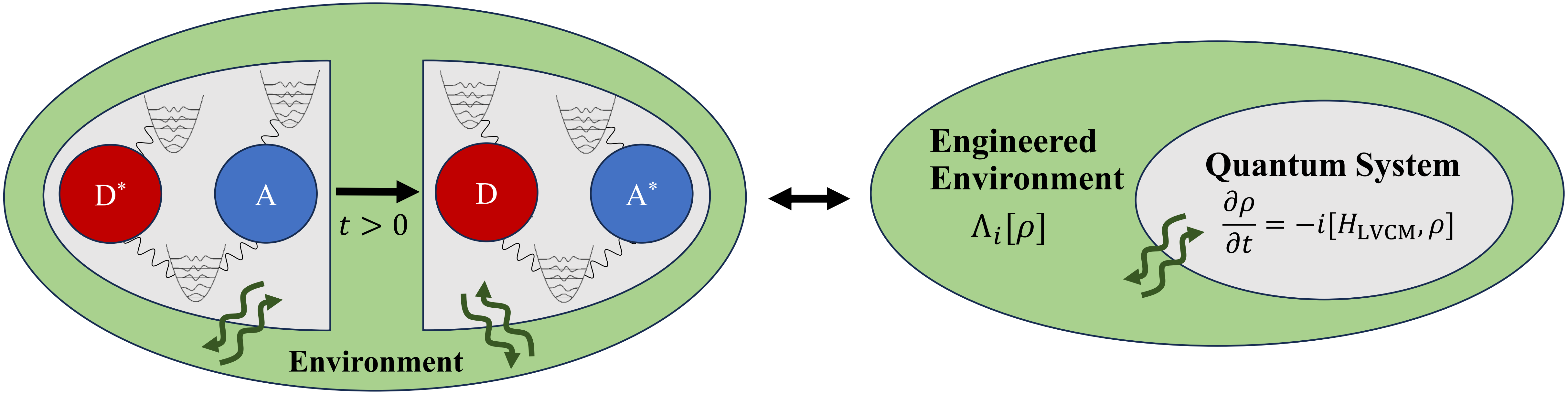
$$\partial_t \rho = -i[H_{\text{LVCM}}, \rho] + \sum_i \Lambda_i[\rho],$$

$$\Lambda_i[\rho] = \gamma_i(\bar{n}_i + 1)\mathcal{L}_{a_i}[\rho] + \gamma_i \bar{n}_i \mathcal{L}_{a_i^\dagger}[\rho],$$

$$\mathcal{L}_c[\rho] = c\rho c^\dagger - \frac{1}{2}\{c^\dagger c, \rho\}.$$

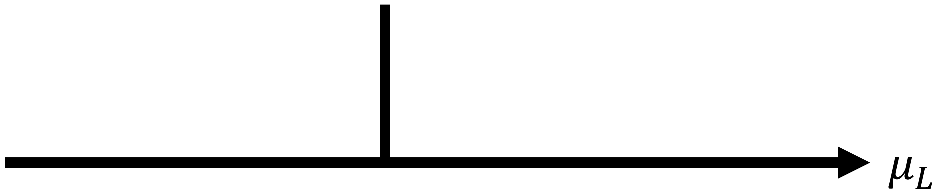
A. Lemmer et al., *New J. Phys.* **20**, 073002 (2018)

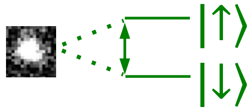
Open-system Quantum Simulation of LVCMs



Open-system Quantum Simulation of LVCMs

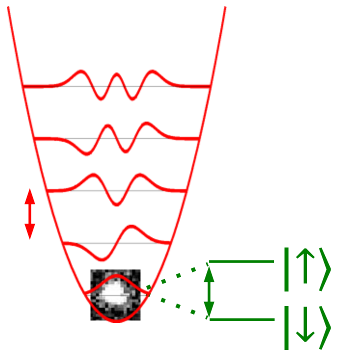
- Trapped ions: $\frac{\partial \rho}{\partial t} = -i[H_{\mathrm{LVCM}}, \rho]$
  - Internal states (electronic sites/configurations)

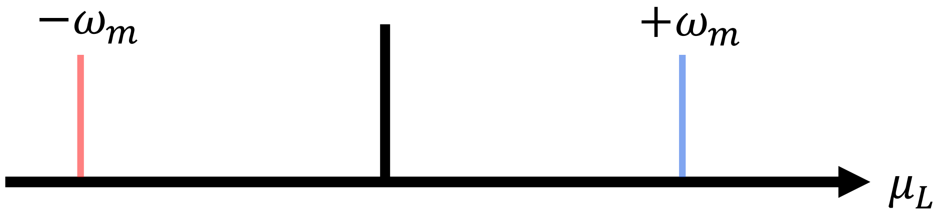




Open-system Quantum Simulation of LVCMs

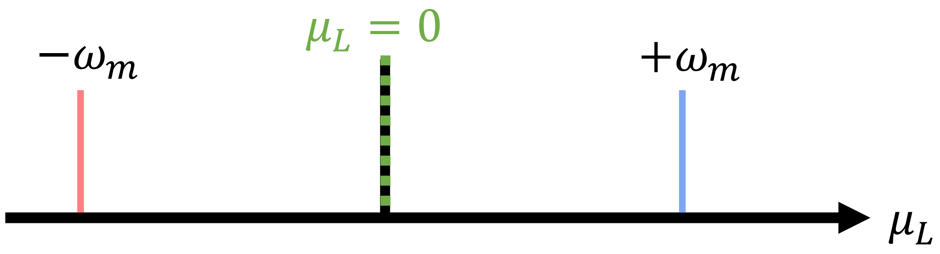
- Trapped ions: $\frac{\partial \rho}{\partial t} = -i[H_{\mathrm{LVCM}}, \rho]$
  - Internal states (electronic sites/configurations)
  - External harmonic oscillator modes (vibrations)

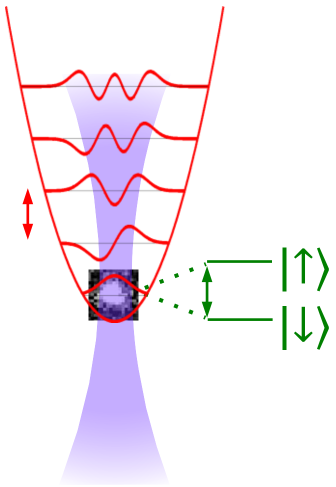


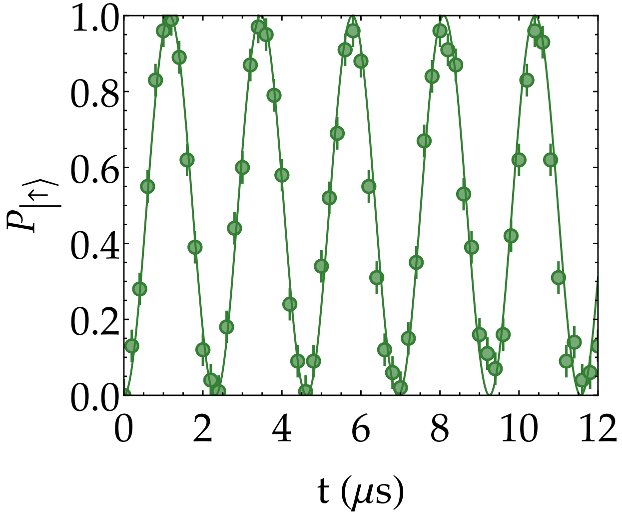


Open-system Quantum Simulation of LVCMs

- Trapped ions: $\frac{\partial \rho}{\partial t} = -i[H_{\mathrm{LVCM}}, \rho]$
  - ➢ Internal states (electronic sites/configurations)
  - ➢ External harmonic oscillator modes (vibrations)
  - ➢ Light-ion interactions (H_{LVCM})







$$H = \sum_i \frac{\Omega_i}{2} \sigma^i_{\phi_i}, \quad \sigma^i_{\phi_i} = \sigma^i_x \cos\phi_i + \sigma^i_y \sin\phi_i$$

Open-system Quantum Simulation of LVCMs

- Trapped ions: $\frac{\partial \rho}{\partial t} = -i[H_{\mathrm{LVCM}}, \rho]$
  - Internal states (electronic sites/configurations)
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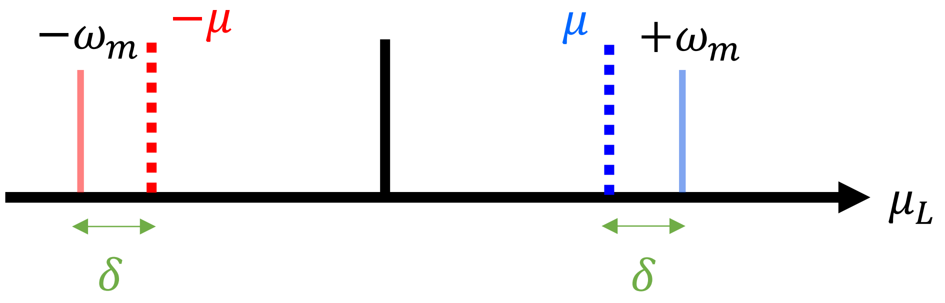

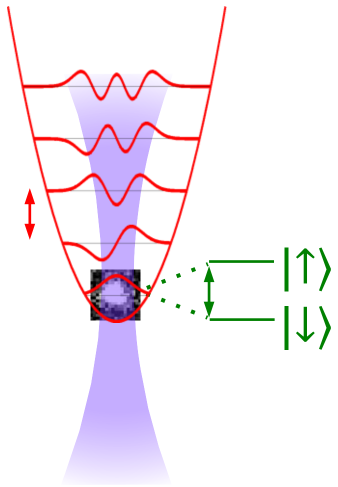

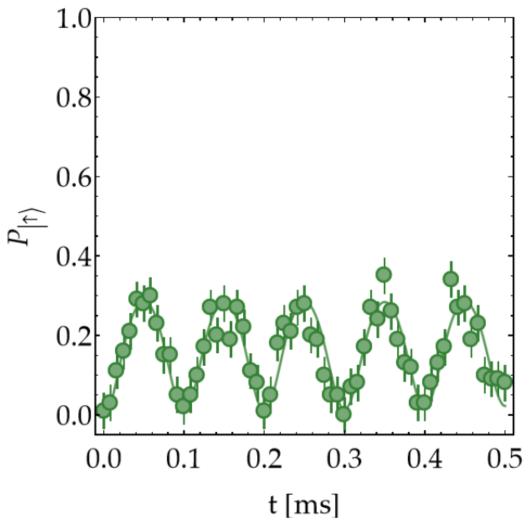

$\mu + \omega_m \gg \delta$ and $\delta \sim \eta_{im}\Omega_i$:

$$H = \frac{\eta_{im}\Omega_i}{2}\sigma^i_{\phi_i}\left(a_m e^{-i\psi_i} + a_m^\dagger e^{i\psi_i}\right) + \delta a_m^\dagger a_m$$

Open-system Quantum Simulation of LVCMs

- Trapped ions: $\frac{\partial \rho}{\partial t} = -i[H_{\mathrm{LVCM}}, \rho]$
  - ➢ Internal states (electronic sites/configurations)
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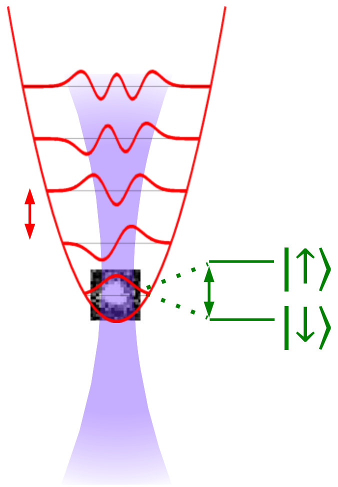
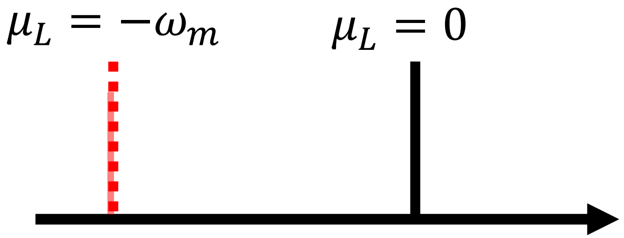
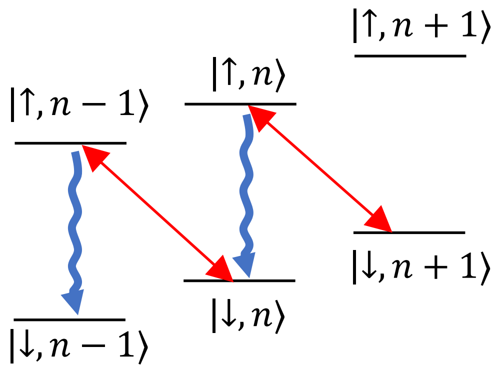
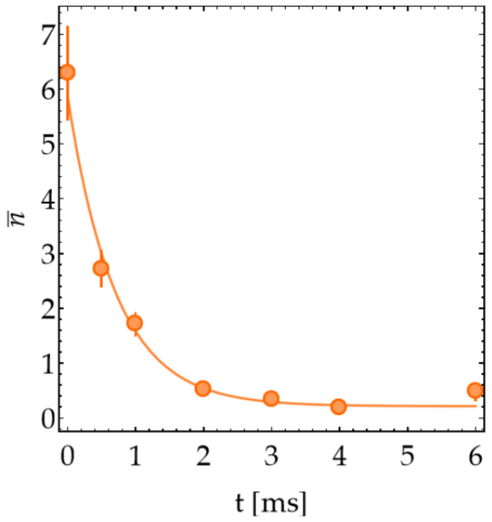
  - ➢ Light-ion interactions (H_{LVCM})



- Resolved-sideband cooling:
  $\Lambda_i[\rho]$ with tunable γ_i and $\bar{n}_i \sim 0$







Experimental implementation

- Donor-acceptor + one damped vibrational mode ($g \gtrsim \omega$):

$$H_{1\mathrm{M}} = \frac{\Delta E}{2}\sigma_z + V\sigma_x + \frac{g}{2}\sigma_z\left(a + a^\dagger\right) + \omega a^\dagger a$$

$$\partial_t \rho = -i[H_{1\mathrm{M}}, \rho] + \Lambda\,[\rho]$$

  - $\Delta E > 0$: exothermic reaction

Donor-acceptor system: two electronic sites

$$\{|\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle\} \rightarrow \{|\uparrow\rangle_z, |\downarrow\rangle_z\} \equiv \{|D\rangle, |A\rangle\}$$

F. Schlawin et al., *PRX Quantum* **2**, 010314 (2021)

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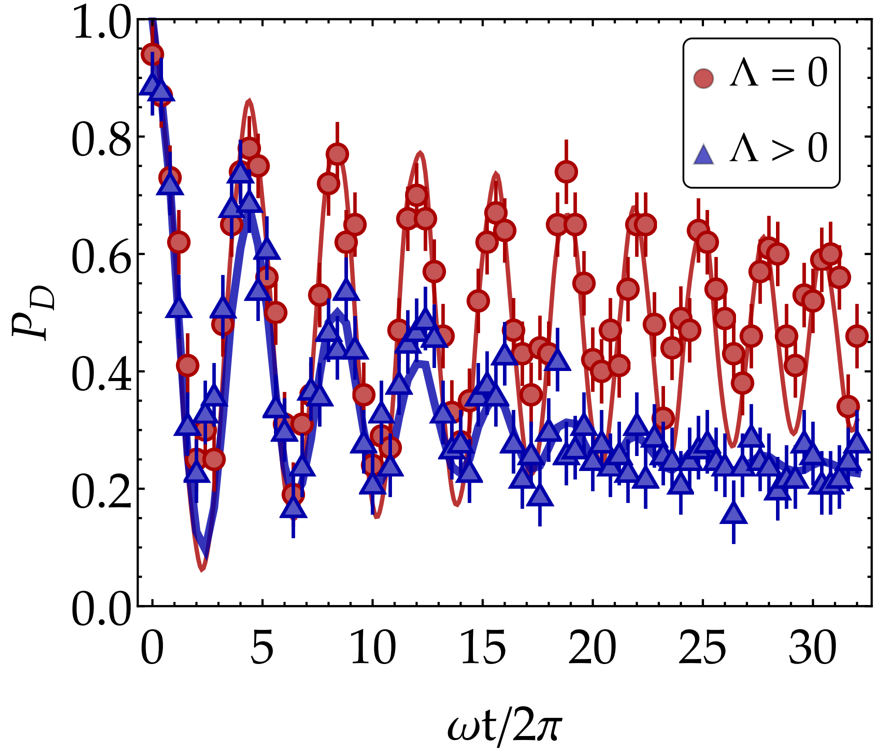
  - ➢ $\Delta E > 0$: exothermic reaction
  - ➢ $\Lambda > 0$: irreversible transfer



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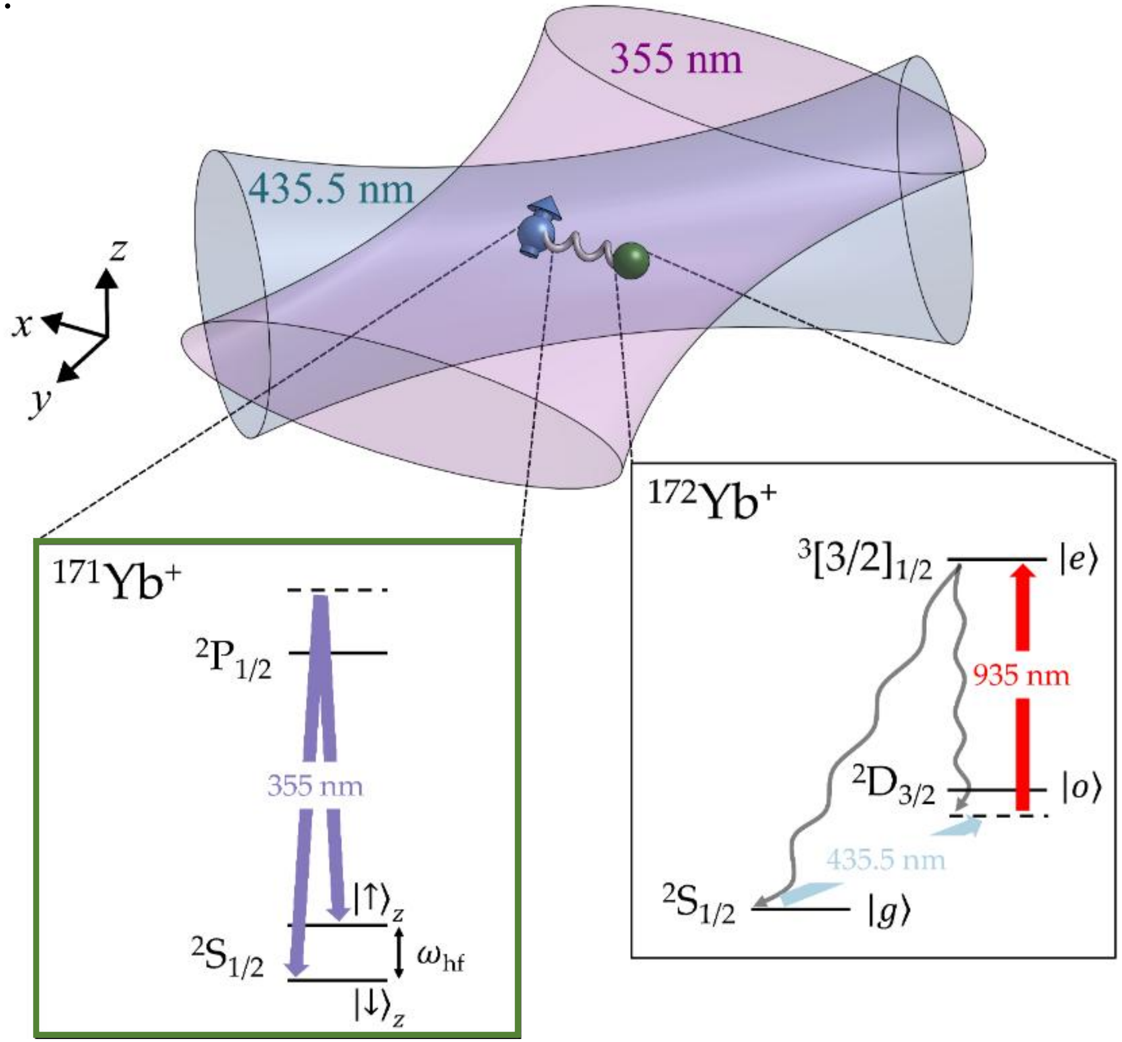
- Dual-species chain and its shared collective modes:
  - ➢ Qubit $^{171}\mathrm{Yb}^+$: 355 nm Raman laser tones ($H_{1\mathrm{M}}$: system parameters)



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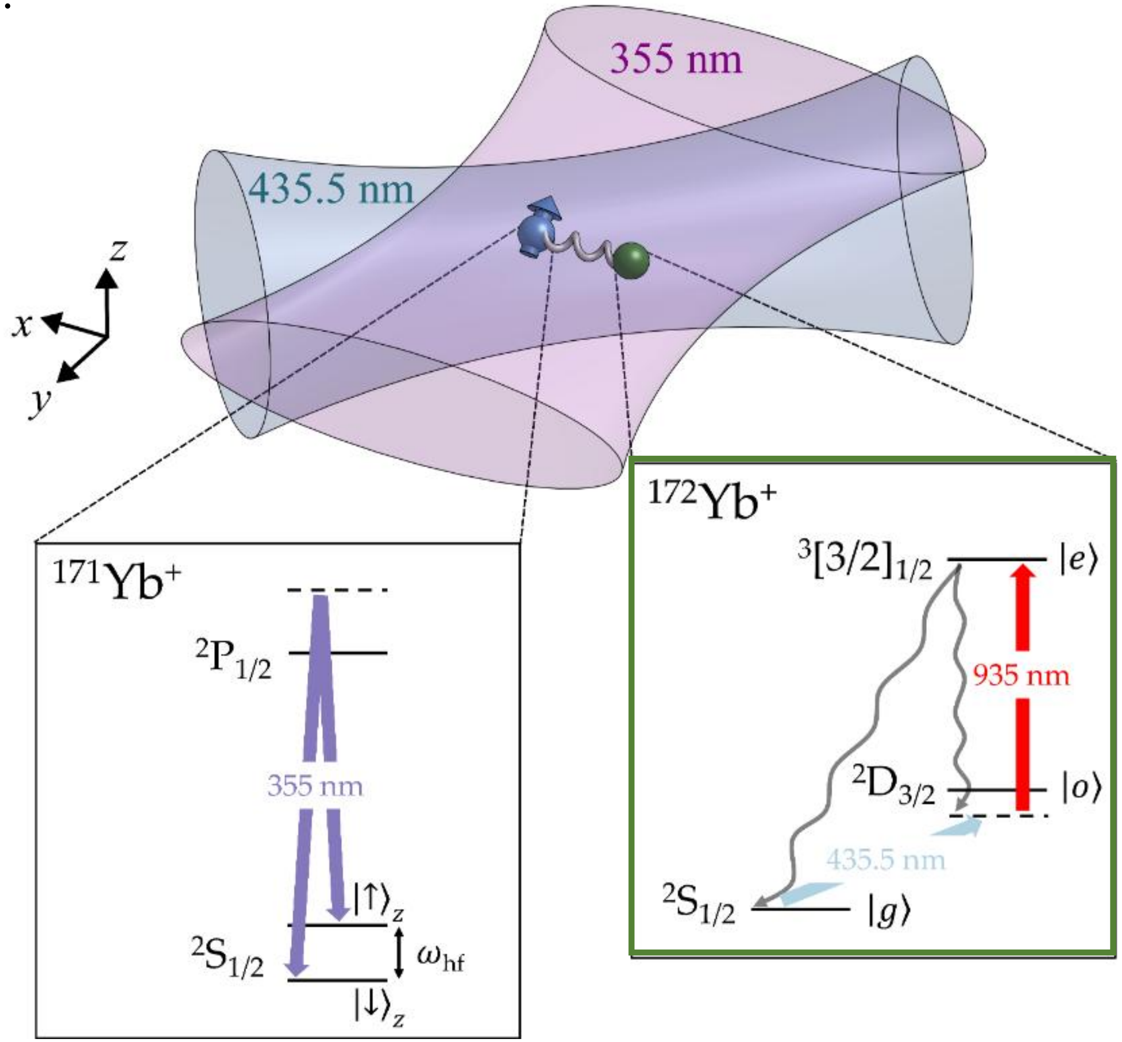
  - $\Lambda > 0$: irreversible transfer

- Dual-species chain and its shared collective modes:
  - Qubit $^{171}\mathrm{Yb}^+$: 355 nm Raman laser tones ($H_{1\mathrm{M}}$: system parameters)
  - Coolant $^{172}\mathrm{Yb}^+$: 435.5 nm laser tones ($\Lambda[\rho]$: dissipation rate)



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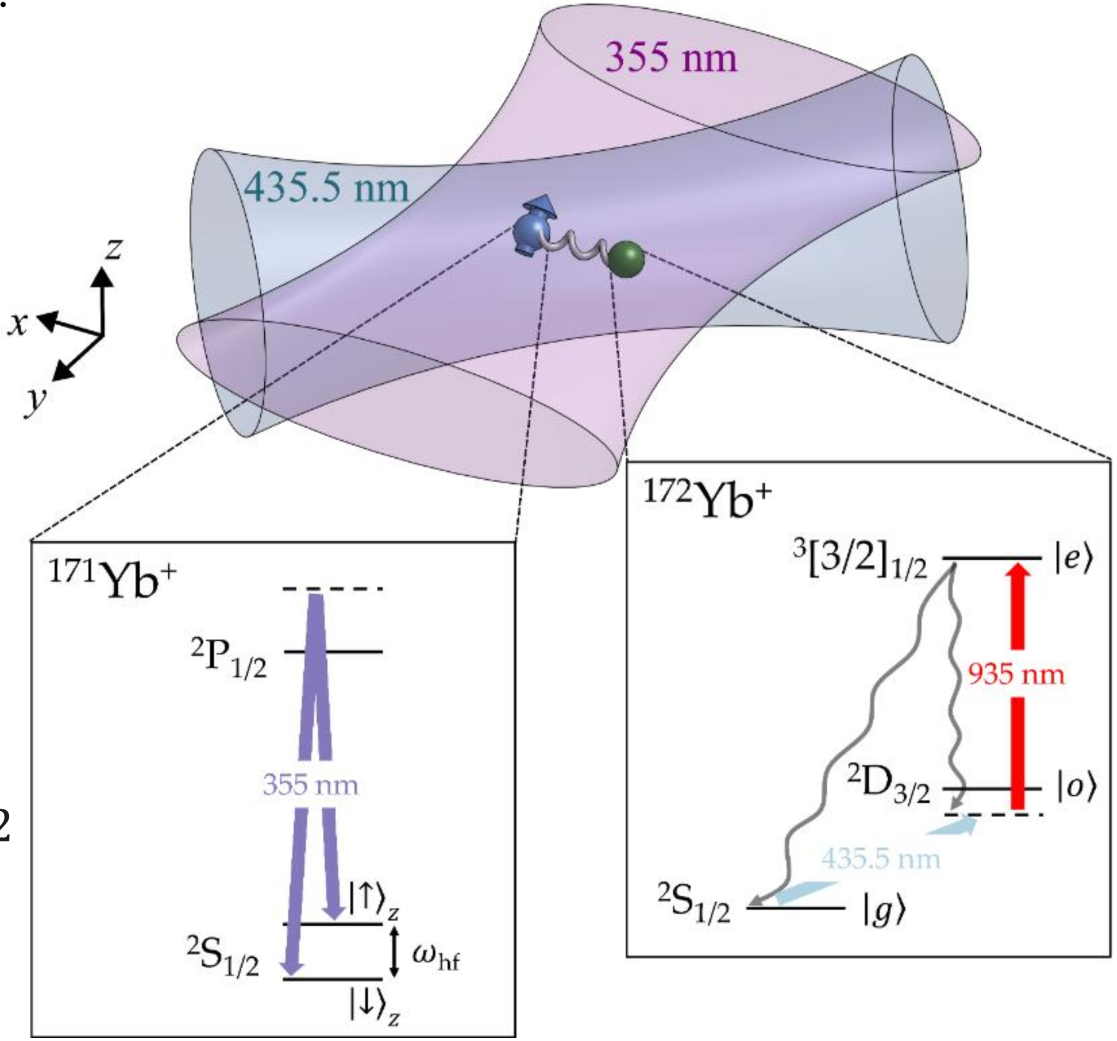
- Evolve the system and measure the transfer rate (k_T):
$$k_T = \int P_D(t)dt \Big/ \int t P_D(t)dt, \qquad P_D(t) = (\langle \sigma_z(t) \rangle + 1)/2$$



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Electron/Charge Transfer

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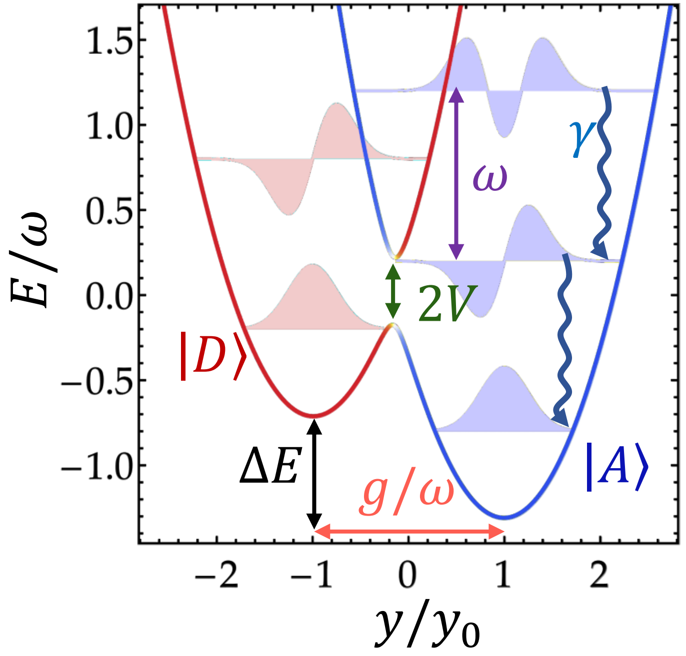
$$\partial_t \rho = -i[H_{1\mathrm{M}}, \rho] + \Lambda\,[\rho]$$

- $y = \frac{y_0}{2}(a + a^\dagger)$ with $y_0 = \frac{1}{\sqrt{2m\omega}}$
- $\lambda = g^2/\omega$: reorganization energy
- Regimes of adiabaticity:
  - **Nonadiabatic regime: $\boldsymbol{V \lesssim \gamma,\ \ V < \lambda/4}$**
    - Localized donor and acceptor energy surfaces



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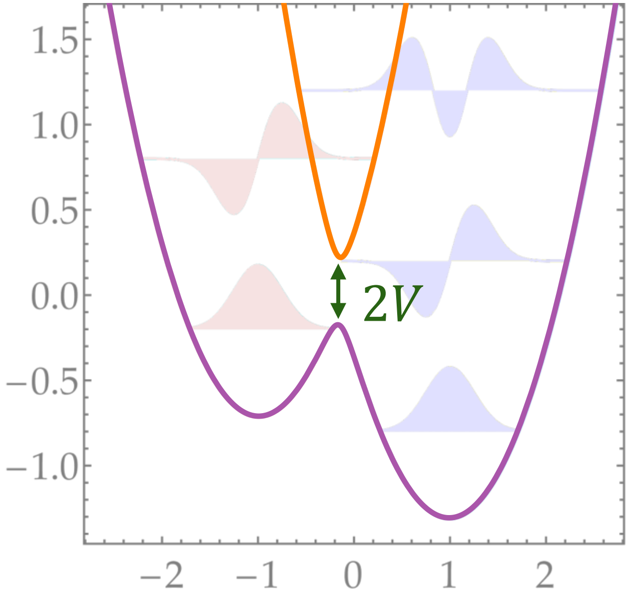
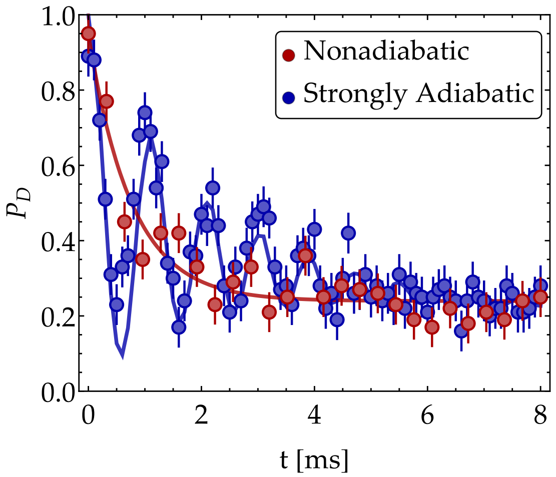
- $y = \frac{y_0}{2}(a + a^\dagger)$ with $y_0 = \frac{1}{\sqrt{2m\omega}}$

- $\lambda = g^2/\omega$: reorganization energy

- Regimes of adiabaticity:
  - **Nonadiabatic regime: $V \lesssim \gamma$, $V < \lambda/4$**
    - Localized donor and acceptor energy surfaces
  - **Strongly adiabatic: $V > \gamma$, $V \sim \lambda/4$**
    - Upper and lower hybridized (adiabatic) energy surfaces





$\Delta E = \omega$

Nonadiabatic Regime

- $V \ll \lambda/4$, Fermi's golden rule:

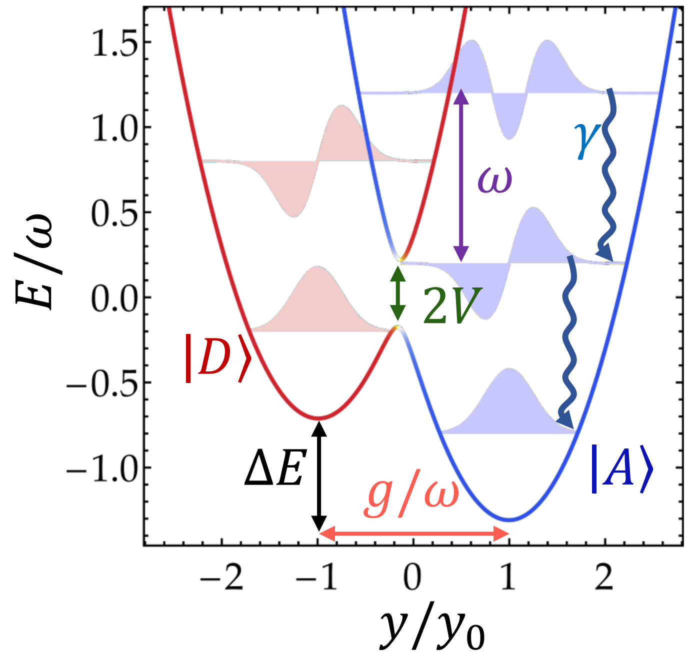
$$k_T = 2\pi|V|^2 \sum_{n_-,n_+} p_{n_-} \mathrm{FC}_{n_-,n_+} \delta(E_{D,n_-} - E_{A,n_+})$$

Franck-Condon factors: $\mathrm{FC}_{n_-,n_+} = |\langle n_-|n_+\rangle|^2$

$$H_{1\mathrm{MU}} = \frac{\Delta E}{2}\sigma_z + \frac{g}{2}\sigma_z(a + a^\dagger) + \omega a^\dagger a$$

Uncoupled vibronic states: $|D\rangle|n_-\rangle$, $|A\rangle|n_+\rangle$, where

$$|n_\pm\rangle = \mathcal{D}\left(\pm\frac{g}{2\omega}\right)|n\rangle$$



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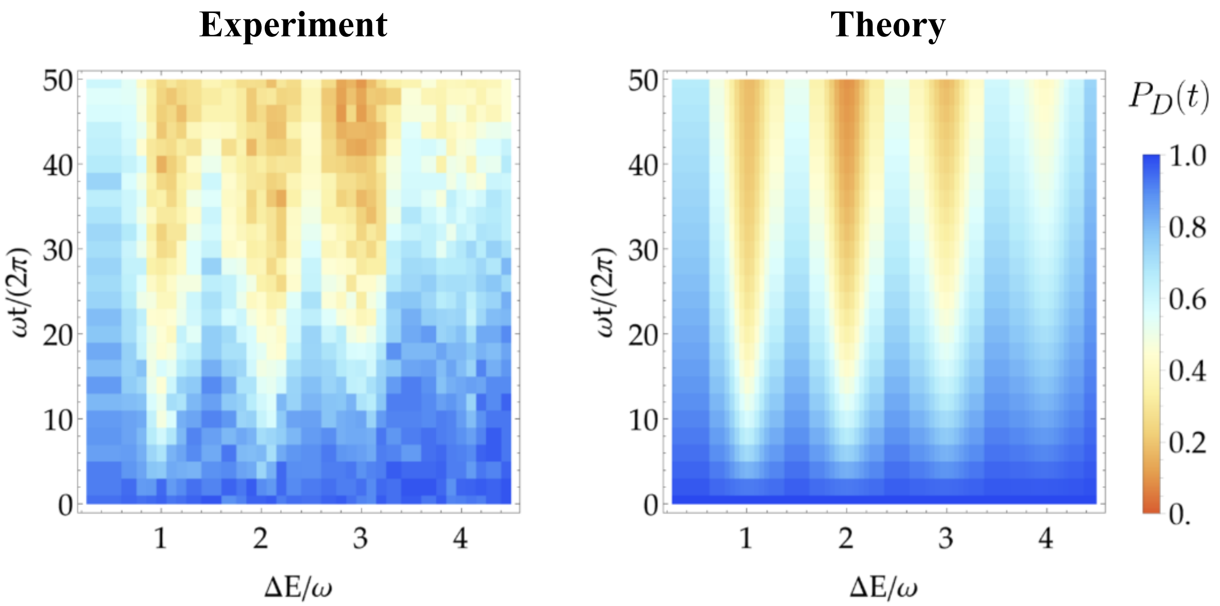
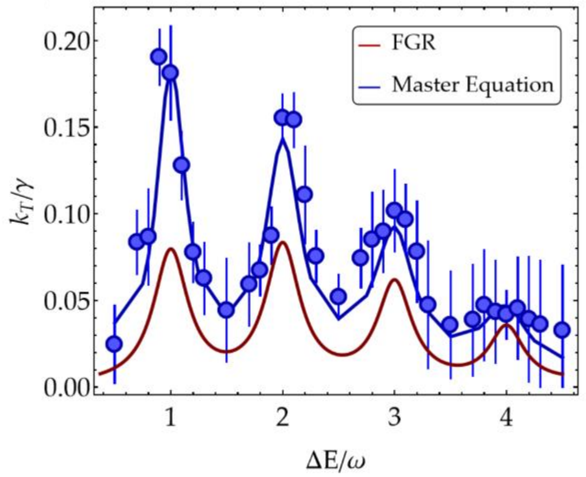
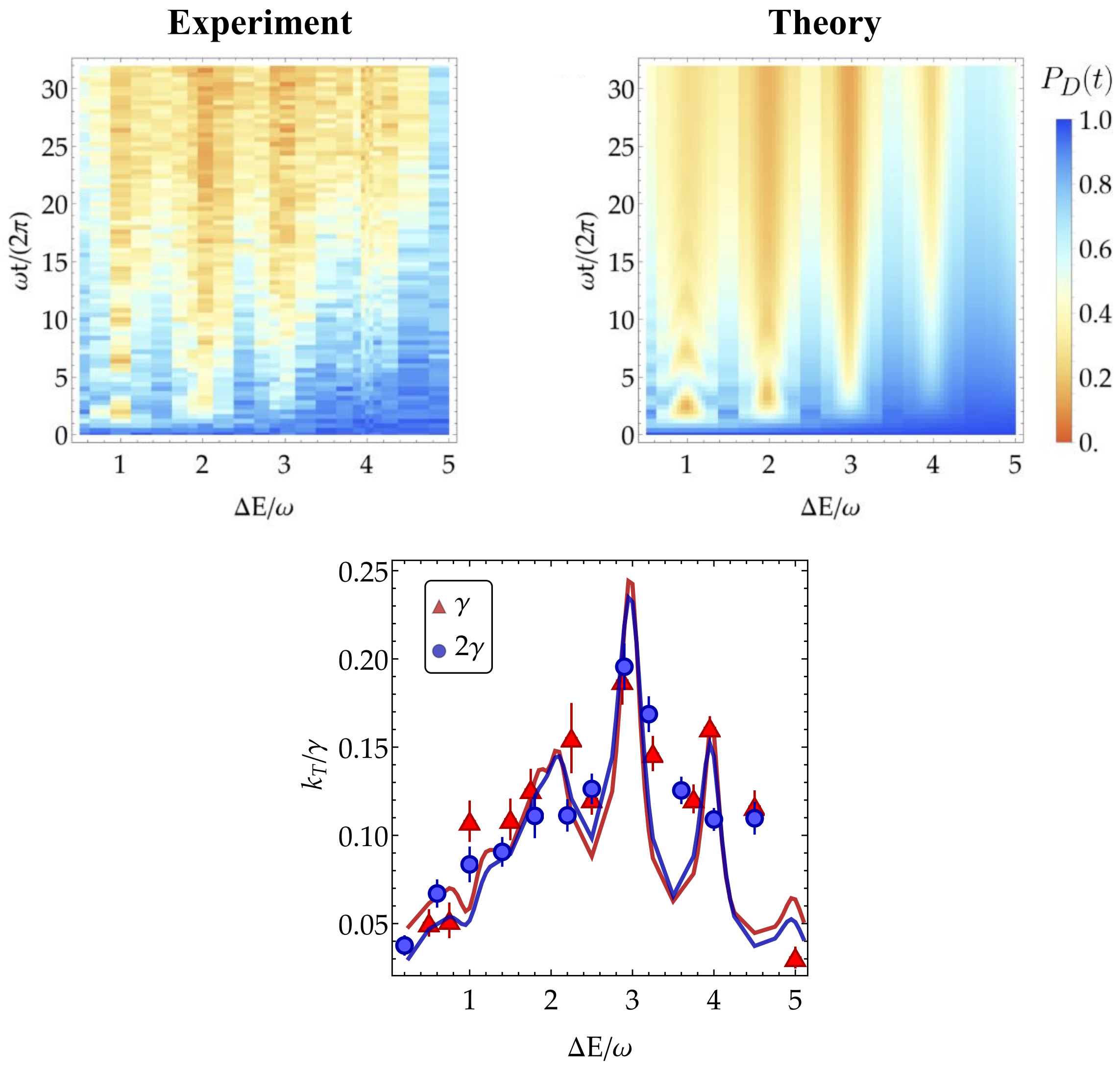
- Transfer spectrum ~ vibrational mode structure
  - ➢ Distinct resonances at $\Delta E = l\omega$, $l \in \mathbb{N}$
  - ➢ γ ~ Lorentzian FWHM





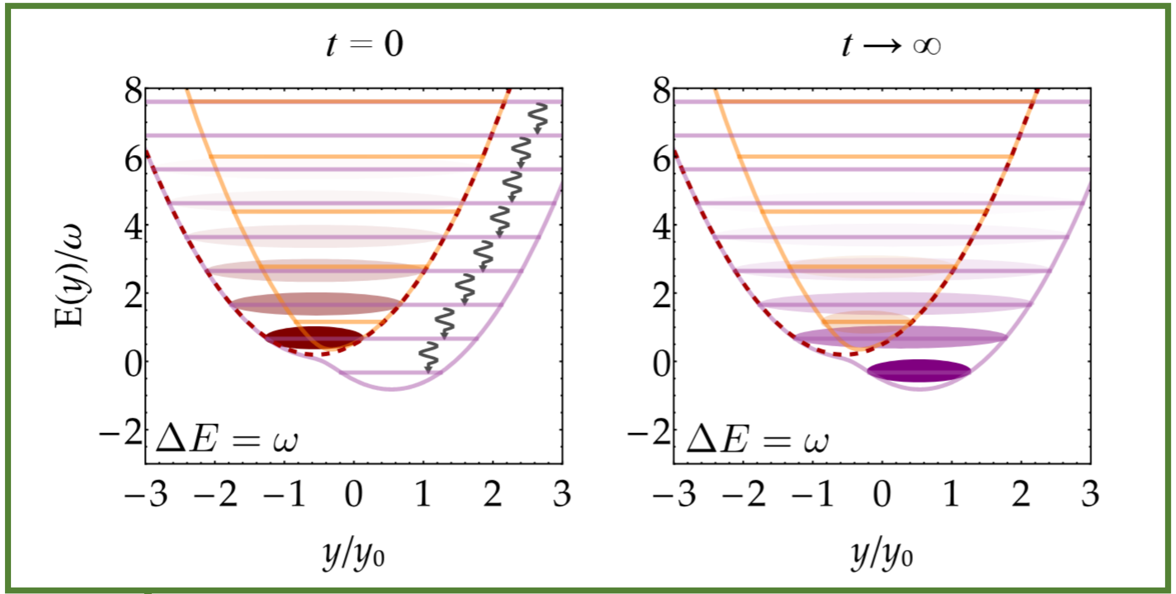
Strongly Adiabatic Regime

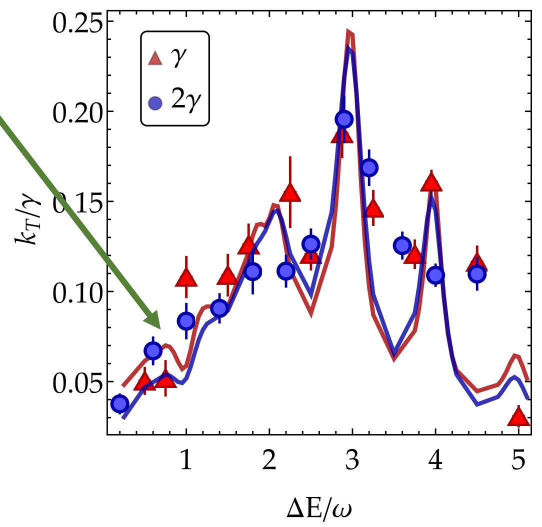
- $k_T \propto \gamma$



Strongly Adiabatic Regime

- $k_T \propto \gamma$
- Transfer rate spectrum:
  - $\Delta E < 2\omega$: no distinct resonance peaks

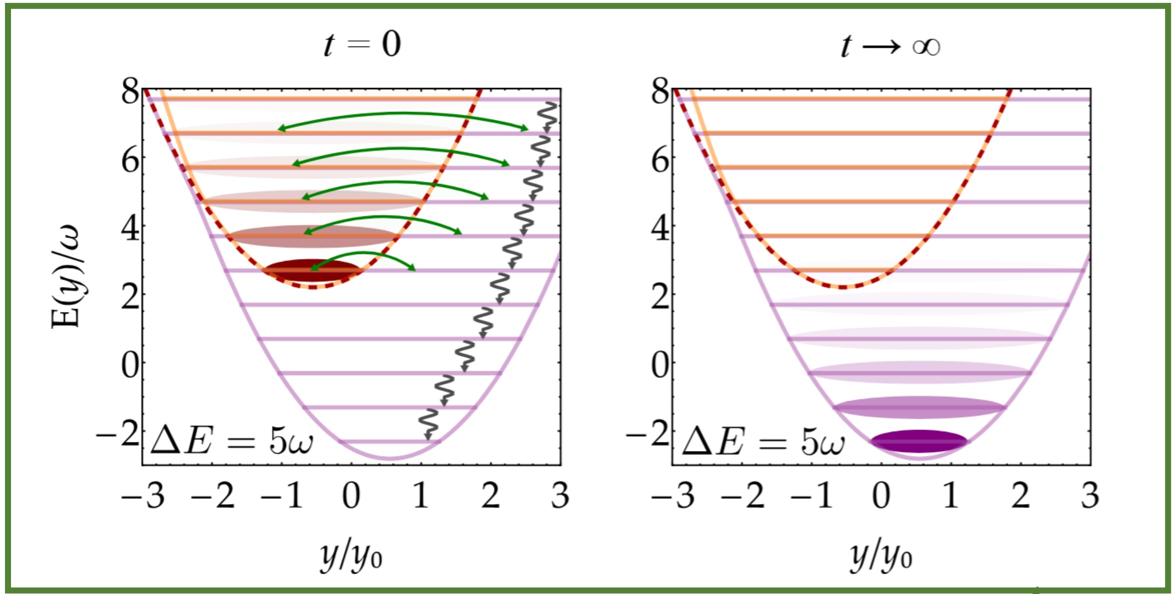


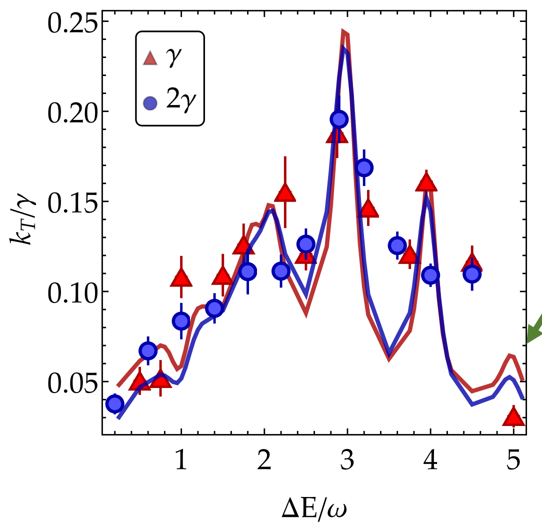


Strongly Adiabatic Regime

- $k_T \propto \gamma$

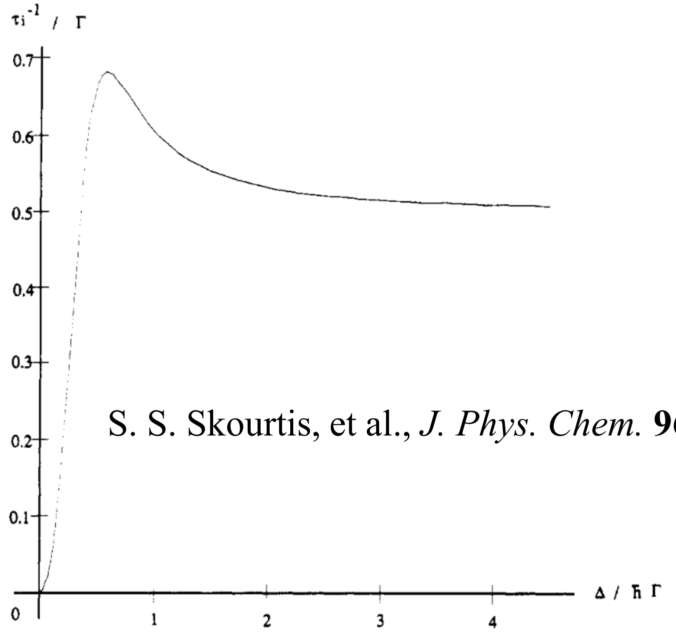
- Transfer rate spectrum:
  - ➢ $\Delta E < 2\omega$: no distinct resonance peaks
  - ➢ $\Delta E > 2\omega$: release of the initial state localized in the upper hybridized surface
  - ➢ $\Delta E > 3\omega$: $k_T \downarrow$ ("inverted regime")



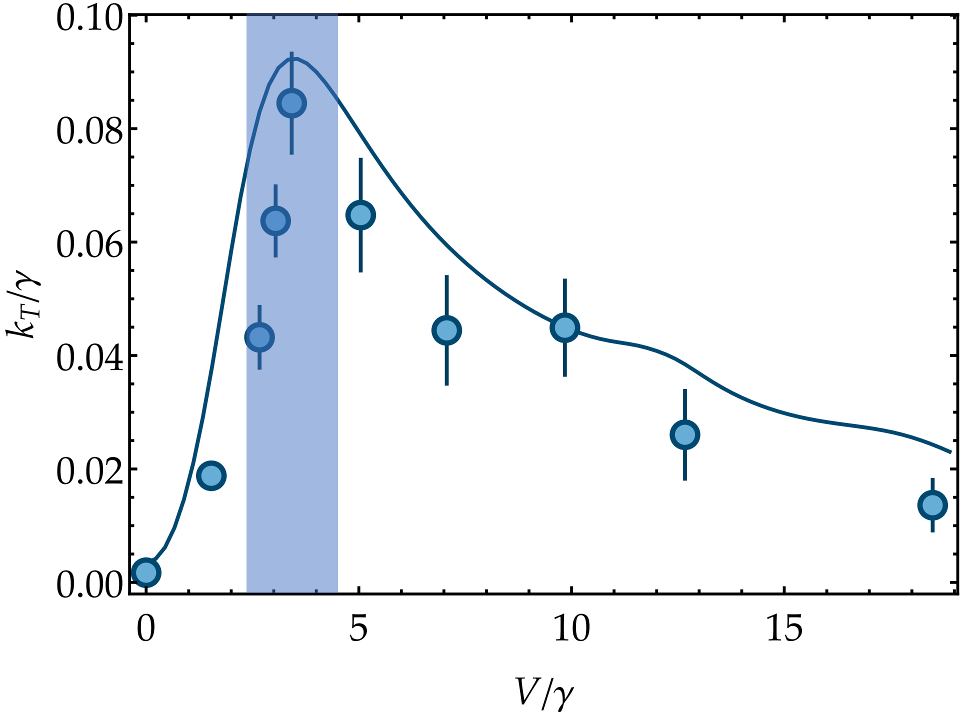


Optimal Transfer with V/γ

- Scanning V/γ on resonance:
  - ➢ Optimal transfer rate



S. S. Skourtis, et al., *J. Phys. Chem.* **96**, 20 (1992)



D. E. Logan and P. G. Wolynes, *Phys. Rev. B* **36**, 4135 (1987)
C. Maier, et al., *Phys. Rev. Lett.* **122**, 050501 (2019)
M. B. Plenio and S. F. Huelga, *New J. Phys.* **10**, 113019 (2008)
P. Rebentrost, et al., *New J. Phys.* **11**, 033003 (2009)
A. W. Chin, et al., *New J. Phys.* **12**, 065002 (2010)

What happens to multi-mode systems?

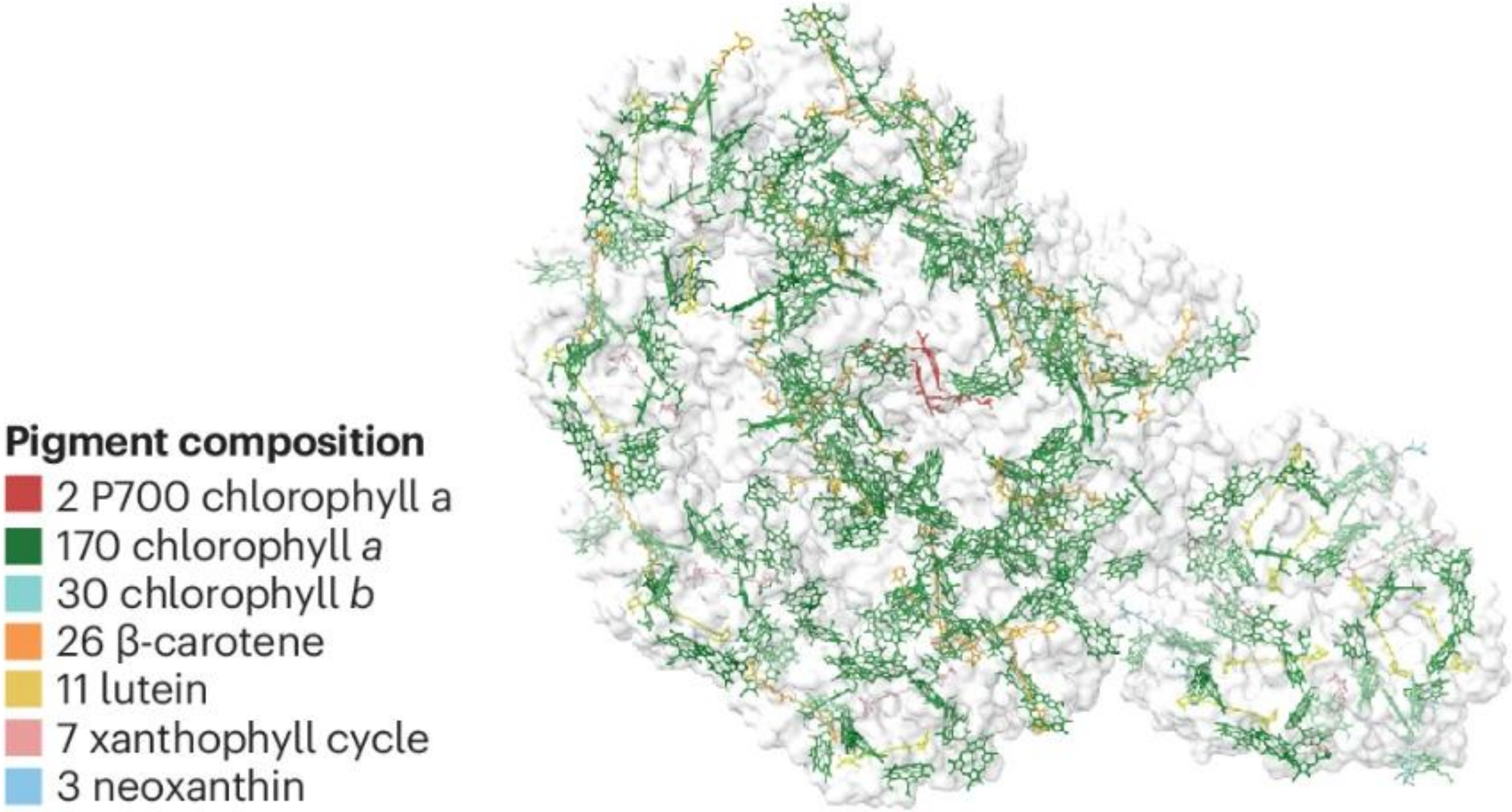


Image: M. P. Johnson, *Nat. Mol. Cell Biol.* **26**, 667-690 (2025)

Minimal multi-mode donor-acceptor system

$$H_{2\mathrm{M}} = \frac{\Delta E}{2}\sigma_z + V\sigma_x + \sum_{i=1}^{2}\left\{\frac{g_i}{2}\sigma_z\left(a_i + a_i^\dagger\right) + \omega_i a_i^\dagger a_i\right\}$$

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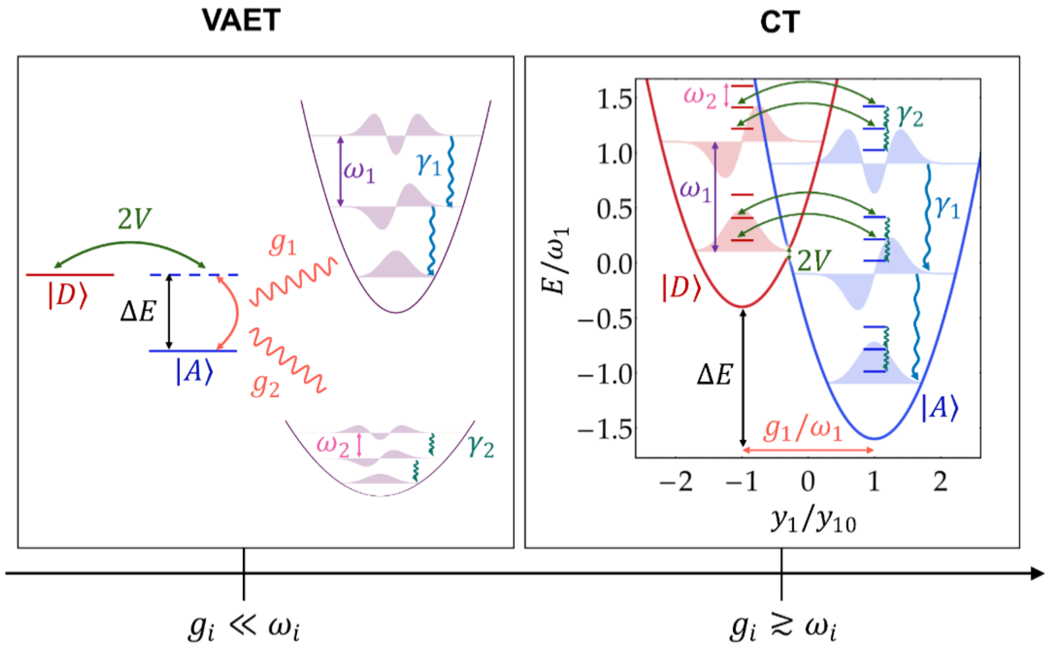

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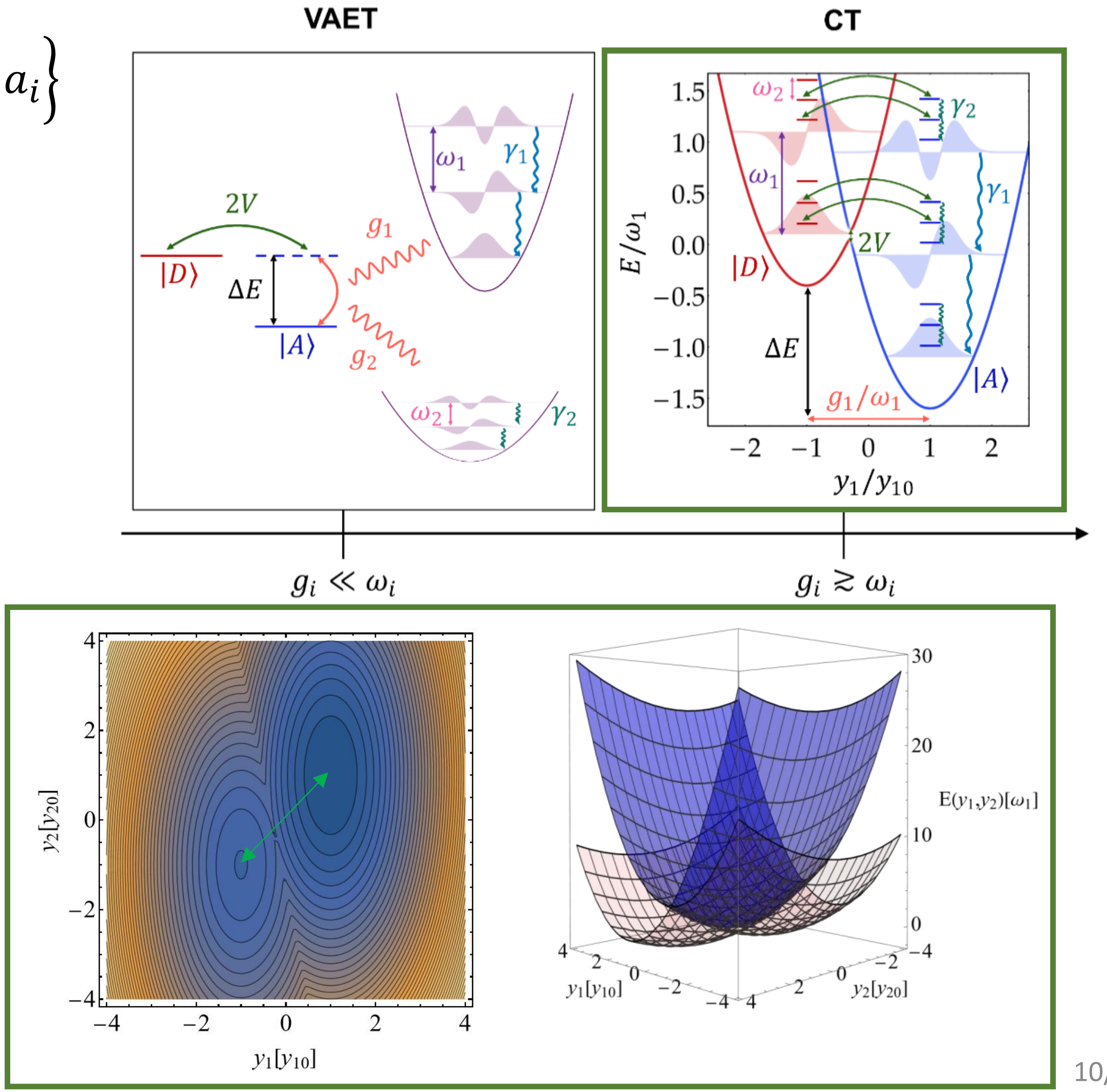

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- **Electron/Charge Transfer (CT):**
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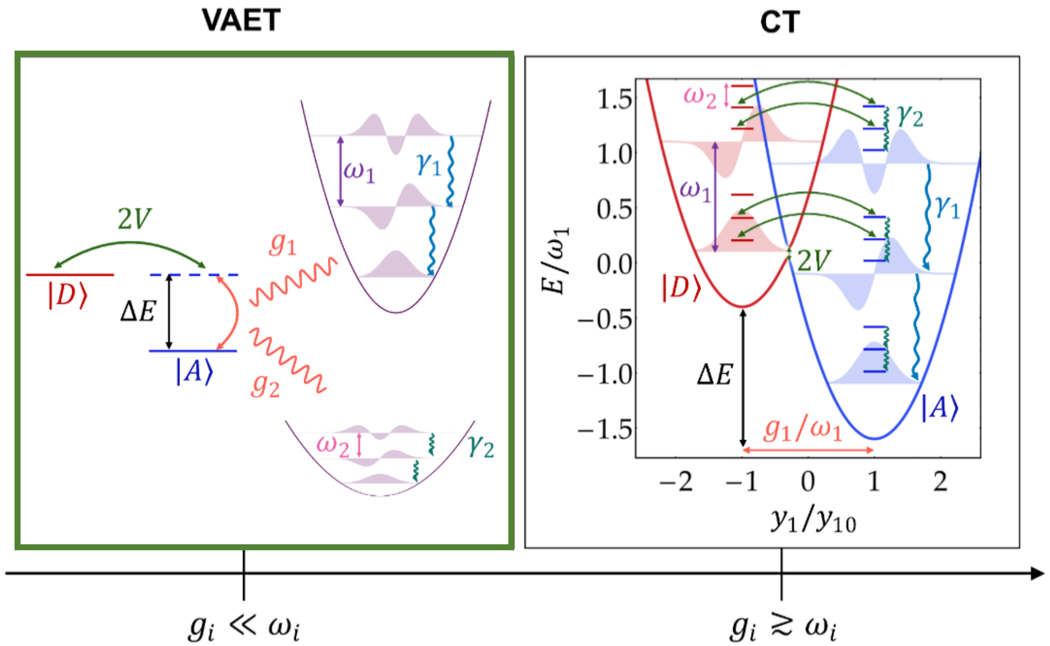
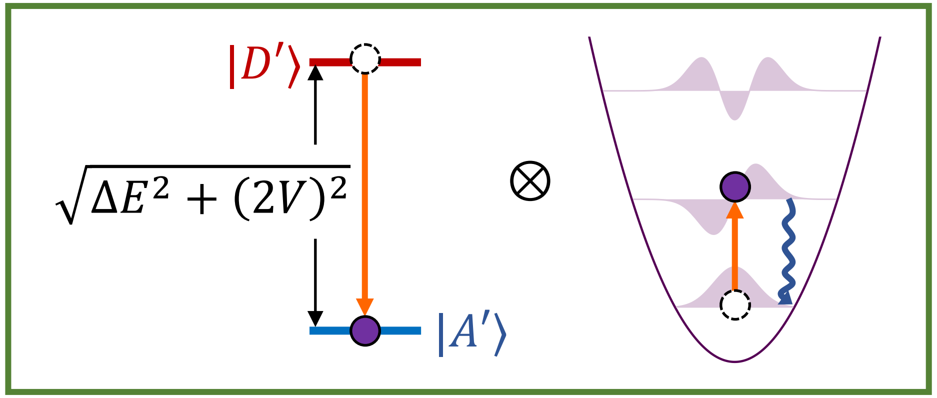
- **Vibrationally Assisted Exciton Transfer (VAET):**
  - ➢ Vibrational modes are weakly coupled to electronic sites → energy exchange between electronic sites and vibrational degrees of freedom (reservoirs)

$$|D'\rangle \otimes |0\rangle \underset{g}{\rightarrow} |A'\rangle \otimes |1\rangle \underset{\gamma}{\rightarrow} |A'\rangle \otimes |0\rangle$$





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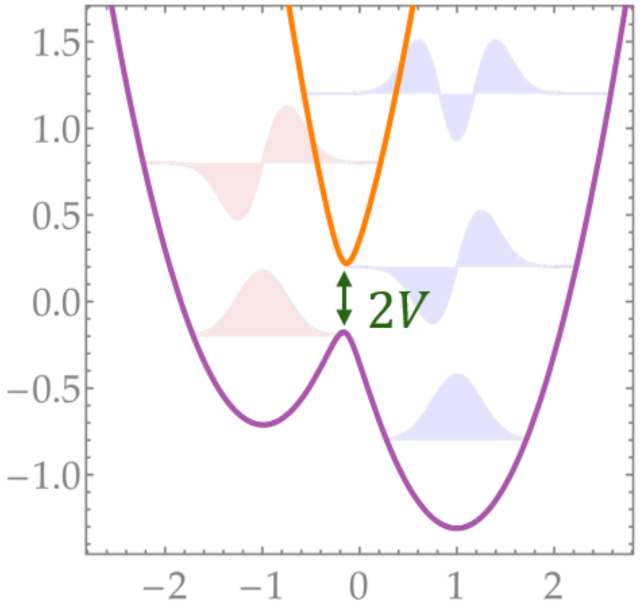
- Strong electronic coupling: $V \sim \lambda_i/4$
  - Hybridization of the donor and acceptor energy surfaces



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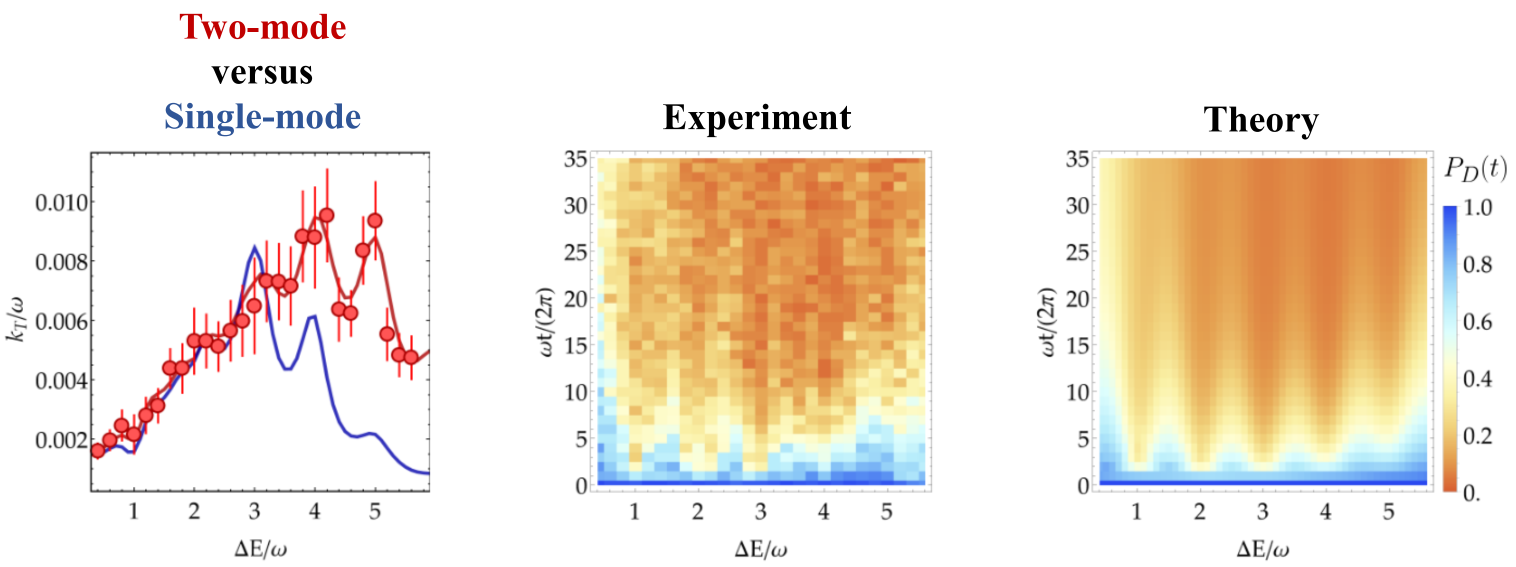

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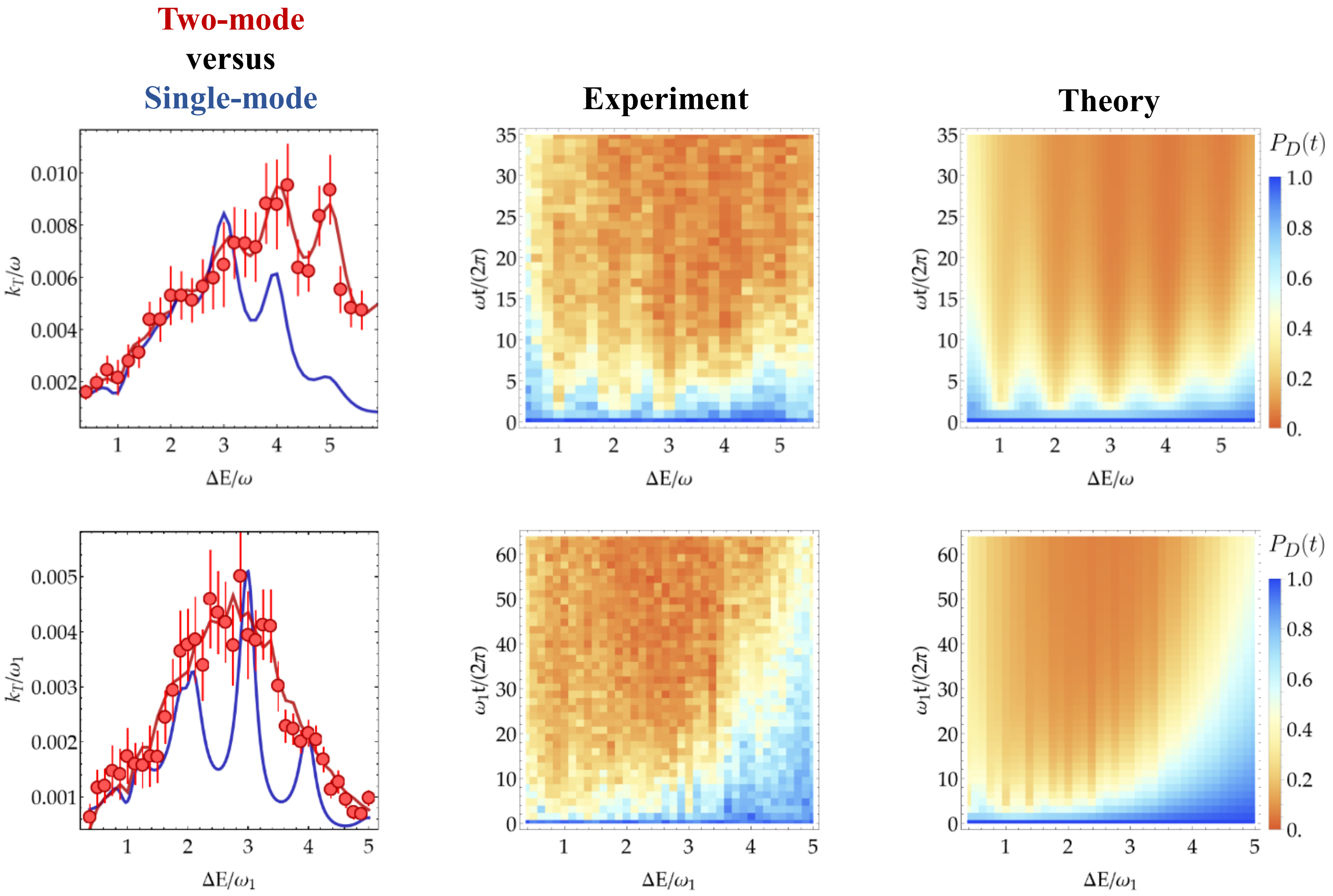
- Non-degenerate case ($\omega_1 > \omega_2$):
  - ➢ Delocalized states are spread out



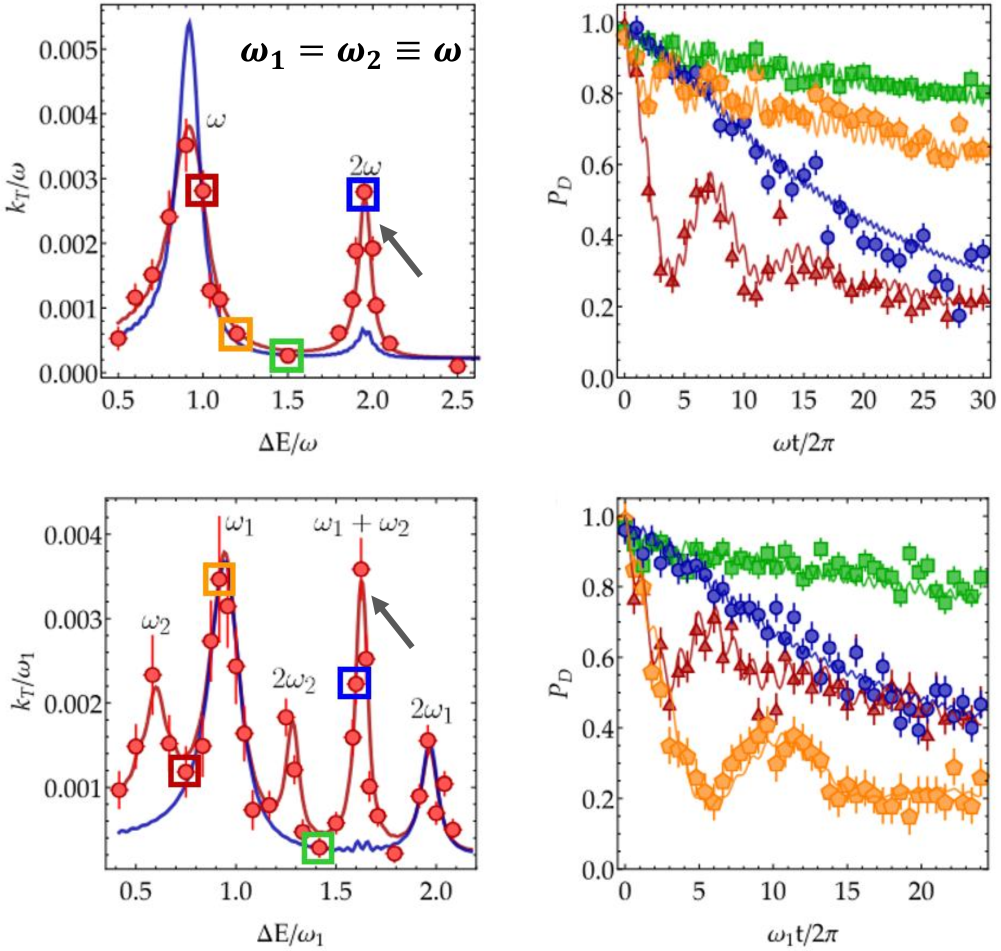
Vibrationally Assisted Exciton Transfer (VAET)

- Well-resolved resonances:

$$\Delta E \approx \sqrt{(l_1\omega_1 + l_2\omega_2)^2 - (2V)^2},\ (l_1, l_2 \in \mathbb{Z})$$

- Both cases of mode degeneracy:
  - ➢ Low-temperature processes: 1st-order (single-phonon exchange) and 2nd-order (two-phonon exchange)

Two-mode
versus
Single-mode



D. J. Gorman et al., *PRX* **8**, 011038 (2018)
Z. Z. Li et al., *New J. Phys.* **23**, 073012 (2021)
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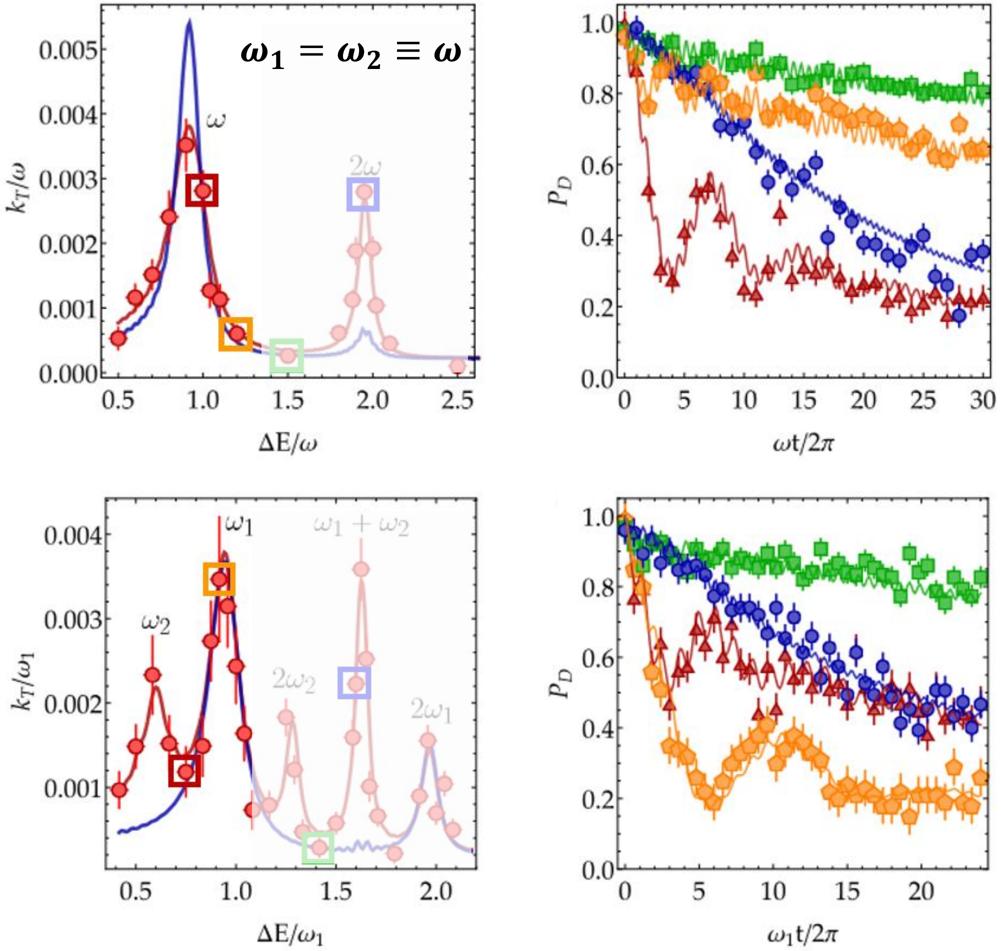

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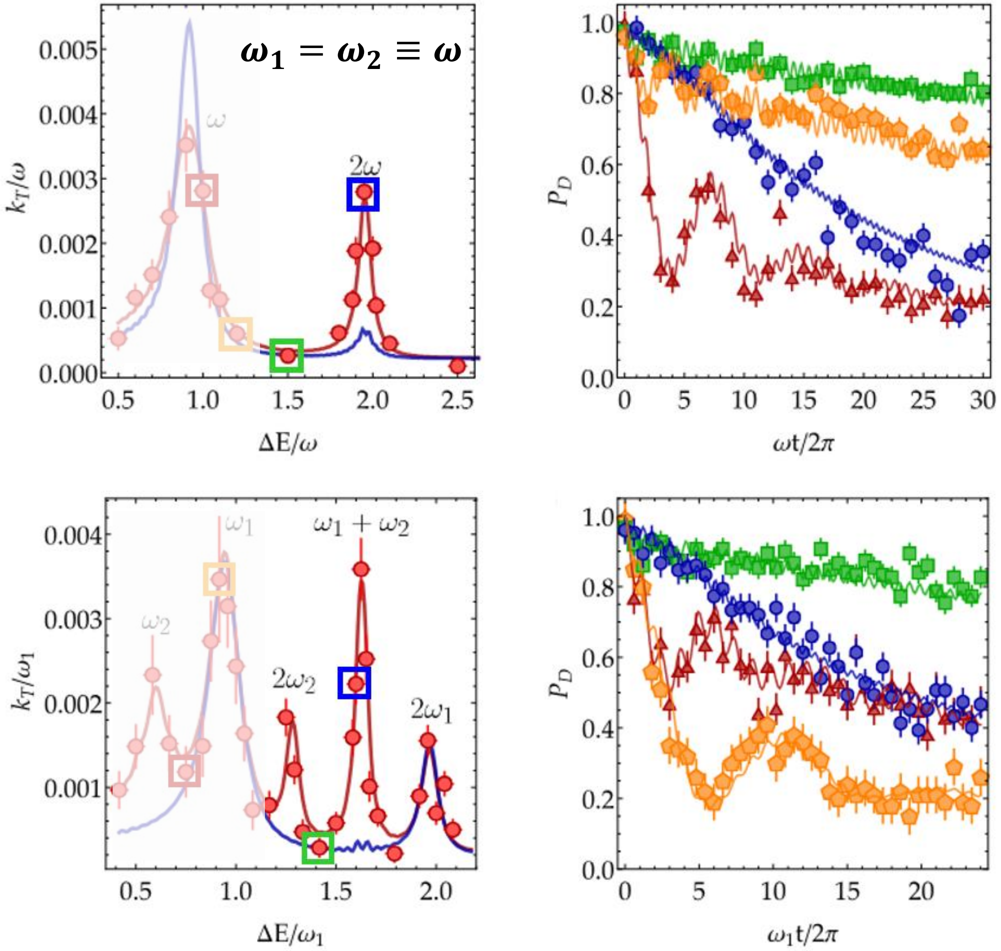

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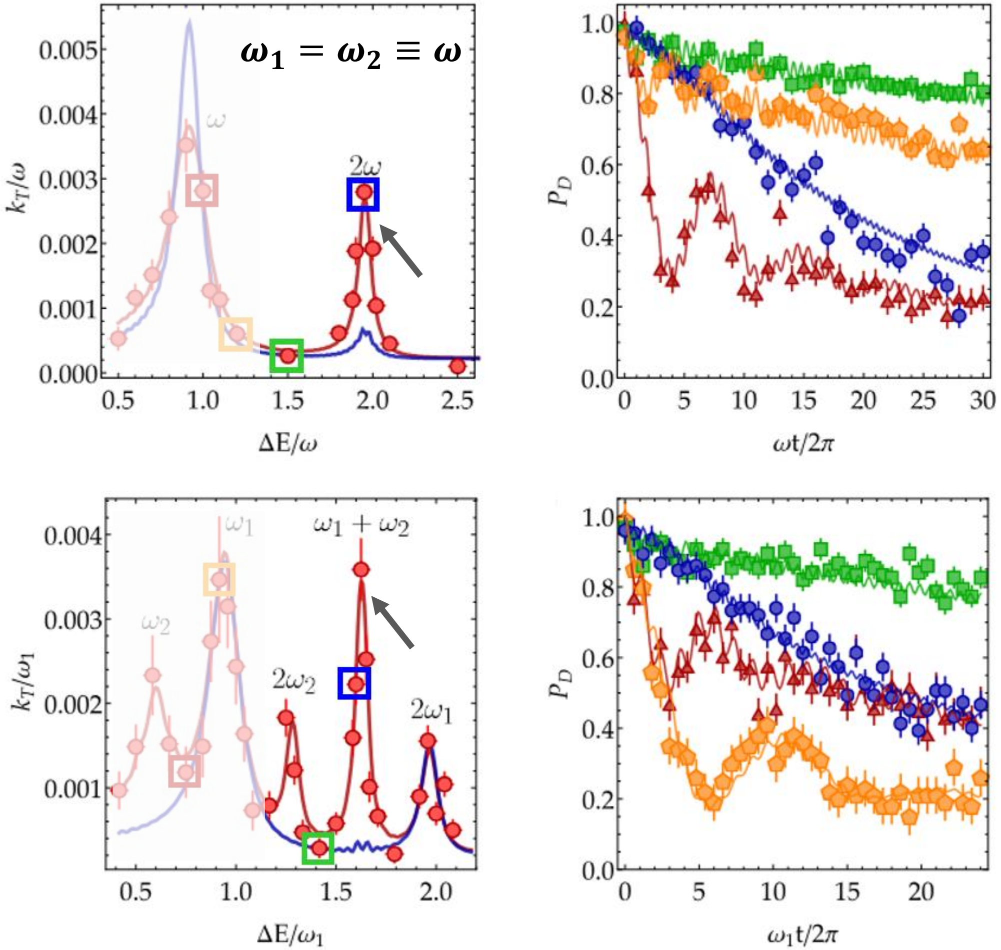
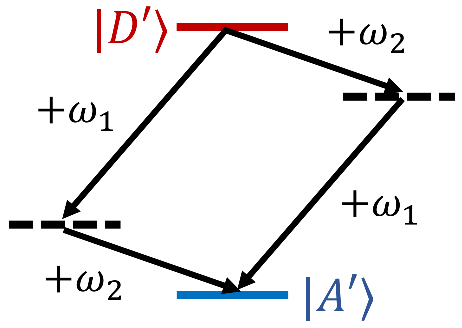
  - ➢ $\omega_1 + \omega_2$ exchange with constructively interfering pathways

Two-mode
versus
Single-mode



$\omega_1 + \omega_2$ process



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Z. Z. Li et al., *New J. Phys.* **23**, 073012 (2021)
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What about the temperature?

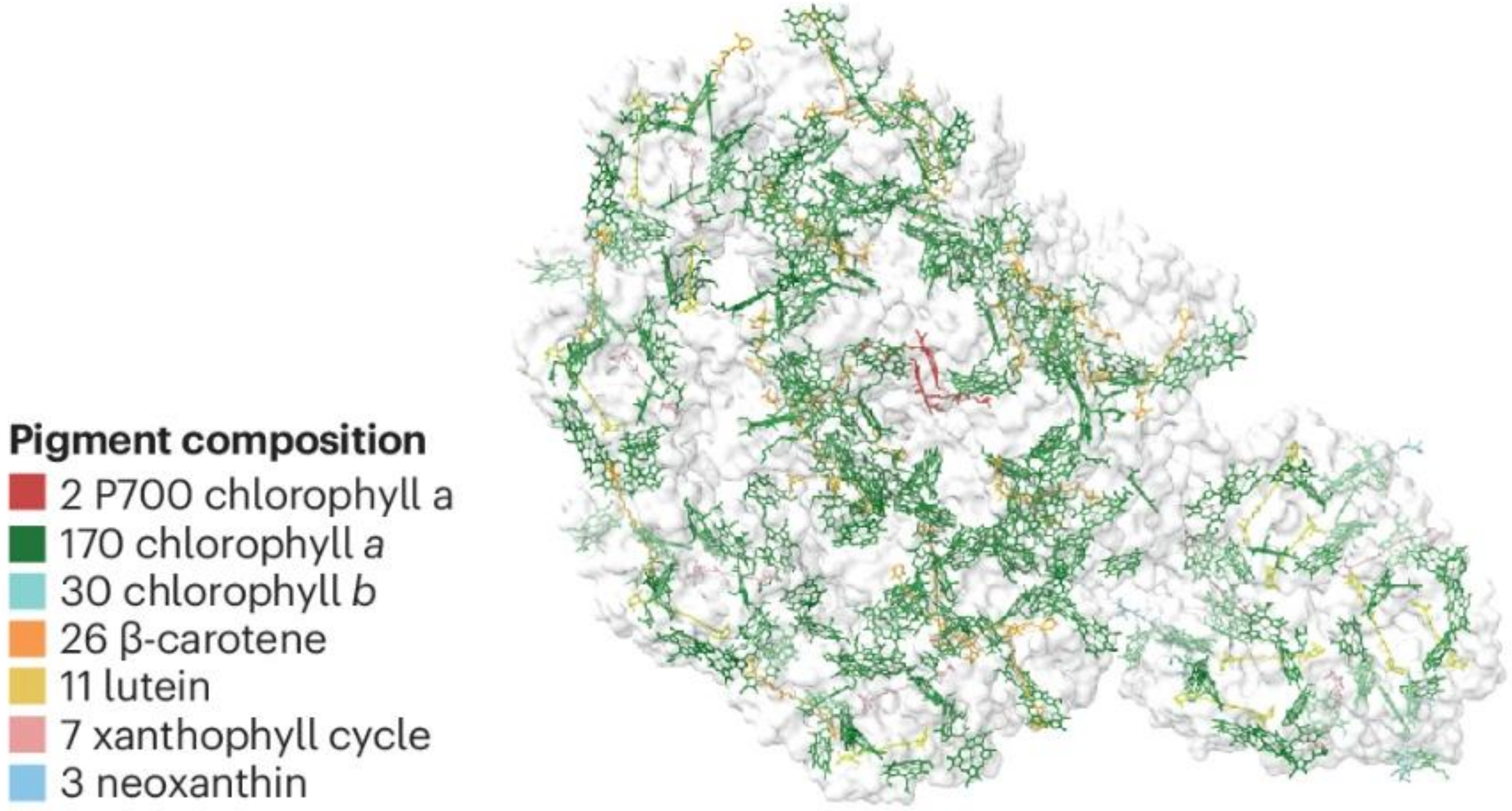
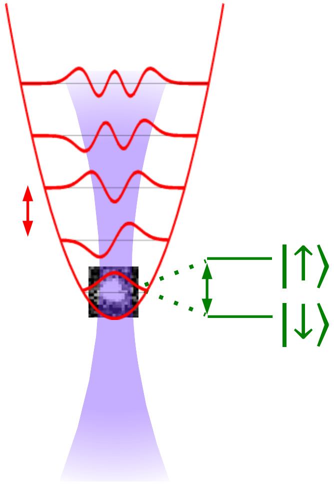


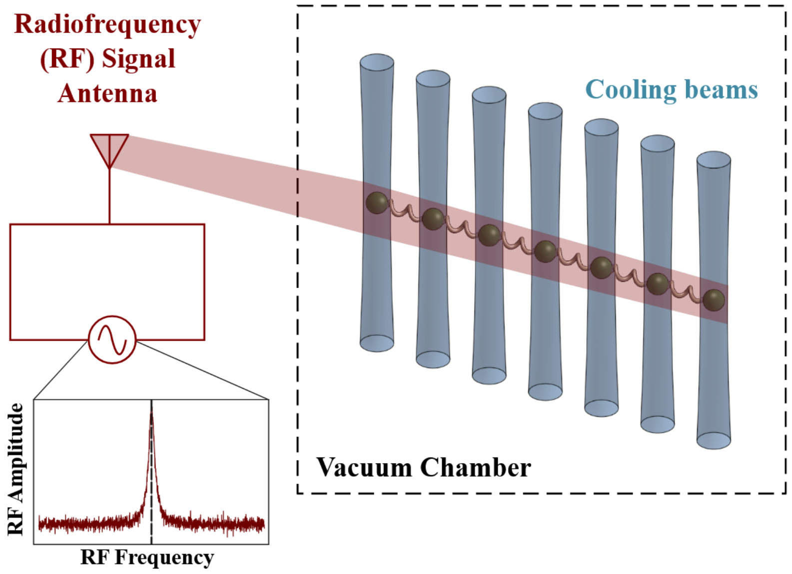
Image: M. P. Johnson, *Nat. Mol. Cell Biol.* **26**, 667-690 (2025)

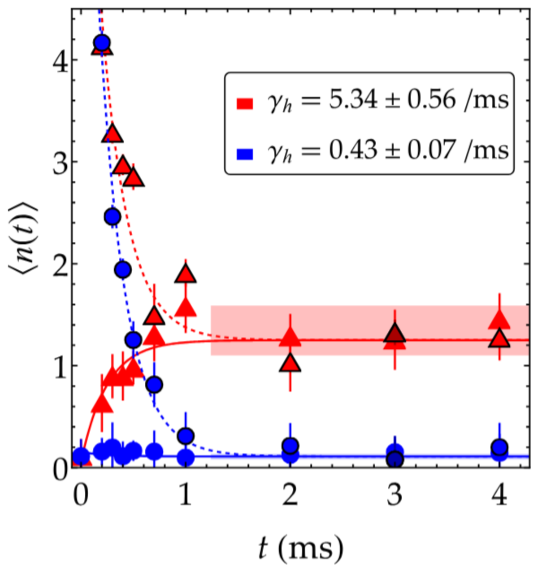
Open-system Quantum Simulation of LVCMs

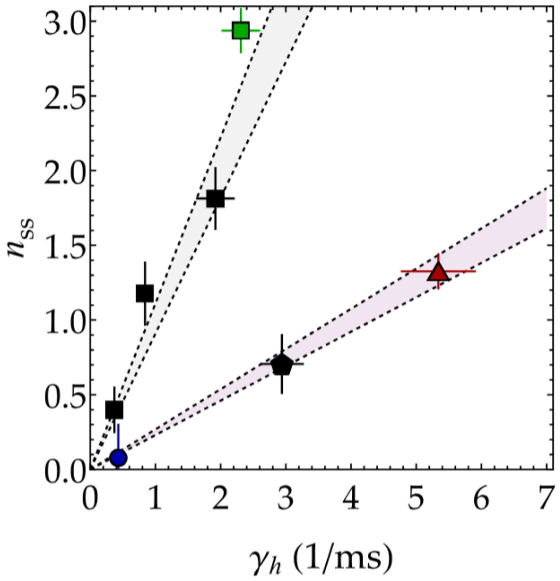
- Trapped ions: $\frac{\partial \rho}{\partial t} = -i[H_{\mathrm{LVCM}}, \rho]$
  - Internal states (electronic sites/configurations)
  - External harmonic oscillator modes (vibrations)
  - Light-ion interactions (H_{LVCM})



- Resolved-sideband cooling <u>+ electric-field noise broadcast</u>: $\Lambda_i[\rho]$ with <u>independently</u> tunable γ_i and $\bar{n}_i = \gamma_{hi}/\gamma_i$

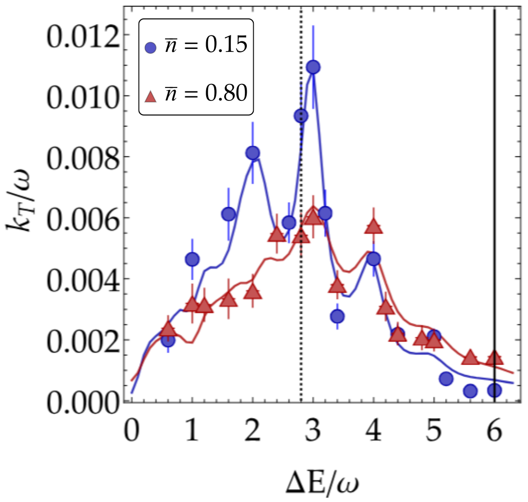


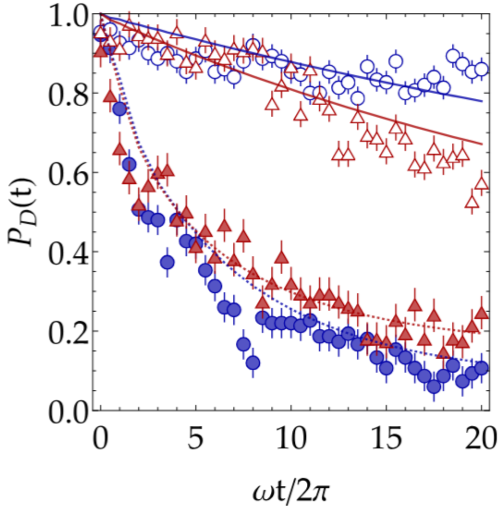




Thermal Effects in Excitation Transfer

- Redistribution of phonon population
- Single-mode electron/charge transfer
  - Broadening of the transfer rate spectrum
  - Different from Classical Marcus Theory





Thermal Effects in Excitation Transfer

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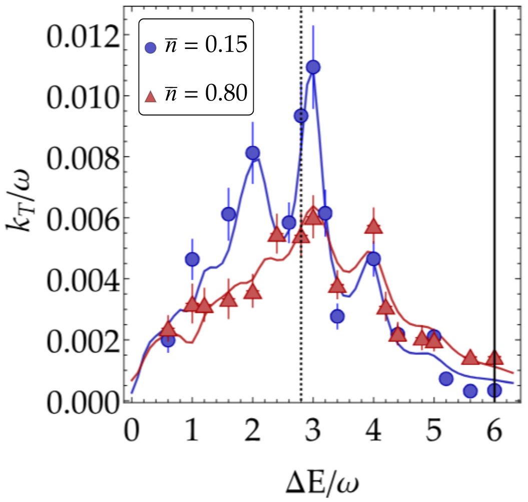
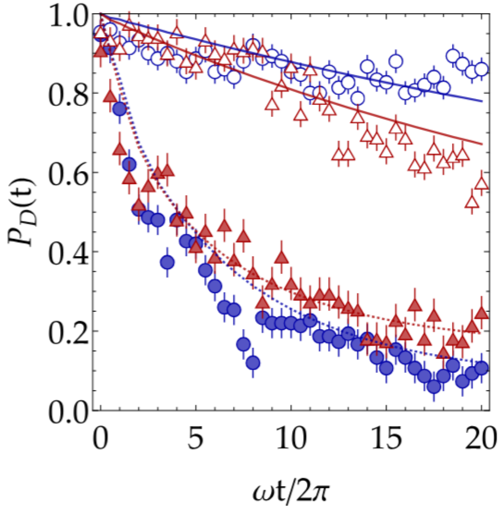
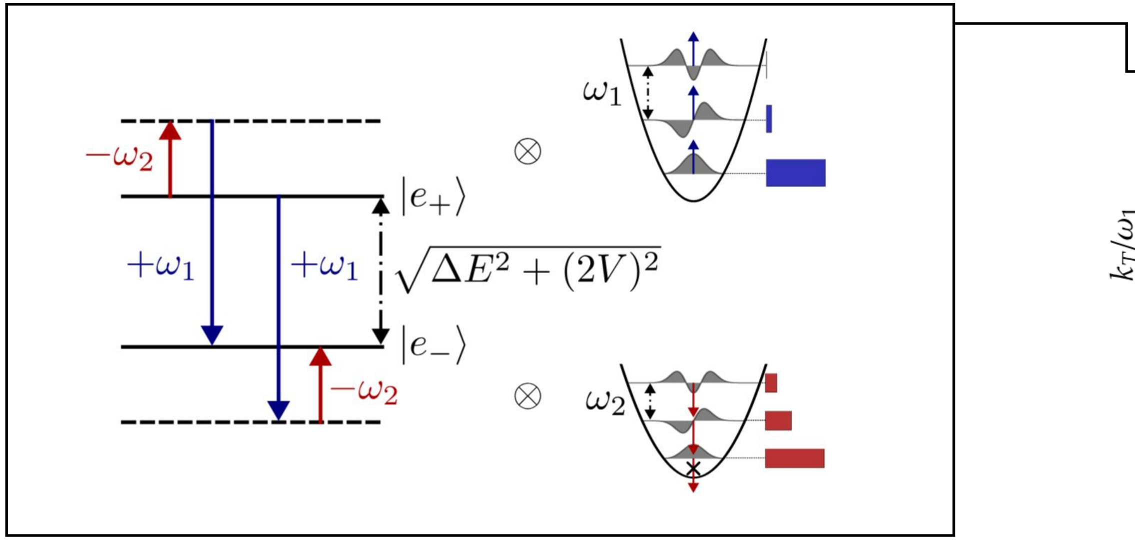
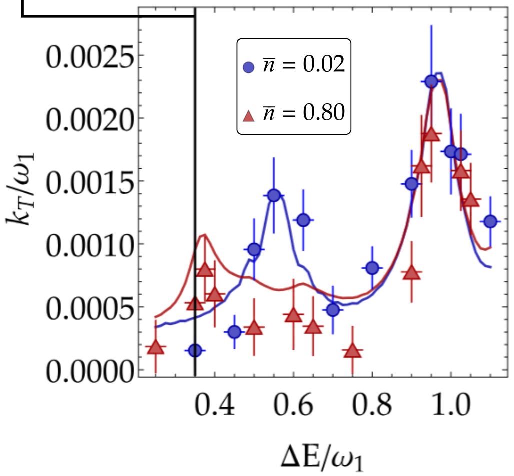
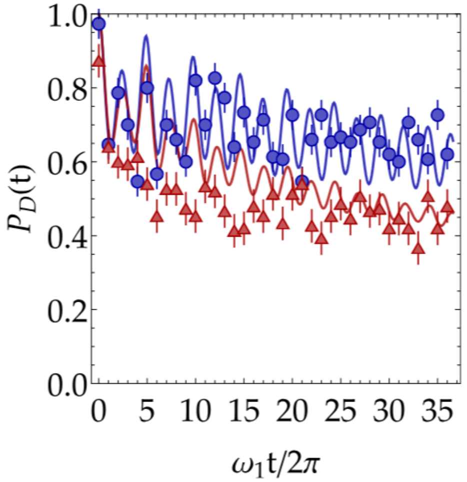
  - ➢ Different from Classical Marcus Theory
- Two-mode vibrationally assisted exciton transfer
  - ➢ Thermally activated transfer pathways











Summary

- Open single-mode LVCM: Electron/Charge Transfer with tunable dissipation
  - Access different regimes of adiabaticity
  - Identify optimal transfer conditions
- Open two-mode LVCM: Charge Transfer and Vibrationally Assisted Exciton Transfer
  - Measure enhanced transfer rates
  - Observe constructive interference effect in VAET pathways
  - Apply to the same class of LVCM systems with $i > 2$
- Thermal-bath engineering
  - Broadening effect in ET/CT spectrum
  - Uncover thermally activated transfer pathways

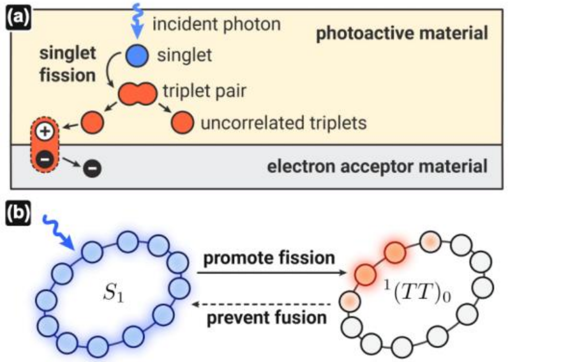
Key Takeaway:

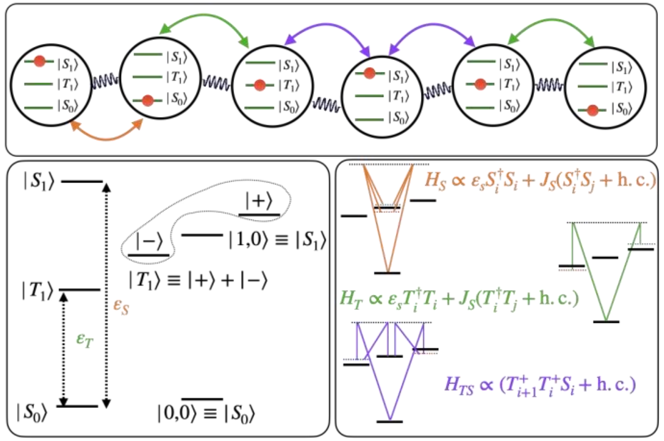
Hardware-efficient approach to simulating spin-boson models with controlled environment
→ near-term qualitative advantage over classical methods?

Outlook and Open Questions

Singlet Fission

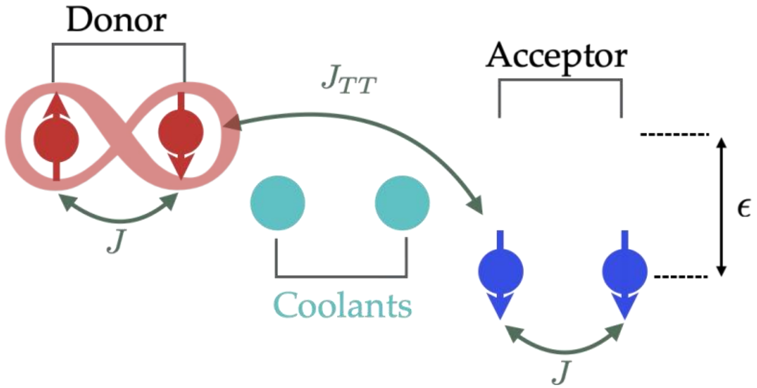
F. Campaioli et al., *PRX Energy* **3**, 043003 (2024)





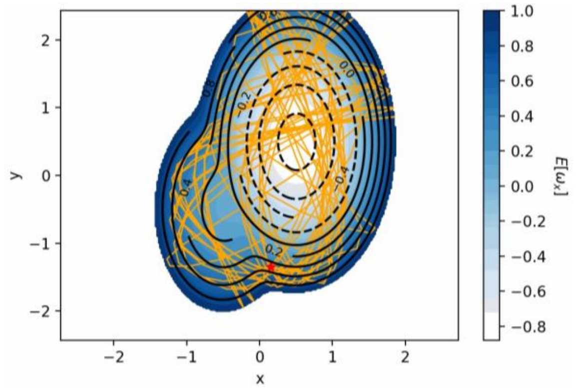
Delocalized Excitation Transport

D. Fallas Padilla, **VS**, et al., *PRX Quantum* **6** (4),040301 (2025)



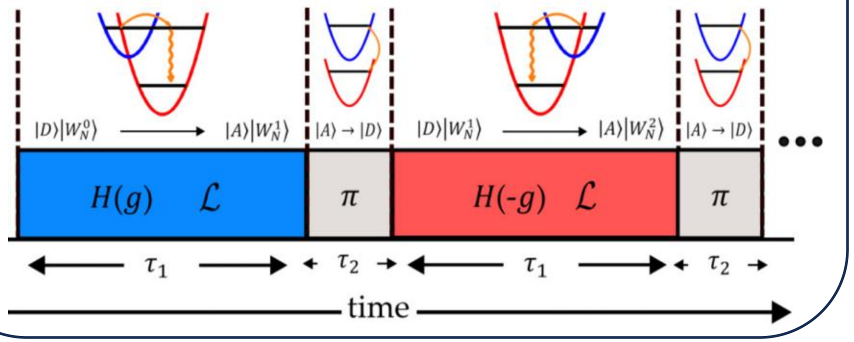
Anharmonicity and Chaos

C. Zhang et al., *PNAS* **120**, e2221690120 (2023)



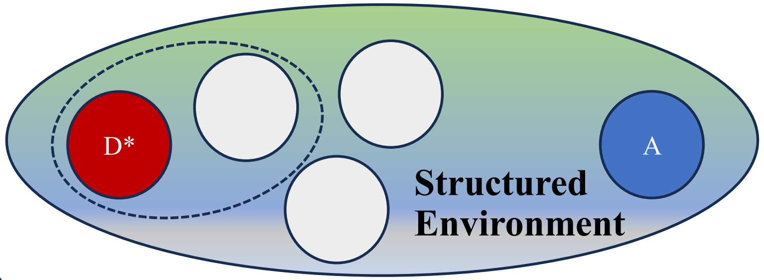
ET-inspired Quantum-state Engineering

M. Zhu, **VS**, et al., *Phys. Rev. A* **112**, 012617 (2025)



Structured Environment

A. Lemmer et al., *New J. Phys.* **20**, 073002 (2018)



AND MORE …

Outlook and Open Questions

Polaron Physics? Fermion-Boson-Gauge Theories? Others!

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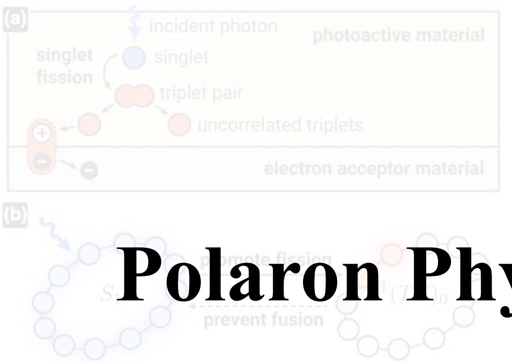

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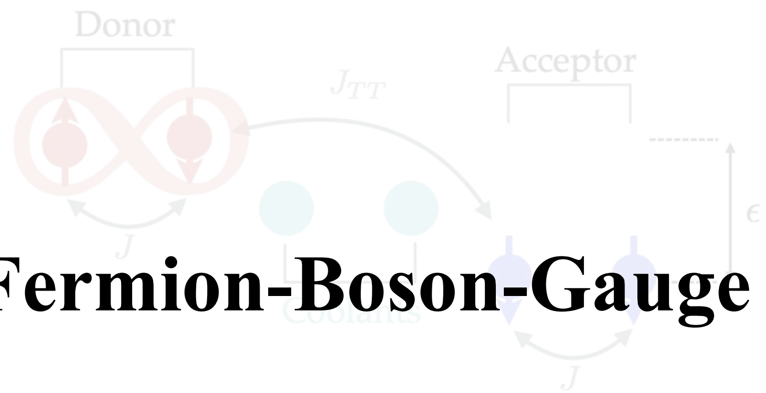

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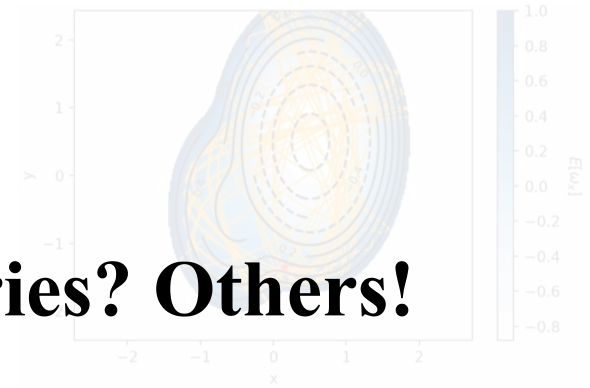

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