Quantum work statistics at strong reservoir coupling

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Thanks to Owen Diba ,Harry Miller, Jake Iles-Smith

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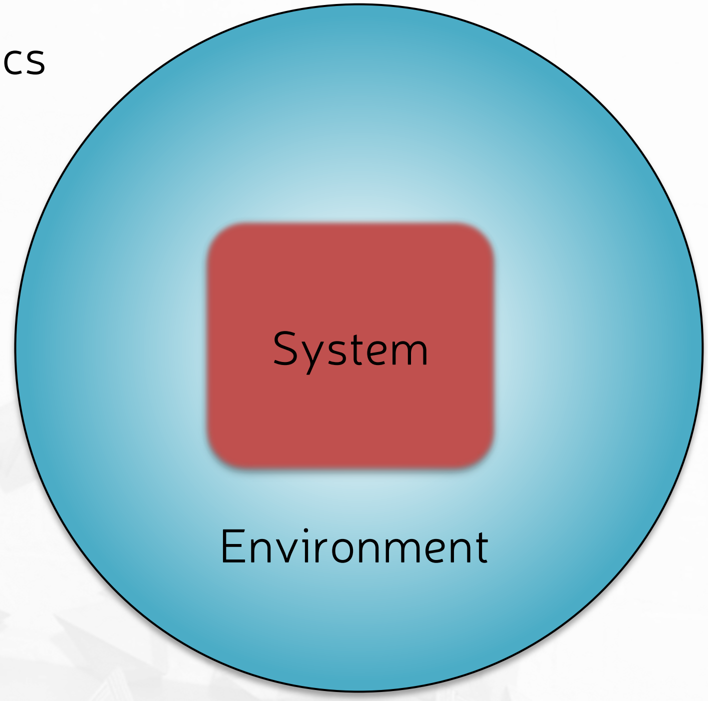
Outline

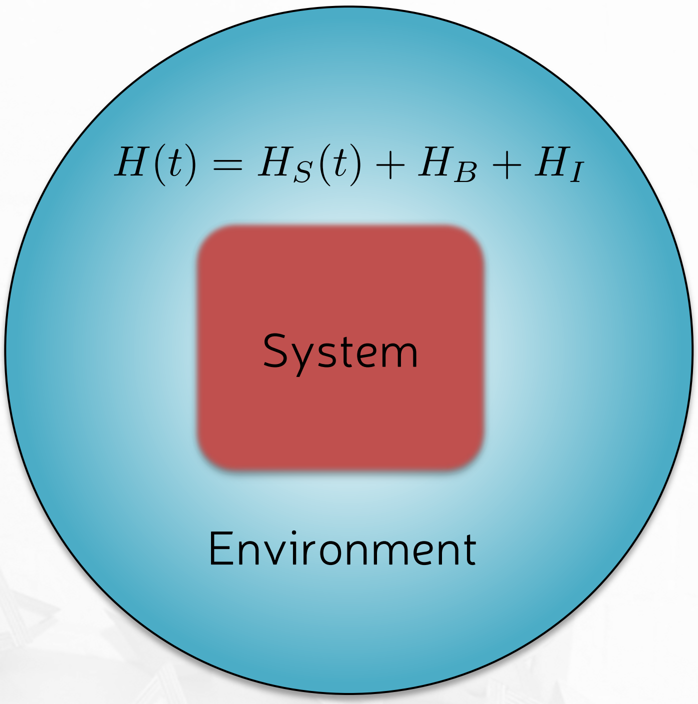
- **Two-point measurement protocol for work**
  - Work probability distribution
  - Characteristic function and counting statistics
- **Adiabatic dynamics**
  - Master equation
  - Counting statistics
- **Beyond weak reservoir coupling**
  - Polaron approach
- **Why polaron?**
  - Experiments on controlled quantum dots
- **Work counting statistics examples**
  - Landau-Zener protocol
  - Weak-coupling vs polaron
- **Future directions**



Motivation

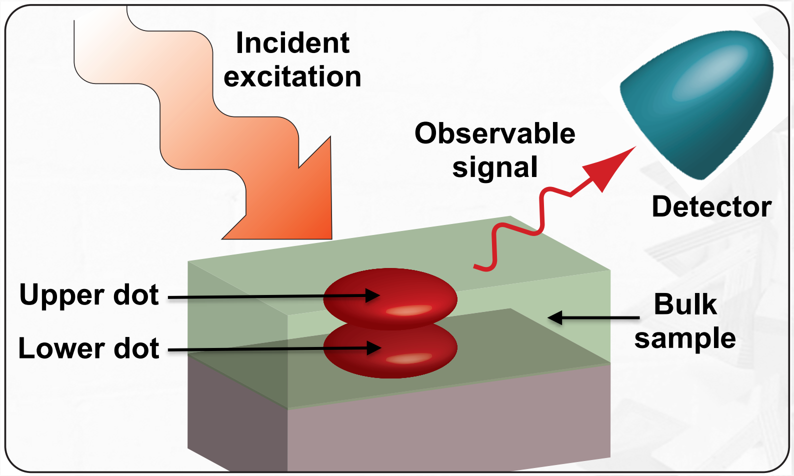
Strong-coupling thermodynamics

- Here we focus on calculating the full work distribution for a driven open system
- Standard approaches generally assume system-reservoir interactions play negligible role
- Determining statistics of work in strong coupling regimes is a **formidable task**
  - Requires calculation of full eigenspectrum of system and reservoir
- We will circumvent this issue using a unitary polaron transformation
  - Maps our open system to a new frame where a weak-coupling-like theory can be applied
  - Application to a Landau-Zener protocol



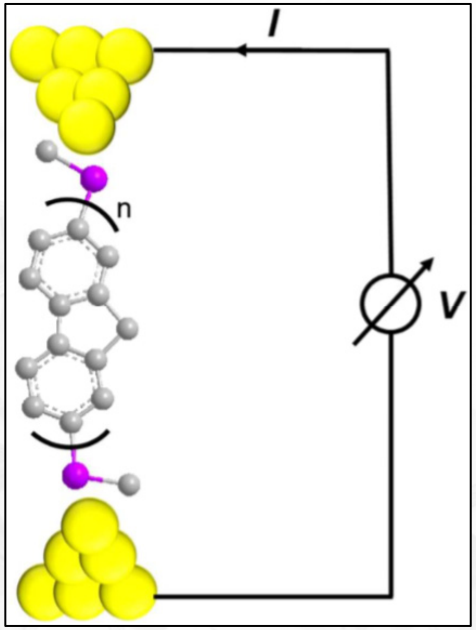
Example open quantum systems

Semiconductor Nanostructures



- **Strong** coupling to phonons
- Weak coupling to the electromagnetic field

Molecular Nanojunctions



B. Chen and K. Xu, Nano 14, 1930007 (2019)

- **Strong** coupling to vibrations
- Weak tunnel coupling to the leads

Non-additivity of multiple environments

H. Maguire, J. Iles-Smith, and AN, PRL 123, 093601 (2019)

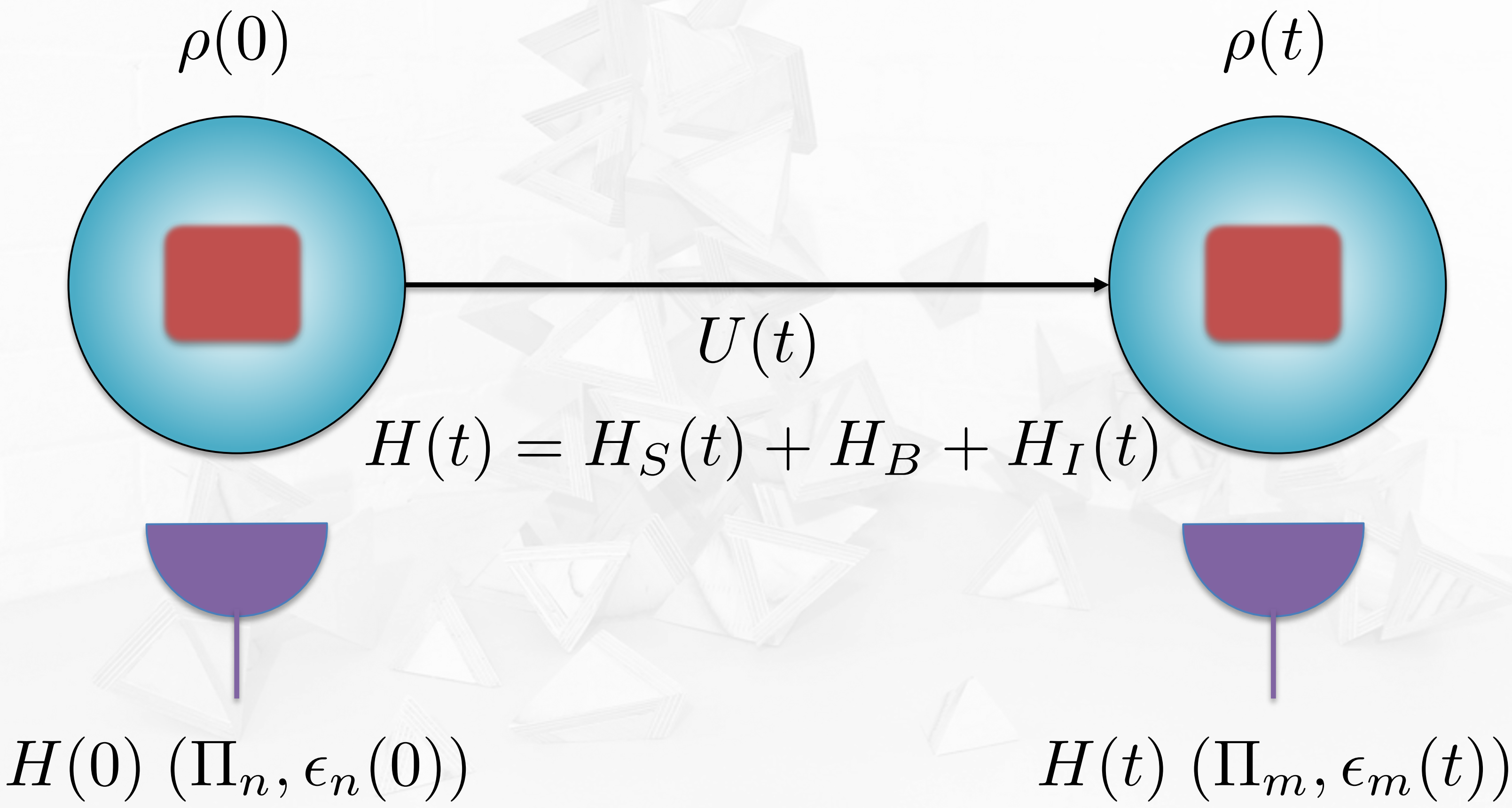
C. McConnell and AN, JCP 151, 054104 (2019)

C. McConnell and AN, NJP 24, 025002 (2022)

Work: two-point measurement

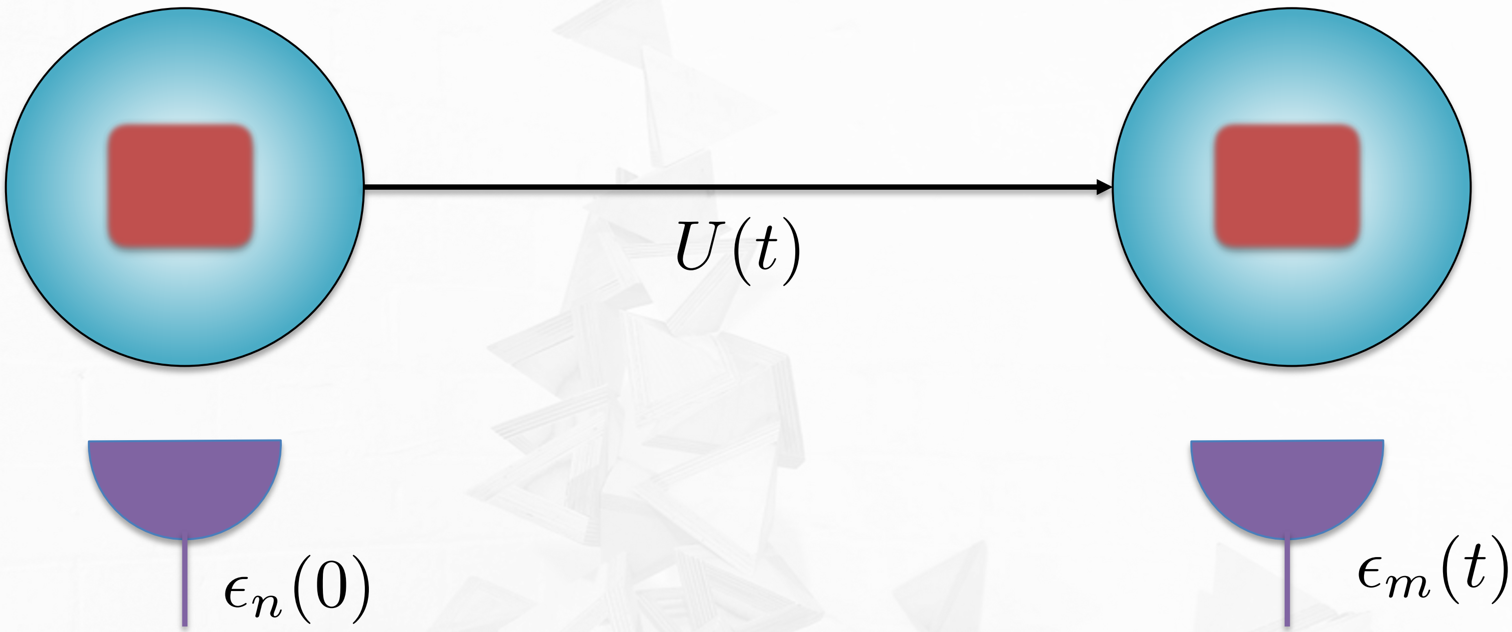
We characterise (stochastic) work via the two-point measurement protocol

- Consider projective energy measurements performed on **combined system and environment**, which is closed and evolves unitarily under the action of an external force



P. Talkner, E. Lutz, P. Hanggi, Phys. Rev. E 75, 050102(R) (2007)

Work probability density



$$p(n) = \mathrm{tr}(\Pi_n \rho(0))$$

$$p(m,t|n) = \frac{\mathrm{tr}(\Pi_m U(t) \Pi_n \rho(0) \Pi_n U^\dagger(t))}{p(n)}$$

Work done on system is measured energy difference, leading to probability density

$$p(w) = \sum_{n,m} p(n) p(m,t|n) \delta(w - [\epsilon_m(t) - \epsilon_n(0)])$$

P. Talkner, E. Lutz, P. Hanggi, Phys. Rev. E 75, 050102(R) (2007)

Work characteristic function

For practical purposes, it is easier to work with the characteristic function

$$\Phi(\chi) = \int dw e^{i\chi w} p(w)$$

Contains all statistical information about the work performed on our closed system+environment

$$\langle w^k \rangle = (-i)^k \frac{\partial^k \Phi(\chi)}{\partial \chi^k}\bigg|_{\chi=0}$$

Characteristic function can be written in terms of a counting-field dependent density operator

$$\Phi(\chi) = \mathrm{tr}(\rho(\chi,t)) = \mathrm{tr}_S(\rho_S(\chi,t))$$

With reduced density operator (which we look to approximate)

$$\rho_S(\chi,t) = \mathrm{tr}_B(\rho(\chi,t))$$

Work counting statistics

Counting-field dependent density operator obeys an equation of motion of the form

$$\dot{\rho}(\chi,t) = -i(H(\chi,t)\rho(\chi,t) - \rho(\chi,t)H(-\chi,t))$$

With a transformed Hamiltonian

$$H(\chi,t) = H(t) + i\partial_t(e^{i\chi H(t)/2})e^{-i\chi H(t)/2}$$

Reduced density operator obeys a generalised master equation

$$\boxed{\dot{\rho}_S(\chi,t) = \mathcal{L}(\chi,t)\rho_S(\chi,t)}$$

Form of the Liouvillian depends on the approximations made, e.g.

- Weak coupling
- Slow time dependence (adiabatic)

M. Esposito, U. Harbola, and S. Mukamel, Rev. Mod. Phys. 81, 1665 (2009),
Rev. Mod. Phys. 86, 1125 (2014)

Adiabatic Markovian master equations

Dealing with arbitrary time-dependence can be difficult, so we will consider the adiabatic limit of slow external driving and static interactions

$$H(t) = H_S(t) + H_B + H_I$$

Following Albash et al. we can derive a Markovian Lindblad master equation under the Born-Markov-secular approximations:

$$\dot{\rho}_s(t) = \mathcal{L}^{\mathrm{ad}}(t)\rho_S(t) = -i[H_S(t) + H_{\mathrm{LS}}(t), \rho_S(t)] + \mathcal{D}(t)\rho_S(t)$$

$$\mathcal{D}(t)\rho_S(t) = \sum_{\alpha\beta}\sum_{\omega}\gamma_{\alpha\beta}(\omega(t))\left[L_{\omega,\beta}(t)\rho_S(t)L^{\dagger}_{\omega,\alpha}(t) - \frac{1}{2}\{L^{\dagger}_{\omega,\alpha}(t)L_{\omega,\beta}(t), \rho_S(t)\}\right]$$

Applying the same approximations to the counting-field dependent density operator, and **ignoring interaction contributions** to energy measurements, we obtain an adiabatic weak-coupling form

$$\dot{\rho}_S(\chi, t) = \mathcal{L}^{\mathrm{ad}}(\chi, t)\rho_S(\chi, t)$$

Albash et al., New J. Phys. 14 123016 (2012)
F. Liu, Phys. Rev. E 90, 032121 (2014)

Moving beyond weak coupling: solid-state quantum optics

How do we modify standard quantum optics to model solid-state devices?

- e.g. what effect do lattice vibrations (phonons) have on system properties?

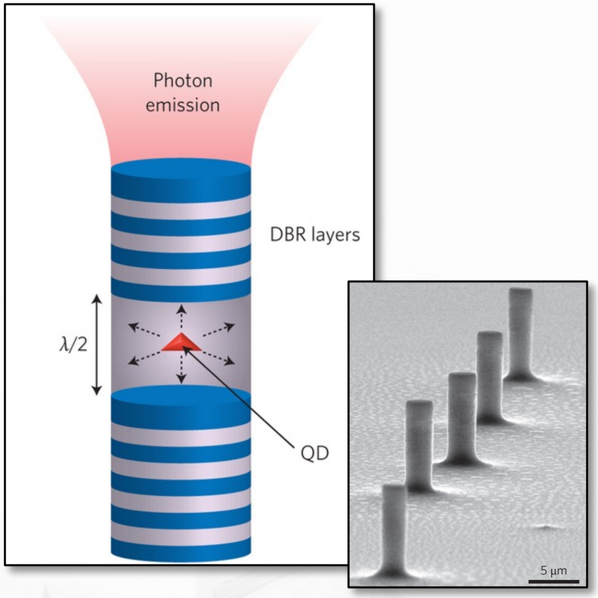
Model

- two-level system
- coherent manipulations through external laser addressing (adiabatic)
- excitation of single electron from valence to conduction band
- oscillations damped by phonon interactions

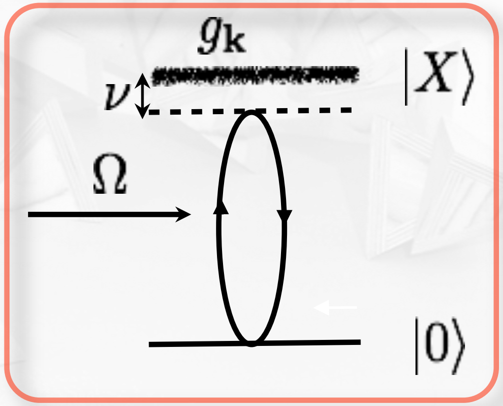
$$H_S(t) = \frac{\omega_0}{2}\sigma_z + \Omega(e^{-i\omega_l t}\sigma_+ + e^{i\omega_l t}\sigma_-)$$

$$H_B = \sum_k \omega_k b_k^\dagger b_k$$

$$H_I = \sigma_z \sum_k g_k (b_k^\dagger + b_k)$$



R. Oulton, Nature Nano. 9, 169 (2014)

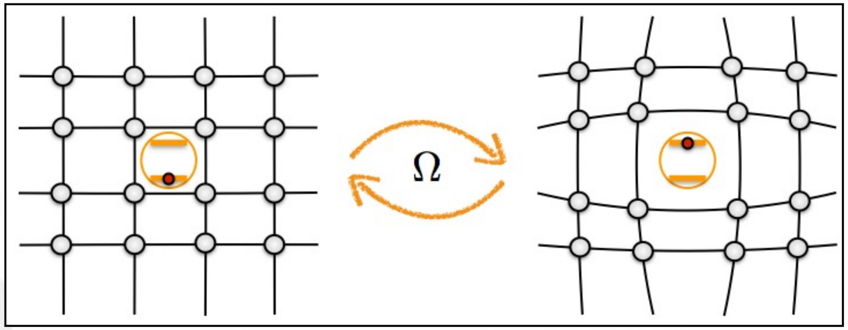


Phonon interactions

Lattice displaces in response to changes in charge configuration

- polaron formation – new boundary
- we incorporate this physics into our master equation via a unitary transformation
- allows strong electron-phonon interactions
- direct expt-theory comparisons

$$H_P = e^S H e^{-S}$$



Topical Review: AN and D. P. S. McCutcheon, JPCM 28, 103002 (2016)

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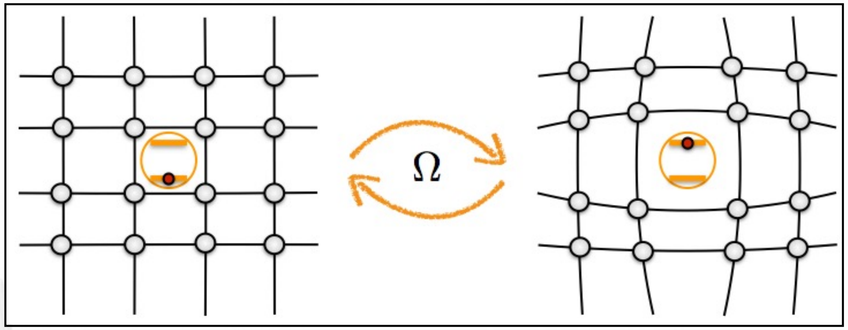

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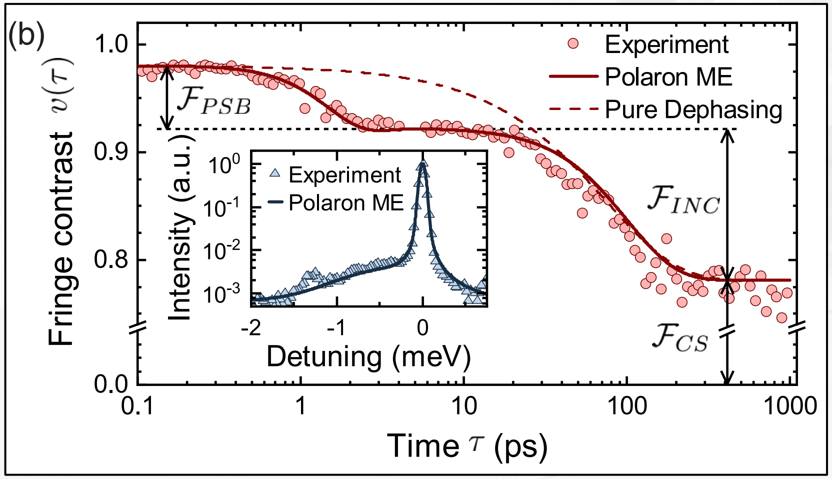
Damping of coherence



A. Brash et al., Phys. Rev. Let. 123, 167403 (2019)

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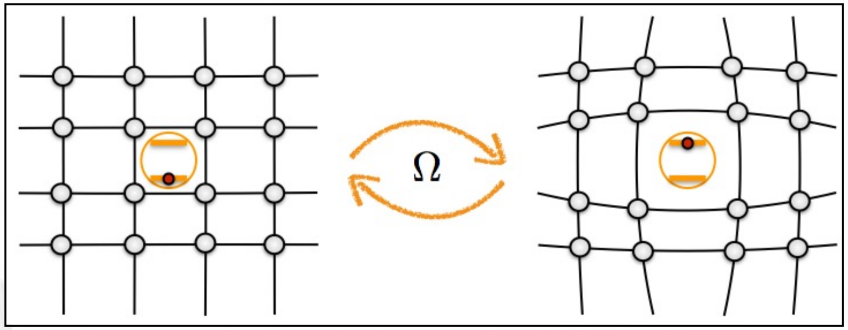

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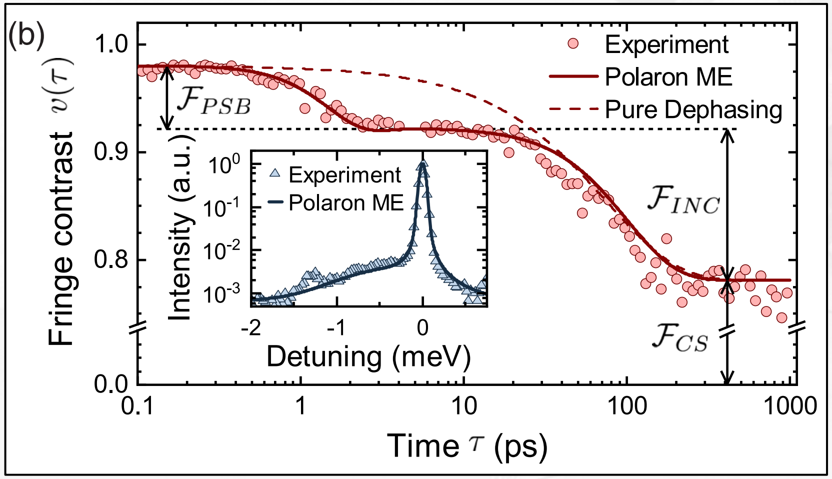
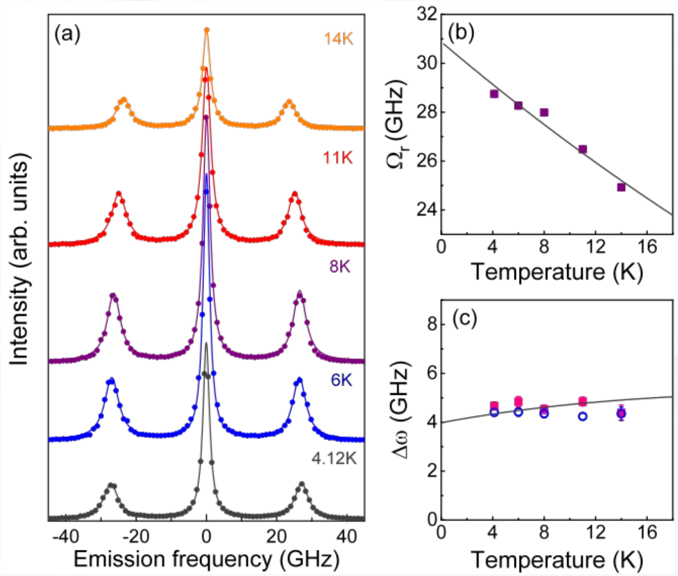


A. Brash et al., Phys. Rev. Let. 123, 167403 (2019)

Temp. dependence in resonance fluorescence



Y. Wei et al., PRL 113, 097401 (2014)
D. P. S. McCutcheon and AN, PRL 110, 217401 (2013)

Polaron transformation

We perform a unitary polaron transformation to our Hamiltonian to identify a new perturbation term

$$H_P(t) = e^S H(t) e^{-S},\ S = \sigma_z \sum_k (g_k/\omega_k)(b_k^\dagger - b_k)$$

This leads to a non-perturbative temperature and coupling strength dependent renormalisation of system driving

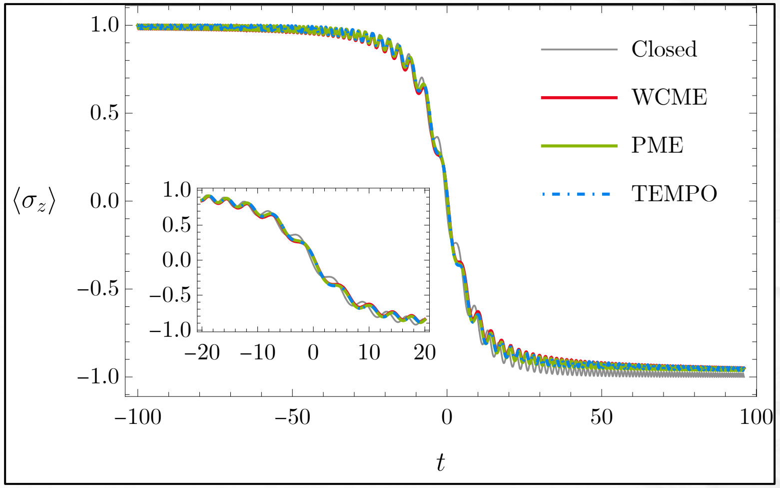
$$H_{PS}(t) = \frac{1}{2}\nu t \sigma_z + \frac{1}{2}\Delta\kappa\sigma_x,\ 0 \le \kappa \le 1$$

System now couples through raising and lowering operators to environmental **displacements**.

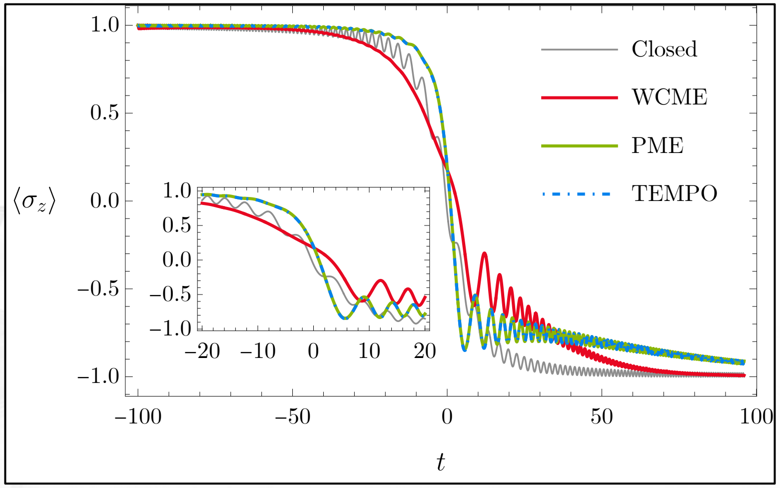
Following the same adiabatic, Markovian procedure in the **polaron frame** we obtain a generalised polaron mater equation

$$\dot{\rho}_{P_S}(\chi, t) = \mathcal{L}_P^{\mathrm{ad}}(\chi, t)\rho_{P_S}(\chi, t)$$

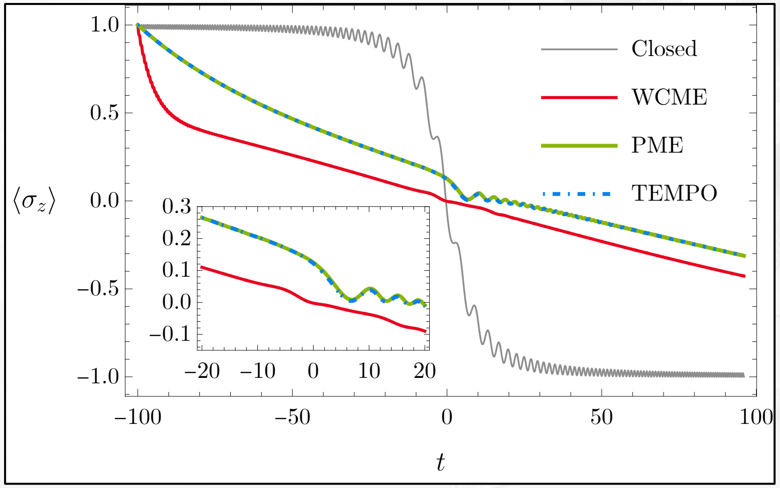
Benchmarking – Landau-Zener



$\alpha = 0.02, \Delta\beta = 1$



$\alpha = 0.4, \Delta\beta = 1$



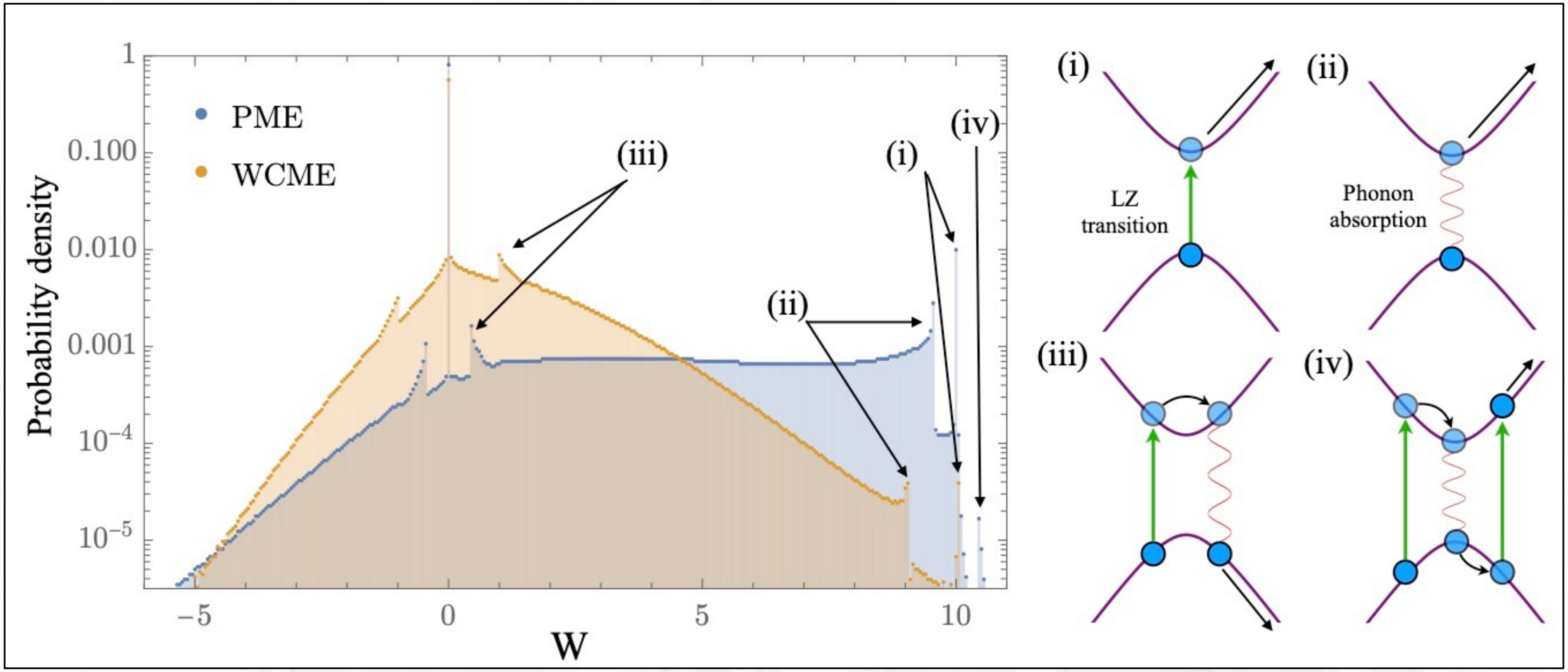
$\alpha = 0.4, \Delta\beta = 0.1$

Benchmark dynamics against numerically exact TEMPO method

Spectral density – system-bath coupling strength weighted by bath density of states

$$J(\omega) = \alpha \frac{\omega^3}{\omega_c^2} e^{-\omega/\omega_c}$$

Work distributions

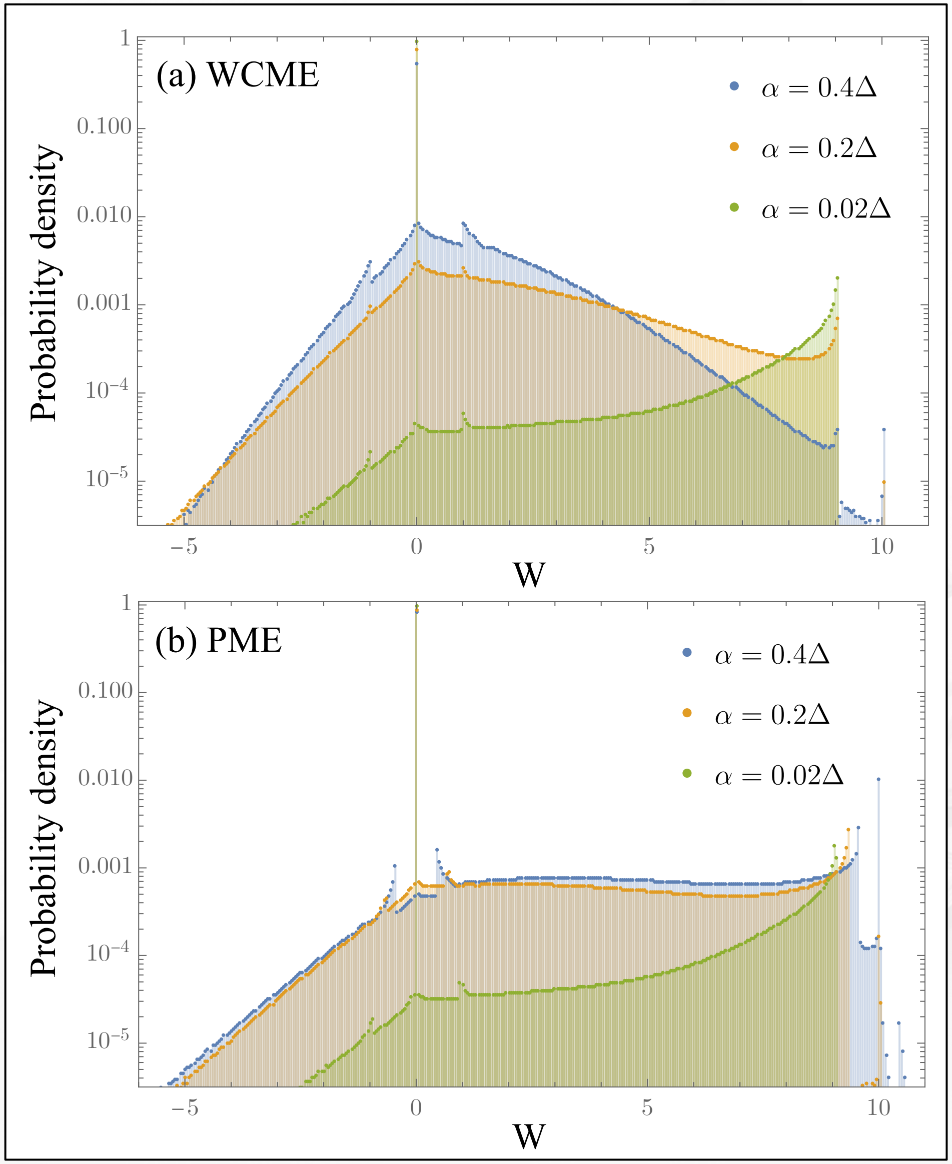


$$\alpha = 0.4, \Delta\beta = 1$$

Jarzynski fluctuation relation also reproduced, consistent with laws of stochastic thermodynamics

$$\langle e^{-\beta W} \rangle = e^{-\beta \Delta F_{PS}}$$

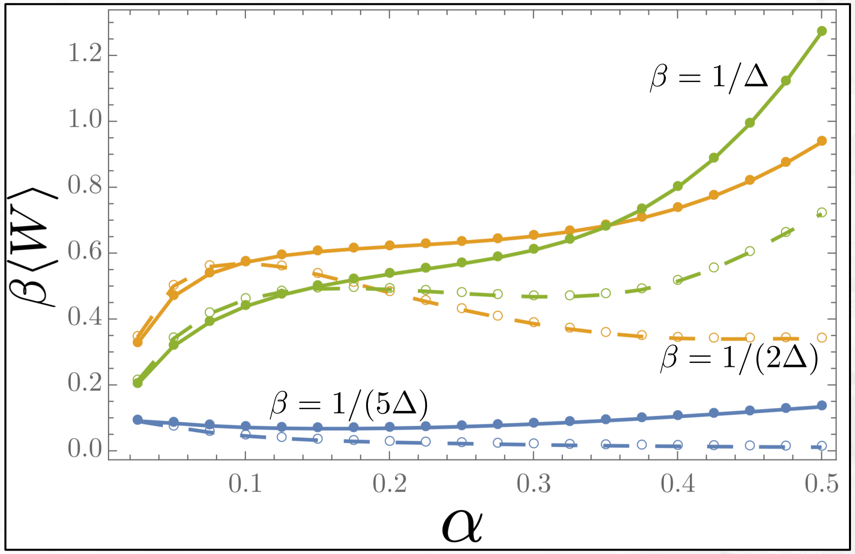
Effects of renormalisation

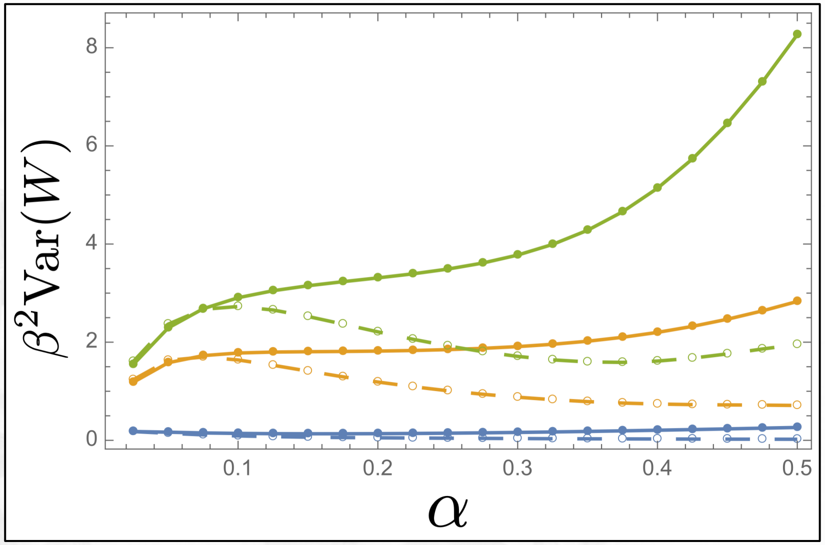


Peak positions incorrectly independent of coupling strength in weak-coupling theory

Polaron theory captures renormalisation of the energy gap, leading to peak shifts

Work average and variance

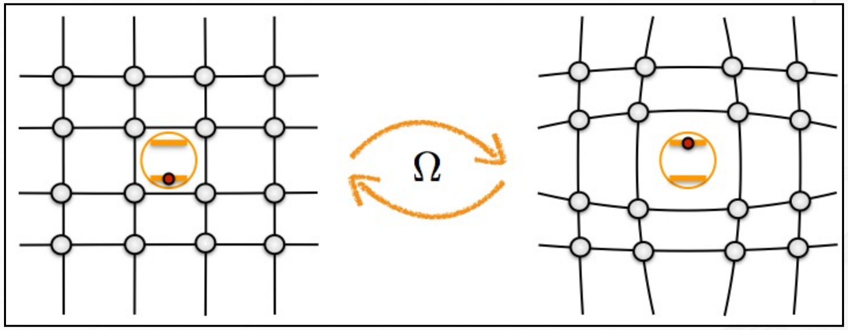




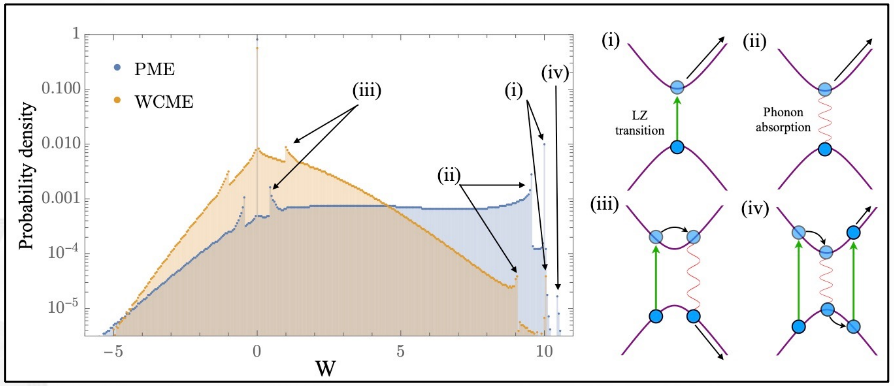
Polaron – solid lines
Weak-coupling – dashed lines

Weak-coupling theory tends to underestimate the average work done and its variance, except at very small couplings

Summary and future work



Polaron transformation



Adiabatic work probability distribution

arXiv:2302.08395

Ongoing

- How do we probe these work distributions experimentally?
- Extension to non-adiabatic, periodically driven systems
- Shortcuts to adiabaticity
- Reaction coordinates and other non-perturbative theories

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- Ali Raza Mirza (Surrey)

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The University of Manchester
Photon Science Institute

Thank You

Aside: Heat

Heat can be characterised in a similar manner

- Consider projective energy measurements performed only on the (static) environment