Numerically Exact Path-Integral Approach for non-equilibrium quantum systems

Bijay Kumar Agarwalla

IISER PUNE

Collaboration:

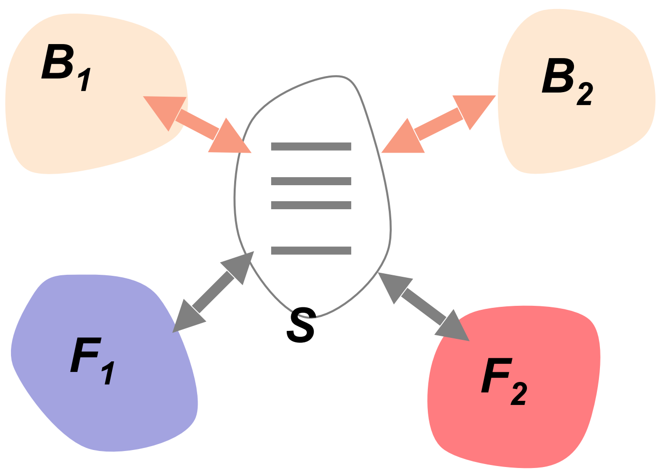
Dvira Segal (Univ of Toronto)

Indian Statistical Physics Meeting, ICTS Bangalore—2018

Exact Numerical Scheme for Open Quantum Systems

Iterative Influence functional Path-Integral approach

Makri et al Chem. Phys. Lett (1994)
Segal et al PRB (2010), PRB (2013)



Reduced Density Matrix

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

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

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 and linear coupling

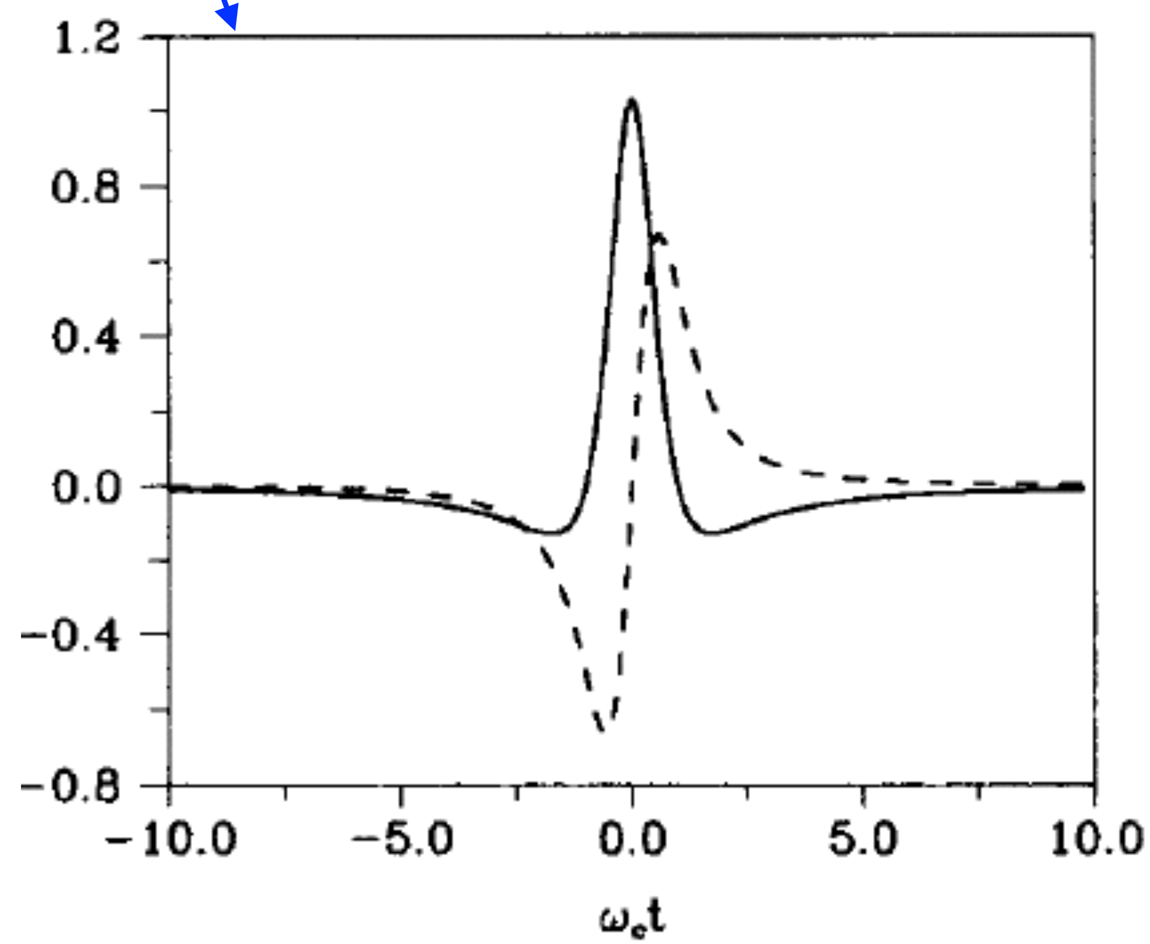
$$I^{har}(s_0^{\pm} \cdots s_N^{\pm}) = \exp\left[-\sum_{k=0}^{N} \sum_{k'=0}^{k} (s_k^+ - s_k^-)(\eta_{k,k'} s_{k'}^+ - \eta_{k,k'}^* s_{k'}^-) \right]$$

Bath correlation functions

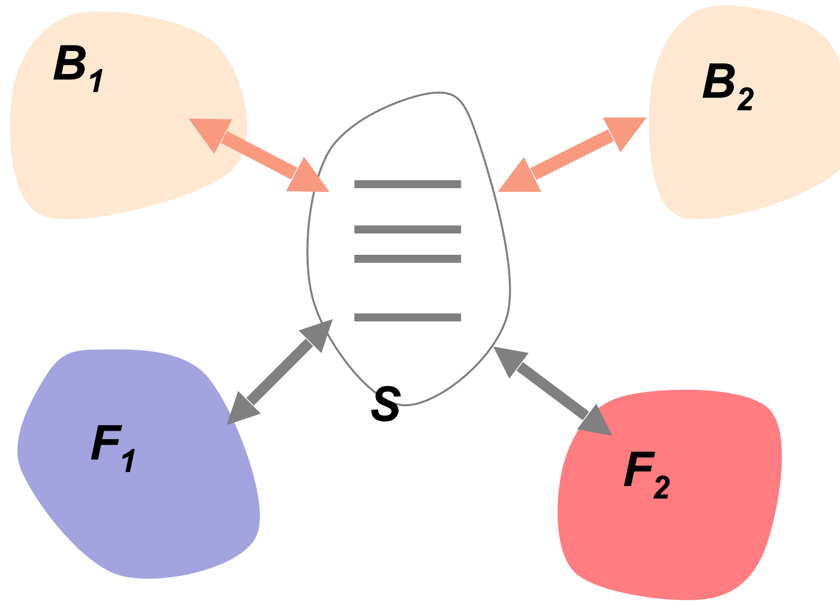
Influence Functional **(non-local in time)** can be truncated beyond a memory time

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

Iterative time-evolution scheme



Full-Statistics of Integrated Current



$$Q_L(t,\, t_0) = \int_{t_0=0}^{t} I_L(t')\,\mathrm{d}t' = H_L(0) - H_L^H(t)$$

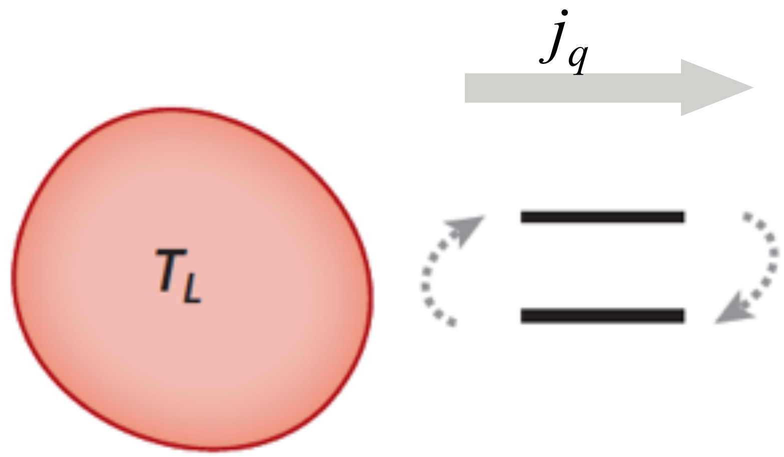
Generating function for energy current

$$\mathcal{Z}(\xi) = \left\langle \mathrm{e}^{\mathrm{i}\xi H_L}\, \mathrm{e}^{-\mathrm{i}\xi H_L^H(t)} \right\rangle$$

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

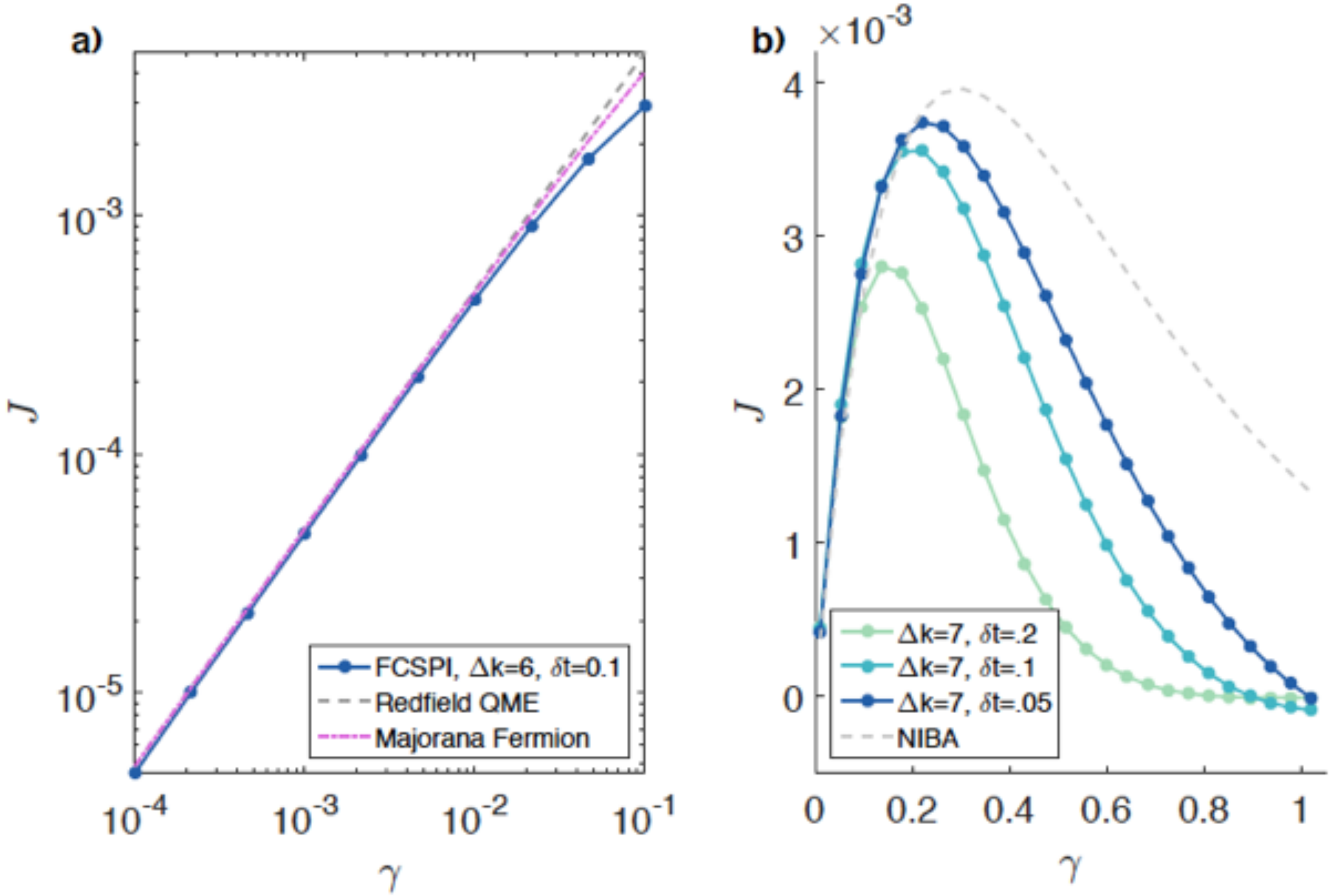
- The entire system evolves with new dressed Hamiltonian.
- The influence functional now gets auxiliary field dependent terms.

Example: Non-equilibrium Spin Boson Model



$$H = \frac{\hbar\Delta}{2}\sigma_x + \sum_{j,\nu}\hbar\omega_{j,\nu} b^\dagger_{j,\nu} b_{j,\nu} + \sigma_z \sum_{j,\nu}\hbar\lambda_{j,\nu}(b_{j,\nu} + b^\dagger_{j,\nu})$$

Some preliminary results:



M. Kilgour, B. K. Agarwalla, D. Segal (Ongoing)

Analytical Results

Analytical Results: Non-equilibrium Spin Boson Model

Weak coupling regime: Redfield quantum master equation approach

Nicolin, Segal PRB (2011)

Majorana Fermion representation (NEGF):

$$\vec{\sigma} = -\frac{i}{2}\vec{\eta} \times \vec{\eta}$$

Agarwalla, Segal NJP (2017).

Cumulant Generating Function:

$$\mathcal{G}(\xi) \equiv \lim_{t\to\infty} \frac{1}{t} \ln \mathcal{Z}(\xi) = \lim_{t\to\infty} \frac{1}{t} \sum_{n=1}^{\infty} \frac{(\mathrm{i}\xi)^n}{n!} \langle\langle Q^n \rangle\rangle$$

$$\mathcal{G}(\xi) = \int_{-\infty}^{\infty} \frac{d\omega}{4\pi} \frac{\Delta^2}{\omega^2} \ln\left[1 + \mathcal{T}(\omega, T_L, T_R) F(\xi, T_L, T_R)\right]$$

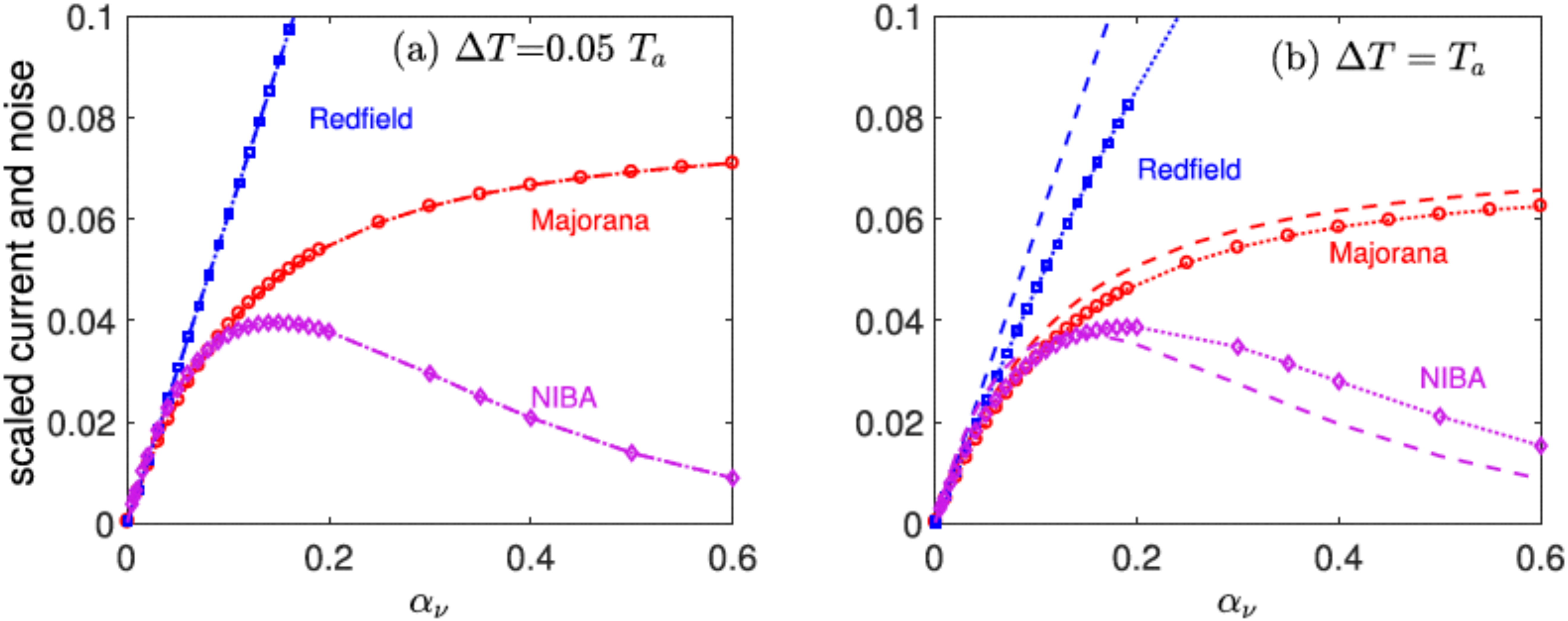
$$F(\xi, T_L, T_R) = \left[n_L(\omega)\bar{n}_R(\omega)\left(e^{i\xi\omega} - 1\right) + n_R(\omega)\bar{n}_L(\omega)\left(e^{-i\xi\omega} - 1\right)\right]$$

Gallovatti-Cohen Fluctuation Symmetry

$$\mathcal{G}(\xi) = \mathcal{G}(-\xi + \mathrm{i}(\beta_R - \beta_L))$$

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

Non-equilibrium Spin Boson Model

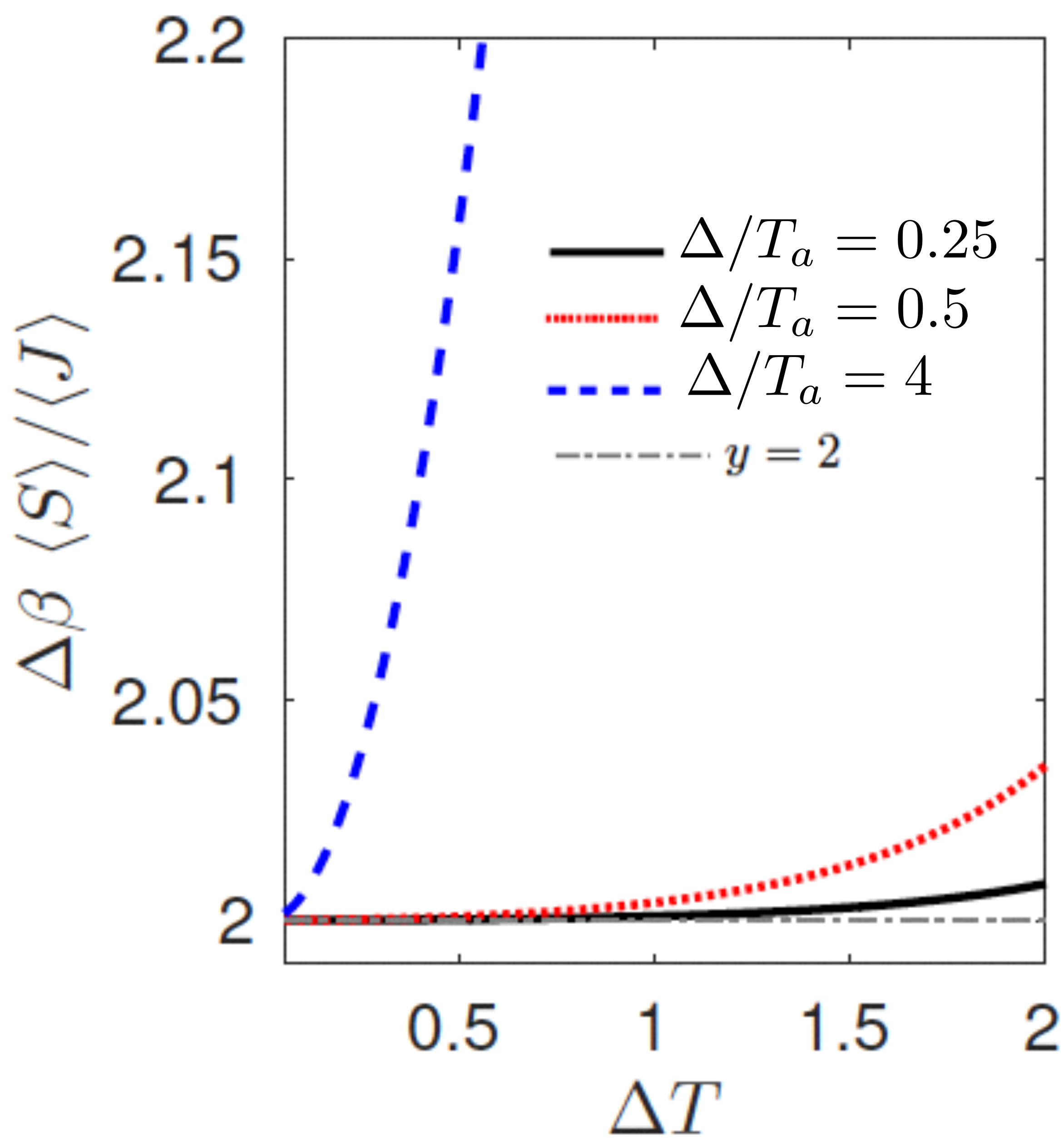


Scaled current $\langle I \rangle / \Delta T$ (dashed lines) and noise $\langle S \rangle / 2T_a^2$ (symbols)

$$\Delta = T_a = 1, T_{L,R} = T_a \pm \Delta T/2, \omega_c = 10\Delta, \text{and } \alpha_L = \alpha_R$$

Thermodynamic Uncertainty relation

$$\frac{\langle S \rangle}{\langle J \rangle} \Delta\beta \geq 2k_B$$



Quantum thermodynamics from weak to strong system-bath coupling

H. Friedmann, B. K. Agarwalla, D. Segal, arXiv: 1802.00511

Thank you!

Additional Slides

Harmonic bath and linear coupling

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

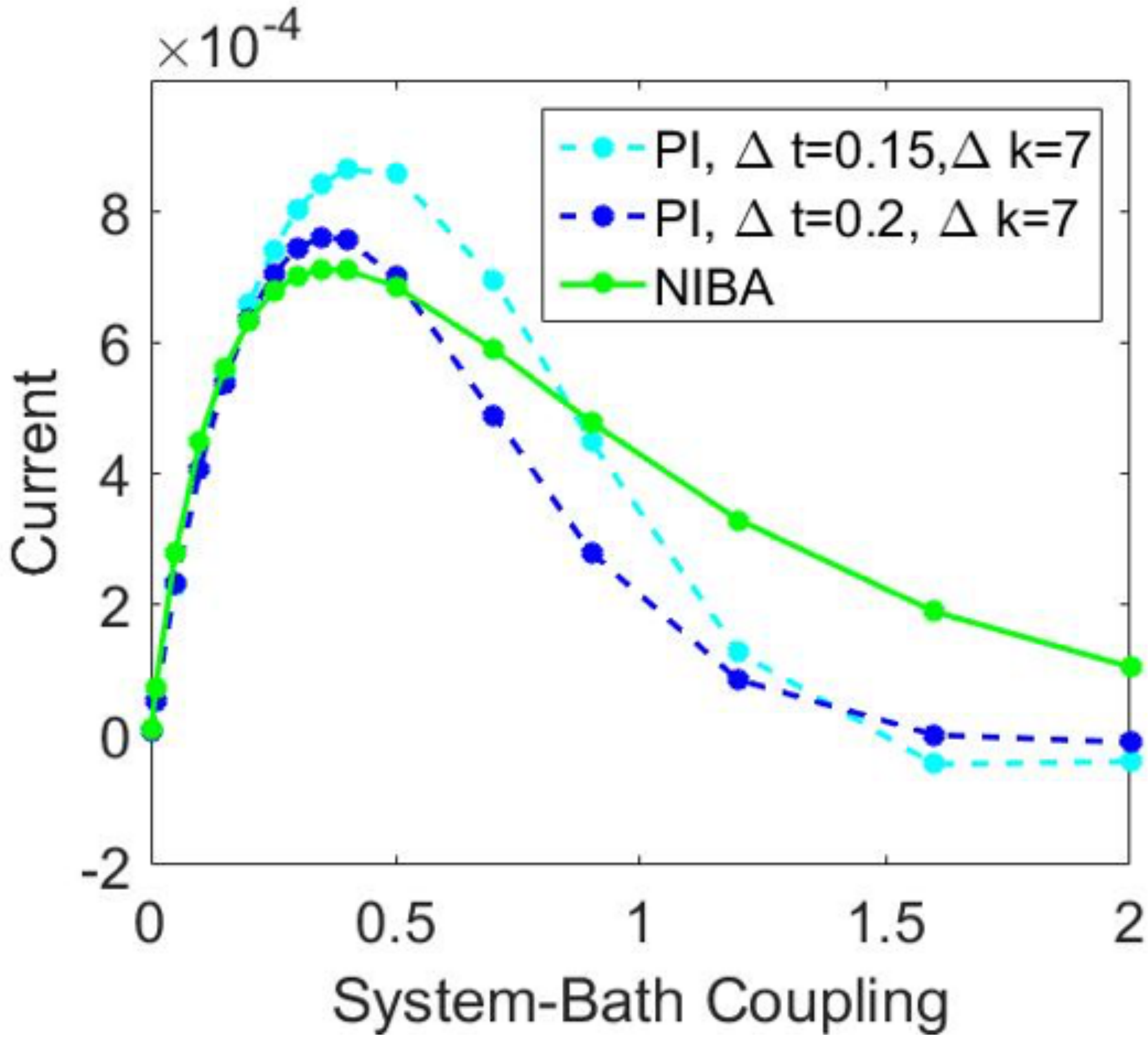
Bath correlation functions

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

Generating function for current

Results: Non-equilibrium spin-boson model

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

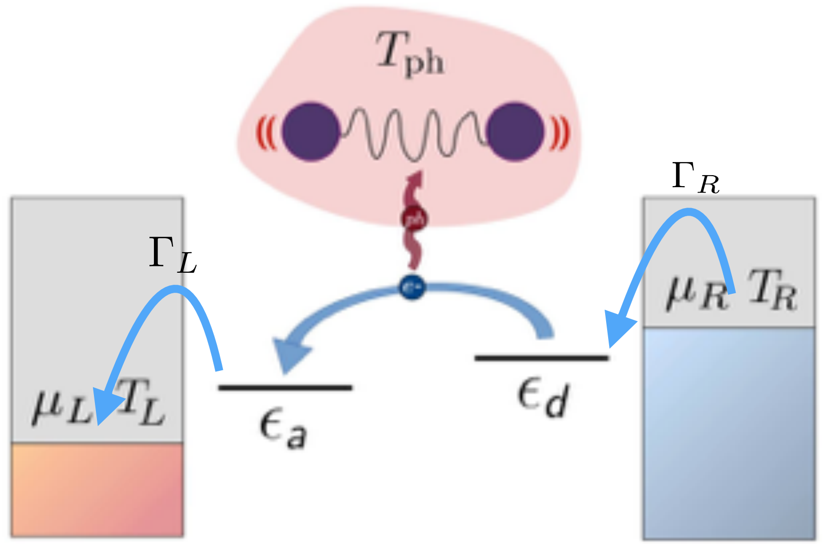


Summary:

- 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



Summary:

- 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

Dvira Segal
Univ of Toronto

Hava Friedman
(grad)

Michael Kilgour
(grad)