Transport and Counting Statistics with Inchworm Monte Carlo

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Quantum Matter: Computation Meets Experiments
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Outline

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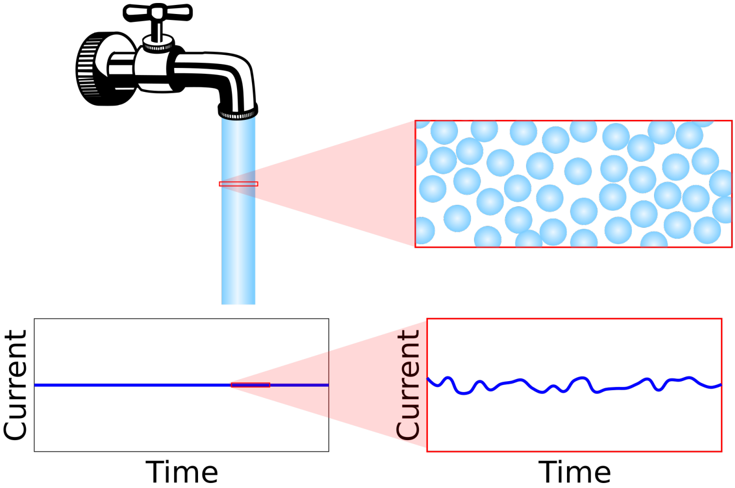
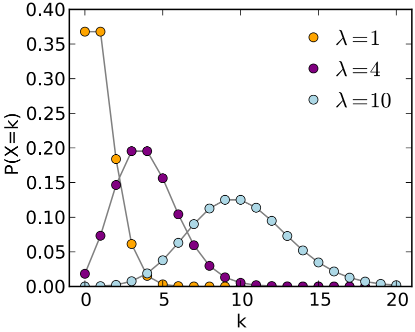
Flow: from continuum to microscopics



Classical uncorrelated flow

- Assume particles enter the flow at a constant, uncorrelated rate $\Leftrightarrow$ Poisson distribution $\Leftrightarrow \sigma^2 = S \sim |I|$.
- Walter Schottky, working on vacuum tubes in 1918, found $S = 2e|I|$.



Shot noise provides information about charge carriers

$$e_{\mathrm{eff}} \equiv \frac{S}{2|I|}.$$

Quantum uncorrelated flow

- For noninteracting fermion transport (here at zero temperature), Landauer formula:

$$I = \frac{e^2}{\pi\hbar} \int_{\mu-\frac{V}{2}}^{\mu+\frac{V}{2}} T(\omega)\,\mathrm{d}\omega.$$

- 70 years after Schottky, it turned out that:[1]

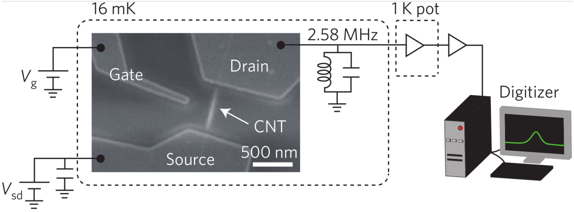
$$S = \frac{2e^3}{\pi\hbar} \int_{\mu-\frac{V}{2}}^{\mu+\frac{V}{2}} T(\omega)\left[1 - T(\omega)\right]\mathrm{d}\omega \neq 2e\left|I\right|.$$

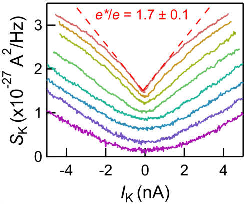
- At $T \to 0$, this reduces to classical Poisson limit.
- At $T \to 1$, quantum noise is fully suppressed.

[1] L. S. Levitov and G. B. Lesovik, JETP Lett. 58, 230 (1993).

Correlated quantum systems: many open questions

- For interacting systems, only a few results in special limits are known.
- Experiments[2] ahead of theory: only fermi liquid limit[3] understood.





[2] M. Ferrier, T. Arakawa, T. Hata, R. Fujiwara, R. Delagrange, R. Weil, R. Deblock, R. Sakano, A. Oguri, and K. Kobayashi, Nat Phys 12, 230 (2016).

[3] E. Sela, Y. Oreg, F. von Oppen, and J. Koch, Phys. Rev. Lett. 97, 086601 (2006).

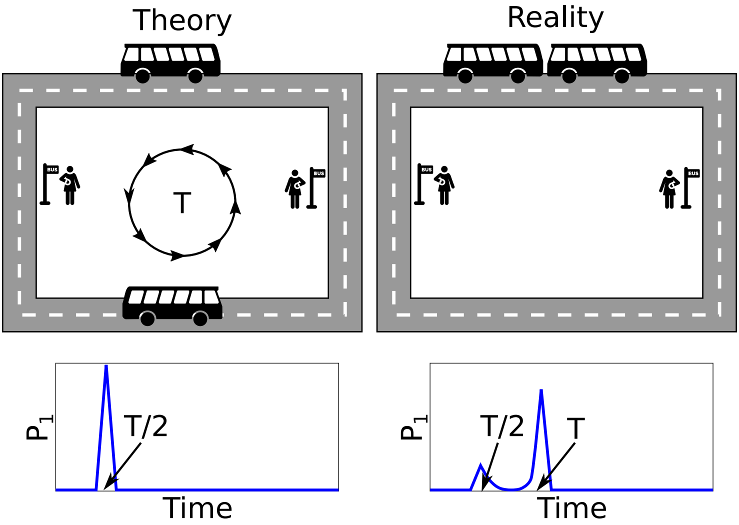
Full counting statistics: definition

- Can measure not just populations, currents and noise; but also higher-order moments.
- The (population) full counting statistics generating function describes all moments:

$$\boxed{Z(\lambda,t) \equiv \left\langle e^{i\lambda\Delta n(t)} \right\rangle = \sum_{n=0}^{\infty} \frac{(i\lambda)^j}{j!} \left\langle [\Delta n(t)]^j \right\rangle}.$$

- Current: $I = \lim_{t\to\infty} \frac{\mathrm{d}}{\mathrm{d}t} \langle \Delta n(t) \rangle$.
- Noise: $S = \lim_{t\to\infty} \frac{\mathrm{d}}{\mathrm{d}t} \langle \Delta n^2(t) \rangle$.
- Wealth of information about Fano factors, entanglement entropy, waiting-time distributions, efficiency fluctuations...

Beyond shot noise: bus bunching and waiting times



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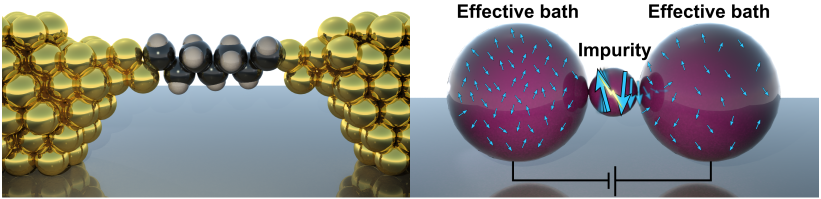
Transport in junctions

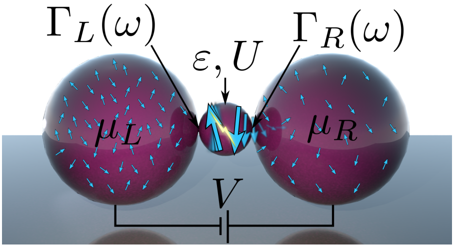


$$\hat{H} = \hat{H}_{dot} + \hat{H}_{leads} + \hat{H}_{hyb}$$

We would like to understand:

Electronic populations and transport; the effects of many-body correlation; magnetic and optical properties; elastic properties and heat transport; ...

An example: the Anderson impurity model



$$
\begin{aligned}
H &= \hat{H}_{dot} + \hat{H}_{leads} + \hat{H}_{hyb} \\
&= \sum_{\sigma} \varepsilon_\sigma d_\sigma^\dagger d_\sigma + U d_\uparrow^\dagger d_\uparrow d_\downarrow^\dagger d_\downarrow + \sum_{\sigma k} \sum_{\ell \in \{L,R\}} \varepsilon_{\sigma \ell k} a_{\sigma \ell k}^\dagger a_{\sigma \ell k} \\
&+ \sum_{\sigma k} \sum_{\ell \in \{L,R\}} t_{\sigma \ell k} a_{\sigma \ell k}^\dagger d_\sigma + t_{\sigma \ell k}^* d_\sigma^\dagger a_{\sigma \ell k}.
\end{aligned}
$$

Nonequilibrium Monte Carlo methods

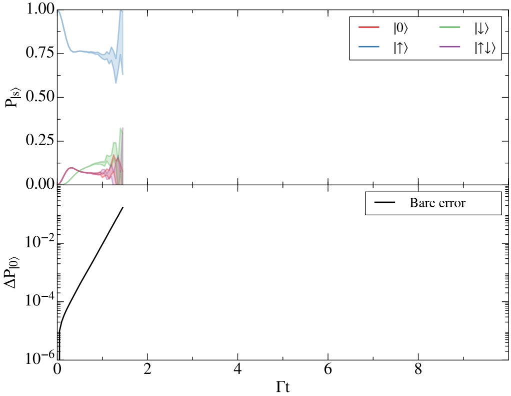
- Continuous time solvers can be formulated in real time (expand $e^{\pm iHt}$).[4, 5, 6]

Nonequilibrium / exact dynamics require real time QMC

This results in dynamical sign problems.

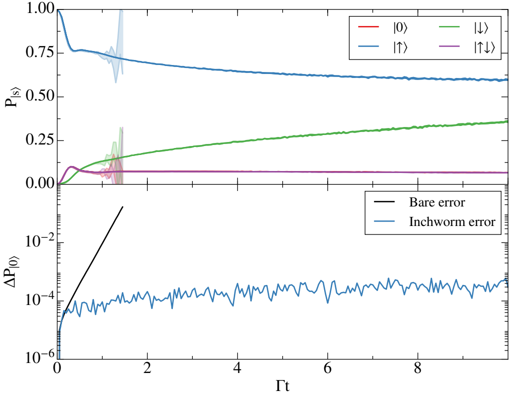
[4] Mühlbacher, L. & Rabani, 2008, E. Phys. Rev. Lett. 100, 176403.
[5] Werner, P., Oka, T., Millis, A.J., 2009. Phys. Rev. B 79, 035320.
[6] Schiró, M., Fabrizio, M., 2009. Phys. Rev. B 79, 153302.

What a dynamical sign problem looks like



G. Cohen, E. Gull, D. R. Reichman, A. J. Millis, PRL 115 (26), 266802.

Getting around the dynamical sign problem



$$U = 8\Gamma,\ \beta_K \Gamma \simeq 50.$$

G. Cohen, E. Gull, D. R. Reichman, A. J. Millis, PRL 115 (26), 266802.

Hybridization expansion

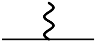
Partitioning the Hamiltonian

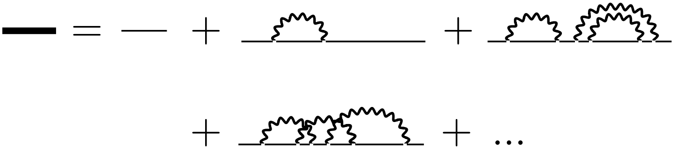
- We separate the Hamiltonian into:
  - V: the hybridization between the dot and the fermionic leads.
  - H_0: everything else.
- To evaluate an auxiliary propagator $G(t) \equiv \langle e^{iHt} \rangle$, we expand it in a Dyson series:

$$G(t) = \mathrm{Tr}\left\{\rho_0 \mathrm{T}\left(U^\dagger(t) e^{-iH_0 t}\right)\right\},$$

$$U(t) = \sum_{n=0}^{\infty}\left(-\frac{i}{\hbar}\right)^n \int_0^t ds_1 \int_0^{s_1} ds_2 \ldots \int_0^{s_{n-1}} ds_n \times V_I(s_1) V_I(s_2) \ldots V_I(s_n).$$

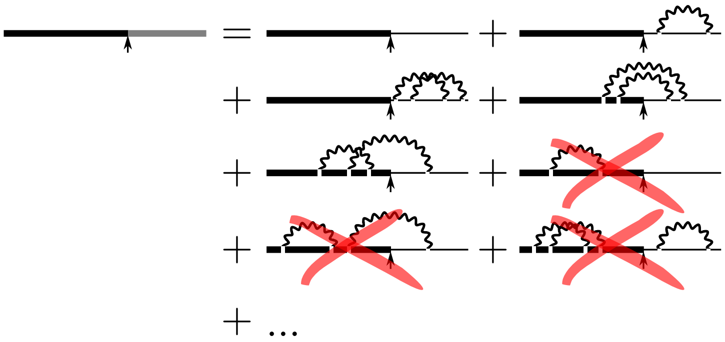
Simplified diagrammatic notation

$G :$  $G^{(0)} :$ $V :$ 

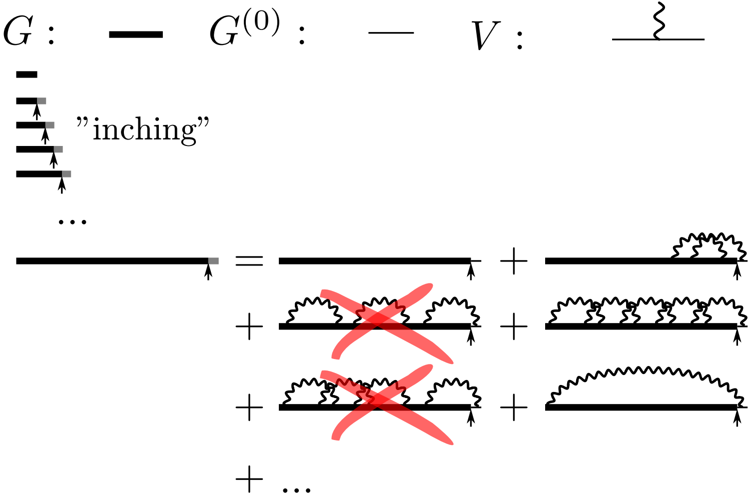


Partitioning propagators: segment-proper diagrams

G : $G^{(0)}$: V :



The Inchworm algorithm

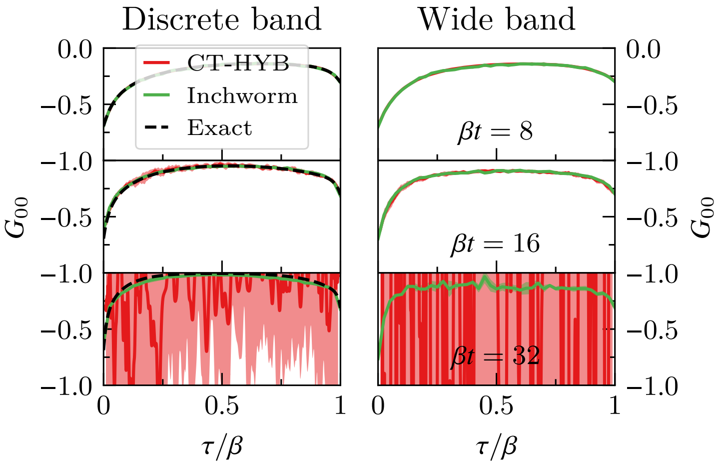


Extensions to larger impurities?

- Interacting local Hamiltonian has dimension $2^{N_{\text{spins}}}$.
- Therefore, adding a Hubbard site (two spin orbitals): $\dim H \to 4 \dim H$.
- Contribution to computation (local matrix products): $\times 4^3 = 64$.
- Symmetries can greatly reduce this; also, not dominant contribution.
- Effect on sign problem unknown, but seems small in imaginary time.[7]

[7] arXiv:1907.08570

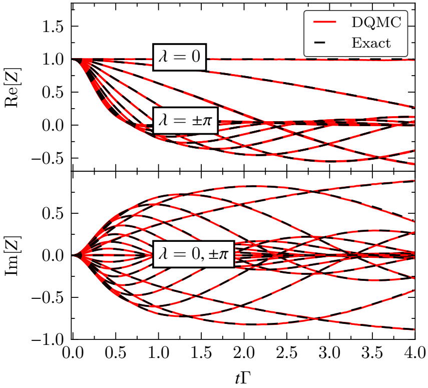
Two-orbital Kanamori model



Outline

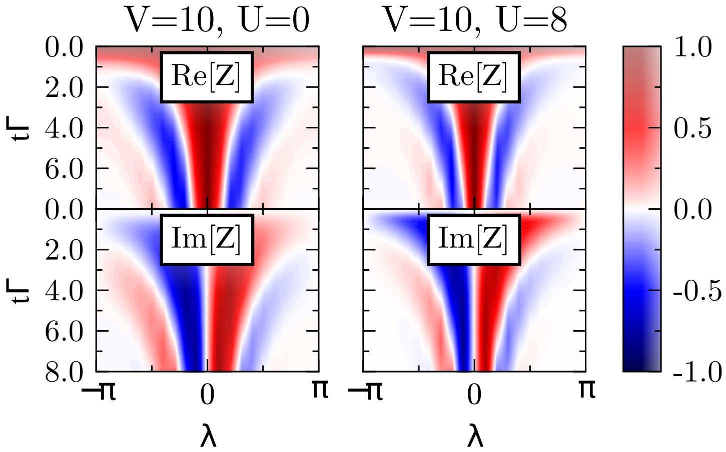
Full counting statistics: noninteracting

- Noninteracting benchmarks for generating function $Z(\lambda, t) = \left\langle e^{i\lambda\Delta n(t)} \right\rangle$:



$U = 0$; $V = 10\Gamma$, $\beta = 50/\Gamma$.

Full counting statistics: interacting



$U = 0,\ 5\Gamma;\ V = 10\Gamma,\ \beta = 50/\Gamma.$

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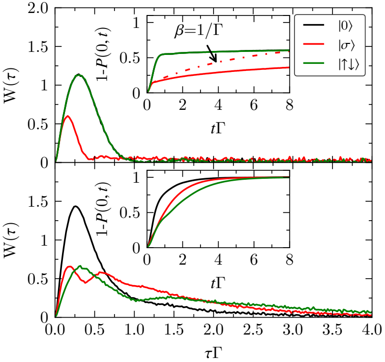
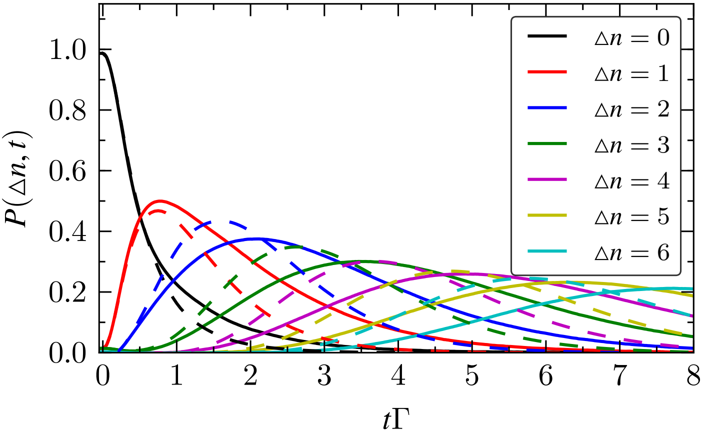
Full counting statistics: first passage time distribution

- Generating function describes distributions
  $P(\Delta n, t) = \int_{-\pi}^{\pi} \frac{\mathrm{d}\lambda}{2\pi} Z(\lambda, t) e^{-i\lambda \Delta n}$.



$U = 8\Gamma$; $V = 0, 10\Gamma$, $\beta = 50/\Gamma$.

Full counting statistics: *n*-electron passage



$U = 0, 8\Gamma;\ V = 10\Gamma,\ \beta = 50/\Gamma.$

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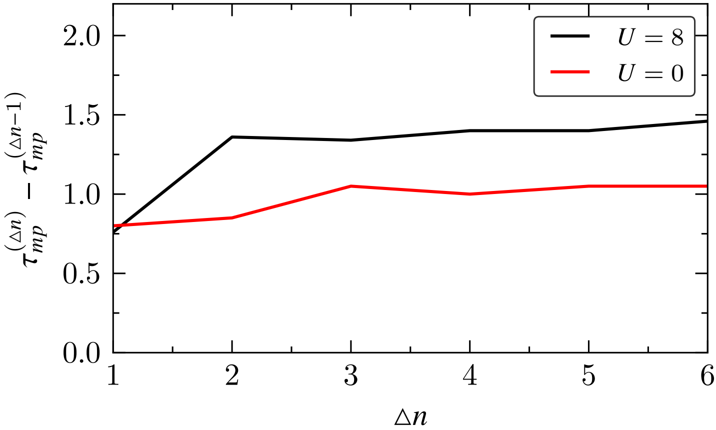
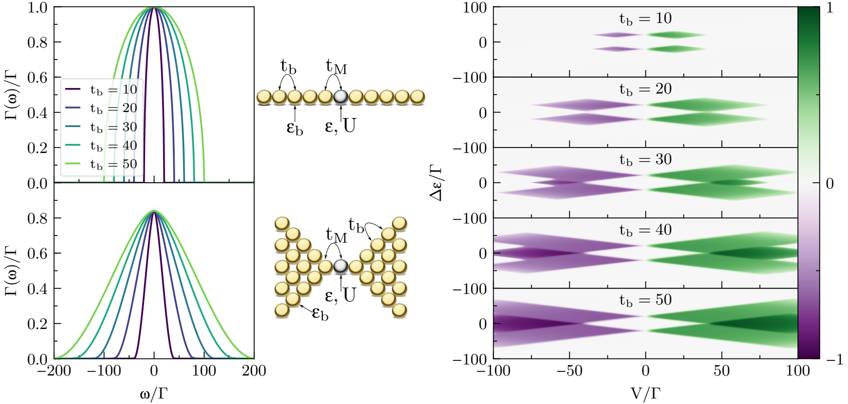
Full counting statistics: typical time between events



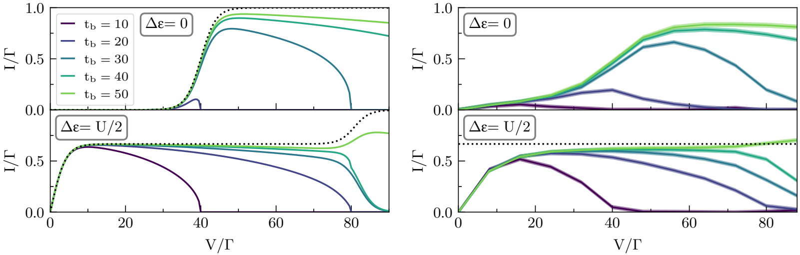
$U = 0, 8\Gamma$; $V = 10\Gamma$, $\beta = 50/\Gamma$.

Lead geometry



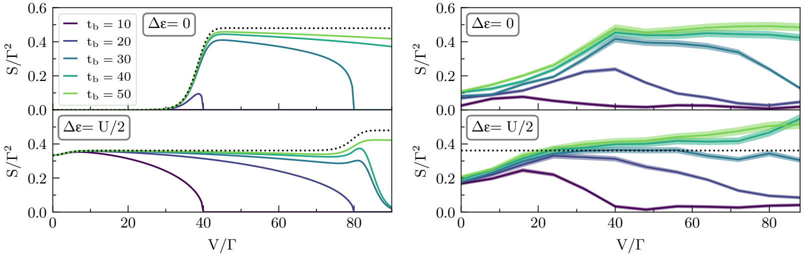
$$U = 40\Gamma;\ \beta = 1/\Gamma.$$

Lead geometry: currents



$$U = 40\Gamma;\, \beta = 1/\Gamma.$$

Lead geometry: noise



$$U = 40\Gamma;\ \beta = 1/\Gamma.$$

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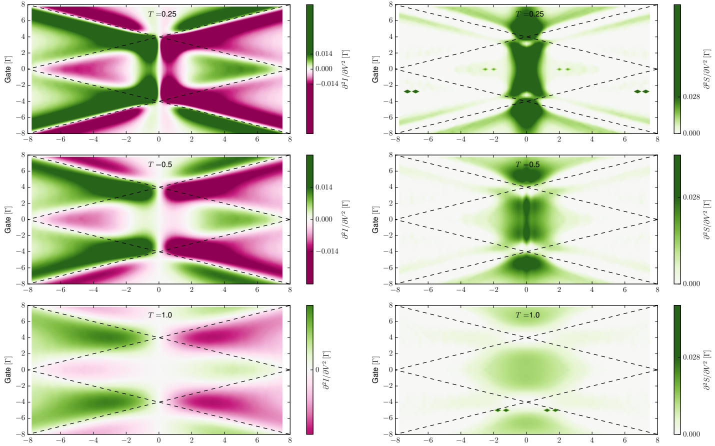
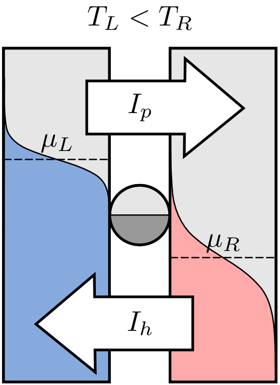
Approaching Kondo regime (NCA, preliminary)



$U = 8\Gamma$, wide band limit, $\beta\Gamma = 10, 4, 1$.

Energy counting statistics



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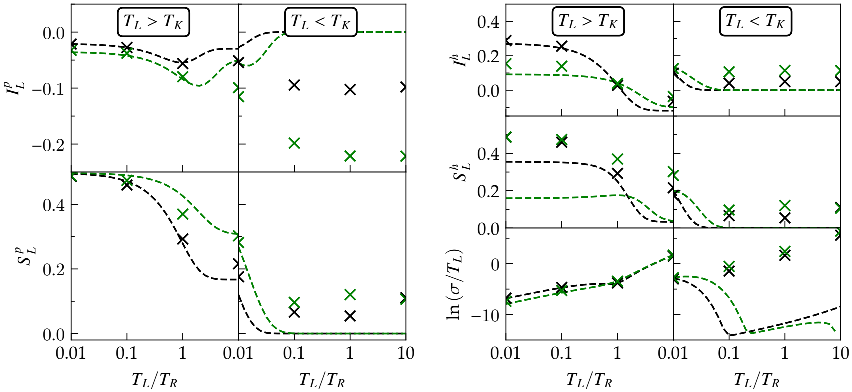
Energy counting statistics



$U = 8\Gamma, 4\Gamma;\ V = 1\Gamma.$

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Conclusions

- **The Inchworm algorithm** eliminates the dynamical sign problem quite generally in several kinds of impurity models and expansions.[8,9]
- Arbitrary band structures[10] and multiorbital impurity models[11] are accessible.
- Access to populations; currents and correlation functions;[12] and even high-order moments and cumulants (full counting statistics) of charge[13] and energy.[14]

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[8] G. Cohen, E. Gull, D. R. Reichman, and A. J. Millis, Phys. Rev. Lett. 115, 266802 (2015)

[9] H.-T. Chen, G. Cohen, and D. R. Reichman, The Journal of Chemical Physics 146, 054105 (2017)

[10] M. Ridley, E. Gull, and G. Cohen, J. Chem. Phys. 150, 244107 (2019)

[11] E. Eidelstein, E. Gull, and G. Cohen, ArXiv:1907.08570

[12] A. E. Antipov, Q. Dong, J. Kleinhenz, G. Cohen, and E. Gull, Phys. Rev. B 95, 085144 (2017).

[13] M. Ridley, V. N. Singh, E. Gull, and G. Cohen, Phys. Rev. B 97, 115109 (2018)

[14] M. Ridley, M. Galperin, E. Gull, and G. Cohen, Phys. Rev. B 100, 165127 (2019)