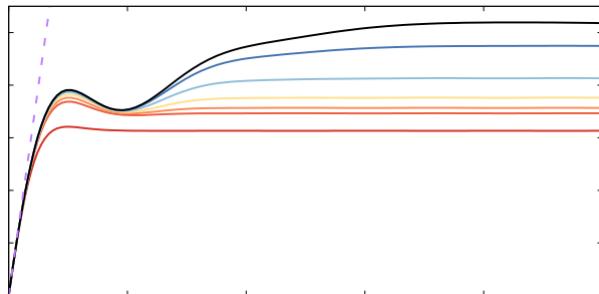


Temperature Flow Renormalization Group for Open Quantum Systems



$$-i \frac{\partial \Sigma}{\partial T} = \text{Diagram 1} + \text{Diagram 2} + \text{Diagram 3}$$

The equation shows the derivative of the self-energy Σ with respect to temperature T . The right side consists of three Feynman-like diagrams: Diagram 1 shows a horizontal line with a dot at one end and an open circle at the other; Diagram 2 shows a horizontal line with a dot at both ends; Diagram 3 shows a horizontal line with a dot at one end and a closed circle at the other.

Konstantin Nestmann
Marie Curie Postdoctoral Fellow

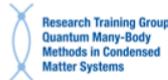
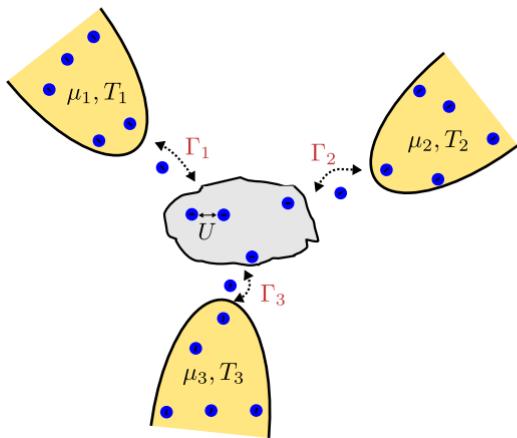


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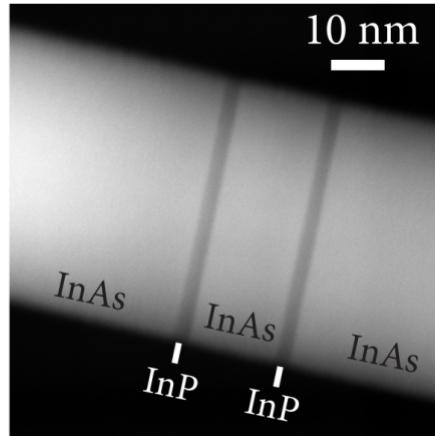
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1 Open quantum systems & quantum transport

Theorists' view...



Experimental realization...



Anderson quantum dot as simplest transport model with interaction:

$$H_{\text{tot}} = \varepsilon(n_\uparrow + n_\downarrow) + U n_\uparrow n_\downarrow + \sum_{r\sigma} \int d\omega (\omega + \mu_r) a_{r\sigma}^\dagger(\omega) a_{r\sigma}(\omega) + \sum_{r\sigma} \sqrt{\frac{\Gamma}{2\pi}} \int d\omega (d_\sigma^\dagger a_{r\sigma}(\omega) + a_{r\sigma}^\dagger(\omega) d_\sigma)$$

1. Picture from Josefsson, Svilans, Burke, *et al.* *Nature Nanotech* **13**, 920–924 (2018)

2 Theoretical setup

- Open quantum systems approach: focus on $\rho(t) := \text{Tr}_R |\psi\rangle\langle\psi|_{\text{tot}}(t)$
- If $\rho_{\text{tot}}(0) = \rho_0 \otimes \rho_R$, then

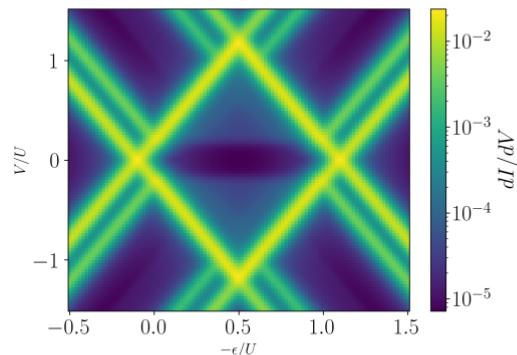
$$\rho(t) = \Pi(t)\rho_0, \quad \text{and} \quad \frac{\partial}{\partial t}\Pi(t) = -i\mathcal{L}\Pi(t) - i\int_0^t ds \mathcal{K}(t-s)\Pi(s)$$

where $\mathcal{L} = [H, \bullet]$, Π and \mathcal{K} are superoperator-valued.

- Memory kernel approach well-developed²
 - Keldysh or superoperator formulation
 - Time or frequency space
- QmeQ: Open source python implementation perturbation theory in Γ

$$-i\mathcal{K} = \begin{array}{c} \text{---} \\ | \\ \text{---} \end{array} + \begin{array}{c} \text{---} \\ | \\ \text{---} \\ | \\ \text{---} \end{array} + \begin{array}{c} \text{---} \\ | \\ \text{---} \\ | \\ \text{---} \\ | \\ \text{---} \end{array}$$

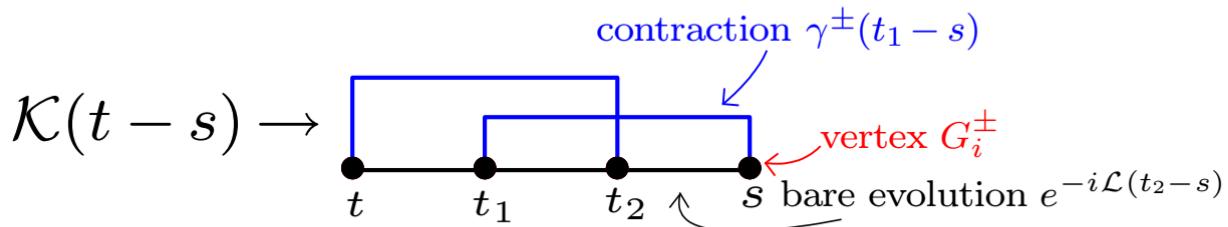
→ stationary state from $[\mathcal{L} + \hat{\mathcal{K}}(0)] \rho_{\text{stat}} = 0$



$T = 10\Gamma$, $U = 500\Gamma$, $B = 100\Gamma$

2. Schoeller and König, Phys. Rev. Lett. **84**, 3686 (2000), Schoeller, Eur. Phys. J. Spec. Top. **168**, 179–266 (2009)

3 Superfermionic perturbation theory



Clever definition superfermions:³

$$G_1^{p=\pm} \sigma := \frac{1}{\sqrt{2}} \left(d_1 \sigma + p (-1)^n \sigma (-1)^n d_1 \right)$$

	Superfermion	Ordinary fermion	
Anticommutation	$\{G_1^+, G_2^+\} = 0$ $\{G_1^-, G_2^+\} = \delta_{12}$	$\{d_{\sigma_1}^\dagger, d_{\sigma_2}^\dagger\} = 0$ $\{d_{\sigma_1}, d_{\sigma_2}^\dagger\} = \delta_{\sigma_1 \sigma_2}$	$\gamma^+(t) = \Gamma \delta(t)$
Pauli principle	$(G_1^+)^2 = 0$	$(d_\sigma^\dagger)^2 = 0$	$\gamma^-(t) \propto \frac{\Gamma \textcolor{red}{T}}{\sinh(\pi t \textcolor{red}{T})}$
Vacuum state	$G_1^- \mathbb{1} = 0$	$d_\sigma 0\rangle = 0$	

3. Saptsov and Wegewijs, Phys. Rev. B **90**, 045407 (2014)

4 Renormalized perturbation theory around $T = \infty$

Step 1. Exact limit $T \rightarrow \infty$: all $\gamma^- \rightarrow 0$, only time-local $\gamma_1^+(t) \propto \delta(t)$ contractions remain !

$$\lim_{T \rightarrow \infty} \Pi = \underline{\quad} + \underline{\text{---}} + \underline{\text{---}} \underline{\text{---}} + \underline{\text{---}} \underline{\text{---}} \underline{\text{---}} + \dots = e^{-i\mathcal{L}_\infty t}$$

$$\begin{aligned}\lim_{T \rightarrow \infty} \mathcal{K}(t) &= \Sigma_\infty \bar{\delta}(t) \\ \mathcal{L}_\infty &= \mathcal{L} + \Sigma_\infty\end{aligned}$$

Step 2. At finite T : systematically resum infinite T contributions⁴

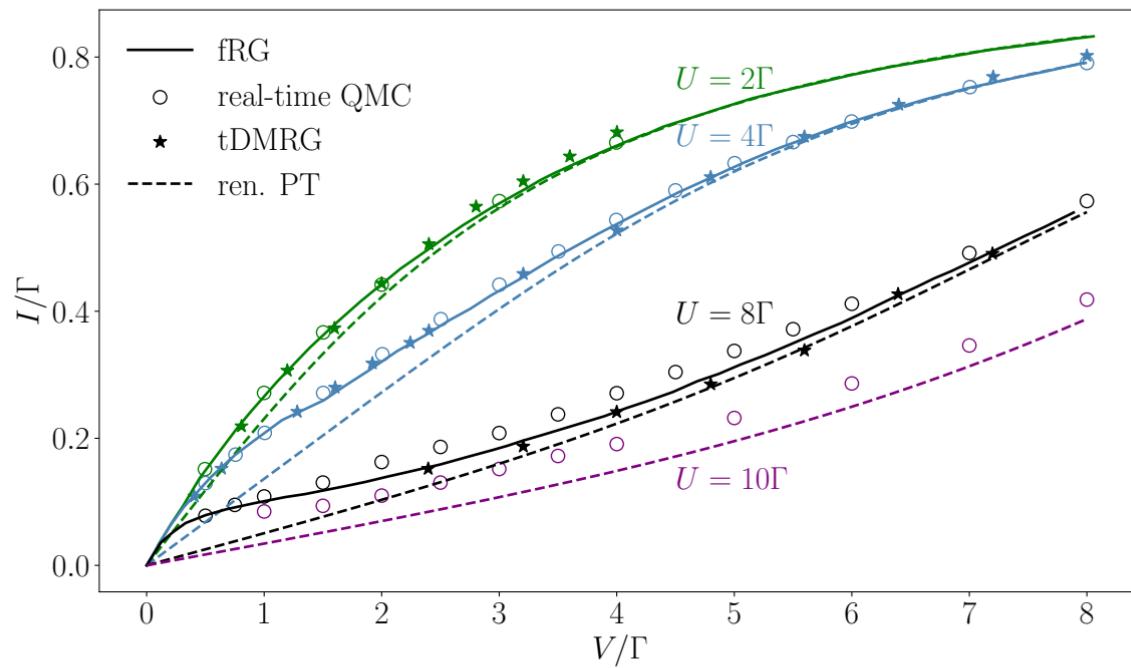
$$\mathcal{K}(t) = \Sigma_\infty \bar{\delta}(t) + \Sigma(t)$$

Same diagrammatics for Σ as bare perturbation theory but:

- Replace bare Liouvillean $\mathcal{L} = [H, \bullet] \longrightarrow \mathcal{L}_\infty = \mathcal{L} + \Sigma_\infty$ with infinite temperature Liouvillian
- Only creation superoperators G_1^+ allowed as vertices, G_1^- absorbed into renormalized intermediate propagators
- Resulting PT is exact for $\Gamma \rightarrow 0$, $T \rightarrow \infty$ and **terminates for $U = 0$!**

4. Saptsov and Wegewijs, Phys. Rev. B **90**, 045407 (2014)

I - V characteristic: renormalized perturbation theory at $T=0$, $\varepsilon=-U/2$



Compare with Eckel *et al*, New J. Phys. **12**, 043042 (2010) + Werner *et al*, Phys. Rev. B **81**, 035108 (2010)

5 T -flow renormalization group

Idea:

- Problem pert. theory: goes $T = \infty \rightarrow 0$ in one step
- Instead: use many small steps δT in RG transformation $\Sigma_{T-\delta T} = \mathcal{F}[\Sigma_T]$
- Temperature the inverse correlation time reservoirs
→ flow from short-ranged correlations ($\gamma_{T=\infty}^- = 0$) to long-ranged ones ($\gamma_{T=0}^- \propto \Gamma/t$)
- Lower T & reduce thermal fluctuations → generate effective higher-order coupling

On a technical level: computing $\partial_T \Sigma$ better-behaved than computing Σ itself:

$$\gamma^-(t) \propto \frac{\Gamma T}{\sinh(\pi t T)} \quad \text{but} \quad \frac{\partial \gamma^-}{\partial T}(t) \approx t T \Gamma e^{-\pi t T} \implies \boxed{\left. \frac{\partial \Sigma}{\partial T} \right|_{T=0} = 0}$$

Note: we don't change temperature as function of time !

5 T -flow renormalization group

Step 1. Derive self-consistent expression for Σ (technical inspiration “ E -flow”⁵)

Resum connected subblocks to full propagators [$\Pi = \text{=====}$]

$$-i\Sigma = \text{---} + \text{---} + \text{---} + \dots$$

Define effective vertices:

$$\text{---} = \text{---} + \text{---} + \text{---} + \dots, \quad \text{---} = \text{---} + \text{---} + \text{---} + \dots$$

We recognize:

$$\boxed{-i\Sigma = \text{---}, \quad \text{---} = \text{---} + \text{---} + \text{---} + \text{---}}$$

5. Pletyukhov and Schoeller, Phys. Rev. Lett. **108**, 260601 (2012)

5 T -flow renormalization group

Step 2. Take T -derivative:

$$-i \frac{\partial \Sigma}{\partial T} = \begin{array}{c} \text{Diagram: two horizontal lines, one with a vertical line segment above it, both ends black dots} \end{array} + \begin{array}{c} \text{Diagram: two horizontal lines, one with a vertical line segment below it, both ends black dots} \end{array} + \begin{array}{c} \text{Diagram: two horizontal lines, one with a vertical line segment to its right, both ends black dots} \end{array} \quad \text{where} \quad \frac{\partial \Pi}{\partial T} = -i \Pi * \frac{\partial \Sigma}{\partial T} * \Pi$$

$$\boxed{} = \frac{\partial}{\partial T} \left[\begin{array}{c} \text{Diagram: three horizontal lines, top and middle have vertical segments above them, bottom has a vertical segment below it, all ends black dots} \end{array} + \begin{array}{c} \text{Diagram: three horizontal lines, top and middle have vertical segments below them, bottom has a vertical segment above it, all ends black dots} \end{array} + \begin{array}{c} \text{Diagram: three horizontal lines, top and middle have vertical segments to their right, bottom has a vertical segment to its right, all ends black dots} \end{array} \right]$$

Step 3. Cutoff hierarchy:

- 1-loop

$$-i \frac{\partial \Sigma}{\partial T} = \begin{array}{c} \text{Diagram: three horizontal lines, top and middle have vertical segments above them, bottom has a vertical segment below it, all ends black dots} \end{array} + \mathcal{O}(G^{+4})$$

$$\boxed{} = 0 + \mathcal{O}(G^{+3})$$

5 T -flow renormalization group

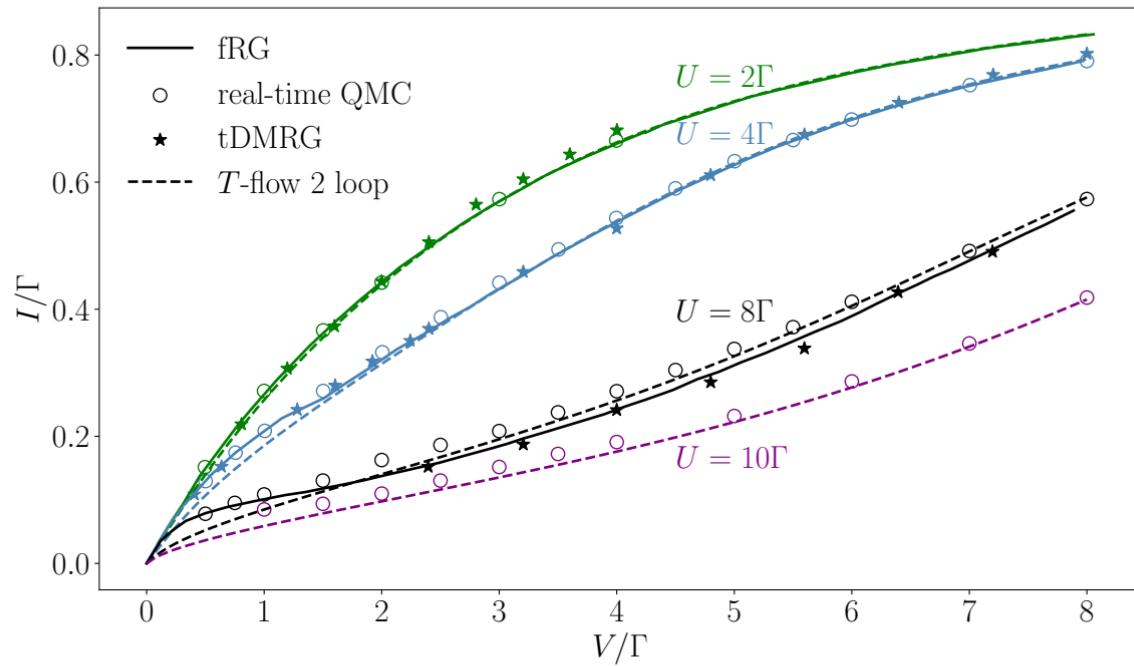
- 2-loop

$$-i \frac{\partial \Sigma}{\partial T} = \begin{array}{c} \text{Diagram: two horizontal lines with a diagonal line from top-left to bottom-right} \\ \text{Diagram: two horizontal lines with a diagonal line from top-right to bottom-left} \\ \text{Diagram: two horizontal lines with a diagonal line from top-left to bottom-right} \end{array} + \mathcal{O}(G^{+5})$$

- 3-loop

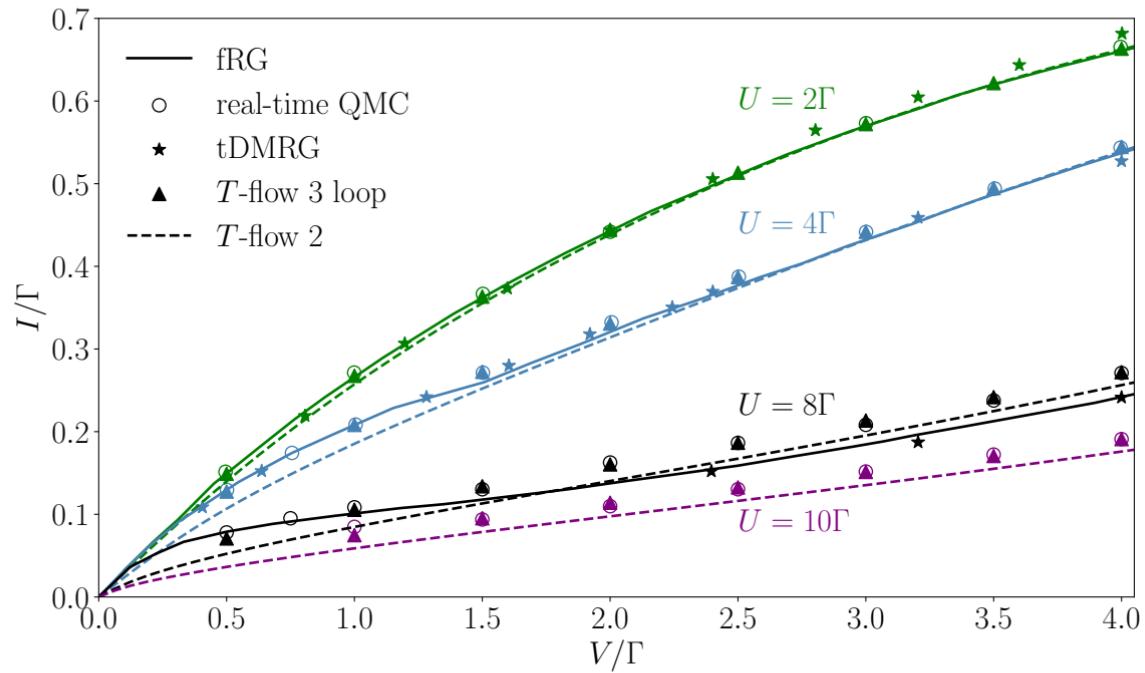
$$\begin{aligned} -i \frac{\partial \Sigma}{\partial T} &= \begin{array}{c} \text{Diagram: two horizontal lines with a diagonal line from top-left to bottom-right} \\ \text{Diagram: two horizontal lines with a diagonal line from top-right to bottom-left} \\ \text{Diagram: two horizontal lines with a diagonal line from top-left to bottom-right} \end{array} \\ \begin{array}{c} \text{Diagram: three horizontal lines with a diagonal line from top-left to bottom-right} \\ \text{Diagram: three horizontal lines with a diagonal line from top-right to bottom-left} \\ \text{Diagram: three horizontal lines with a diagonal line from top-left to bottom-right} \\ \text{Diagram: three horizontal lines with a diagonal line from top-right to bottom-left} \\ \text{Diagram: three horizontal lines with a diagonal line from top-left to bottom-right} \\ \text{Diagram: three horizontal lines with a diagonal line from top-right to bottom-left} \end{array} &= + \mathcal{O}(G^{+7}), \\ \begin{array}{c} \text{Diagram: four horizontal lines with a diagonal line from top-left to bottom-right} \\ \text{Diagram: four horizontal lines with a diagonal line from top-right to bottom-left} \end{array} &= + \mathcal{O}(G^{+6}) \end{aligned}$$

I - V characteristic: 2-loop T -flow at $T = 0$, $\varepsilon = -U/2$



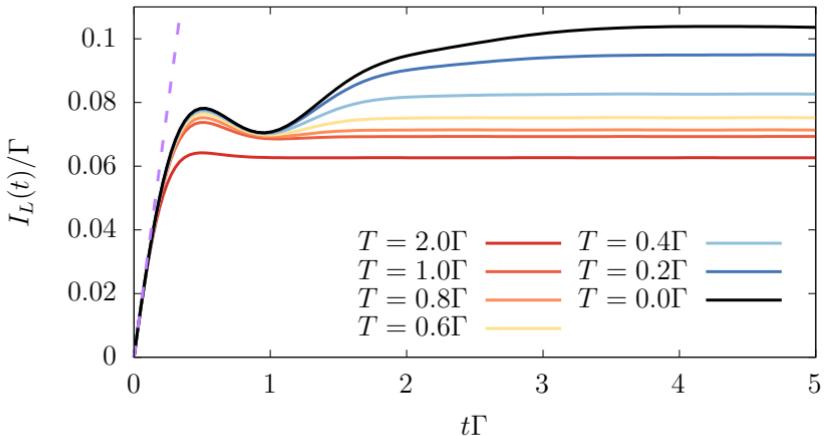
Compare with Eckel *et al*, New J. Phys. **12**, 043042 (2010) + Werner *et al*, Phys. Rev. B **81**, 035108 (2010)

I - V characteristic: 3-loop T -flow at $T = 0$, $\varepsilon = -U/2$

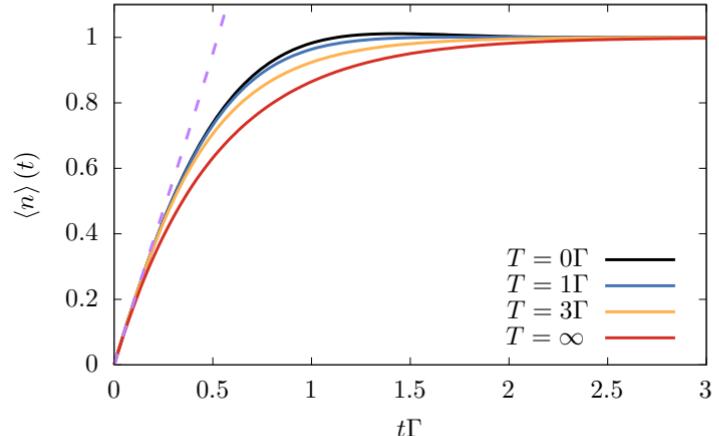


Compare with Eckel *et al*, New J. Phys. **12**, 043042 (2010) + Werner *et al*, Phys. Rev. B **81**, 035108 (2010)

Short-time dynamics: T independent !



$$\varepsilon = -U/2 = -4\Gamma, V = \Gamma, \rho_0 = |\uparrow\rangle\langle\uparrow|$$



$$\varepsilon = -U/2 = -2\Gamma, V = \Gamma, \rho_0 = |0\rangle\langle 0|$$

Short time:

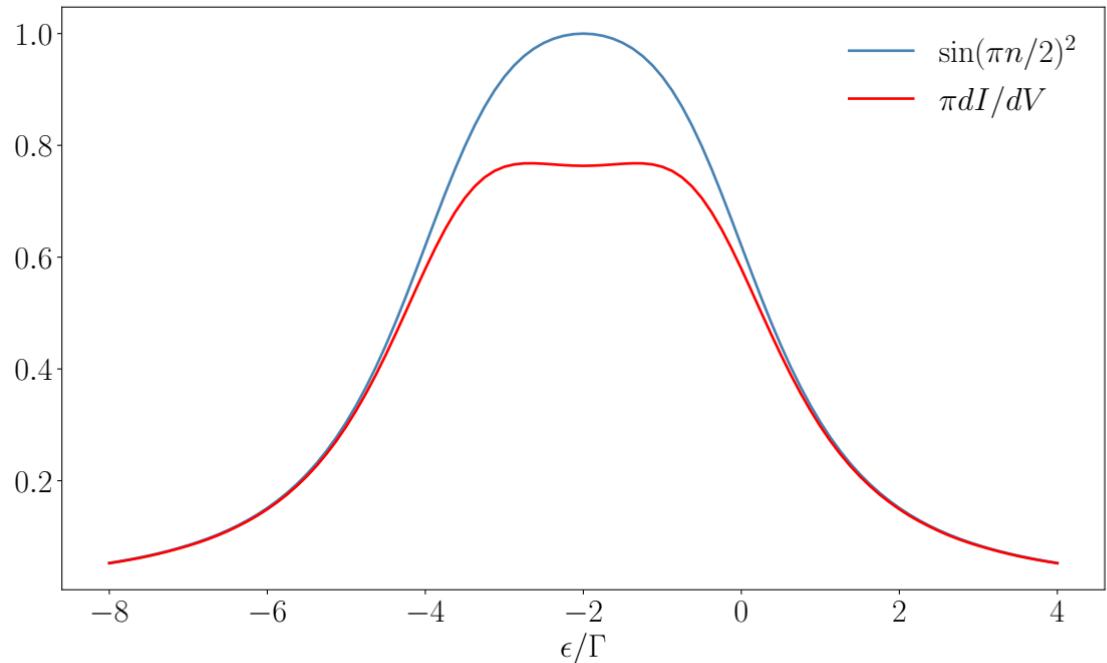
$$\begin{aligned} \frac{I(\delta t)}{\Gamma} &= (V - U - 2\varepsilon) \frac{\delta t}{\pi} \\ &\quad + (1 - \langle n \rangle_{\rho_0}) \left[1 + (U - 2\pi\Gamma) \frac{\delta t}{\pi} \right] + \mathcal{O}(\delta t^2) \end{aligned}$$

$$\langle n \rangle(\delta t) = 1 - e^{-2\Gamma\delta t} (1 - \langle n \rangle_{\rho_0}) + \mathcal{O}(\delta t^2)$$

Friedel sum rule, 2 loop

From Fermi liquid theory:

$$\frac{dI}{dV} \Big|_{V=0} = \frac{1}{2\pi} \sum_{\sigma} \sin^2(\pi \langle n_{\sigma} \rangle)$$

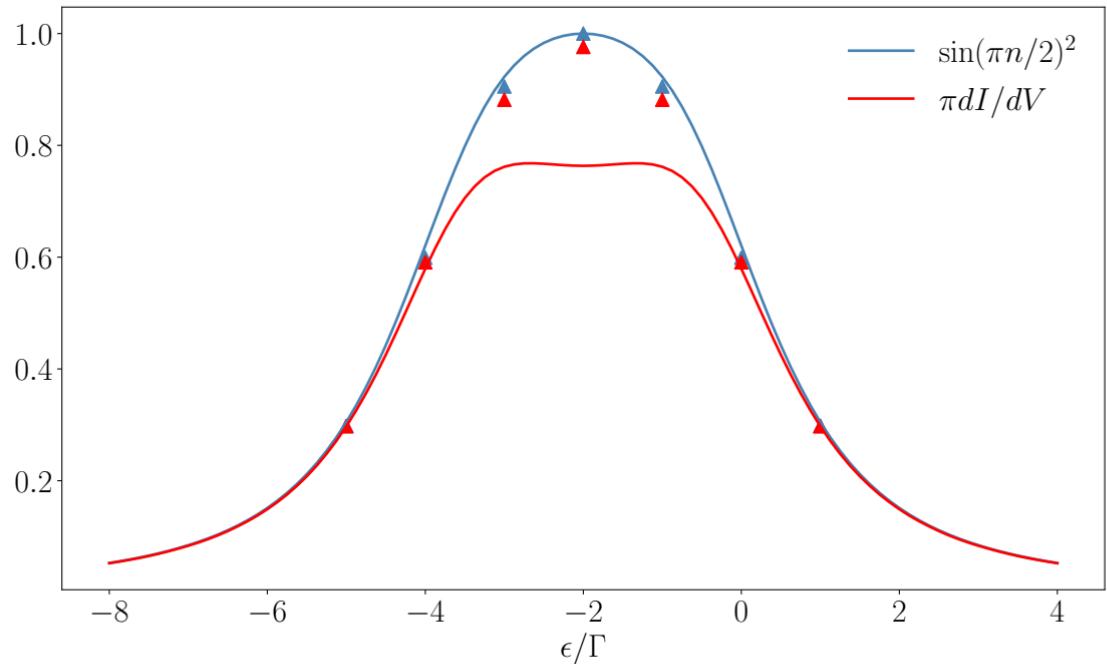


$$\begin{aligned} T &= 0 \\ U &= 4\Gamma \\ t_{\max} &= 20\Gamma^{-1} \\ V &= 0 \end{aligned}$$

Friedel sum rule, 3 loop

From Fermi liquid theory:

$$\frac{dI}{dV} \Big|_{V=0} = \frac{1}{2\pi} \sum_{\sigma} \sin^2(\pi \langle n_{\sigma} \rangle)$$



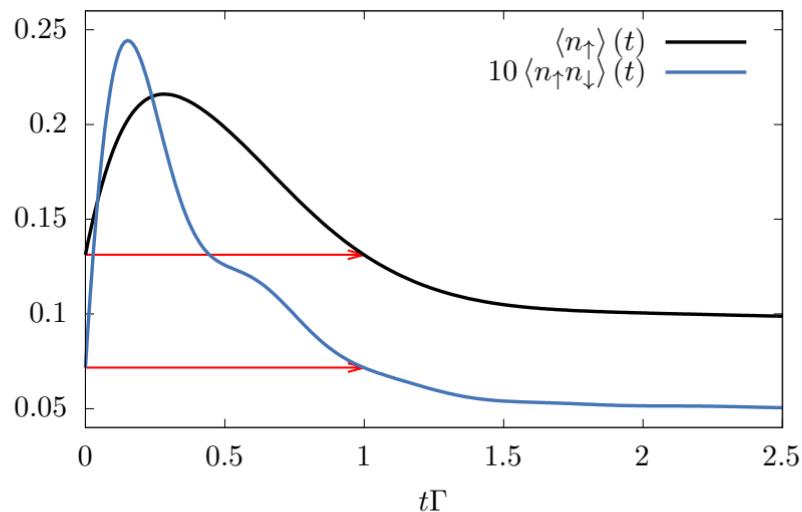
$$\begin{aligned} T &= 0 \\ U &= 4\Gamma \\ t_{\max} &= 20\Gamma^{-1} \\ V &= 0 \end{aligned}$$

Application: Reentrant states

For every time t_r the propagator Π has a fixed point $\rho_1(t_r)$:

$$\Pi(t_r) \rho_1(t_r) = \rho_1(t_r) \quad \text{with} \quad \rho_1(t_r) \geq 0 \quad \text{and} \quad \text{Tr} \rho_1(t_r) = 1.$$

\Rightarrow prepare system at $t=0$ in $\rho_1(t_r) \Rightarrow$ all local observables will return to initial value at time t_r



Reentrant effect. $U = 8\Gamma$, $\varepsilon = 2.75\Gamma$, $V = \Gamma$, $T = 0$.

Thank you for your attention !

Summary:

- Main reference: Nestmann, Wegewijs, SciPost Phys. **12**, 121 (2022)
- Goal: compute non-equilibrium open-system dynamics
- Use T itself as flow parameter to access low-temperature memory kernel
—> no wasted work, each intermediate step gives physical finite T evolution
- Alternative flow scheme: V -flow (?)
- Supermap-formalism (?)