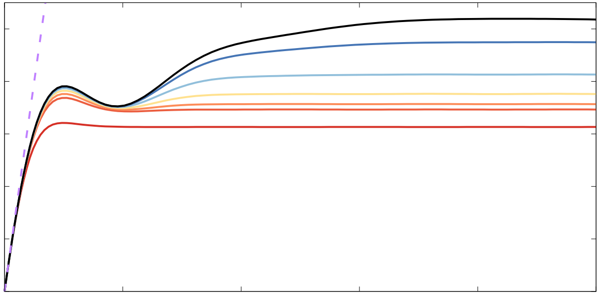
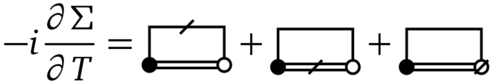
Temperature Flow
Renormalization Group for Open Quantum Systems





Konstantin Nestmann
Marie Curie Postdoctoral Fellow

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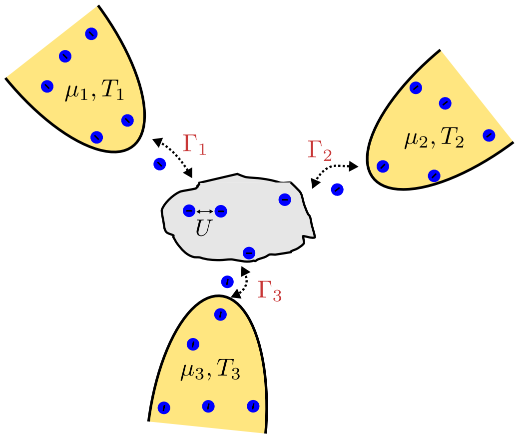
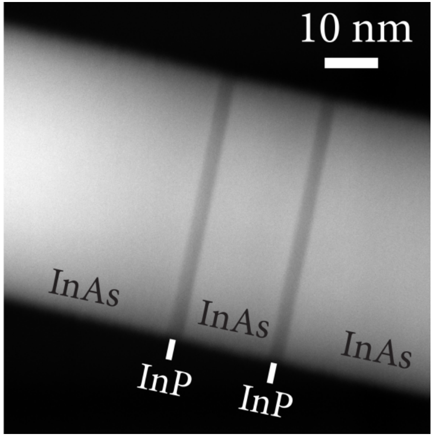
1 Open quantum systems & quantum transport

Theorists' view...



Experimental realization...



Heterostructured nanowire[1]

Anderson quantum dot as simplest transport model with interaction:

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

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

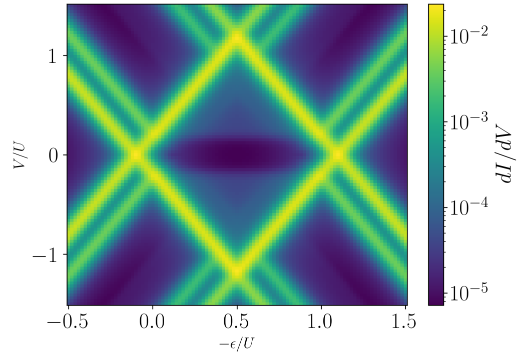
2 Theoretical setup

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

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

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

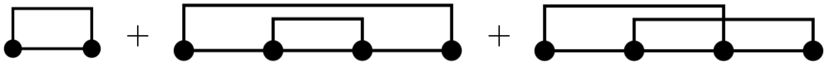
- Memory kernel approach well-developed[2]
  - Keldysh or superoperator formulation
  - Time or frequency space



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

- QmeQ: Open source python implementation perturbation theory in Γ

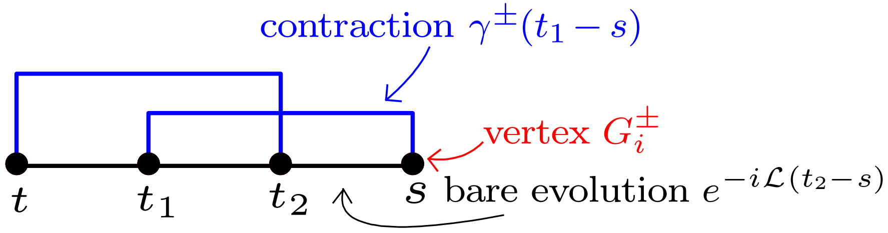
$-i\mathcal{K}$ =



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

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

3 Superfermionic perturbation theory

$\mathcal{K}(t-s) \rightarrow$ 

Clever definition superfermions:[3]

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

	Superfermion	Ordinary fermion
Anticommutation	$\{G_1^+, G_2^+\} = 0$	$\{d_{\sigma_1}^\dagger, d_{\sigma_2}^\dagger\} = 0$
	$\{G_1^-, G_2^+\} = \delta_{12}$	$\{d_{\sigma_1}, d_{\sigma_2}^\dagger\} = \delta_{\sigma_1\sigma_2}$
Pauli principle	$(G_1^+)^2 = 0$	$(d_\sigma^\dagger)^2 = 0$
Vacuum state	$G_1^-\,\mathbb{1} = 0$	$d_\sigma\lvert 0\rangle = 0$

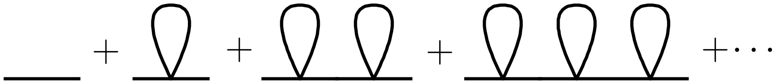
$$\gamma^+(t) = \Gamma\,\delta(t)$$
$$\gamma^-(t) \propto \frac{\Gamma\,T}{\sinh(\pi\,t\,T)}$$

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

4 Renormalized perturbation theory around $T = \infty$

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

$$\lim_{T\to\infty}\Pi =$$



$$= e^{-i\mathcal{L}_\infty t}$$

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

Step 2. At finite T: systematically resum infinite T contributions[4]

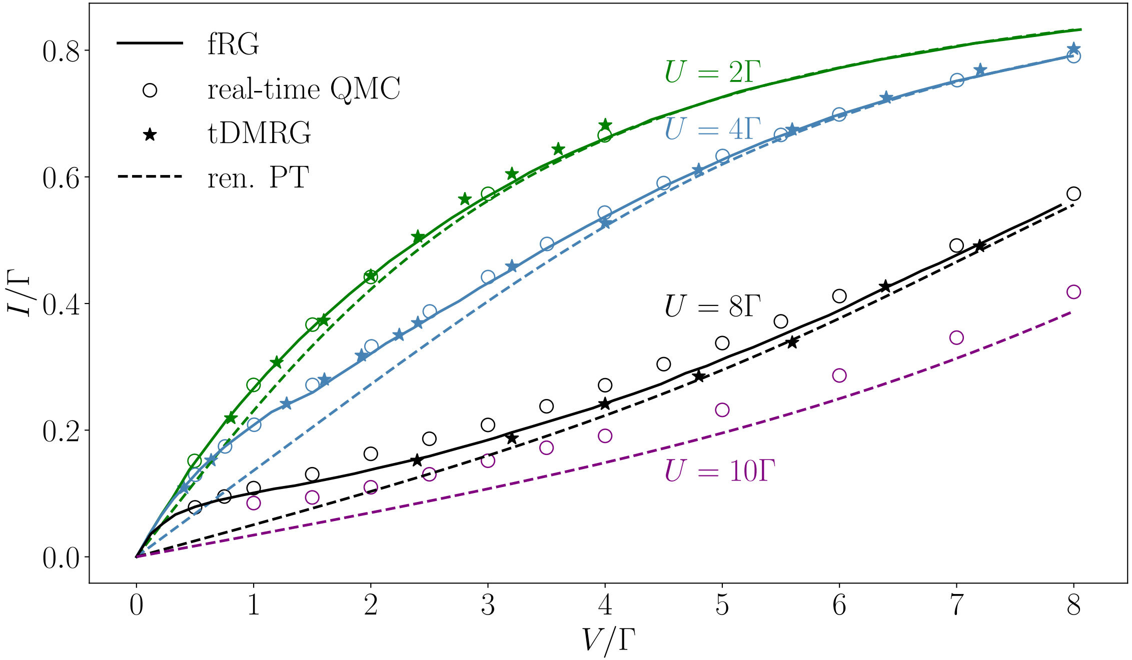
$$\mathcal{K}(t) = \Sigma_\infty \bar{\delta}(t) + \Sigma(t)$$

Same diagrammatics for Σ as bare perturbation theory but:

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

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 $T = \infty \to 0$ 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
  $\rightarrow$ flow from short-ranged correlations ($\gamma^-_{T=\infty} = 0$) to long-ranged ones ($\gamma^-_{T=0} \propto \Gamma / t$)
- Lower T & reduce thermal flucuations $\longrightarrow$ generate effective higher-order coupling

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

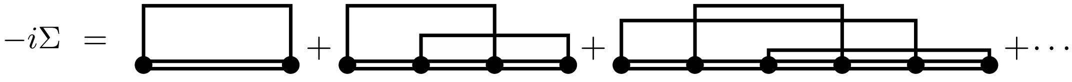
$$\gamma^-(t) \;\propto\; \frac{\Gamma\, T}{\sinh(\pi\, t\, T)} \qquad \text{but} \qquad \frac{\partial \gamma^-}{\partial T}(t) \;\approx\; t\, T\, \Gamma\, e^{-\pi t T} \quad \Longrightarrow \quad \boxed{\left.\frac{\partial \Sigma}{\partial T}\right|_{T=0} = 0}$$

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

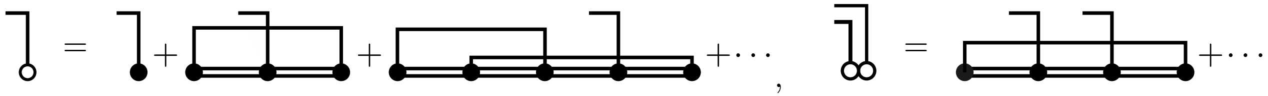
5 T-flow renormalization group

Step 1. Derive self-consistent expression for Σ (technical inspiration "E-flow"[5])

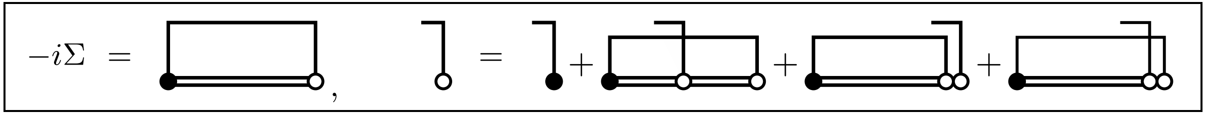
Resum connected subblocks to full propagators [$\Pi =$ ]



Define effective vertices:



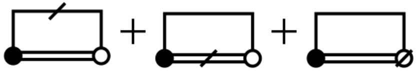
We recognize:

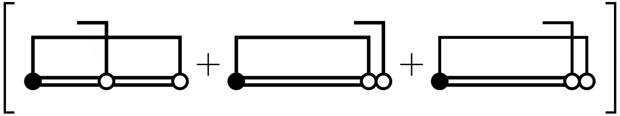


5. Pletyukhov and Schoeller, Phys. Rev. Lett. **108**, 260601 (2012)

5 T-flow renormalization group

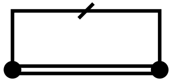
Step 2. Take T-derivative:

$$-i\,\frac{\partial\Sigma}{\partial T} \;=$$  where $$\frac{\partial\Pi}{\partial T} = -i\,\Pi * \frac{\partial\Sigma}{\partial T} * \Pi$$

 $$= \frac{\partial}{\partial T}$$ 

Step 3. Cutoff hierarchy:

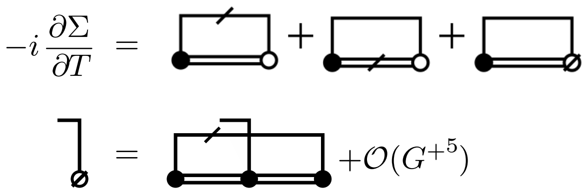
- 1-loop

$$-i\,\frac{\partial\Sigma}{\partial T} \;=$$  $$+\mathcal{O}(G^{+4})$$

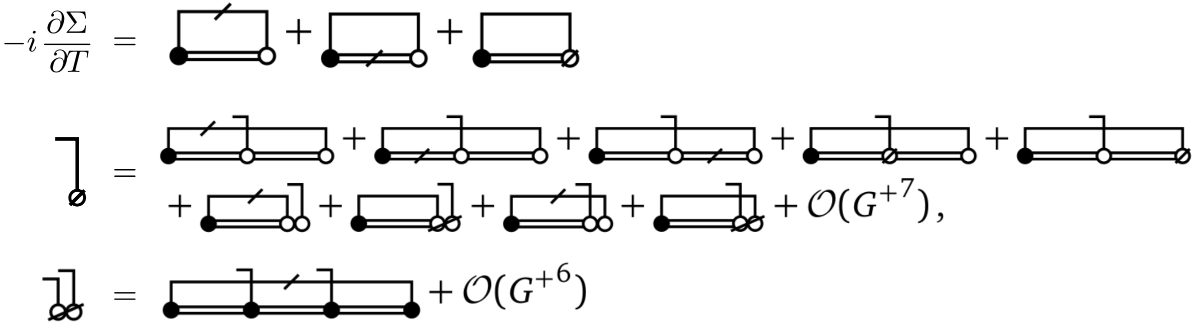
 $$= 0 + \mathcal{O}(G^{+3})$$

5 *T*-flow renormalization group

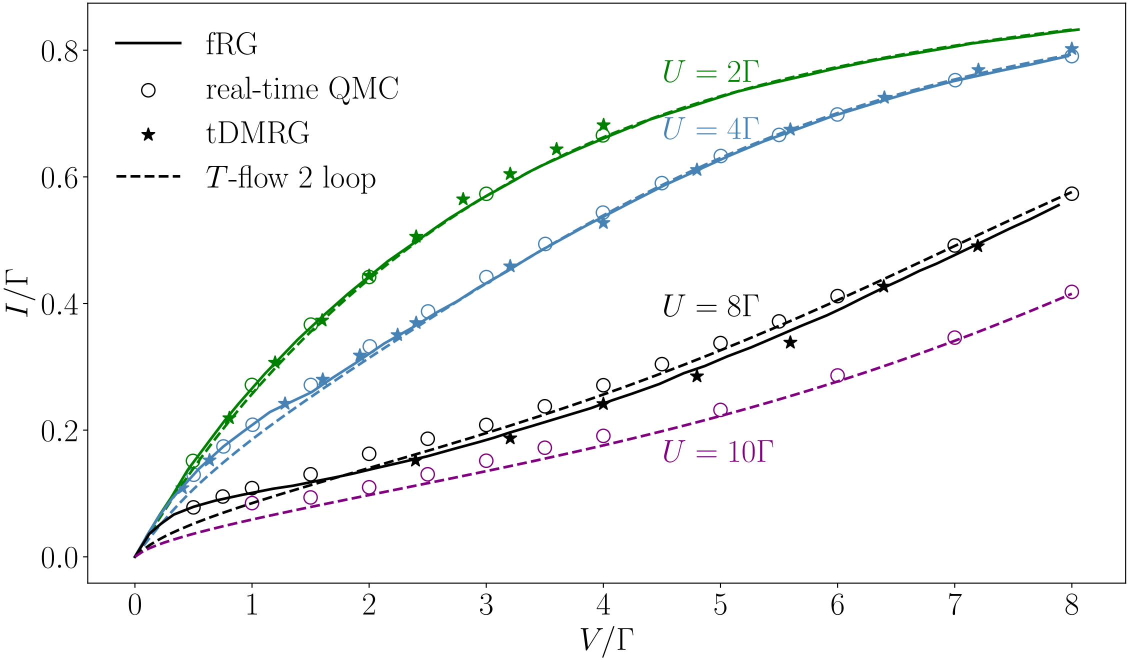
- 2-loop



- 3-loop

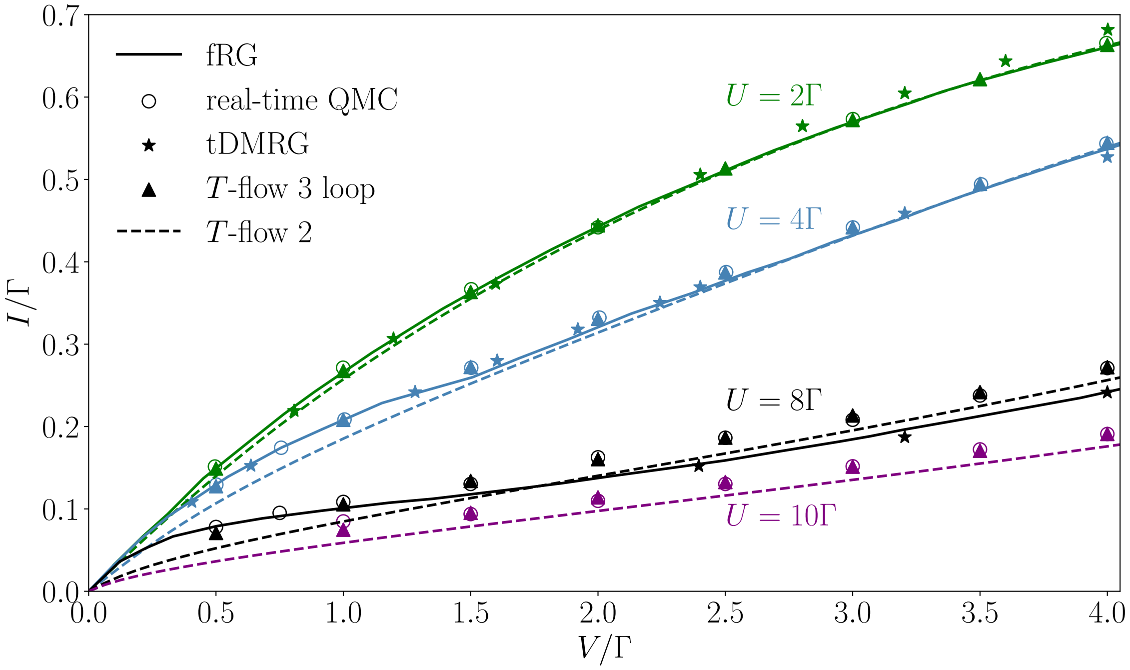


I-V characteristic: 2-loop T-flow at $T = 0$, $\varepsilon = -U/2$



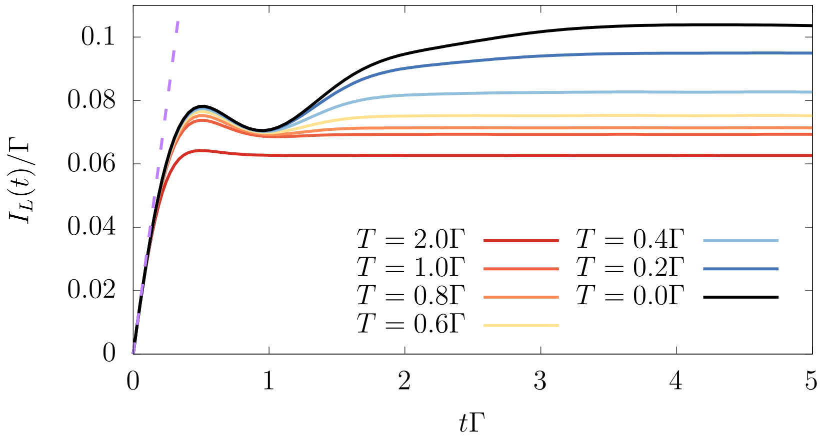
Compare with Eckel *et al*, New J. Phys. **12**, 043042 (2010) + Werner *et al*, Phys. Rev. B **81**, 035108 (2010)

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

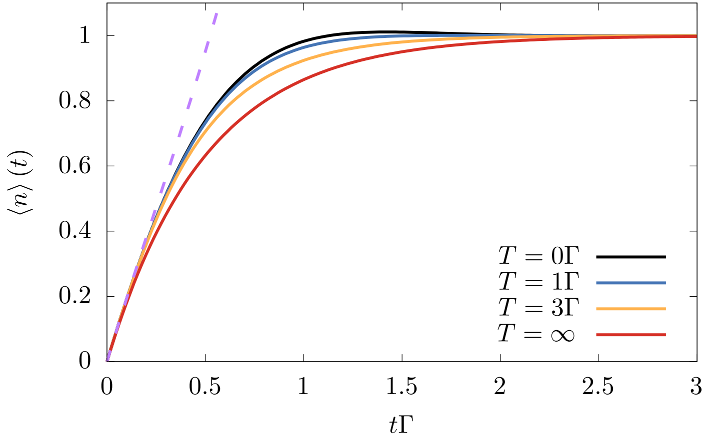


Compare with Eckel *et al*, New J. Phys. **12**, 043042 (2010) + Werner *et al*, Phys. Rev. B **81**, 035108 (2010)

Short-time dynamics: T independent !



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



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

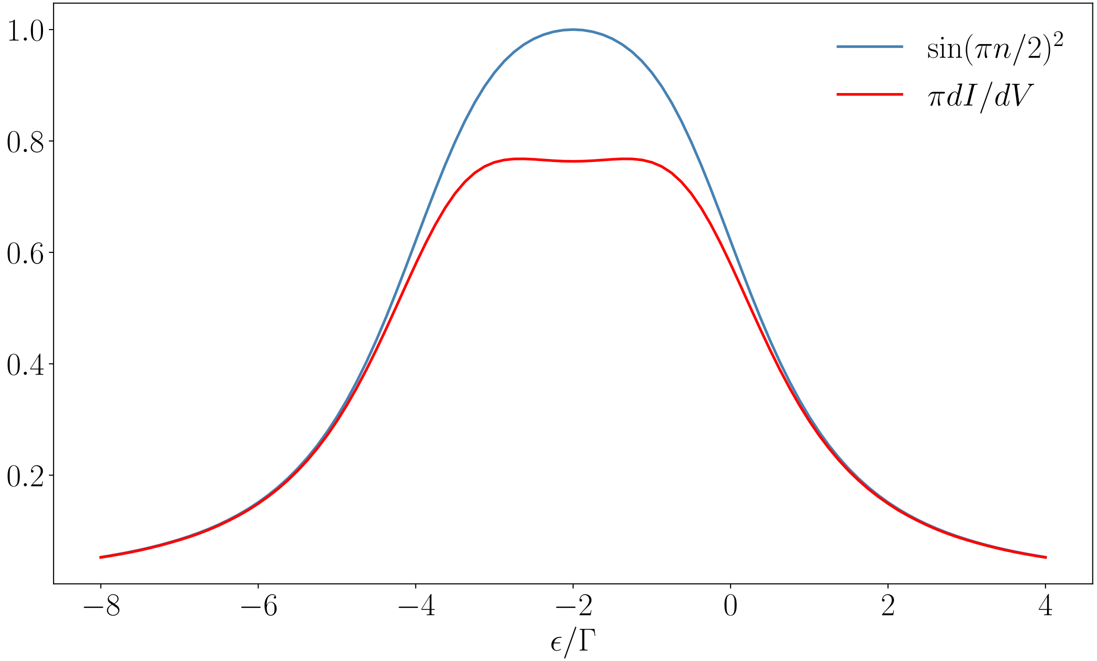
Short time:

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

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

Friedel sum rule, 2 loop

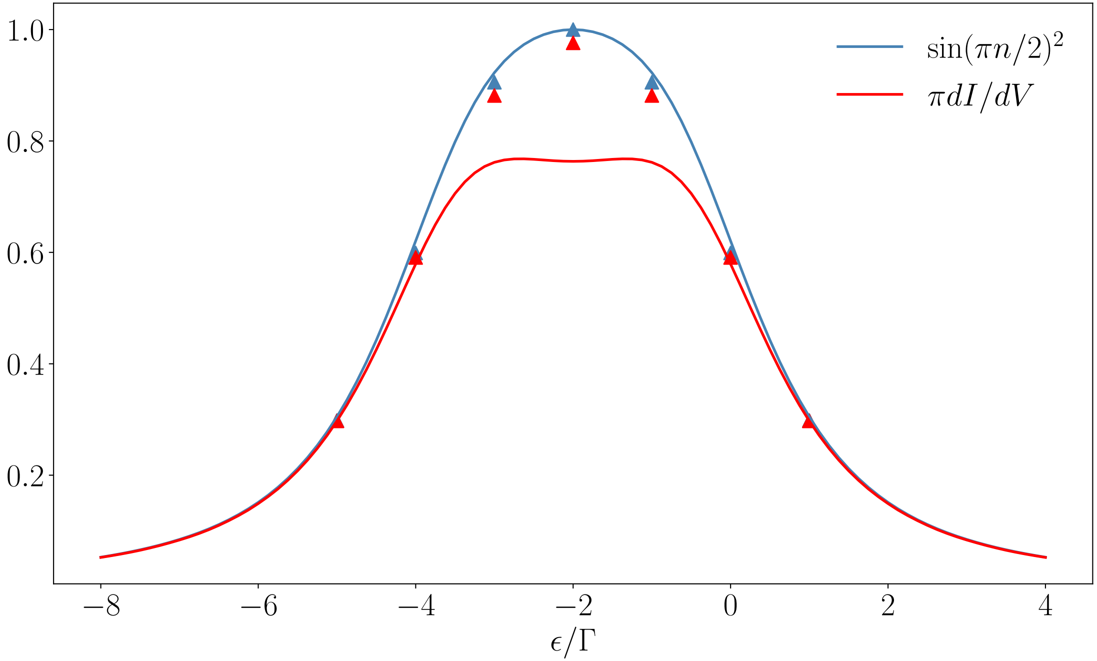
From Fermi liquid theory:
$$\left.\frac{\mathrm{d}I}{\mathrm{d}V}\right|_{V=0} = \frac{1}{2\pi}\sum_{\sigma} \sin^2\big(\pi\langle n_\sigma\rangle\big)$$



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

Friedel sum rule, 3 loop

From Fermi liquid theory: $$\left.\frac{\mathrm{d}I}{\mathrm{d}V}\right|_{V=0} = \frac{1}{2\pi}\sum_{\sigma}\sin^2\left(\pi\langle n_\sigma\rangle\right)$$



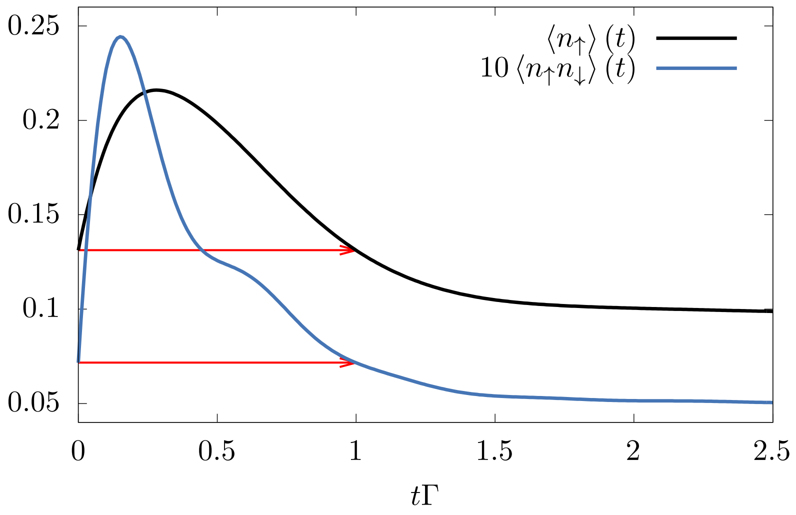
$T = 0$
$U = 4\Gamma$
$t_{\max} = 20\Gamma^{-1}$
$V = 0$

Application: Reentrant states

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

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

$\Longrightarrow$ prepare system at $t = 0$ in $\rho_1(t_r)$ $\Longrightarrow$ all local observables will return to inital 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
  $\longrightarrow$ no wasted work, each intermediate step gives physical finite T evolution
- Alternative flow scheme: V-flow (?)
- Supermap-formalism (?)