QTD 2019

W. Talarico

A microscopic viewpoint to energy transport in many-body systems

TCQP

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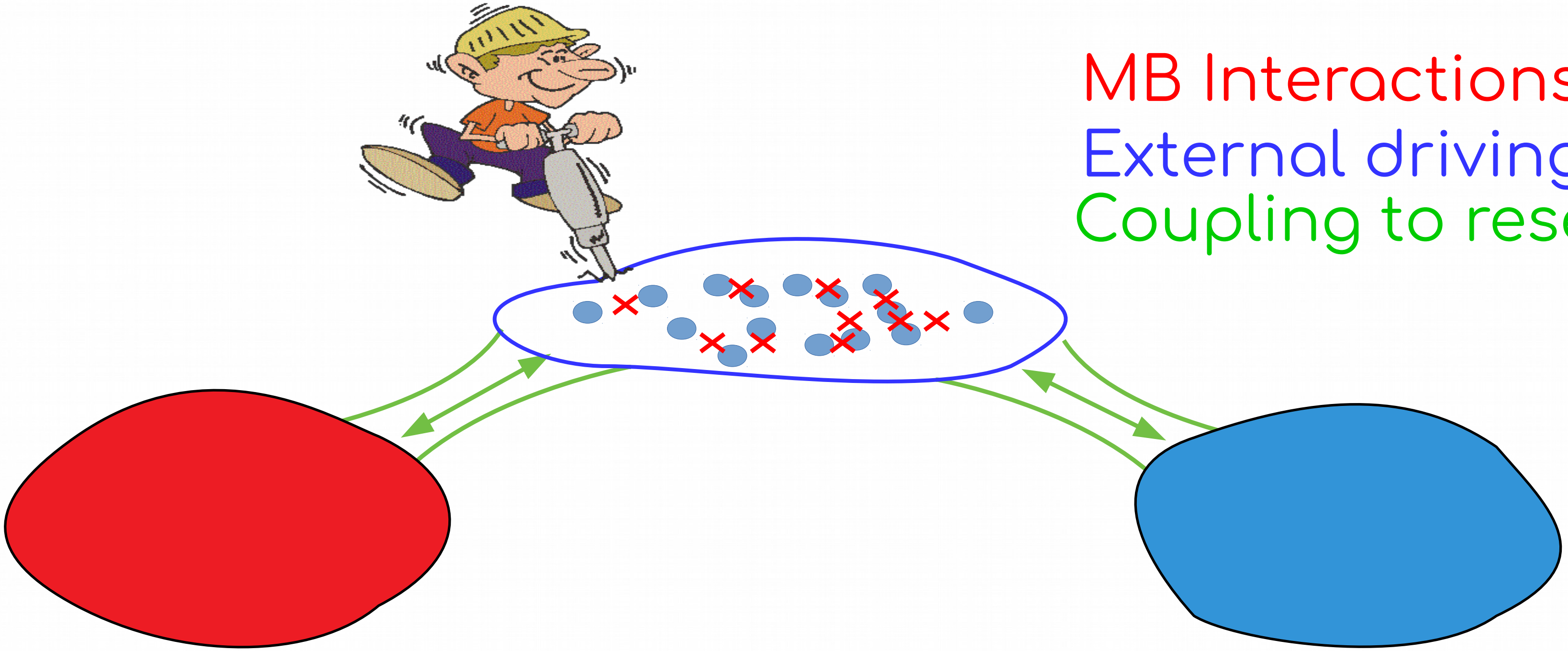
Many-body quantum systems

MB Interactions

External driving

Coupling to reservoirs



Particles on a contour

$$\hat{H} = \hat{H}_0 + \hat{V} + \hat{H}_{SL}$$

$$\hat{H}_0 = \sum_{i,j} h_{ij} \hat{d}_i^\dagger \hat{d}_j$$

Free

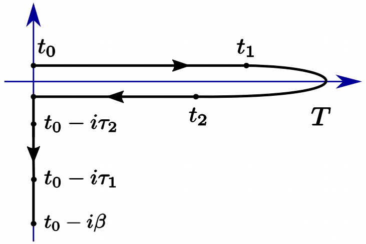
$$\hat{V} = \sum_{i,j,i',j'} v_{iji'j'} \hat{d}_i^\dagger \hat{d}_{i'}^\dagger \hat{d}_{j'} \hat{d}_j$$

MB Interactions

$$\hat{H}_{SL} = \sum_{\alpha} \sum_{ki} g_{ki}^{\alpha} \hat{D}_{\alpha,k}^\dagger \hat{d}_i + h.c.$$

Coupling to reservoirs

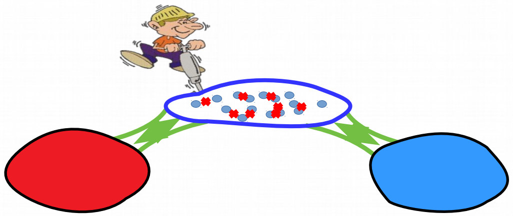
Keldysh-Schwinger contour



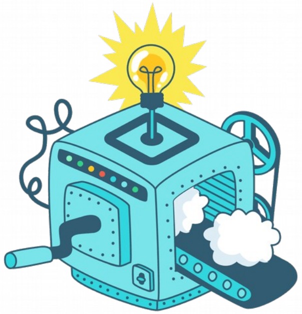
Single particle Green's function

$$G_{ij}(z; z') = -\imath \langle T_\gamma \hat{d}_i(z) \hat{d}_j(z') \rangle$$

NEGFs



- Choose a self-energy
- Apply the machinery of NEGFs
- Get the SP Green's



Pros and cons

- ✔ Interactions
- ✔ Access to spectral properties
- ✔ Leads are treated non-perturbatively
- ✔ Any spectral function
- ✔ Drive
- ✔ Linear scaling with size

- ✗ Interactions are treated perturbatively
- ✗ Computationally demanding

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An example: SIAM

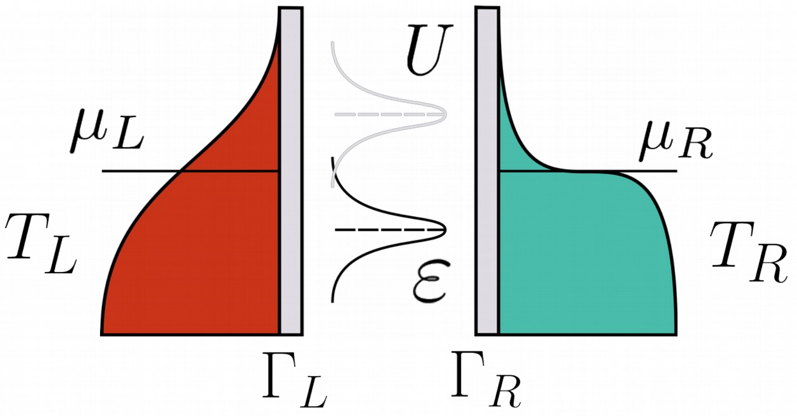
The model

$$\hat{H} = \hat{H}_0 + \hat{V} + \hat{H}_{SL}$$

$$\hat{H}_0 = \sum_n \epsilon\, \hat{n}_\sigma$$

$$\hat{V} = U \hat{n}_\uparrow \hat{n}_\downarrow$$

$$\hat{H}_{LS} = \sum_\alpha \sum_{k_\alpha \sigma} T_{k_\alpha \sigma,\alpha} \left[\hat{d}^\dagger_\sigma \hat{c}_{k_\alpha \sigma,\alpha} + \hat{c}^\dagger_{k_\alpha \sigma,\alpha} \hat{d}_\sigma \right]$$



Strong Correlations

$$\frac{U}{\Gamma} \gg 1$$

Low Temperature

$$T < T_K$$

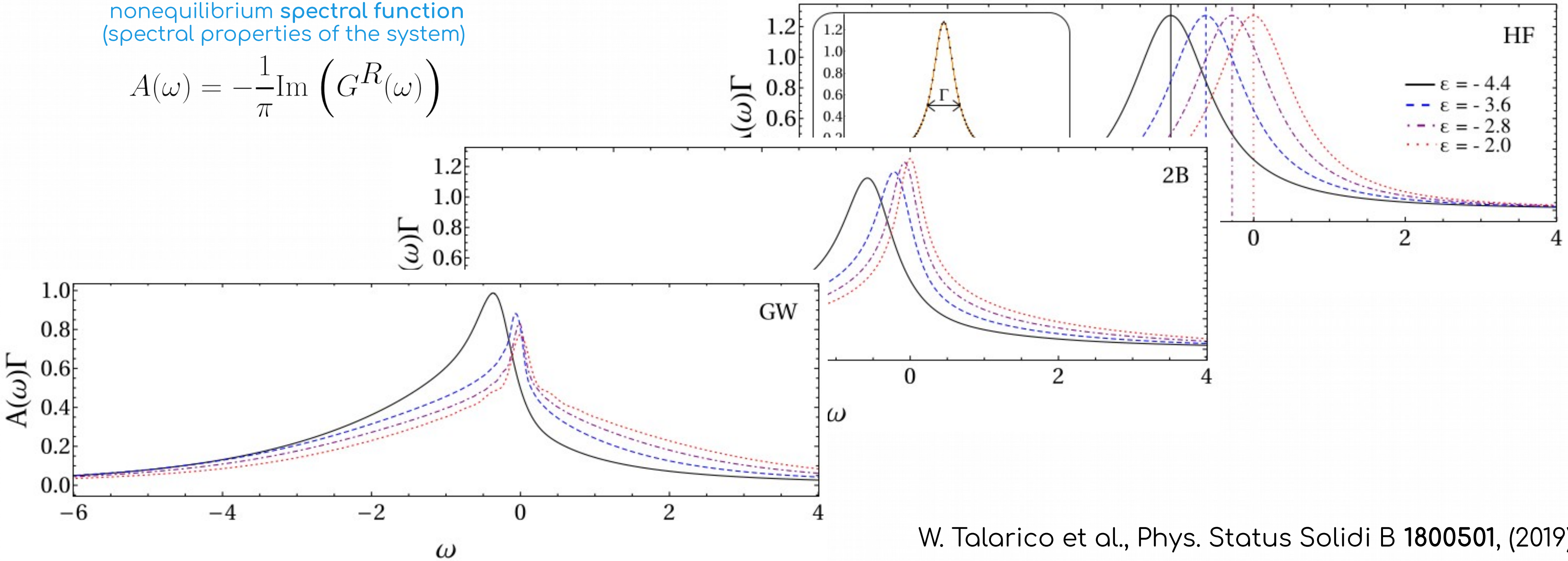
Kondo Regime

W. Talarico et al., Phys. Status Solidi B **1800501**, (2019)

A signature of the Kondo regime

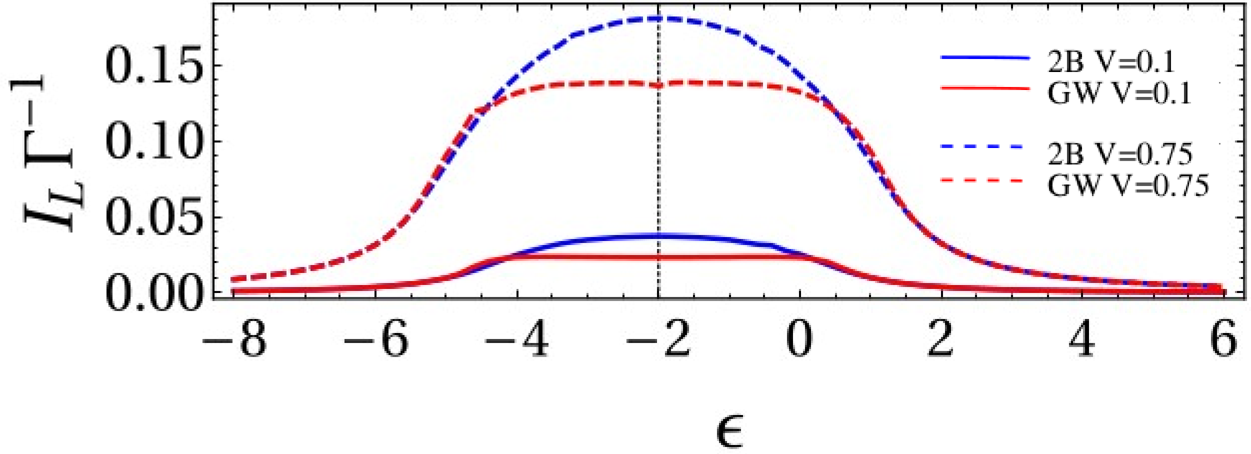
nonequilibrium **spectral function**
(spectral properties of the system)

$$A(\omega) = -\frac{1}{\pi}\mathrm{Im}\left(G^R(\omega)\right)$$



W. Talarico et al., Phys. Status Solidi B **1800501**, (2019)

A signature of the Kondo regime

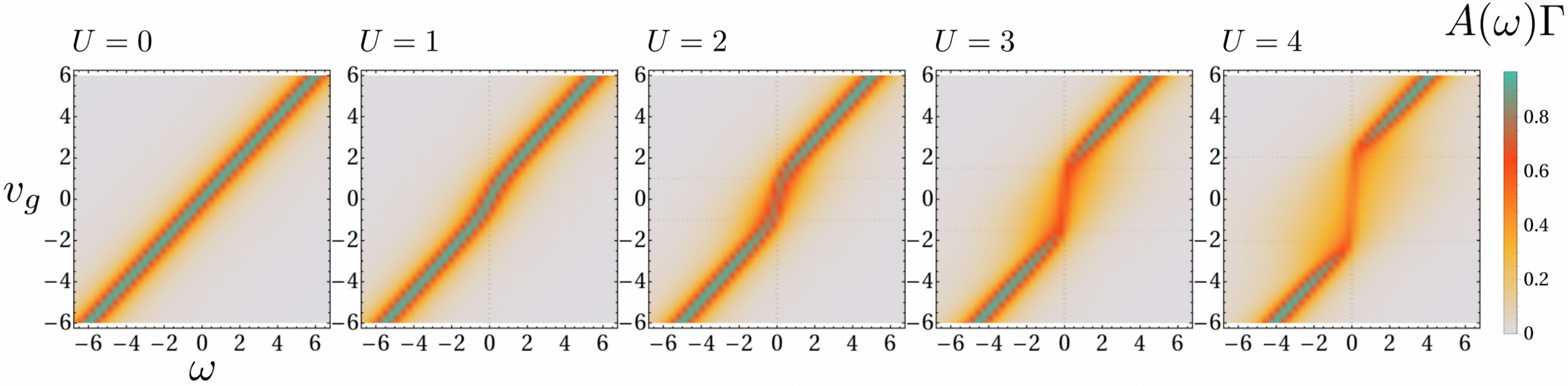


W. Talarico et al., Phys. Status Solidi B **1800501**, (2019)

A signature of the Kondo regime

$$A(\omega) = -\frac{1}{\pi}\mathrm{Im}\left(G^R(\omega)\right)$$

Within the **GW** approximation
it is possible to explore
Kondo correlations effects



Energy current

Particle (charge) current

$$\frac{d\langle \hat{N}(t)\rangle}{dt} = i\langle[\hat{H}, \hat{N}(t)]\rangle$$

From Dyson equation

$$\mathcal{I}_\alpha(z) = 2Re\left\{\int d\mathbf{x}_1 d\bar{1}\; G(1,\bar{1})\Sigma_\alpha(\bar{1},1^+)\right\}$$

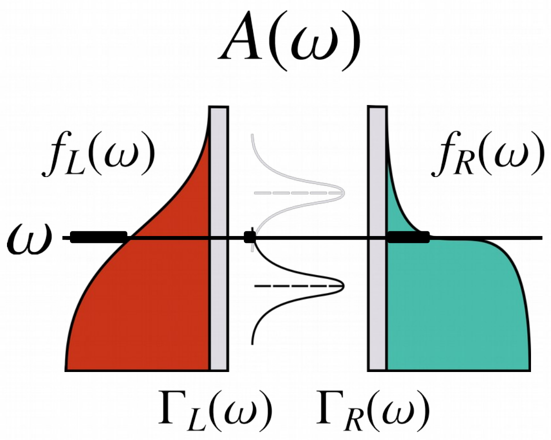
Embedding Self-Energy

Stationary Limit

Meir-Wingreen

$$\mathcal{I}_\alpha^{(S)} = \int d\omega \Gamma(\omega)[f_\alpha(\omega) - f_{\bar{\alpha}}(\omega)]A(\omega)$$

$$\Gamma(\omega) = \frac{\Gamma_L(\omega)\Gamma_R(\omega)}{\Gamma_L(\omega)+\Gamma_R(\omega)}$$



Energy current

$$\frac{d\langle \hat{H}_C(t)\rangle}{dt} = i\langle[\hat{H}, \hat{H}_C(t)]\rangle$$

$$\frac{d\langle \hat{H}_\alpha(t)\rangle}{dt} = i\langle[\hat{H}, \hat{H}_\alpha(t)]\rangle$$

Interaction complicates things

The energy variation in the system equals the sum in the energy variation of the leads

Stationary state

"Meir-Wingreen"

$$\mathcal{J}_\alpha^{(S)} = \int d\omega \Gamma(\omega)(\omega - \mu_\alpha)[f_\alpha(\omega) - f_{\bar{\alpha}}(\omega)]A(\omega)$$

Particles flowing into the lead carry charge AND energy

Where did the interaction go?

Energy current

$$\frac{d\langle \hat{H}_C(t)\rangle}{dt} = i\langle[\hat{H}, \hat{H}_C(t)]\rangle$$

Interaction complicates things

$$\mathcal{J}_C^{(\alpha)}(t) = 2\mathrm{Re}\left\{\int d\mathbf{x}_1 d\bar{1} d\bar{2} \left[h(1)\delta(1,\bar{1}) + \Sigma(1,\bar{1})\right] G(\bar{1},\bar{2})\Sigma_\alpha(\bar{2},1^+)\right\}_{z_1=t}$$

SP Energy

Interaction Energy

“Particle current”

It is consistent with the approximations made

$$\Sigma(1,1') \to G(1,1')$$

Energy current : SIAM

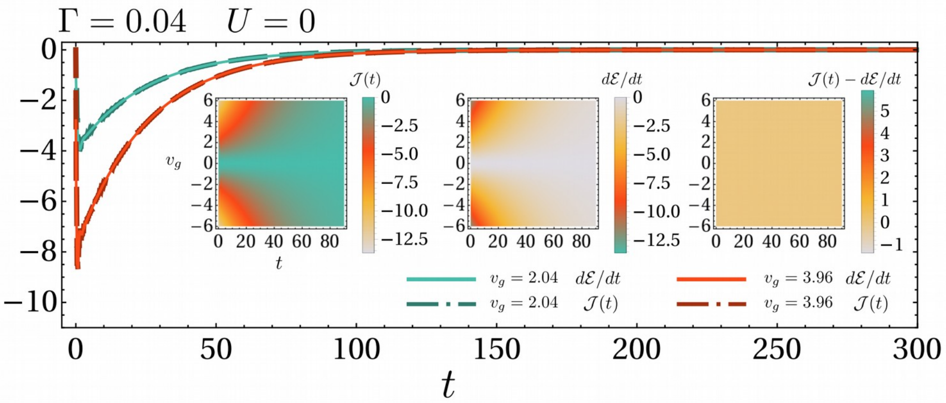
$$\mu_L = \mu_R = 0 \qquad T_L > T_R$$

GW conserving approximation

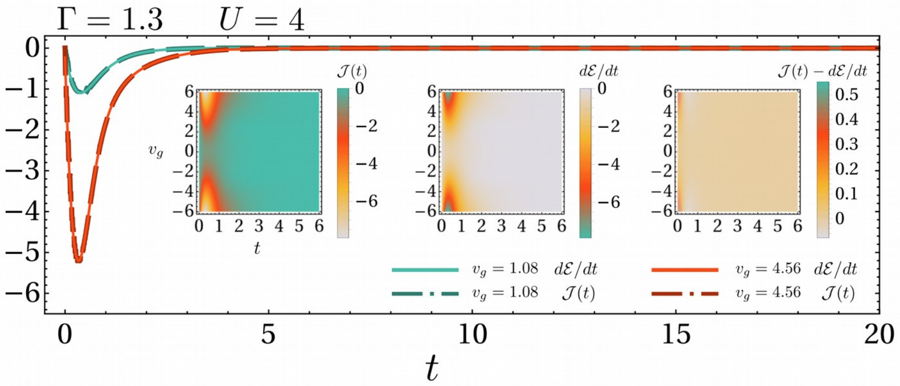
Macroscopic conservation laws are built into the **MBPT**

$$\frac{d\mathcal{E}(t)}{dt} = \sum_{\alpha} \mathcal{J}_C^{(\alpha)}(t)$$

Weak coupling



Strong coupling



Energy current : stationarity

Time-dependent expressions
for the particle and energy currents
obtained from the **MBPT**

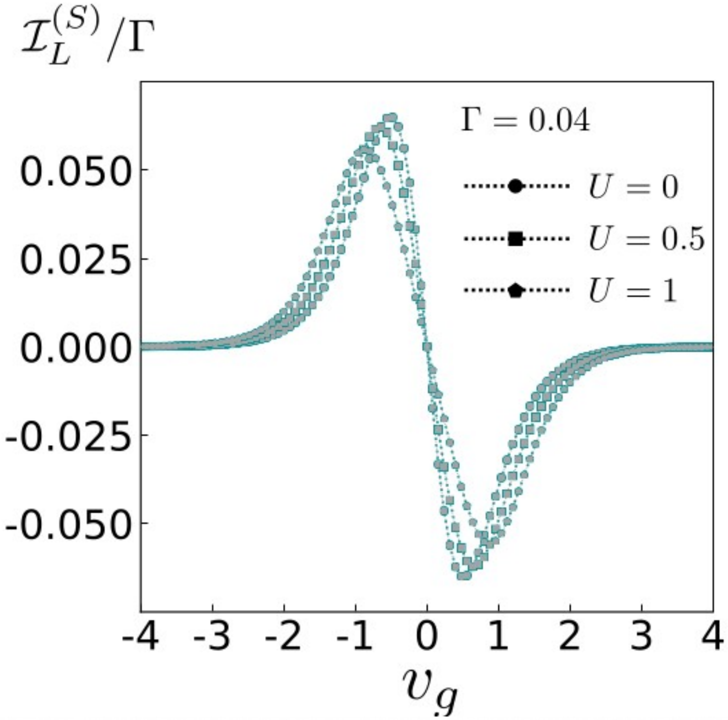
Steady-state values
of the particle and energy currents:
Meir-Wingreen formulae

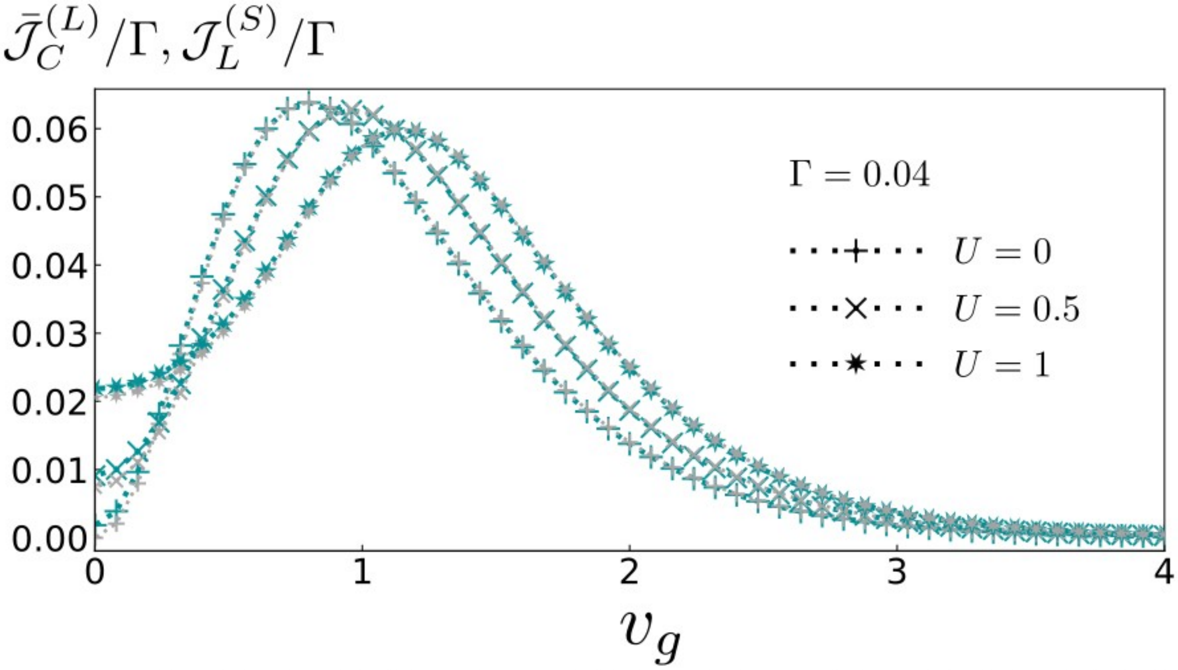
$$\mathcal{I}_\alpha(z) = 2Re\left\{\int d\mathbf{x}_1 d\bar{1}\; G(1,\bar{1})\Sigma_\alpha(\bar{1},1^+)\right\} \quad \xrightarrow{t\to\infty} \quad \mathcal{I}^{(S)}_\alpha = \int d\omega \Gamma(\omega)[f_\alpha(\omega) - f_{\bar{\alpha}}(\omega)]A(\omega)$$

$$\mathcal{J}^{(\alpha)}_C(t) = 2\mathrm{Re}\left\{\int d\mathbf{x}_1 d\bar{1} d\bar{2}\; [h(1)\delta(1,\bar{1}) + \Sigma(1,\bar{1})]\, G(\bar{1},\bar{2})\Sigma_\alpha(\bar{2},\bar{1}^+)\right\}_{z_1=t} \qquad \mathcal{J}^{(S)}_\alpha = \int d\omega \Gamma(\omega)(\omega - \mu_\alpha)[f_\alpha(\omega) - f_{\bar{\alpha}}(\omega)]A(\omega)$$

SIAM at Stationarity $\mu_L = \mu_R = 0 \quad T_L > T_R$

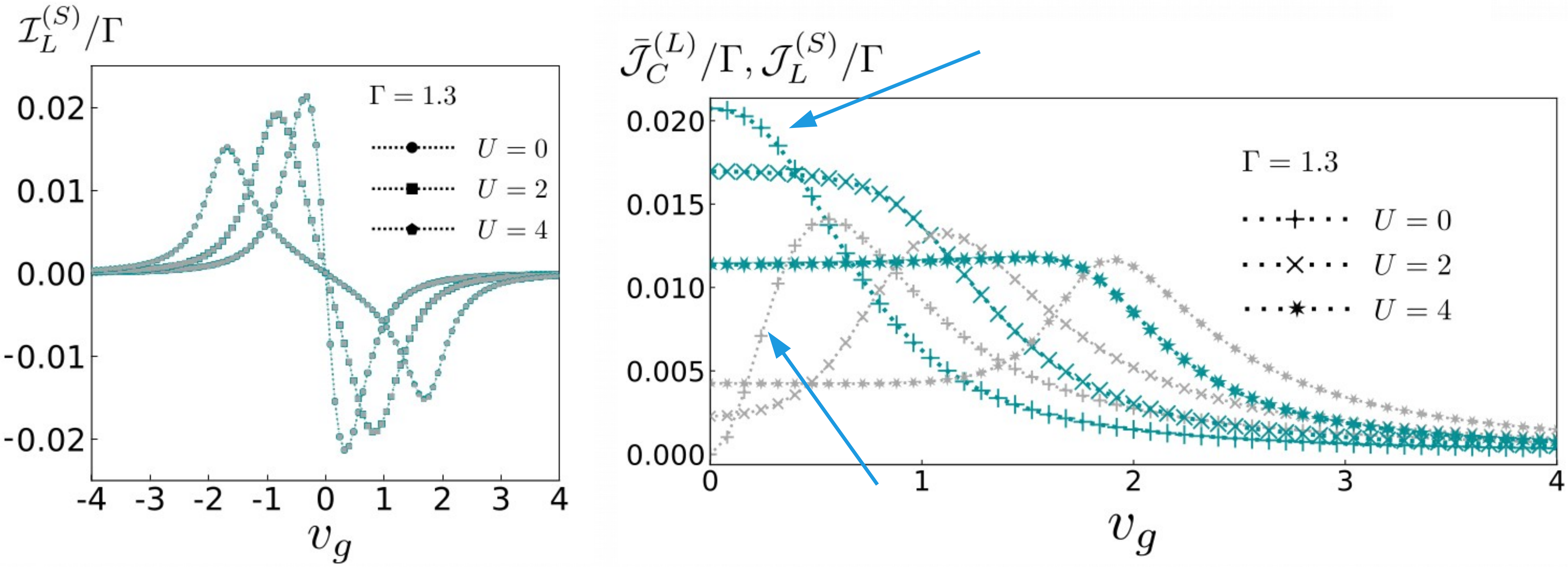
Weak coupling





SIAM at Stationarity $\mu_L = \mu_R = 0 \quad T_L > T_R$

Strong coupling



The missing term

Coupling term

$$\frac{d}{dt}\langle \hat{V}_C^{(\alpha)}(t)\rangle = -J_\alpha(t) - J_C^{(\alpha)}(t) - \Delta J_\alpha(t) + \frac{\partial}{\partial t}\langle \hat{V}_C^{(\alpha)}(t)\rangle$$

$$\mathcal{J}_\alpha^{(S)} = \int d\omega \Gamma(\omega)(\omega - \mu_\alpha)[f_\alpha(\omega) - f_{\bar{\alpha}}(\omega)]A(\omega)$$

$$\mathcal{J}_C^{(\alpha)}(t) = 2\mathrm{Re}\left\{\int d\mathbf{x}_1 d\bar{1} d\bar{2}\; [h(1)\delta(1,\bar{1}) + \Sigma(1,\bar{1})]\, G(\bar{1},\bar{2})\Sigma_\alpha(\bar{2},\bar{1}^+)\right\}_{z_1=t}$$

No drive (DC)

$$\frac{d}{dt}\langle \hat{V}_C^{(\alpha)}(t)\rangle = 0$$

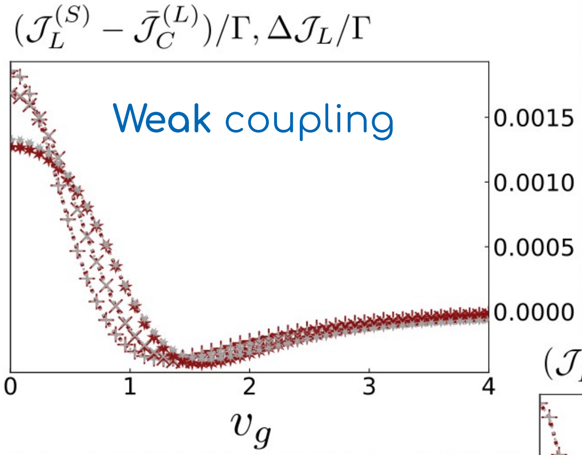
M.F. Ludovico, L. Arrachea, M. Moskalets, and D. Sanchez, Entropy 18, 419 (2016)

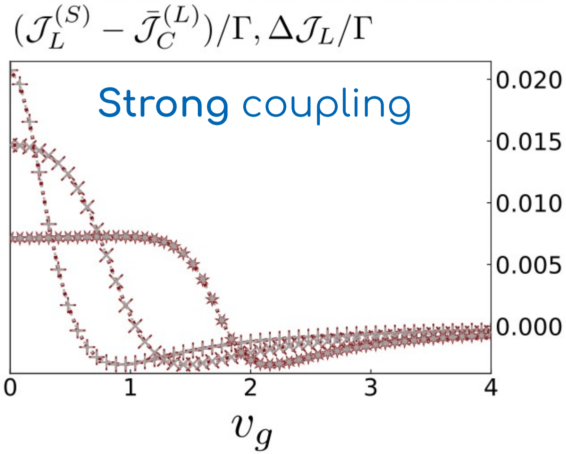
The missing term

$$\Delta J_\alpha(t) = \sum_{\beta\neq\alpha} \int d\mathbf{x}_1 T_\beta(1) G_{\beta\alpha}(1;1^+) T^*_\alpha(1) \Big|_{z_1=t}$$

Leads-leads propagator

$$G_{\beta\alpha}(1,1') = \int d\bar{1} d\bar{2}\; g_\beta(1;\bar{1}) T^*_\beta(\bar{1}) G(\bar{1};\bar{2}) T_\alpha(\bar{2}) g_\alpha(\bar{2};1')$$

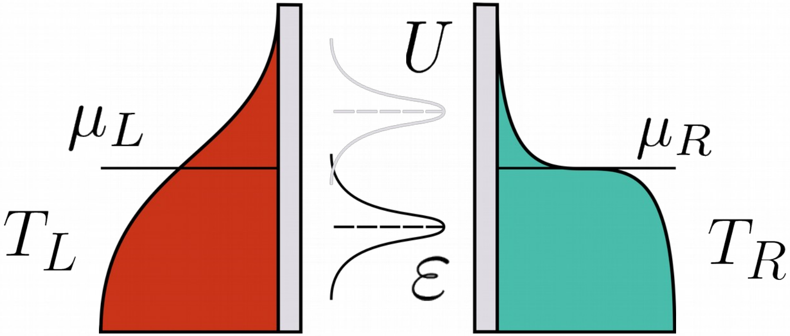


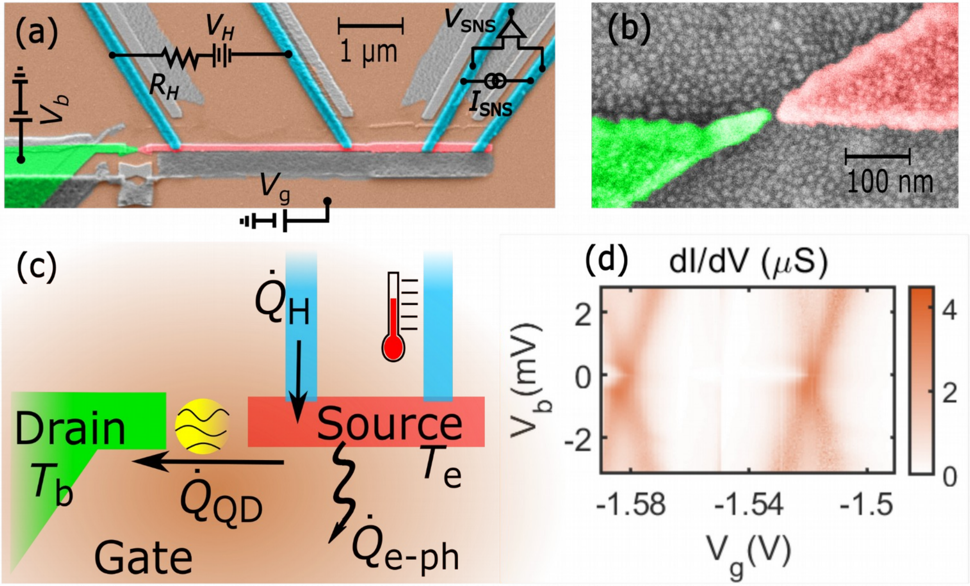


N. W. Talarico, S. Maniscalco, and N. Lo Gullo arXiv:1906.10000

Probing the leads

A single level quantum dot





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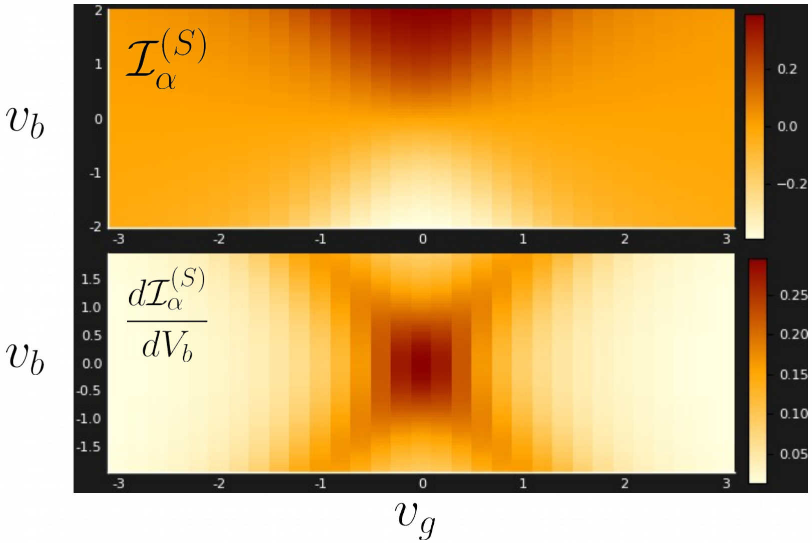
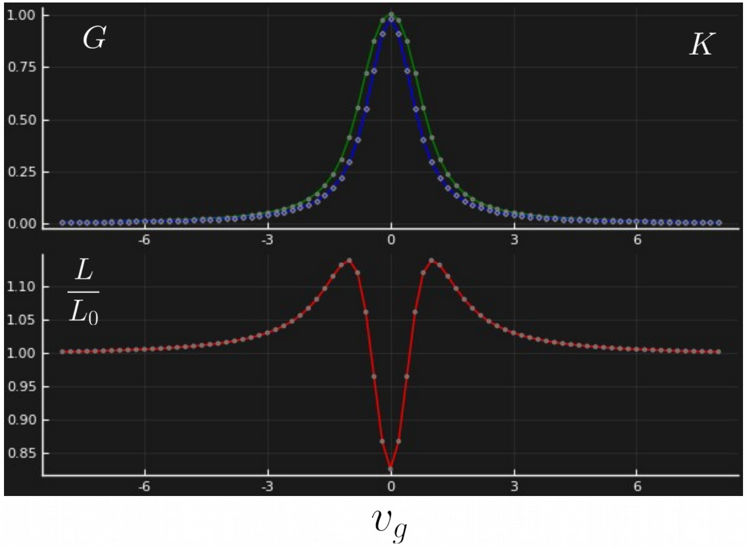
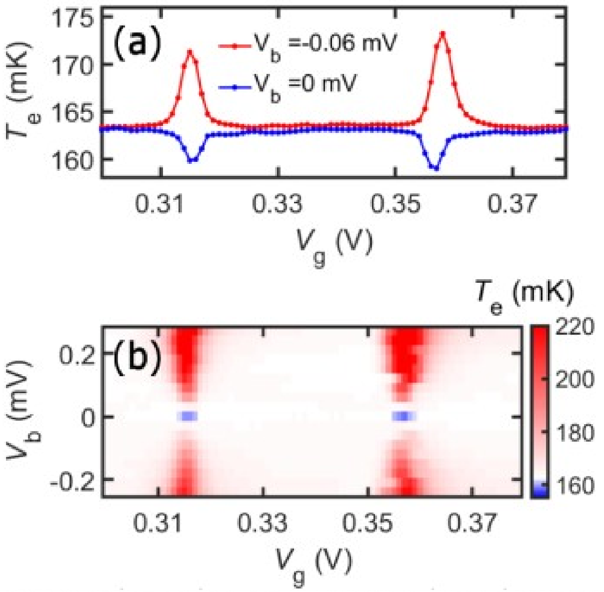
(violation of) Wiedemann-Franz

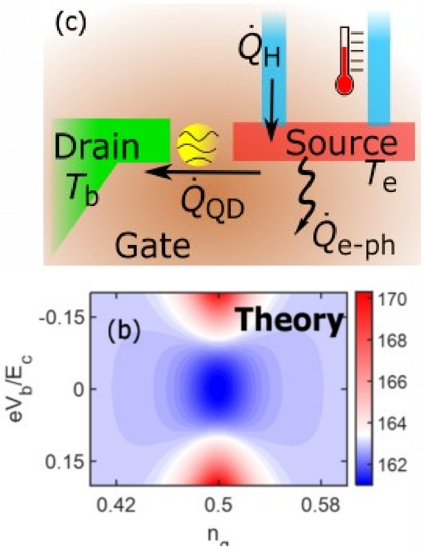
$$L = \frac{K}{TG} \qquad G(T,V) = \frac{\partial I}{\partial V}\bigg|_{\Delta T=0} \qquad K(T,V) = \frac{\partial J}{\partial \Delta T}\bigg|_{I=0}$$





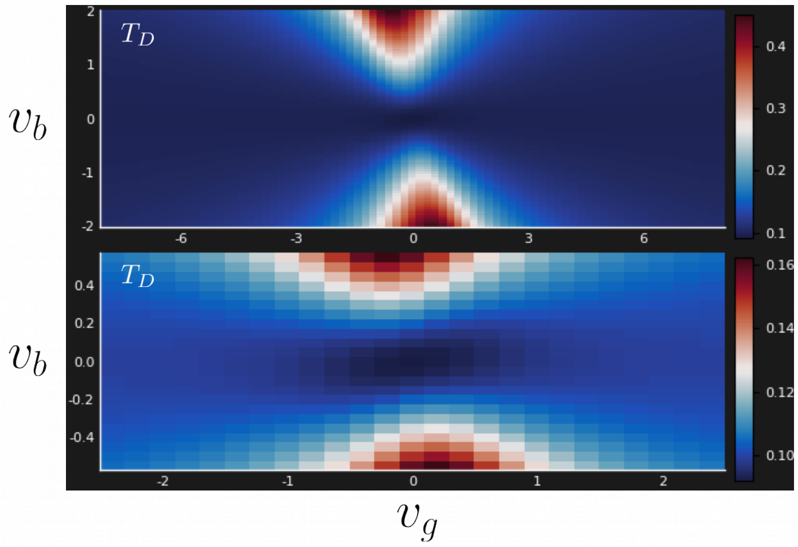
Leads at stationarity





$$\dot{Q}_H - \dot{Q}_{e-ph} - \dot{Q}_{QD} + \dot{Q}_J = 0$$

NEGF theory



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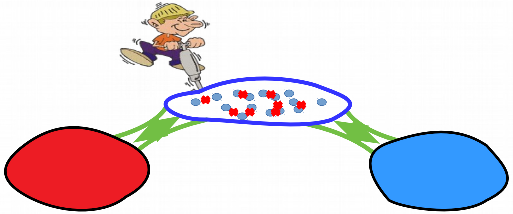
Summary

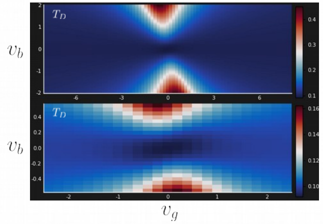
- NEGFs is a versatile tool to study transport in interacting systems



- Energy and particle currents are different

$$\Delta J_\alpha(t) = \sum_{\beta\neq\alpha} \int d\mathbf{x}_1 T_\beta(1) G_{\beta\alpha}(1;1^+) T^*_\alpha(1) \Big|_{z_1=t}$$

- Leads contain information too



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Computational facilities

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materiali, tecnologie e ricerca avanzata

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