Time-dependent Meir-Wingreen expression for energy current

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Outline

- Motivation
- Theoretical approach to quantum transport (NEGF)
- Derivation of the Energy Current
- Application and Results
- Conclusion

Motivation

How does the interaction influence the thermoelectric properties?

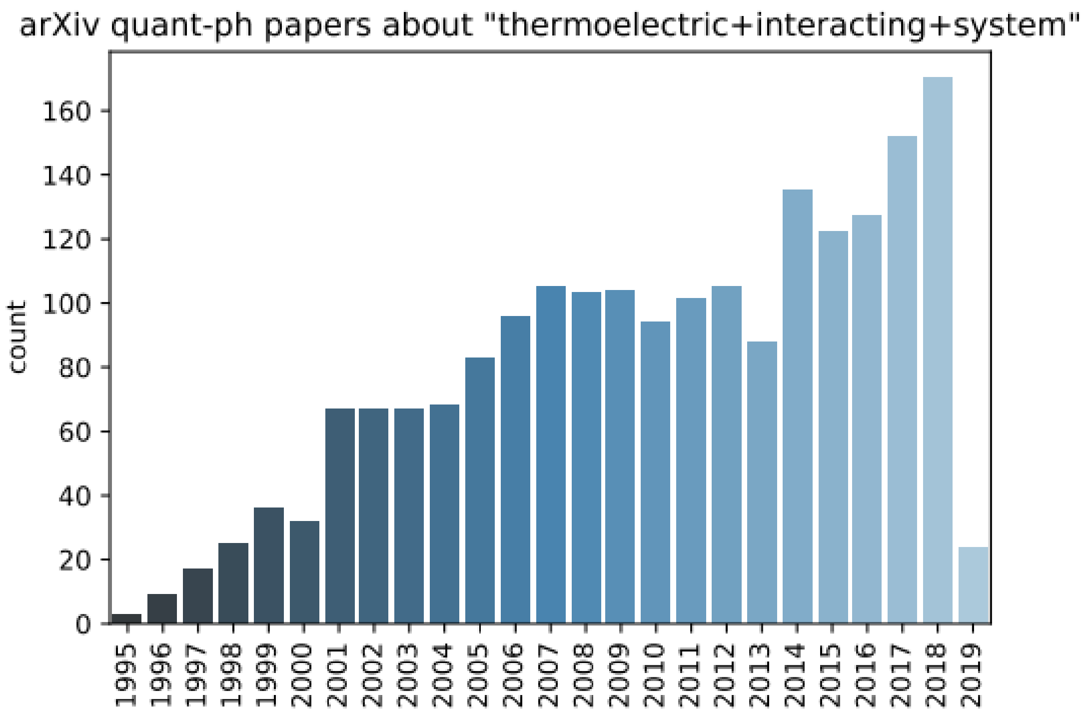
$$G(T,V) = \left.\frac{\partial I}{\partial V}\right|_{\Delta T=0}$$ **Electric Conductance**

$$K(T,V) = \left.\frac{\partial J}{\partial \Delta T}\right|_{I=0}$$ **Thermal Conductance**

Wiedemann-Franz Law

$$L(T,V) = \frac{K(T,V)}{TG(T,V)}$$

Violated!



Motivation

PHYSICAL REVIEW B **92**, 115402 (2015)

Time-dependent heat flow in interacting quantum conductors

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We derive the frequency-resolved heat current expression in the linear-response regime for a setup composed of a reservoir, an interacting central site, and a tunneling barrier under the action of a time-dependent electrical signal. We exploit the frequency parity properties of response functions to obtain the heat current expression for interacting quantum conductors. Importantly, the corresponding heat formula, valid for arbitrary ac frequencies, can describe photon-assisted heat transport. In particular, we analyze the heat transfer for an interacting multilevel conductor (a carbon nanotube quantum dot) coupled to a single reservoir. We show that the electrothermal admittance can reverse its sign by properly tuning the ac frequency.

DOI: 10.1103/PhysRevB.92.115402 PACS number(s): 72.10.Bg, 72.15.Jf, 73.63.Kv

Motivation

PHYSICAL REVIEW LETTERS **121,** 206801 (2018)

Thermoelectric Characterization of the Kondo Resonance in Nanowire Quantum Dots

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We experimentally verify hitherto untested theoretical predictions about the thermoelectric properties of Kondo correlated quantum dots (QDs). The specific conditions required for this study are obtained by using QDs epitaxially grown in nanowires, combined with a recently developed method for controlling and measuring temperature differences at the nanoscale. This makes it possible to obtain data of very high quality both below and above the Kondo temperature, and allows a quantitative comparison with theoretical predictions. Specifically, we verify that Kondo correlations can induce a polarity change of the thermoelectric current, which can be reversed either by increasing the temperature or by applying a magnetic field.

DOI: 10.1103/PhysRevLett.121.206801

NEGF (Closed System)

Consider the system…….

$$\hat{H}_C(z) = \underbrace{\int d\mathbf{x}_1 \, \hat{\psi}^\dagger(1) h(1) \hat{\psi}(1)}_{\text{One-body}} + \underbrace{\frac{1}{2}\int d1' d\mathbf{x}_1 \, \hat{\psi}^\dagger(1)\hat{\psi}^\dagger(1') v(1,1') \hat{\psi}(1')\hat{\psi}(1)}_{\text{Two-body (interacting)}}$$

Legend: $1 = (\mathbf{x}_1, z_1), \;\; \mathbf{x} = (\mathbf{r}, \sigma), \;\; z \in \gamma$

$$G(1,1') = -i \left\langle \mathcal{T}_\gamma \hat{\psi}(1) \hat{\psi}^\dagger(1') \right\rangle_0$$

Non-equilibrium Green's function

Contains information about **single particle quantities** such as density, momentum distribution, density-of-states, currents.

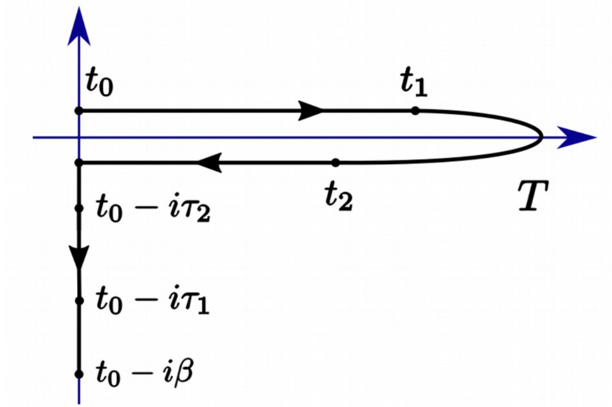


Fig. 1 The **Keldysh-Schwinger** contour γ

NEGF (Closed System)

The dynamics of the **1p-negf** is described by

$$G(1,1') = g(1,1') + i\int d\bar{1}d\bar{2}\; g(1,\bar{1})v(\bar{1},\bar{2})G_2(\bar{1},\bar{2},1',\bar{2}^+)$$

Non-interacting (Hartree-Fock)

2p-negf

$$G_2(1,2,3,4) = (-i)^2\langle\mathcal{T}_\gamma\hat{\psi}(1)\hat{\psi}(2)\hat{\psi}^\dagger(4)\hat{\psi}^\dagger(3)\rangle$$

Dyson Equation

Is the formal solution for the equation of the 1p-negf. The latter is part of a set of integro-differential equations (**Martin-Schwinger hierarchy**).

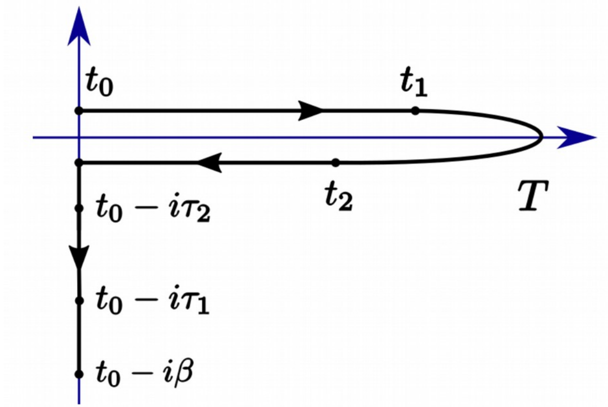


Fig. 1 The **Keldysh-Schwinger** contour γ

NEGF (Closed System)

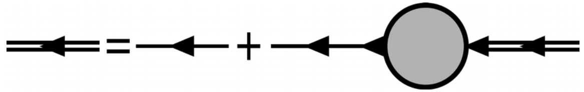
Truncation of the hierarchy (**many body perturbation theory**):

$$i\int d\bar{2}v(\bar{1},\bar{2})G_2(\bar{1},\bar{2},1',\bar{2}^+) = \int d\bar{2}\Sigma(\bar{1},\bar{2})G(\bar{2},1')$$

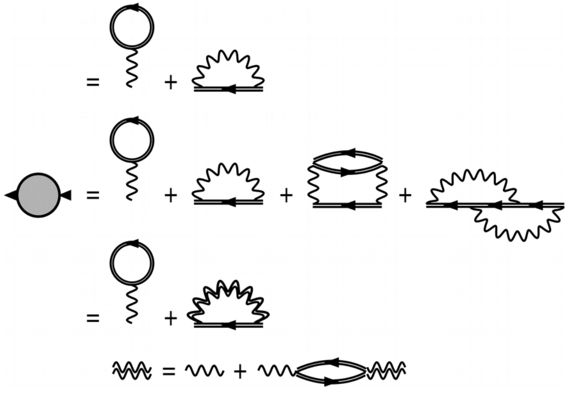
Self-Energy

Contains only necessary information about the **two-body interaction**

DE revisited $G(1,1') = g(1,1') + \int d\bar{1}d\bar{2}\; g(1,\bar{1})\Sigma(\bar{1},\bar{2})G(\bar{2},1')$



$\Sigma(G, v)$



Hartree-Fock

2^{nd} Born

GW

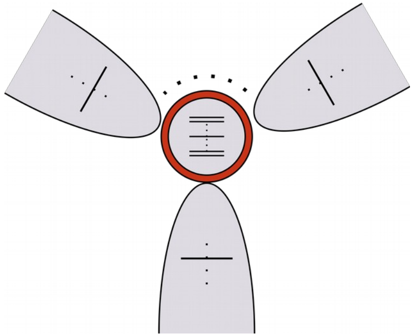
Conserving Approximation

Self consistent solution of DE

NEGF (Open System)

Now consider…….

$$\hat{H}(z) = \hat{H}_C(z) + \sum_{\alpha=1}^{N} \hat{H}_\alpha(z) + \hat{H}_T(z)$$



$$\hat{H}_\alpha(z) = \int d\mathbf{x}_1 \hat{\psi}^\dagger_\alpha(1) h_\alpha(1) \hat{\psi}_\alpha(1)$$

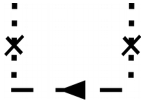
$$\hat{H}_T(z) = \int d\mathbf{x}_1 \left[\hat{\psi}^\dagger(1) T_\alpha(1) \hat{\psi}_\alpha(1) + h.c.\right]$$

How to include the effect of the **external baths** ?

Embedding self-energy

It is a correction to the **atomic levels** of the system due to the presence of **coupling** with the baths

$$\Sigma_{em}(1,1') = \sum_\alpha T_\alpha(1) g_\alpha(1,1') T_\alpha(1')$$



DE revisited v2

$$G(1,1') = g(1,1') + \int d\bar{1} d\bar{2}\; g(1,\bar{1})[\Sigma(\bar{1},\bar{2}) + \Sigma_{em}(\bar{1},\bar{2})]G(\bar{2},1')$$

Energy-Current

The **energy-current** through the interacting region is.....

$$\mathcal{J}(z) \equiv \frac{d}{dz}\langle \hat{H}_C(z)\rangle = i\langle[\hat{H}(z), \hat{H}_C(z)]\rangle$$

⋮ Lengthy algebra

$$\mathcal{J}(z) = \sum_\alpha \left[2Re\left\{ \int d\mathbf{x}_1 h(1) T^*(1^+) G^{C\alpha}(1,1^+) \right\} + 2Re\left\{ i \int d\mathbf{x}_1 d\bar{1} v(1,\bar{1}) T^*(\bar{1}^+) G_2^{CCC\alpha}(\bar{1},1;1^+,\bar{1}^+) \right\} \right]$$

1p and 2p mixed **Green's functions**

$$G^{C\alpha}(1,1') = -i\langle \mathcal{T}_\gamma \hat{\psi}(1)\hat{\psi}^\dagger_\alpha(1')\rangle \qquad G_2^{CCC\alpha}(1,2,3,4) = (-i)^2\langle \mathcal{T}_\gamma \hat{\psi}(1)\hat{\psi}(2)\hat{\psi}^\dagger_\alpha(4)\hat{\psi}^\dagger(3)\rangle$$

Using the S-matrix expansion in the int. picture of the tunneling Hamiltonian and Wick's Theorem for the bath-operators

$$G^{C\alpha}(1,1') = \int d\bar{1} G(1,\bar{1}) T(\bar{1}) g_\alpha(\bar{1},1') \qquad G_2^{CCC\alpha}(1,2,3,4) = \int d\bar{1} G_2(1,2,3,\bar{1}) T(\bar{1}) g_\alpha(\bar{1},4)$$

Energy-Current

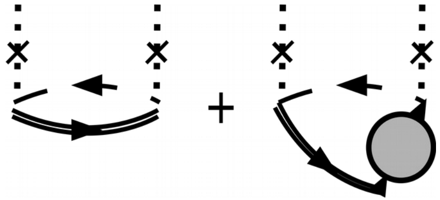
$$\mathcal{J}(z) = \sum_{\alpha}\left[2Re\left\{\int d\mathbf{x}_1 d\bar{1} h(1)G(1,\bar{1})\Sigma_\alpha(\bar{1},1^+)\right\} + 2Re\left\{-i\int d\mathbf{x}_1 d\bar{1}d\bar{2}v(1,\bar{1})G_2(1,\bar{1},\bar{2},1^+)\Sigma_\alpha(\bar{2},\bar{1}^+)\right\}\right]$$

Recall the **MBPT** assumption for the **2p-negf** and **self-energy**.....

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

Time-dependent Meir-Wingreen expression for energy current

First term: the transport of the **single-particle energy.**
Second term: transport of the energy stored in the **particle-particle interaction**



Energy-Current

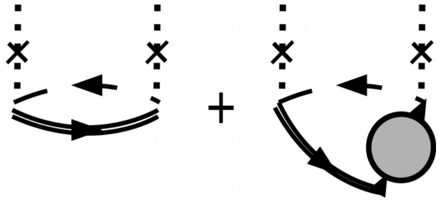
On the conservation of **energy…….**

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

$$\frac{d\mathcal{E}}{dz} = \frac{d}{dz} \langle \hat{H}_C(z) \rangle = \frac{d}{dz} \left[i \int d\mathbf{x}_1 d\bar{1} \left(h(1)\delta(1,\bar{1}) + \frac{1}{2}\Sigma(1,\bar{1}) \right) G(\bar{1},1^{+}) \right]$$

Conservation of energy

The sum of the currents that flow into the baths has to be equal to the time derivative of the **total energy** of the interacting system



Applications (Single Impurity Anderson Model)

"Examples are like cans of over-strength lager.
One is both too many and never enough."

$$\hat{H} = \sum_{\sigma} \varepsilon_\sigma \hat{d}^\dagger_\sigma \hat{d}_\sigma + U \hat{d}^\dagger_\uparrow \hat{d}_\uparrow \hat{d}^\dagger_\downarrow \hat{d}_\downarrow + \sum_{\alpha,k\sigma} (\varepsilon_{\alpha k\sigma} + \mu_\alpha) \hat{c}^\dagger_{\alpha k\sigma} \hat{c}_{\alpha k\sigma} - g \sum_{\alpha,k\sigma} (\hat{c}_{\alpha k\sigma} \hat{d}^\dagger_\sigma + h.c.)$$

System

U charging energy

$v_g = \varepsilon + U/2$ gate voltage

2-Terminals $\alpha = L, R$

Fermionic reservoir in local thermodynamic equilibrium

$$f_\alpha(\varepsilon_k) = [1 + e^{(\varepsilon_k - \mu_\alpha)/k_B T_\alpha}]^{-1}$$

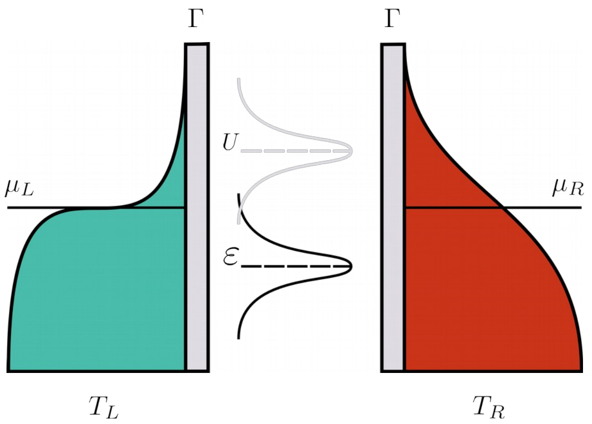
$$\mu = \mu_L = \mu_R = 0$$

$$\Delta T = T_L - T_R \neq 0$$

Flat density of states (WBLA)

Hybridization

$$\Gamma = |g|^2$$



Applications (SIAM)

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

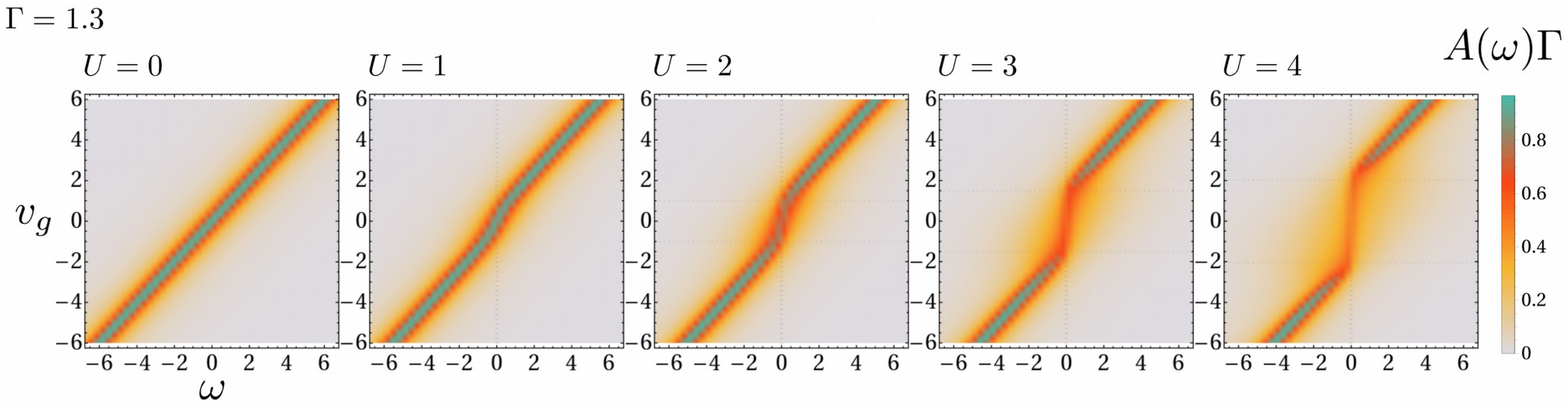
$U/\Gamma \gg 1$ Strong **Coulomb** correlations

$$T \ll T_K \propto \sqrt{2\Gamma U} exp[\varepsilon(\varepsilon + U)/(2\Gamma U)]$$

Kondo temperature

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

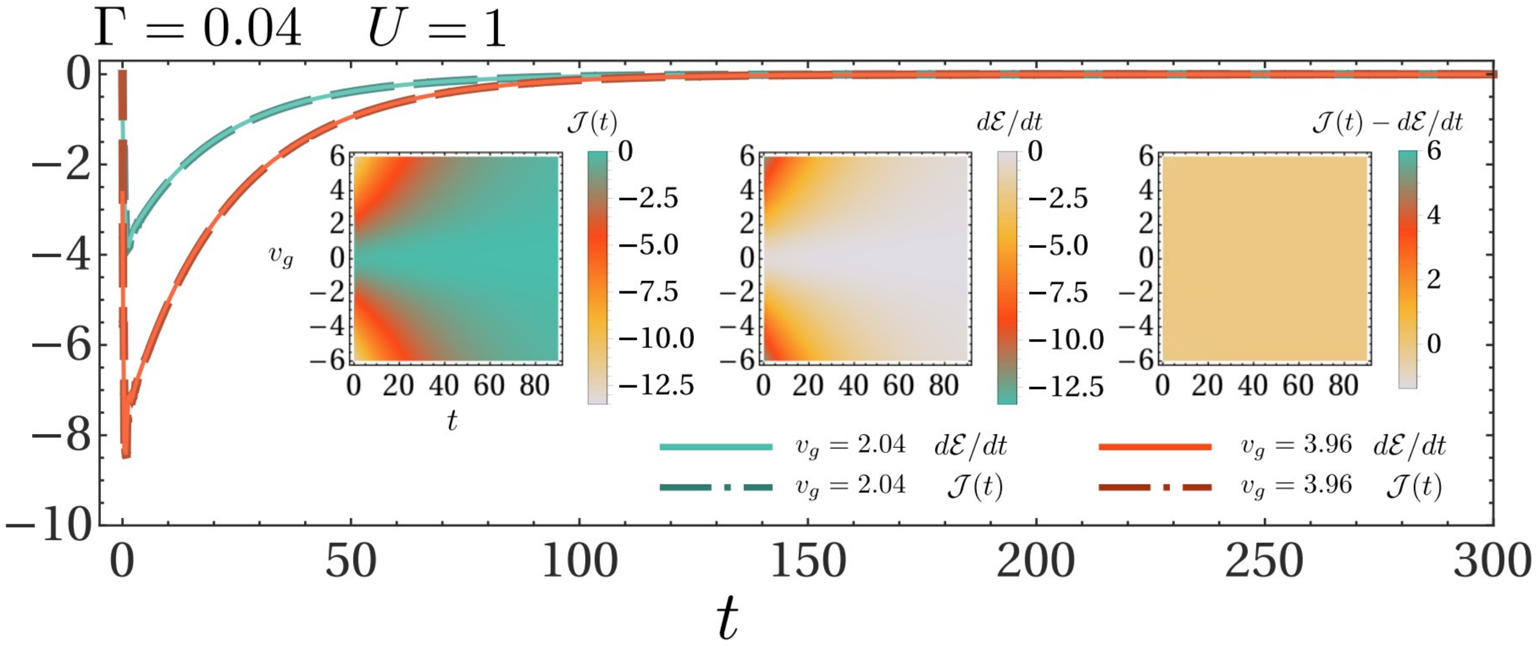
$$A(\omega) = i[G^R(\omega) - G^A(\omega)]$$



Results (SIAM)

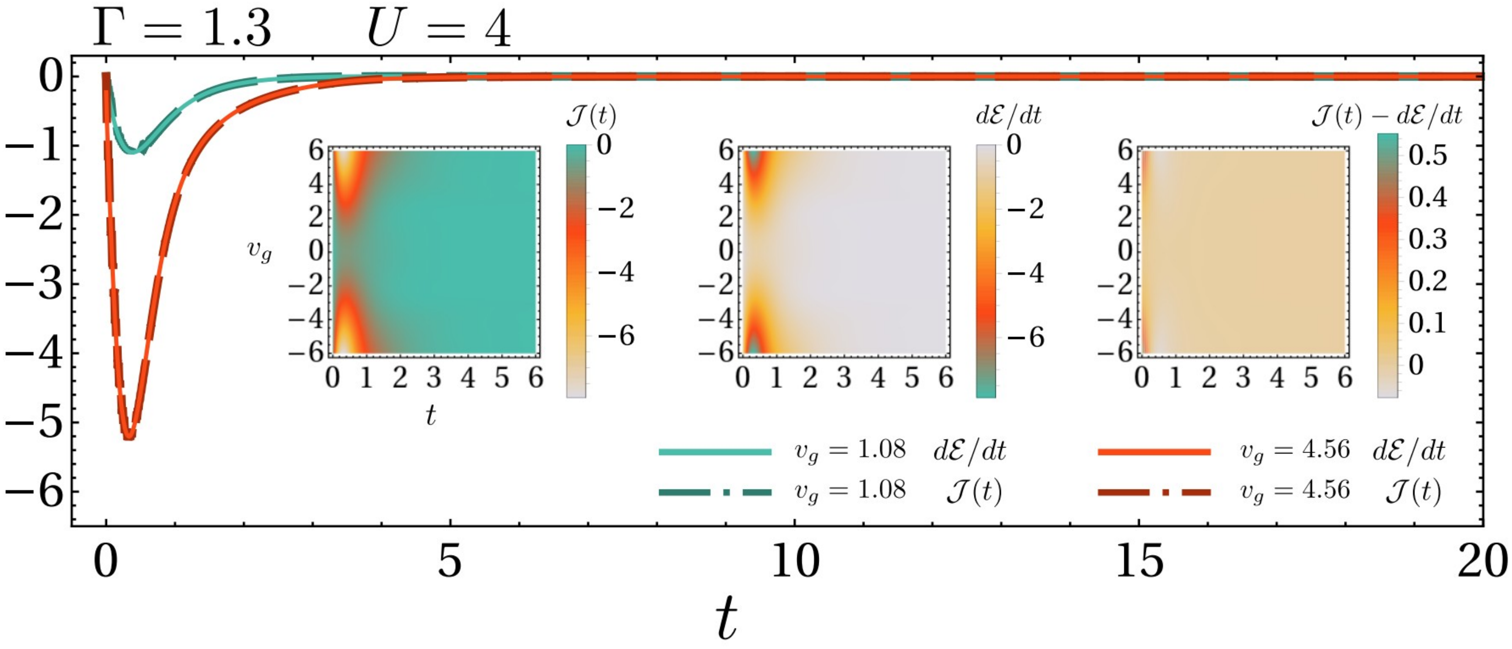
GW conserving approximation → Guarantees that the macroscopic conservation laws are satisfied and automatically built into the **MBPT**

Weak coupling



Results (SIAM)

Strong coupling



Results (SIAM)

Comparison with standard results…….

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

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

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

$$t \rightarrow \infty$$

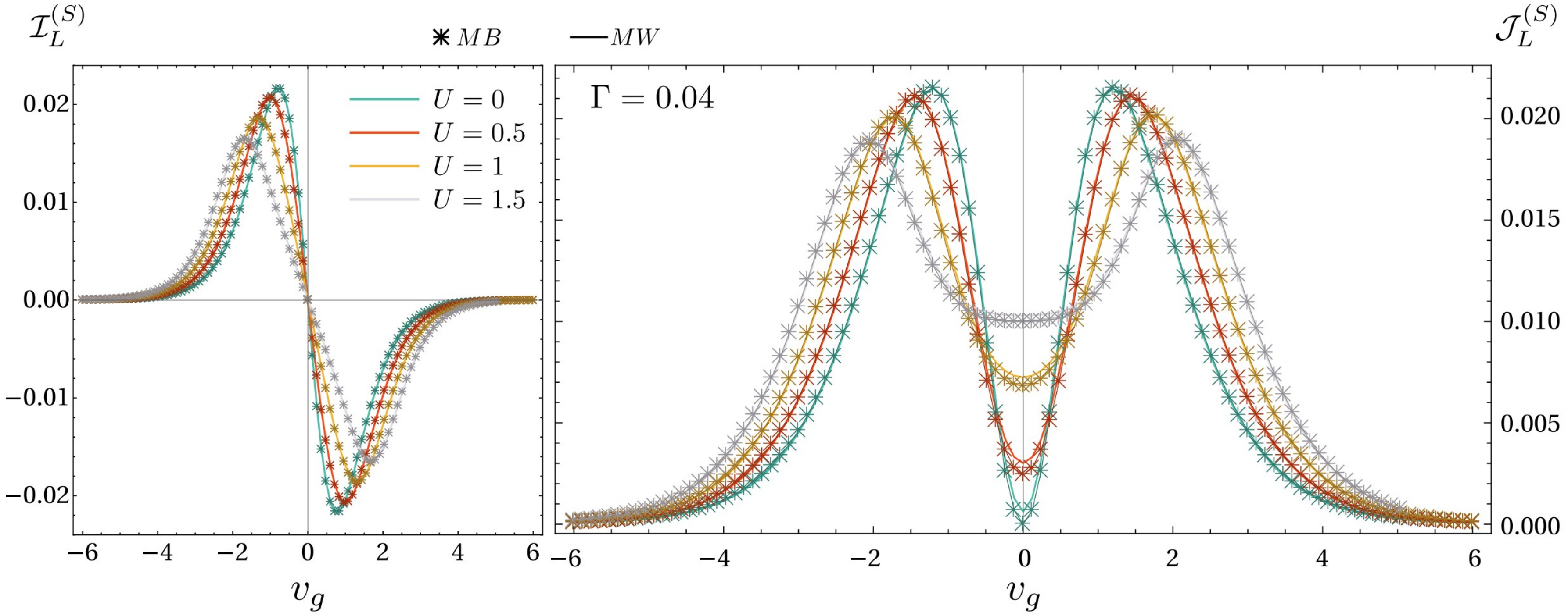
$$\mathcal{I}_\alpha^{(S)} = \int d\omega\Gamma(\omega)[f_\alpha(\omega) - f_{\bar{\alpha}}(\omega)]A(\omega)$$

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

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

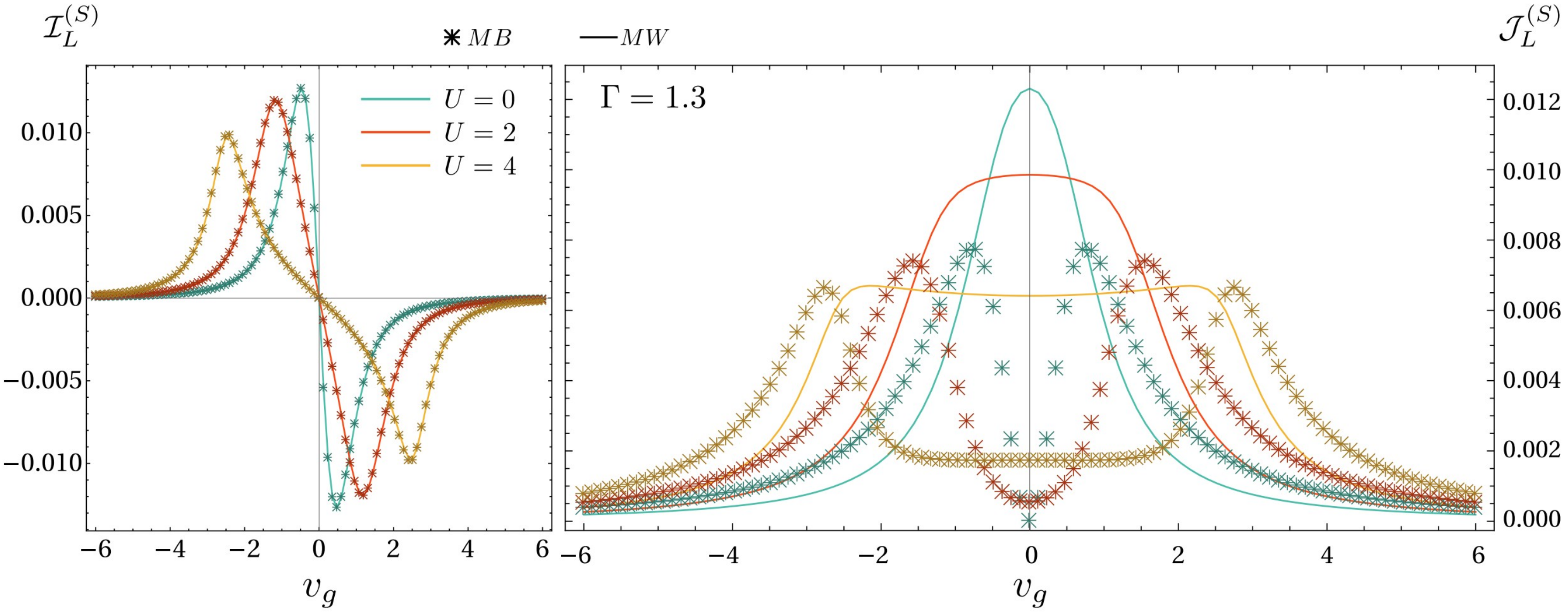
Time-independent **steady-state** values of the particle and energy currents:
Meir-Wingreen formula

Weak coupling



Results (SIAM)

Strong coupling



Results

Why does this happen??

$$0 \equiv \frac{d}{dz}\langle \hat{H}(z)\rangle \rightarrow \frac{d}{dz}\langle \hat{H}_C(z)\rangle = -\sum_\alpha \frac{d}{dz}\langle \hat{H}_\alpha(z)\rangle - \frac{d}{dz}\langle \hat{H}_T(z)\rangle$$

total energy balance equation

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

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

The derivation of “MW” formula for the energy current doesn’t take into account the **tunneling Hamiltonian**

$$\lim_{t\to\infty} \mathcal{J}_\alpha(t) = \mathcal{J}_\alpha^{(S)} \longrightarrow \hat{H}_T \rightarrow 0$$

weak coupling regime

Summary and Conclusion

- We've derived a time-dependent expression for the **energy-current** within the **NEGF** and **MBPT**
- We've seen that, if computed from a **conserving self-energy** approx., the energy-current is a conserved quantity at any time
- We can now explore regimes (**strong coupling** and **correlations)** where the standard techniques fail to capture some physical features
- We can characterize extensively the **thermoelectric** properties in such regimes

Thank you
for your attention !

S-Matrix Expansion

Interaction picture of the tunneling Hamiltonian

$$\hat{H}_T(z) = \int d\mathbf{x}_1 \left[\hat{\psi}^\dagger(1)T_\alpha(1)\hat{\psi}_\alpha(1) + h.c.\right]$$

$$G_{C\alpha}(1,1') = -i\left\langle \mathcal{T}_\gamma \hat{\psi}(1)\hat{\psi}_\alpha^\dagger(1')\right\rangle = -i\left\langle \mathcal{T}_\gamma \tilde{\psi}(1)\tilde{\psi}_\alpha^\dagger(1')S\right\rangle$$

S-matrix $$S = \sum_{k=0}^{\infty}\frac{(-i)^k}{k!}\int_\gamma d\bar{z}_1 \cdots \int_\gamma d\bar{z}_k \tilde{H}_T(\bar{1})\ldots\tilde{H}_T(\bar{k})$$

$$G_{C\alpha}(1,1') = \sum_\alpha -i\left\langle \mathcal{T}_\gamma \tilde{\psi}(1)\tilde{\psi}_\alpha^\dagger(1')\sum_{k=0}^{\infty}\frac{(-i)^k}{k!}\int_\gamma\int d\bar{z}_1 d\bar{\mathbf{x}}_1\left(\tilde{\psi}^\dagger(\bar{1})T(\bar{1})\tilde{\psi}_\alpha(\bar{1}) + h.c.\right)\times\cdots\times\int_\gamma d\bar{z}_k\tilde{H}_T(\bar{k})\right\rangle =$$

Wick's Theorem for the bath-operators

$$= \sum_\alpha\int_\gamma\int d\bar{z}_1 d\bar{\mathbf{x}}_1\sum_{k=0}^{\infty}\frac{(-i)^k}{k!}(-i)\left\langle \mathcal{T}_\gamma\tilde{\psi}_\alpha(\bar{1})\tilde{\psi}_\alpha^\dagger(1')\right\rangle T(\bar{1})\left\langle \mathcal{T}_\gamma\tilde{\psi}(1)\tilde{\psi}^\dagger(\bar{1})\times\cdots\times\int_\gamma d\bar{z}_k\tilde{H}_T(\bar{k})\right\rangle + (\text{remaining } k-1 \text{ terms})$$

$$= \sum_\alpha\int_\gamma\int d\bar{1}(-i)\left\langle \mathcal{T}_\gamma\sum_{k=0}^{\infty}\frac{(-i)^{k-1}}{(k-1)!}\tilde{\psi}(1)\tilde{\psi}^\dagger(\bar{1})\times\cdots\times\int_\gamma dz_k\tilde{H}_T(\bar{k})\right\rangle T(\bar{1})(-i)\left\langle \mathcal{T}_\gamma\tilde{\psi}_\alpha(\bar{1})\tilde{\psi}_\alpha^\dagger(1')\right\rangle$$

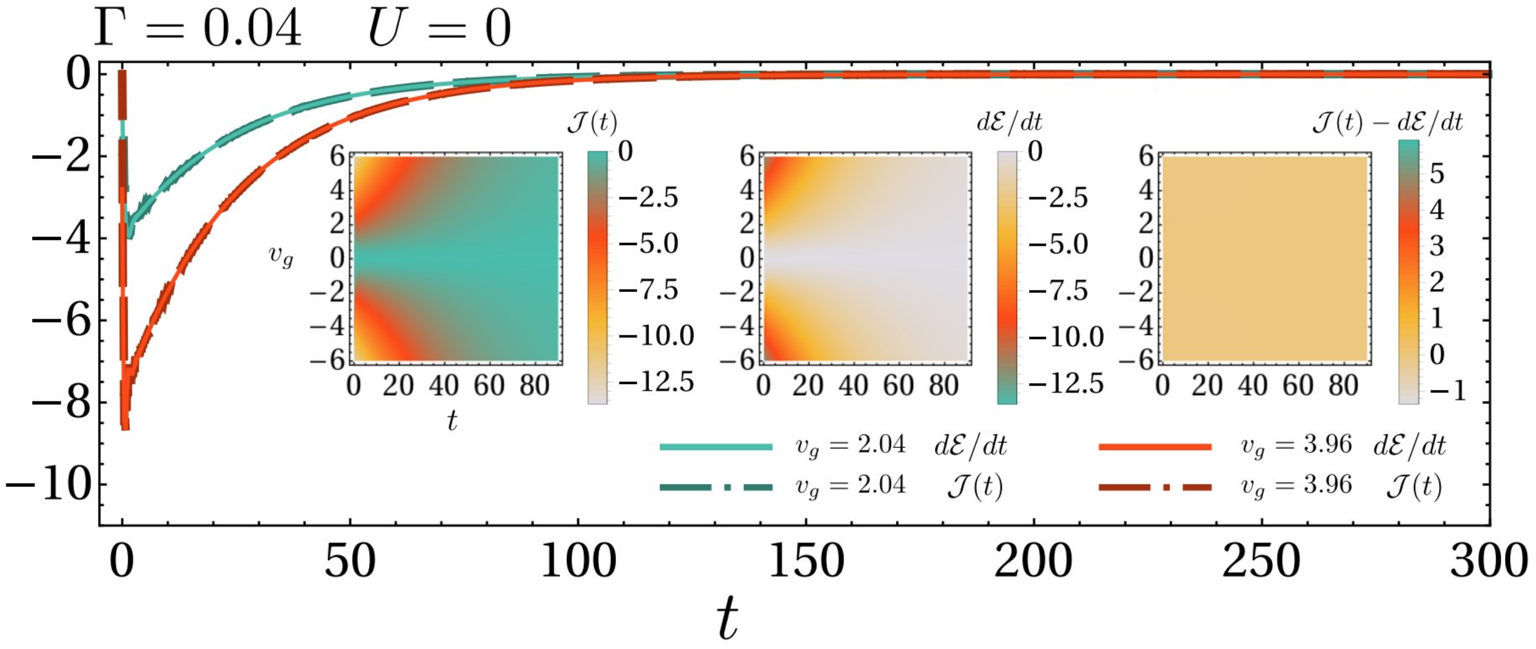
$$= \sum_\alpha\int_\gamma\int d\bar{1}\; G(1,\bar{1})T(\bar{1})g_{\alpha\alpha}(\bar{1},1')$$

A.-P. Jauho, N.S. Wingreen and Y. Meir, Phys. Rev. B 50, 5528 (1994)

Results (SIAM)

GW conserving approximation → Guarantees that the macroscopic conservation laws are satisfied and automatically built into the **MBPT**

Weak coupling



Results (SIAM)

Strong coupling