Unraveling Heat and Charge Transport in Time-Periodic Temperature Driven Interacting Nanoconductors

Minchul Lee

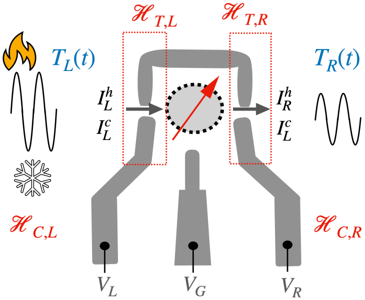
Kyung Hee University, Korea

i-Link Workshop, IFISC, UIB-CSIC
Jun 6, 2023

Collaborators

Rosa Lopéz (UIB-CSIC) and Pascal Simon (Universite Paris-Saclay)

Nanoconductors driven periodically by time-dependent temperature



Objectives

- to adapt the Luttinger's trick to deal with the time-dependent temperature
- to formulate the general forms of the charge and heat currents in terms of QD Green's functions

Temperature-driven systems

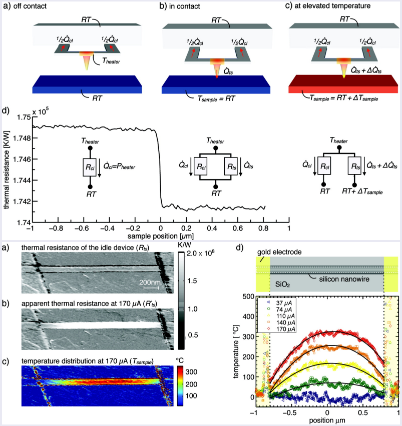
- limitation of Landuauer-Büttiker (LB) formalism

$$I_\alpha = \sum_{\alpha'} \int \frac{d\epsilon}{2\pi\hbar} T_{\alpha\alpha'}(\epsilon)(f_\alpha(\epsilon) - f_{\alpha'}(\epsilon))$$

  - the leads are assumed to be in (local) equilibrium with well-defined temperatures, even though the leads are connected with each other
  - the only place where the different temperatures of the leads enter is in the occupation factor
  - the LB formalism is not adequate for the case where the temperatures at the nanoscale vary in time and space (time scales shorter than the typical equilibrium time)
  - even the Meir-Wingreen formalism, overcoming the mean-field nature of the LB formalism, treats the temperature as a static thermodynamic variable.
- how to convert the temperature, originally defined as a statistical parameter governing the equilibrium of energy exchanges between macroscopic systems, into a dynamical field coupling to mechanical degrees of freedom driven strongly out of equilibrium?

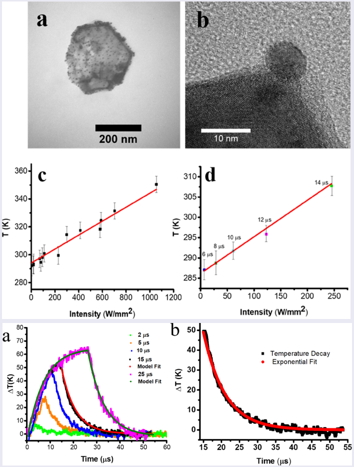
Spatial and temporal resolution of temperature measurement

Scanning thermal microscopy



Menges, Riel, Stemmer, and Gotsmann (2012)

Time-resolved measurement



upconverting nanoparticles
($NaYF_4$:Yb^{3+}:Er^{3+})

Rafiei Miandashti et al. (2019)

Luttinger's Trick

PHYSICAL REVIEW VOLUME 135, NUMBER 6A 14 SEPTEMBER 1964

Theory of Thermal Transport Coefficients*

J. M. LUTTINGER
Department of Physics, Columbia University, New York, New York
(Received 20 April 1964)

A simple proof of the usual correlation-function expressions for the thermal transport coefficients in a resistive medium is given. This proof only requires the assumption that the phenomenological equations in the usual form exist. It is a "mechanical" derivation in the same sense that Kubo's derivation of the expression for the electrical conductivity is. That is, a purely Hamiltonian formalism with external fields is used, and one never has to make any statements about the nature or existence of a local equilibrium distribution function, or how fluctuations regress. For completeness the analogous formulas for the viscosity coefficients and the heat conductivity of a simple fluid are given.

- a space- and time-varying field $\psi(\mathbf{r},t)$ coupled to the energy density

$$\int d^3r\, h(\mathbf{r})\psi(\mathbf{r},t)$$

$\psi(\mathbf{r},t)$ = "gravitational field" (similarity to Einstein's theory of gravity, only in a purely formal sense)
cf) the electric coupling

$$\int d^3r\, \rho(\mathbf{r})\phi(\mathbf{r},t)$$

Luttinger's Trick (cont.)

- electric and energy transport in the linear response regime

$$j^c_\alpha(\mathbf{r}) = L^{(1)}_{\alpha\gamma}\left(E_\gamma - \frac{1}{e}T\nabla_\gamma\left(\frac{\mu}{T}\right)\right) + L^{(2)}_{\alpha\gamma}\left(T\nabla_\gamma\left(\frac{1}{T}\right) - \nabla_\gamma\psi\right)$$
$$j^h_\alpha(\mathbf{r}) = L^{(3)}_{\alpha\gamma}\left(E_\gamma - \frac{1}{e}T\nabla_\gamma\left(\frac{\mu}{T}\right)\right) + L^{(4)}_{\alpha\gamma}\left(T\nabla_\gamma\left(\frac{1}{T}\right) - \nabla_\gamma\psi\right)$$

  where $L^{(i)}$ are the Kubo-formula coefficients.
- thermal analogs of the Einstein relationship: in equilibrium

$$\mathbf{E} = \frac{1}{e}T\nabla_\gamma\left(\frac{\mu}{T}\right) \quad \text{and} \quad \nabla_\gamma\psi = -\frac{\nabla_\gamma T}{T}$$

- dynamical response to $\psi(\mathbf{r}, t)$ = response to (slowly varying) temperature gradient
- extend the concept of thermal response to situations in which the traditional notion of temperature is no longer meaningful
- the gradient of the gravitational field drives the electric/thermal current, just as the gradient of the electric potential drives the electric/thermal current.
- Luttinger's trick requires only the assumption that the phenomenological equations relating the gradient of fields and the corresponing current exist.
  - » ultimately, the validity of the Luttinger's trick should be verified in experiments

Thermal vector potential theory: bulk case

- electric analog

$$\mathbf{j} = \frac{e}{m}\langle \mathbf{p} \rangle - \frac{e^2}{m} n_e \mathbf{A} = (\text{paramagnetic current}) + (\text{diamagnetic current})$$

  - in equilibrium, the two contributions cancel each other.
  - gauge invariance

- thermal case: Using the energy conservation law

$$\partial_t h(\mathbf{r},t) + \nabla \cdot \mathbf{j}^h(\mathbf{r},t) = 0 \quad \text{and} \quad \nabla \Psi = -\nabla T/T$$

one finds

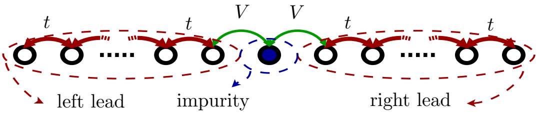
$$\int d^3r\, h(\mathbf{r})\Psi(\mathbf{r},t) = -\int d^3r\, \mathbf{j}^h(\mathbf{r},t) \cdot \mathbf{A}_T(\mathbf{r},t)$$

with

$$\partial_t \mathbf{A}_T = -\frac{\nabla T}{T} \quad \left(\text{more generally, } \nabla\psi + \partial_t \mathbf{A}_T = -\frac{\nabla T}{T}\right)$$

→ elimination of $T = 0$ divergence, incorporation of magnetic currents

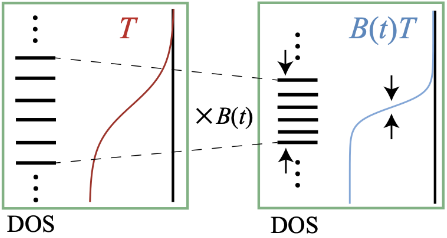
Tatara (2015)



- steady-state behavior: at $t = t_0$, the gravitaional field ψ_α is turned on, or $T \to T_\alpha$
- change of temperature = scaling of lead dispersion

$$\sum_k \epsilon_{\alpha k} a^\dagger_{\alpha k} a_{\alpha k} \to \sum_k \tilde{\epsilon}_{\alpha k} a^\dagger_{\alpha k} a_{\alpha k} = \sum_k (1 + \psi_\alpha)(\epsilon_{\alpha k} + U_\alpha) a^\dagger_{\alpha k} a_{\alpha k}$$

Eich, Principi, Ventra, and Vignale (2014)



$$B(t) = 1 + \psi_\alpha(t)$$

Luttinger-field approach: nanoscale conductors (cont.)

- gravitational field and temperature
  - initially ($t = -\infty$), at equilibrium at (base) temperature T

$$\sum_k f\left(\frac{\epsilon_{\alpha k}}{k_B T}\right) F(\epsilon_{\alpha k})$$

  - rescaling of contact energy: $\epsilon_{\alpha k} \to (1+\psi_\alpha(t))\epsilon_{\alpha k}$

$$\begin{aligned}\sum_k f\left(\frac{\epsilon_{\alpha k}}{k_B T}\right) F(\epsilon_{\alpha k}) &\to \sum_k f\left(\frac{\epsilon_{\alpha k}}{k_B T}\right) F(\epsilon_{\alpha k} \to (1+\psi_\alpha)\epsilon_{\alpha k}) \\ &= \sum_k f\left(\frac{(1+\psi_\alpha)\epsilon_{\alpha k}}{k_B (1+\psi_\alpha) T}\right) F((1+\psi_\alpha)\epsilon_{\alpha k}) \\ &= \sum_k f\left(\frac{\tilde{\epsilon}_{\alpha k}}{k_B T_\alpha}\right) F(\tilde{\epsilon}_{\alpha k})\end{aligned}$$

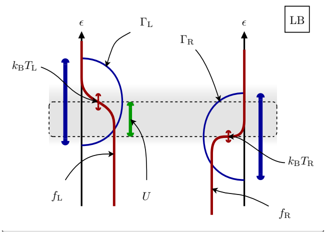
$\to T_\alpha = (1+\psi_\alpha)T$

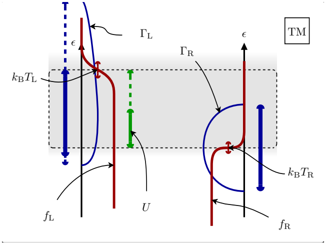
Luttinger-field approach: nanoscale conductors (cont.)

- two differences between LB and Luttinger formalism
  - occupation factors: $T_\alpha = T(1+\psi_\alpha)$

$$f_\alpha^{\rm Luttiner}(\epsilon) = \left\{ \exp\left[\frac{\frac{\epsilon}{1+\psi_\alpha} - U_\alpha}{k_B T} \right] + 1 \right\}^{-1} \text{ vs } f_\alpha^{\rm LB}(\epsilon) = \left\{ \exp\left[\frac{\epsilon - U_\alpha}{k_B T_\alpha} \right] + 1 \right\}^{-1}$$

  - in the linear response regime, both formalisms give rise to the same result.
  - beyond the linear response regime,
    1. $U_\alpha \to (1+\psi_\alpha)U_\alpha$
    2. in the Luttinger's trick, the transmission function $T_{\alpha\beta}(\epsilon)$ also depends on ψ_α

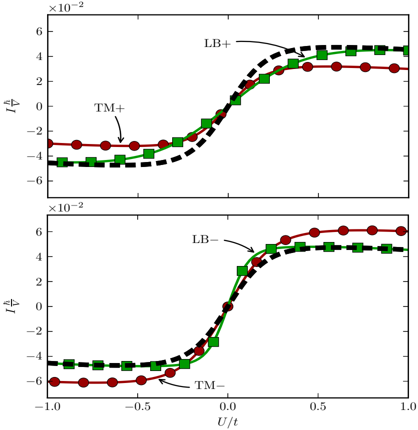




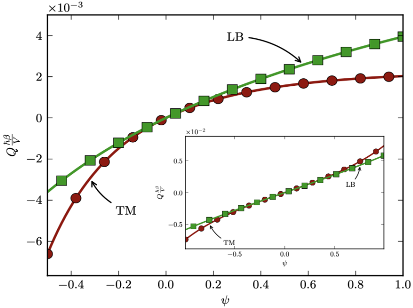
Eich, Principi, Ventra, and Vignale (2014)

Non-linear response

$$\psi_{\mathrm{L}} = \delta T/T = 1$$



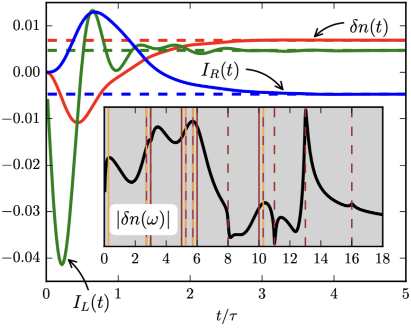
$$\psi_{\mathrm{L}} = \delta T/T = -0.5$$



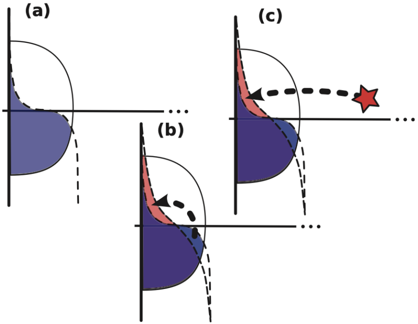
$$U_{\mathrm{L}} - U_{\mathrm{R}} = 0$$
$$\psi = \psi_{\mathrm{L}} - \psi_{\mathrm{R}}$$

Eich, Principi, Ventra, and Vignale (2014)

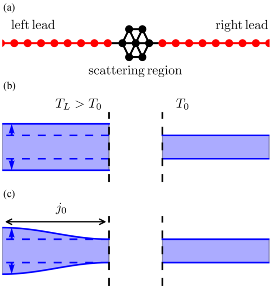
Transient behaviors

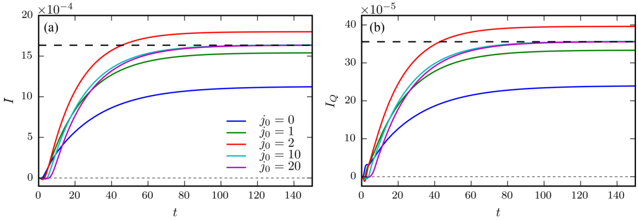


$$\psi_{\rm L} = \delta T/T \to 1$$



Eich, Ventra, and Vignale (2016)

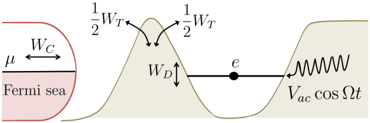




- abrupt spatial change in ψ at the interface
  $\rightarrow$ the addtional scattering
  $\rightarrow$ discrepancy in the steady-state current (in the non-linear regime) and the initial oscillation
- gradual transition of the Luttinger field

Lozej and Rejec (2018)

Dynamic energy transfer in ac-driven quantum systems



- tight-binding model – energy is stored in the barrier

$$\mathcal{H}_{\rm T}$$

- charge flux

$$0 = \frac{d\mathcal{N}}{dt} = J_C(t) + J_D(t), \quad J_i(t) = \frac{i}{\hbar}\langle[\mathcal{H},\mathcal{N}_i]\rangle \ (i = C, D)$$

- energy flux

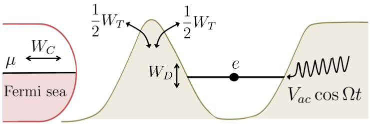
$$\left\langle \frac{d\mathcal{H}}{dt} \right\rangle = \underbrace{W_C(t) + W_T(t) + W_D(t)}_{=0} + \left\langle \frac{\partial\mathcal{H}}{\partial t} \right\rangle, \quad W_i(t) = \frac{i}{\hbar}\langle[\mathcal{H},\mathcal{H}_i]\rangle \ (i = C, T, D)$$

— energy reactance $W_T(t) \neq 0$ $(\overline{W_T} = 0)$

- what is correct definition of energy flux and heat current into the reservoir in the time domain ?

Ludovico, Lim, Moskalets, Arrachea, and Sánchez (2014)

Dynamic energy transfer in ac-driven quantum systems (cont.)



- time-dependent scattering-matrix formalism + Green's function

$$W_E(t) = \frac{\hbar}{4mi}\left[\Psi^*\mathcal{H}\nabla\Psi - \nabla\Psi^*\mathcal{H}\Psi + (h.c)\right]$$

$$= \sum_{n,q} e^{-in\Omega t}\int d\epsilon \frac{\epsilon_q + \epsilon_{n+q}}{2h} S^*(\epsilon_q,\epsilon)S(\epsilon_{n+q},\epsilon)[f(\epsilon_q) - f(\epsilon)] \quad (\epsilon_n = \epsilon + n\hbar\Omega)$$

$\leftarrow$ Fisher-Lee relation ($S \leftrightarrow \mathcal{G}$)

$$= W_C(t) + \frac{1}{2}W_T(t)$$

and

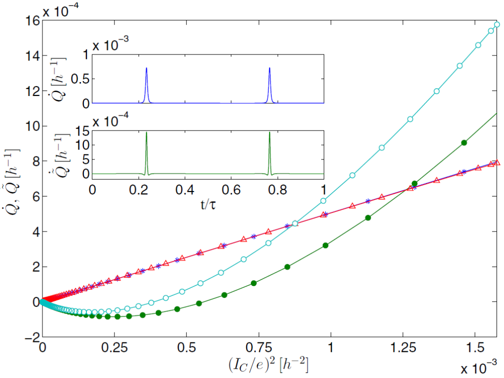
$$I^h \equiv \dot{Q}(t) = W_E(t) - \mu I_C(t)/e$$

Ludovico, Lim, Moskalets, Arrachea, and Sánchez (2014)

Dynamic energy transfer in ac-driven quantum systems (cont.)

- satisfying 2^{nd} law of thermodynamics: for ac current in the adiabatic limit

$$\dot{Q}(t) = W_C(t) + \frac{1}{2}W_T(t) - \mu I_C(t)/e \quad \text{vs} \quad \dot{\tilde{Q}}(t) = W_C(t) - \mu I_C(t)/e$$



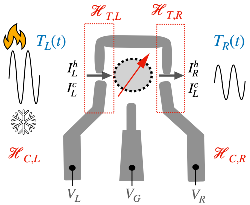
$$\dot{Q}(t) = P = R_q[I_C(t)]^2 \qquad (R_q = R_Q/2 = h/2e^2)$$

Ludovico, Lim, Moskalets, Arrachea, and Sánchez (2014)

Nanoconductor under time-periodic temperature driving: Luttinger’s trick

- unperturbed system: $\ell = \mathrm{L}, \mathrm{R}$

$$\mathcal{H}_{\mathrm{C}} = \sum_{\ell} \mathcal{H}_{\mathrm{C}\ell} = \sum_{\ell} \sum_{\mathbf{k}\sigma} \epsilon_{\ell\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$$
$$\mathcal{H}_{\mathrm{D}} = \sum_{\sigma} \epsilon_{\sigma} d^{\dagger}_{\sigma} d_{\sigma} + U(n_{\uparrow}, n_{\downarrow})$$
$$\mathcal{H}_{\mathrm{T}} = \sum_{\ell} \mathcal{H}_{\mathrm{T}\ell} = \sum_{\ell} \sum_{\mathbf{k}\sigma} \left(t_{\ell\mathbf{k}} d^{\dagger}_{\sigma} c_{\mathbf{k}\sigma} + (h.c.) \right)$$



- dot-contact coupling

$$\Gamma_{\ell} \equiv \frac{\pi \rho_0 |t_{\ell}|^2}{\hbar} \quad \text{and} \quad \Gamma \equiv \sum_{\ell} \Gamma_{\ell}$$

- Luttinger’s trick: gravitational field $\Psi_{\ell}(t)$ coupled to *excess energy*

$$\mathcal{H}_{\mathrm{G}}(t) = \sum_{\ell} \Psi_{\ell}(t) \left(\mathcal{H}_{\mathrm{C}\ell} + \lambda \mathcal{H}_{\mathrm{T}\ell} - \langle \mathcal{H}_{\mathrm{C}\ell} + \lambda \mathcal{H}_{\mathrm{T}\ell} \rangle_0 \right)$$

with

$$\lambda = \frac{1}{2} \quad \text{and} \quad \Psi_{\ell}(t) = \Psi_{\ell} \cos \Omega t \quad (\tau = 2\pi/\Omega)$$

- Contacts at the base temperature T: $f_{\ell}(\omega) = f(\omega)$

Nanoconductor under time-periodic temperature driving: Luttinger's trick

- Total Hamiltonian

$$\begin{aligned}\mathcal{H} &= \mathcal{H}_{\mathrm{C}} + \mathcal{H}_{\mathrm{D}} + \mathcal{H}_{\mathrm{T}} + \mathcal{H}_{\mathrm{G}}(t) \\ &= \mathcal{H}_{\mathrm{C},\Psi}(t) + \mathcal{H}_{\mathrm{D}} + \mathcal{H}_{\mathrm{T},\Psi}(t)\end{aligned}$$

with

$$\begin{aligned}\mathcal{H}_{\mathrm{C},\Psi}(t) &\equiv \sum_\ell \mathcal{H}_{\mathrm{C}\ell,\Psi}(t) = \sum_\ell \left[\mathcal{H}_{\mathrm{C}\ell} + \Psi_\ell(t)(\mathcal{H}_{\mathrm{C}\ell} - \langle \mathcal{H}_{\mathrm{C}\ell}\rangle_0)\right] \\ &= \sum_\ell \underbrace{(1+\Psi_\ell(t))\epsilon_{\ell\mathbf{k}}}_{=\,\epsilon_{\ell\mathbf{k}}(t)} c^\dagger_{\ell\mathbf{k}\sigma} c_{\ell\mathbf{k}\sigma} - \sum_\ell \Psi_\ell(t)\,\langle \mathcal{H}_{\mathrm{C}\ell}\rangle_0\,, \\ \mathcal{H}_{\mathrm{T},\Psi}(t) &\equiv \sum_\ell \mathcal{H}_{\mathrm{T}\ell,\Psi}(t) = \sum_\ell \left[\mathcal{H}_{\mathrm{T}\ell} + \lambda\Psi_\ell(t)(\mathcal{H}_{\mathrm{T}\ell} - \langle \mathcal{H}_{\mathrm{T}\ell}\rangle_0)\right] \\ &= \sum_\ell \sum_{\mathbf{k}\sigma} \Big[\underbrace{(1+\lambda\Psi_\ell(t))t_{\ell\mathbf{k}}}_{=\,t_{\ell\mathbf{k}}(t)} d^\dagger_\sigma c_{\mathbf{k}\sigma} + (h.c.)\Big] - \sum_\ell \lambda\Psi_\ell(t)\,\langle \mathcal{H}_{\mathrm{T}\ell}\rangle_0\end{aligned}$$

QD-lead hybridization should be immune to the gravitational field

- Self energies

$$\Sigma_{\ell\sigma}^{R/A/<}(t,t') \equiv \sum_{\mathbf{k}} \frac{t_{\ell\mathbf{k}}(t)}{\hbar} g_{\ell\mathbf{k}\sigma}^{R/A/<}(t,t') \frac{t_{\ell\mathbf{k}}^{*}(t')}{\hbar}$$

- Retarded/advanced self energies

$$\Sigma_{\ell\sigma}^{R/A}(t,t') = \frac{|t_\ell|^2}{\hbar^2}(1+\lambda\Psi_\ell(t))(1+\lambda\Psi_\ell(t')) \sum_{\mathbf{k}} g_{\ell\mathbf{k}\sigma}^{R/A}(t,t')$$

$$= \mp i\Gamma_\ell \frac{(1+\lambda\Psi_\ell(t))^2}{1+\Psi_\ell(t)} \delta(t-t')$$

$\leftarrow$ QD-contact coupling

$\leftarrow$ contact density of states

- linear response regime

$$\Sigma_{\ell\sigma}^{R/A}(t,t') \approx \mp i\Gamma_\ell(1+(2\lambda-1)\Psi_\ell(t))\delta(t-t')$$

$\rightarrow$ only when $\lambda = 1/2$, $\Sigma_{\ell\sigma}^{R/A}$ is not affected by the gravitational field

- beyond the linear response regime

$$1+\frac{1}{2}\Psi_\ell(t) \rightarrow \sqrt{1+\Psi_\ell(t)}$$

Hasegawa and Kato (2017), Hasegawa and Kato (2018)

Charge Currents

- Charge current in terms of QD Green's functions

$$I_\ell^c(t) = -e\left\langle \frac{d\mathcal{N}_\ell}{dt} \right\rangle = \frac{e}{\hbar}\sum_{\mathbf{k}\sigma} \mathcal{G}^<_{d,\ell\mathbf{k}\sigma}(t,t)t^*_{\ell\mathbf{k}}(t) + (c.c.),$$
$$= e\sum_\sigma \int dt' \left(\mathcal{G}^R_{d\sigma}(t,t')\Sigma^<_{\ell\sigma}(t',t) + \mathcal{G}^<_{d\sigma}(t,t')\Sigma^A_{\ell\sigma}(t',t) \right) + (c.c.)$$
$$I_{\mathrm{D}}^c(t) = -e\left\langle \frac{d\mathcal{N}_{\mathrm{D}}}{dt} \right\rangle = e\sum_\sigma i\frac{d}{dt}\mathcal{G}^<_{d\sigma}(t,t)$$

- Charge conservation:

$$[\mathcal{H}, \sum_\ell \mathcal{N}_\ell + \mathcal{N}_{\mathrm{D}}] = 0 \quad \rightarrow \quad \sum_\ell I_\ell^c(t) + I_{\mathrm{D}}^c(t) = 0$$

Heat Currents

- Heat current and contact energy for lead ℓ

$$I_\ell^h(t) = \frac{dQ_\ell(t)}{dt}$$

with

$$Q_\ell(t) = \langle \mathcal{H}_{\mathrm{C}\ell} + \lambda \mathcal{H}_{\mathrm{T}\ell} \rangle$$

or

$$Q_\ell(t) = \langle \mathcal{H}_{\mathrm{C}\ell,\Psi}(t) + \lambda \mathcal{H}_{\mathrm{T}\ell,\Psi}(t) \rangle$$

The difference between the two definitions,

$$\Psi_\ell(t) \left[\mathcal{H}_{\mathrm{C}\ell} - \langle \mathcal{H}_{\mathrm{C}\ell} \rangle_0 + \lambda^2 (\mathcal{H}_{\mathrm{T}\ell} - \langle \mathcal{H}_{\mathrm{T}\ell} \rangle_0) \right],$$

is of the second order in Ψ_ℓ
$\rightarrow$ the two definitions give rise to the same result in the linear response regime.

Heat Currents (cont.)

- Heat currents in terms of QD Green's functions

$$\begin{aligned}
\langle \mathcal{H}_{\mathrm{C}\ell} \rangle &= -i \sum_{\mathbf{k}\sigma} \epsilon_{\ell\mathbf{k}} \mathcal{G}^{<}_{\ell\mathbf{k},\ell\mathbf{k}\sigma}(t,t) \\
&= E_{\mathrm{C}\ell 0} + \sum_{\sigma} \int dt' \int dt'' \Big(\Xi^{RA}_{\ell\sigma}(t,t',t'') \mathcal{G}^{<}_{d\sigma}(t',t'') \\
&\qquad + \Xi^{R<}_{\ell\sigma}(t,t',t'') \mathcal{G}^{R}_{d\sigma}(t',t'') + \Xi^{<A}_{\ell\sigma}(t,t',t'') \mathcal{G}^{A}_{d\sigma}(t',t'') \Big) \\
\langle \mathcal{H}_{\mathrm{T}\ell} \rangle &= -i \sum_{\mathbf{k}\sigma} \mathcal{G}^{<}_{d,\ell\mathbf{k}\sigma}(t,t) t^{*}_{\ell\mathbf{k}} + (c.c.) \\
&= -\frac{i\hbar}{1+\lambda\Psi_{\ell}(t)} \sum_{\sigma} \int dt' \Big(\mathcal{G}^{R}_{d\sigma}(t,t') \Sigma^{<}_{\ell\sigma}(t',t) + \mathcal{G}^{<}_{d\sigma}(t,t') \Sigma^{A}_{\ell\sigma}(t',t) \Big) + (c.c.)
\end{aligned}$$

with

$$\Xi^{ab}_{\ell\sigma}(t,t',t'') \equiv -i \sum_{\mathbf{k}} \epsilon_{\ell\mathbf{k}} g^{a}_{\ell\mathbf{k}\sigma}(t,t') \frac{t^{*}_{\ell\mathbf{k}}(t')}{\hbar} \frac{t_{\ell\mathbf{k}}(t'')}{\hbar} g^{b}_{\ell\mathbf{k}\sigma}(t'',t)$$

for $a, b = R, A, <$.

Heat Currents (cont.)

- Sum rule:

$$[\mathcal{H}(t), \mathcal{H}(t)] = 0 \quad \to \quad \sum_\ell (W_{C\ell}(t) + W_{T\ell}(t)) + W_D(t) = 0$$

where the energy change rates are defined as

$$\begin{aligned} W_{C\ell}(t) &\equiv \frac{i}{\hbar}[\mathcal{H}(t), \mathcal{H}_{C\ell,\Psi}(t)] = (1 + \Psi_\ell(t)) \frac{d\langle \mathcal{H}_{C\ell} \rangle}{dt} \\ W_{T\ell}(t) &\equiv \frac{i}{\hbar}[\mathcal{H}(t), \mathcal{H}_{T\ell,\Psi}(t)] = (1 + \lambda\Psi_\ell(t)) \frac{d\langle \mathcal{H}_{T\ell} \rangle}{dt} \\ W_D(t) &\equiv \frac{i}{\hbar}[\mathcal{H}(t), \mathcal{H}_D]. \end{aligned}$$

Note that this sum rule can be applied only when the QD Hamiltonian, $\mathcal{H}_D$ is known.

- power supplied by the time-dependent thermal source or the power dissipated

$$P(t) = \left\langle \frac{\partial \mathcal{H}}{\partial t} \right\rangle = \sum_\ell \dot{\Psi}_\ell \left(\langle \mathcal{H}_{C\ell} + \lambda \mathcal{H}_{T\ell} \rangle - \langle \mathcal{H}_{C\ell} + \lambda \mathcal{H}_{T\ell} \rangle_0 \right)$$

Linear Response Regime

- We focus on the linear response regime
- Fouerier transformation: using the periodicity $\mathcal{G}(t,t') = \mathcal{G}(t+\tau, t'+\tau)$

$$\mathcal{G}(t,t') = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega(t-t')} \mathcal{G}(t,\omega),$$
$$\mathcal{G}(t,\omega) = \sum_{n=-\infty}^{\infty} \mathcal{G}(n,\omega) e^{-in\Omega t}.$$

- Expansion of the QD Green's functions: only $n = 0, \pm 1$ components are relevant

$$\mathcal{G}_{d\sigma}^{R/A/<}(n=0,\omega) \approx \mathcal{G}_{d\sigma,\mathrm{eq}}^{R/A/<}(\omega)$$
$$\mathcal{G}_{d\sigma}^{R/A/<}(n=\pm 1,\omega) \propto \Psi_\ell$$

and

$$I_{\ell/\mathrm{D}}^{c/h}(t) = I_{\ell/\mathrm{D}}^{c/h}(\Omega) e^{-i\Omega t} + I_{\ell/\mathrm{D}}^{c/h}(-\Omega) e^{+i\Omega t}$$

Linear Response Regime: Charge Currents

- Charge currents

$$I_{\mathrm{D}}^{c}(\Omega) = e\sum_{\sigma}\omega\int\frac{d\omega}{2\pi}\mathcal{G}_{d\sigma}^{<}(1,\omega)$$

$$I_{\ell}^{c}(\Omega) = e\sum_{\sigma}\int\frac{d\omega}{2\pi}\Big[\Sigma_{\ell\sigma}^{<}(1,\omega)\left(\mathcal{G}_{d\sigma,\mathrm{eq}}^{R}(\omega+\Omega)-\mathcal{G}_{d\sigma,\mathrm{eq}}^{A}(\omega)\right) + f(\omega+\Omega)(2i\Gamma_{\ell})\left(\mathcal{G}_{d\sigma}^{R}(1,\omega+\Omega)-\mathcal{G}_{d\sigma}^{A}(1,\omega)\right)+(2i\Gamma_{\ell})\mathcal{G}_{d\sigma}^{<}(1,\omega)\Big]$$

- The charge currents depend not only on the equilibrium QD Green's functions but also on the dynamical ones, $\mathcal{G}_{d\sigma}^{R/A/<}(1,\omega)$, even though the linear response $(\Psi_{\ell}\to 0)$ is taken. It is obviously because our perturbations are dynamical and the dynamical excitations of the system, even though being small, cannot be described solely in terms of the equilibrium Green's functions.

Linear Response Regime: Charge Currents (cont.)

- Elimination of $\int d\omega\, \mathcal{G}^<_{d\sigma}(1,\omega)$ from the charge conservation

$$\sum_\ell I^c_\ell(t) + I^c_{\mathrm{D}}(t) = 0 \quad \rightarrow \quad \int d\omega\, \mathcal{G}^<_{d\sigma}(1,\omega) = \cdots$$

- Charge currents, free of $\mathcal{G}^<_{d\sigma}(1,\omega)$

$$I^c_\ell(\Omega) = e\sum_\sigma \int \frac{d\omega}{2\pi}\Bigg[\left(\sum_{\ell'} \frac{\Psi_{\ell'}}{2}\frac{2i\Gamma_{\ell'}}{2i\Gamma+\Omega} - \frac{\Psi_\ell}{2}\right)\Delta_f(\omega+\Omega,\omega)\left(\omega+\frac{\Omega}{2}\right)(2i\Gamma_\ell) \times \left(\mathcal{G}^R_{d\sigma,\mathrm{eq}}(\omega+\Omega) - \mathcal{G}^A_{d\sigma,\mathrm{eq}}(\omega)\right) + \frac{\Omega}{2i\Gamma+\Omega} f(\omega+\Omega)(2i\Gamma_\ell)\left(\mathcal{G}^R_{d\sigma}(1,\omega+\Omega) - \mathcal{G}^A_{d\sigma}(1,\omega)\right)\Bigg]$$

with

$$\Delta_f(\omega,\omega') \equiv \frac{f(\omega)-f(\omega')}{\omega-\omega'}$$

Linear Response Regime: Heat Currents

- Heat currents

$$I_\ell^h(\Omega) = \sum_\sigma \hbar \int \frac{d\omega}{2\pi} \left[\frac{\Psi_\ell}{2} \Delta_f(\omega+\Omega,\omega) \left(\omega + \frac{\Omega}{2}\right)^2 (2i\Gamma_\ell) \left(\mathcal{G}^R_{d\sigma,\mathrm{eq}}(\omega+\Omega) - \mathcal{G}^A_{d\sigma,\mathrm{eq}}(\omega) \right) \right.$$
$$- \left(\omega + \frac{\Omega}{2}\right) (2i\Gamma_\ell) \left(f(\omega)\mathcal{G}^R_{d\sigma}(1,\omega) - f(\omega+\Omega)\mathcal{G}^A_{d\sigma}(1,\omega) \right) \Big]$$
$$\left. - \left(\omega + \frac{\Omega}{2}\right) (2i\Gamma_\ell) \mathcal{G}^<_{d\sigma}(1,\omega) \right]$$

- Elimination of $\int d\omega \left(\omega + \frac{\Omega}{2}\right) \mathcal{G}^<_{d\sigma}(1,\omega)$ from the sum rule

$$\sum_\ell (W_{\mathrm{C}\ell}(\Omega) + W_{\mathrm{T}\ell}(\Omega)) + W_{\mathrm{D}}(\Omega) = 0 \quad \to \quad \int d\omega \left(\omega + \frac{\Omega}{2}\right) \mathcal{G}^<_{d\sigma}(1,\omega) = \cdots$$

but, aplplicable only after $\mathcal{H}_{\mathrm{QD}}$ or $W_{\mathrm{D}}(\Omega)$ is specified.

- Time-averaged power

$$\overline{P} = -\sum_\ell \Psi_\ell \,\mathrm{Re}[I_\ell^h(\Omega)]$$

Linear Response Regime: Heat Currents (cont.)

- artefact of Luttinger's trick: an additional unphysical term in $I_\ell^h(t)$

$$\frac{d}{dt}\left((1-\lambda)\Psi_\ell(t)E_{\mathrm{T}\ell 0}\right)$$

$\leftarrow$ an effective energy capacitor which is dynamically driven by the field difference $\Psi_\ell(t) - \lambda\Psi_\ell(t)$ between the contact ℓ and the adjacent tunneling barrier.

Application of Luttinger's scheme: Non-interacting case

- QD Hamitlonian

$$\mathcal{H}_{\rm QD} = \sum_\sigma \epsilon_\sigma d_\sigma^\dagger d_\sigma$$

- QD Green's functions

$$\mathcal{G}^{R/A}_{d\sigma,{\rm eq}}(\omega) = \frac{1}{\omega - \epsilon_\sigma/\hbar \pm i\Gamma} \quad \text{and} \quad \mathcal{G}^{R/A}_{d\sigma}(1,\omega) = 0$$

Note that

$$\mathcal{G}^{<}_{d\sigma}(1,\omega) \neq 0$$

- For the sum rule for energy change rates,

$$W_{\rm D}(t) = \frac{d}{dt}\sum_\sigma \epsilon_\sigma \langle n_\sigma(t)\rangle \quad \rightarrow \quad W_{\rm D}(\Omega) = -\sum_\sigma \epsilon_\sigma \int \frac{d\omega}{2\pi}\Omega \mathcal{G}^{<}_{d\sigma}(1,\omega)$$

- Thermoelectric and thermal admittances

$$\begin{bmatrix} I^c_{\rm L}(\Omega) \\ I^c_{\rm R}(\Omega) \end{bmatrix} = \begin{bmatrix} L_{\rm L}(\Omega) - L_{\rm LR}(\Omega) & L_{\rm LR}(\Omega) \\ L_{\rm RL}(\Omega) & L_{\rm R}(\Omega) - L_{\rm LR}(\Omega) \end{bmatrix} \begin{bmatrix} \Psi_{\rm L}/2 \\ \Psi_{\rm R}/2 \end{bmatrix}$$

and

$$\begin{bmatrix} I^h_{\rm L}(\Omega) \\ I^h_{\rm R}(\Omega) \end{bmatrix} = \begin{bmatrix} K_{\rm L}(\Omega) - K_{\rm LR}(\Omega) & K_{\rm LR}(\Omega) \\ K_{\rm RL}(\Omega) & K_{\rm R}(\Omega) - K_{\rm LR}(\Omega) \end{bmatrix} \begin{bmatrix} \Psi_{\rm L}/2 \\ \Psi_{\rm R}/2 \end{bmatrix}$$

with

$$L_\ell(\Omega) = (2i\Gamma_\ell)\Omega e \sum_\sigma P_{1\sigma}(\Omega), \qquad L_{\rm LR}(\Omega) = 4\Gamma_{\rm L}\Gamma_{\rm R} e \sum_\sigma P_{1\sigma}(\Omega)$$

$$K_\ell(\Omega) = (2i\Gamma_\ell)\Omega(-\hbar) \sum_\sigma P_{2\sigma}(\Omega), \qquad K_{\rm LR}(\Omega) = 4\Gamma_{\rm L}\Gamma_{\rm R}(-\hbar) \sum_\sigma P_{2\sigma}(\Omega)$$

and

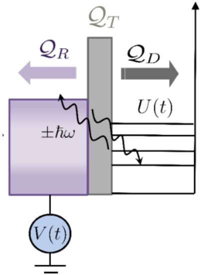
$$P_{n\sigma}(\omega) \equiv \int \frac{d\omega}{2\pi} \Delta_f(\omega+\Omega,\omega) \left(\omega + \frac{\Omega}{2}\right)^n \mathcal{G}^R_{d\sigma,\rm eq}(\omega+\Omega)\mathcal{G}^A_{d\sigma,\rm eq}(\omega)$$

- Onsager reciprocity (micro-reversibility) in the linear-response regime

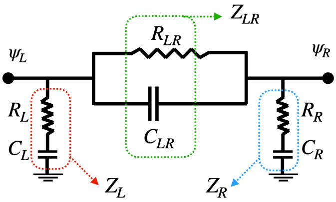
$$L(\Omega) = \frac{\delta I^c(\Omega)}{\delta \Psi(\Omega)} \propto \langle [\frac{d\mathcal{N}}{dt}, \mathcal{Q}] \rangle$$
$$M(\Omega) = \frac{\delta I^h(\Omega)}{\delta V(\Omega)} \propto \langle [\frac{d\mathcal{Q}}{dt}, \mathcal{N}] \rangle$$
$$\rightarrow \quad M(\Omega) = L(\Omega)$$

Both works use the same contact energy

$$\mathcal{Q} = \mathcal{H}_{\mathrm{C}} + \frac{1}{2}\mathcal{H}_{\mathrm{T}}$$



(Rosselló, López, and Lim, 2015)



- Low-frequency ($\hbar\Omega \ll k_B T$) equivalent RC circuit

$$L/K_{\rm LR}(\Omega) = \frac{1}{Z_{L/K,{\rm LR}}(\Omega)} = \frac{1}{R_{L/K,{\rm LR}}} + \frac{1}{1/i\Omega C_{L/K,{\rm LR}}}$$

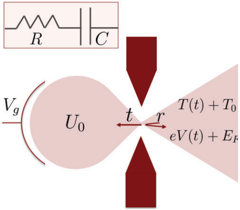
$$L/K_{\ell}(\Omega) = \frac{1}{Z_{L/K,\ell}(\Omega)} = \frac{1}{R_{L/K,\ell} + \frac{1}{i\Omega C_{L/K,\ell}}}$$

Application of Luttinger's scheme: Non-interacting case (cont.)

- fluctuation-dissipation theorem + Kubo formulas + scattering theory

$$K(\Omega) = \frac{1}{\hbar\Omega T}\int_0^\infty dt\, e^{i(\Omega+i0^+)t}\langle[\hat{I}^h(t), \hat{I}^h(0)]\rangle$$
$$L(\Omega) = \frac{1}{\hbar\Omega T}\int_0^\infty dt\, e^{i(\Omega+i0^+)t}\langle[\hat{I}^c(t), \hat{I}^h(0)]\rangle = \frac{M(\Omega)}{T}$$

— in good agreement with our results

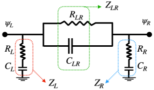


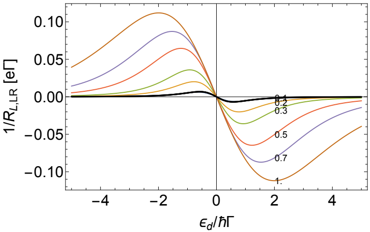
- comparison with previous results
  1. two agreement with previous results → validity of our Luttinger scheme
  2. the fluctuation-dissipation theorem holds for the thermoelectric and thermal transport for non-interacting + linear response

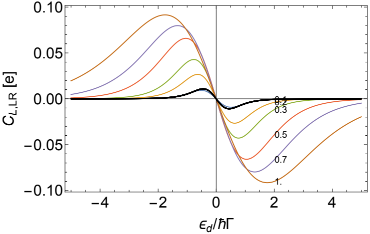
Lim, López, and Sánchez (2013)

Application of Luttinger's scheme: Non-interacting case (cont.)

cross thermoelectric admittace $L_{\rm LR}(\Omega)$ ($\epsilon_\uparrow = \epsilon_\downarrow$)



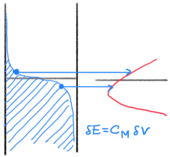




At low temperatures ($k_B T \ll \hbar\Gamma$)

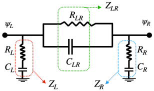
$$\frac{1}{R_{L,\rm LR}} = (-e)hG_{\rm th}T\frac{2\Gamma_{\rm L}\Gamma_{\rm R}}{\Gamma}\sum_\sigma \rho'_\sigma(0)$$

$$C_{L,\rm LR} = (-e)h^2G_{\rm th}T\frac{2\Gamma_{\rm L}\Gamma_{\rm R}}{\Gamma}\sum_\sigma \rho'_\sigma(0)\rho_\sigma(0) \qquad \left(G_{\rm th} = \frac{\pi^2}{3}\frac{k_B^2 T}{h}\right)$$

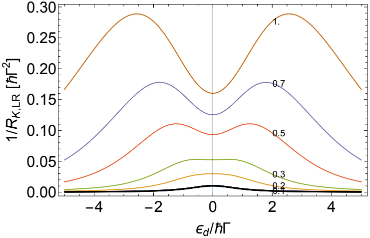


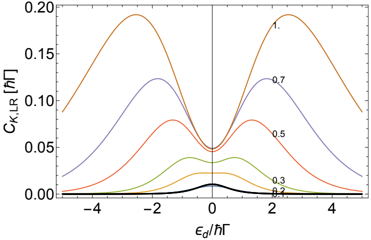
→ the thermodelectric admittance reflects the particle-hole symmetry

Application of Luttinger's scheme: Non-interacting case (cont.)



cross thermal admittance $K_{\rm LR}(\Omega)$



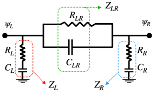


At low temperatures ($k_B T \ll \hbar\Gamma$)

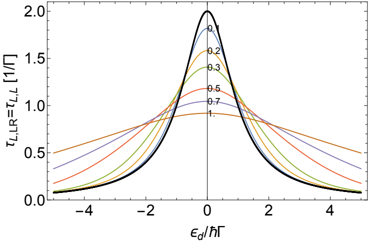
$$\frac{1}{R_{K,\rm LR}} = hG_{\rm th}T\frac{2\Gamma_{\rm L}\Gamma_{\rm R}}{\Gamma}\sum_\sigma \rho_\sigma(0), \qquad C_{K,\rm LR} = \frac{h^2 G_{\rm th}T}{2}\frac{2\Gamma_{\rm L}\Gamma_{\rm R}}{\Gamma}\sum_\sigma [\rho_\sigma(0)]^2$$

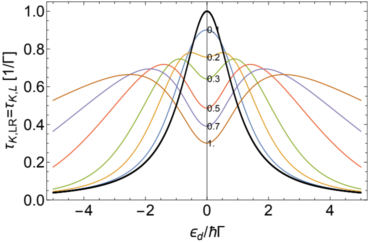
- at low temperatures, $1/R_{K,\rm LR}$ is proportional to the electric conductance
- at high temperatures, large-energy carriers are dominant in the heat transport.

Application of Luttinger's scheme: Non-interacting case (cont.)



RC times or response times





For all temperatures,

$$\tau_{L,\ell} = \tau_{L,\mathrm{LR}} \quad (\leftarrow P_{1\sigma}(\Omega)) \qquad \text{and} \qquad \tau_{K,\ell} = \tau_{K,\mathrm{LR}} \quad (\leftarrow P_{2\sigma}(\Omega))$$

At low temperatures,

$$\tau_{L,\mathrm{LR}} = h\frac{\sum_\sigma [\rho_\sigma(0)]^2}{\sum_\sigma \rho_\sigma(0)} = 2\tau_{K,\mathrm{LR}}$$

Application of Luttinger's scheme: Interacting case

- QD Hamitlonian

$$\mathcal{H}_{\mathrm{QD}} = \sum_{\sigma} \epsilon_{\sigma} d_{\sigma}^{\dagger} d_{\sigma} + U n_{\uparrow} n_{\downarrow}$$

- Hartree approximation

$$\langle\langle n_{\bar{\sigma}} d_{\sigma}, d_{\sigma}^{\dagger} \rangle\rangle(t,t') \approx \langle n_{\bar{\sigma}}(t)\rangle \, \langle\langle d_{\sigma}, d_{\sigma}^{\dagger}\rangle\rangle(t,t') = \langle n_{\bar{\sigma}}(t)\rangle \, \mathcal{G}_{d\sigma}(t,t')$$

- QD Green's functions

$$\mathcal{G}^{R/A}_{d\sigma,\mathrm{eq}}(\omega) = \frac{1}{\omega - \epsilon_{\mathrm{HF},\sigma}/\hbar \pm i\Gamma} \qquad \text{with} \;\; \epsilon_{\mathrm{HF},\sigma} = \epsilon_{\sigma} + U n_{\bar{\sigma},\mathrm{eq}}$$

$$\mathcal{G}^{R/A}_{d\sigma,\mathrm{eq}}(1,\omega) = \frac{U}{\hbar} \mathcal{G}^{R/A}_{d\sigma}(\omega \pm \Omega) n_{\bar{\sigma}}(1,\Omega) \mathcal{G}^{R/A}_{d\sigma}(\omega)$$

- For the sum rule for energy change rates,

$$W_{\mathrm{D}}(t) = \frac{d}{dt}\left(\sum_{\sigma} \epsilon_{\sigma} \langle n_{\sigma}(t)\rangle + U \langle n_{\uparrow}(t)\rangle \langle n_{\downarrow}(t)\rangle \right)$$

$$\rightarrow \quad W_{\mathrm{D}}(\Omega) = -\sum_{\sigma} \epsilon_{\mathrm{HF},\sigma} \int \frac{d\omega}{2\pi} \Omega \mathcal{G}^{<}_{d\sigma}(1,\omega)$$

Application of Luttinger's scheme: Interacting case (cont.)

- Thermoelectric and thermal admittances

$$\begin{bmatrix} I^c_{\rm L}(\Omega) \\ I^c_{\rm R}(\Omega) \end{bmatrix} = \begin{bmatrix} L_{\rm L}(\Omega) - L_{\rm LR}(\Omega) & L_{\rm LR}(\Omega) \\ L_{\rm RL}(\Omega) & L_{\rm R}(\Omega) - L_{\rm LR}(\Omega) \end{bmatrix} \begin{bmatrix} \Psi_{\rm L}/2 \\ \Psi_{\rm R}/2 \end{bmatrix}$$

$$\begin{bmatrix} I^h_{\rm L}(\Omega) \\ I^h_{\rm R}(\Omega) \end{bmatrix} = \begin{bmatrix} K_{\rm L}(\Omega) - K_{\rm LR}(\Omega) & K_{\rm LR}(\Omega) \\ K_{\rm RL}(\Omega) & K_{\rm R}(\Omega) - K_{\rm LR}(\Omega) \end{bmatrix} \begin{bmatrix} \Psi_{\rm L}/2 \\ \Psi_{\rm R}/2 \end{bmatrix}$$

with

$$L_\ell(\Omega) = (2i\Gamma_\ell)\Omega e \sum_\sigma \left[P_{1\sigma}(\Omega) + \frac{2\Gamma U}{\hbar} P_{0\sigma}(\Omega) X_{\bar\sigma}(\Omega) \right]$$

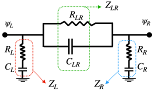
$$L_{\rm LR}(\Omega) = 4\Gamma_{\rm L}\Gamma_{\rm R} e \sum_\sigma \left[P_{1\sigma}(\Omega) + \frac{i\Omega U}{\hbar} P_{0\sigma}(\Omega) X_{\bar\sigma}(\Omega) \right]$$

$$K_\ell(\Omega) = (2i\Gamma_\ell)\Omega(-\hbar) \sum_\sigma \left[P_{2\sigma}(\Omega) + \frac{2\Gamma U}{\hbar} P_{1\sigma}(\Omega) X_{\bar\sigma}(\Omega) \right]$$

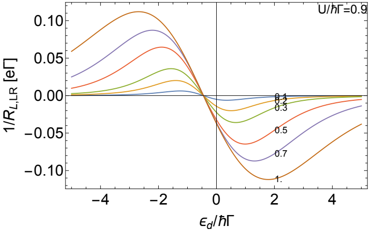
$$K_{\rm LR}(\Omega) = 4\Gamma_{\rm L}\Gamma_{\rm R}(-\hbar) \sum_\sigma \left[P_{2\sigma}(\Omega) + \frac{i\Omega U}{\hbar} P_{1\sigma}(\Omega) X_{\bar\sigma}(\Omega) \right]$$

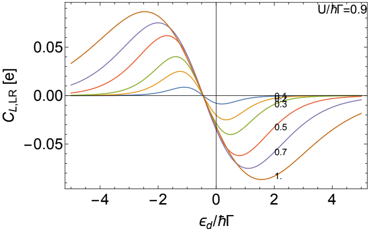
and

$$X_\sigma(\Omega) = \frac{P_{1\sigma}(\Omega) + \frac{2\Gamma U}{\hbar} P_{0\sigma}(\Omega) P_{1\bar\sigma}(\Omega)}{1 - \left(\frac{2\Gamma U}{\hbar}\right)^2 P_{0\sigma}(\Omega) P_{0\bar\sigma}(\Omega)} \approx P_{1\sigma}(\Omega)$$

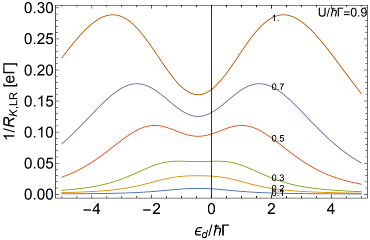


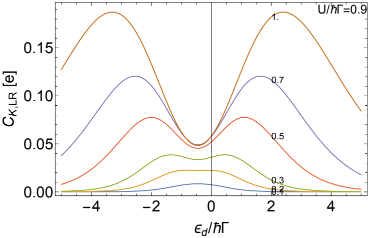
cross thermoelectric admittances

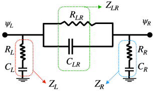




thermal admittances

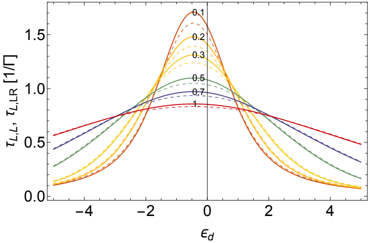


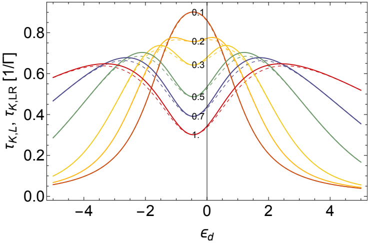


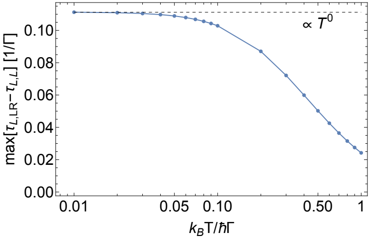


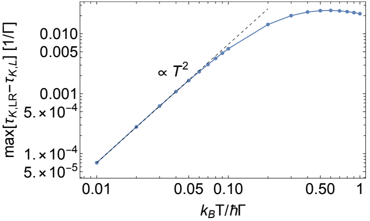
RC times or response times

$$\tau_{L,\ell} \neq \tau_{L,\mathrm{LR}} \quad \text{and} \quad \tau_{K,\ell} \neq \tau_{K,\mathrm{LR}}$$



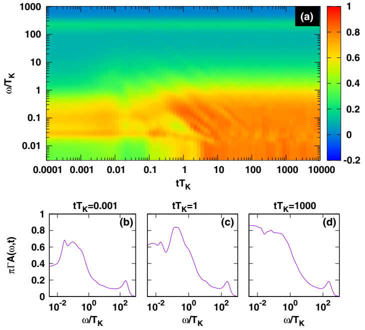




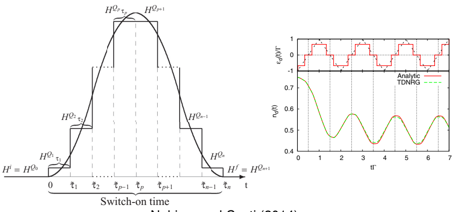


Further applications of Luttinger scheme

- Non-interacting case
  - multi-levels in QD
  - spin-orbit interaction
  - non-trivial geometry: Aharnonov-Bohm interferometer
- Interacting case
  - equation-of-motion method: Coulomb blockade (Meir-Wingreen approximation)
  - time-dependent numerical renormalization group (td-NRG)



Nghiem and Costi (2017)



Nghiem and Costi (2014)

F G Eich, A Principi, M Di Ventra, and G Vignale. Luttinger-field approach to thermoelectric transport in nanoscale conductors. *Phys. Rev. B*, 90(11):115116, sep 2014. doi: 10.1103/PhysRevB.90.115116.

Jong Soo Lim, Rosa López, and David Sánchez. Dynamic thermoelectric and heat transport in mesoscopic capacitors. *Physical Review B*, 88(20):201304, nov 2013. ISSN 1098-0121. doi: 10.1103/PhysRevB.88.201304. url: http://link.aps.org/doi/10.1103/PhysRevB.88.201304.

Č. Lozej and T. Rejec. Time-dependent thermoelectric transport in nanosystems: Reflectionless Luttinger field approach. *Physical Review B*, 98(7):075427, aug 2018. ISSN 2469-9950. doi: 10.1103/PhysRevB.98.075427. url: https://link.aps.org/doi/10.1103/PhysRevB.98.075427.

María Florencia Ludovico, Jong Soo Lim, Michael Moskalets, Liliana Arrachea, and David Sánchez. Dynamical energy transfer in ac-driven quantum systems. *Physical Review B*, 89(16):161306, apr 2014. ISSN 1098-0121. doi: 10.1103/PhysRevB.89.161306. url: http://link.aps.org/doi/10.1103/PhysRevB.89.161306.

Fabian Menges, Heike Riel, Andreas Stemmer, and Bernd Gotsmann. Quantitative Thermometry of Nanoscale Hot Spots. *Nano Letters*, 12(2):596–601, feb 2012. ISSN 1530-6984. doi: 10.1021/nl203169t. url: http://pubs.acs.org/doi/10.1021/nl203169t.

H. T. M. Nghiem and T. A. Costi. Time-dependent numerical renormalization group method for multiple quenches: Application to general pulses and periodic driving. *Physical Review B*, 90(3):035129, jul 2014. ISSN 1098-0121. doi: 10.1103/PhysRevB.90.035129. url: https://link.aps.org/doi/10.1103/PhysRevB.90.035129. Available from arXiv:1406.3444v2.

H. T. M. Nghiem and T. A. Costi. Time Evolution of the Kondo Resonance in Response to a Quench. *Physical Review Letters*, 119 (15):156601, oct 2017. ISSN 0031-9007. doi: 10.1103/PhysRevLett.119.156601. url: https://link.aps.org/doi/10.1103/PhysRevLett.119.156601. Available from 1701.07558.

Ali Rafiei Miandashti, Larousse Khosravi Khorashad, Alexander O. Govorov, Martin E. Kordesch, and Hugh H. Richardson. Time-Resolved Temperature-Jump Measurements and Theoretical Simulations of Nanoscale Heat Transfer Using NaYF 4 :Yb 3+ :Er 3+ Upconverting Nanoparticles. *The Journal of Physical Chemistry C*, 123(6):3770–3780, feb 2019. ISSN 1932-7447. doi: 10.1021/acs.jpcc.8b11215. url: https://pubs.acs.org/doi/10.1021/acs.jpcc.8b11215.

Guillem Rosselló, Rosa López, and Jong Soo Lim. Time-dependent heat flow in interacting quantum conductors. *Physical Review B*, 92(11):115402, sep 2015. ISSN 1098-0121. doi: 10.1103/PhysRevB.92.115402. url: https://link.aps.org/doi/10.1103/PhysRevB.92.115402. Available from 1509.05756.

Gen Tatara. Thermal Vector Potential Theory of Transport Induced by a Temperature Gradient. *Physical Review Letters*, 114(19): 196601, may 2015. ISSN 0031-9007. doi: 10.1103/PhysRevLett.114.196601. url: https://link.aps.org/doi/10.1103/PhysRevLett.114.196601. Available from 1502.00347.