Thermoelectrics of interacting nanosystems

Exploiting fermion-parity superselection instead of time-reversal symmetry

Janine Splettstößer

CHALMERS
UNIVERSITY OF TECHNOLOGY

Applied Quantum Physics, MC2
Chalmers University of Technology, Gothenburg, Sweden

Quantum Thermodynamics and Transport, SPICE Mainz, 8 May 2018

Outline

- Motivation – Nanoscale electronic systems for heat engines and thermoelectrics
- Fermion-parity duality relation for time-evolution kernels
- Consequences from duality for the thermoelectric response of a weakly coupled quantum dot

J. Schulenborg, A. Di Marco, J. Vanherck, M. R. Wegewijs, and J. Splettstoesser, Entropy **19**, 668 (2017).

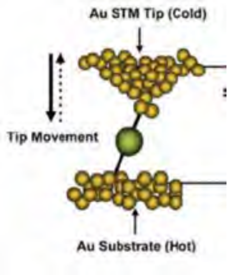
J. Schulenborg, R. B. Saptsov, F. Haupt, J. Splettstoesser, and M. R. Wegewijs, Phys. Rev. B **93**, 081411(R) (2016).

J. Vanherck, J. Schulenborg, R. B. Saptsov, J. Splettstoesser, and M. R. Wegewijs, Phys. Status solidi B **254**, 1600614 (2017).

Read also: Jens Schulenborg, Licentiate Thesis, 2016

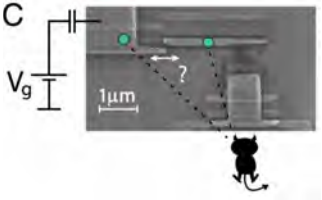
Nanoscale systems as heat engines and thermoelectric devices

Molecular thermoelectrics



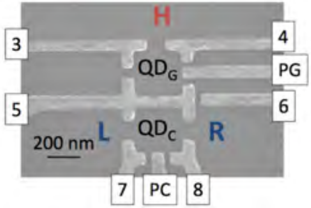
P. Reddy, S.-Y. Jang, R. A. Segalman, A. Majumdar: Science **315**, 1568 (2007).

Single-electron cyclic heat engines



J. V. Koski, V. F. Maisi, J. P. Pekola, D. V. Averin: PNAS **111**, 13786 (2014).

Quantum dot thermocouple

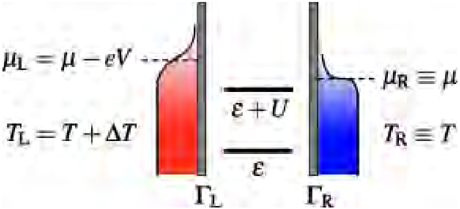


H. Thierschmann, R. Sánchez, B. Sothmann, F. Arnold, C. Heyn, W. Hansen, H. Buhmann, L. W. Molenkamp: Nat. Nanotechnol. **10**, 854 (2015).

- Discrete level spectrum (energy filter)
- Spin physics
- Controllability via gates
- Coulomb interaction (for energy transfer)
- Smaller than thermalization length. . .

Simple – prototype – system

Single-level quantum dot in contact with (several) electronic reservoirs

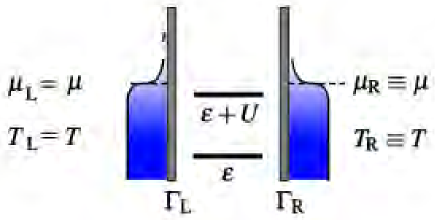


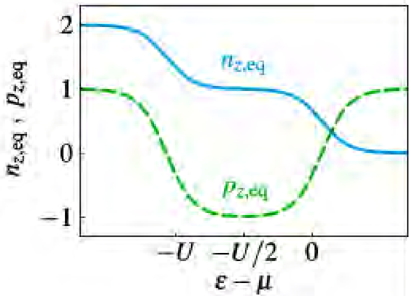
Quantum dot Hamiltonian: $H_{\mathrm{dot}} = \sum_\sigma \epsilon\, d_\sigma^\dagger d_\sigma + U \hat{n}_\uparrow \hat{n}_\downarrow$

with eigenstates $|0\rangle, |1\rangle, |2\rangle$

weakly coupled to electrodes (energy-independent): $\Gamma_{\alpha\sigma} = 2\pi\nu_0 |t_{\alpha\sigma}|^2 \ll k_B T$

Simple – prototype – system





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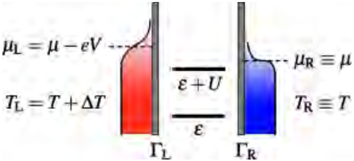
weakly coupled to electrodes (energy-independent): $\Gamma_{\alpha\sigma} = 2\pi\nu_0 |t_{\alpha\sigma}|^2 \ll k_\mathrm{B} T$

Puzzling results for a simple system....

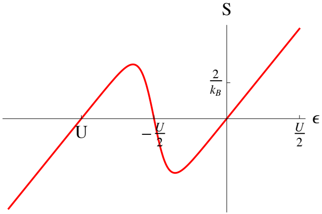
Surprising features in energy-transport already for this simple model!

J. Schulenborg, R. B. Saptsov, F. Haupt, J. Splettstoesser, and M. R. Wegewijs, Phys. Rev. B **93**, 081411(R) (2016).

Example from stationary thermoelectrics:



Seebeck coefficient:



Typically treated as crossover...

Goal:

Demonstrate how a new symmetry-relation can help us to analyse and understand the thermoelectric response of fermionic open systems.

Time evolution and observables

Charge and energy currents

$$I_N^\alpha = -\frac{\partial}{\partial t}\langle \hat{N}_\alpha \rangle \qquad I_E^\alpha = -\frac{\partial}{\partial t}\langle \hat{H}_\alpha \rangle$$

Time evolution and observables

Here: focus on a weakly coupled fermionic open system.

Charge and energy currents

$$I_N^\alpha = -\frac{\partial}{\partial t}\langle \hat{N}_\alpha \rangle = (N|W_\alpha|\rho) \qquad I_E^\alpha = -\frac{\partial}{\partial t}\langle \hat{H}_\alpha \rangle = (H_{\text{dot}}|W_\alpha|\rho)$$

Time-evolution of reduced density matrix

$$\frac{\partial}{\partial t}|\rho) = W|\rho) \quad \text{with} \quad W = \sum_\alpha W_\alpha$$

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Charge and energy currents with the short notation

$$I_N^\alpha = -\frac{\partial}{\partial t}\langle \hat{N}_\alpha \rangle = (N|W_\alpha|\rho) = \text{Tr}\left\{\hat{N}\, W_\alpha\, \hat{\rho}\right\}$$

$$I_E^\alpha = -\frac{\partial}{\partial t}\langle \hat{H}_\alpha \rangle = (H_{\text{dot}}|W_\alpha|\rho)$$

with $\rho = \sum_i p_i |i\rangle\langle i|$

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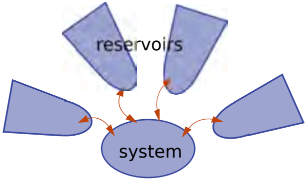
Obviously helpful: eigenmode decomposition. . .

Eigenmode decomposition – open vs. closed system

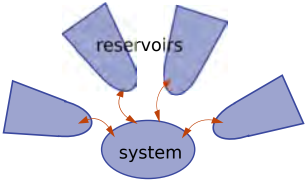


Formally for time-evolution Kernels:

$$W_\alpha = -\sum_{m_\alpha} \gamma_{m\alpha} |m_\alpha)(m'_\alpha|$$

$$W = -\sum_{m} \gamma_m |m)(m'|$$

Eigenmode decomposition – open vs. closed system



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<u>Time evolution in a **closed** system</u>

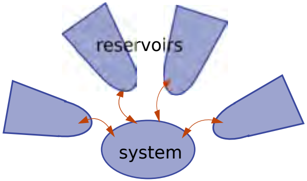
$$|\Psi(t)\rangle = e^{iHt}|\Psi_0\rangle$$

Expand in energy-eigenstates:

$$|\Psi(t)\rangle = \sum_i e^{iE_it}|E_i\rangle\langle E_i|\Psi_0\rangle$$

$\left(H|\Psi\rangle\right)^\dagger = \langle\Psi|H \;\Rightarrow$ Left/right eigenstates are the same.

Eigenmode decomposition – open vs. closed system



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$$W = -\sum_{m} \gamma_{m} |m)(m'|$$

But

$$W^\dagger \neq W$$

How to understand eigenmodes?

Time evolution in a **closed** system

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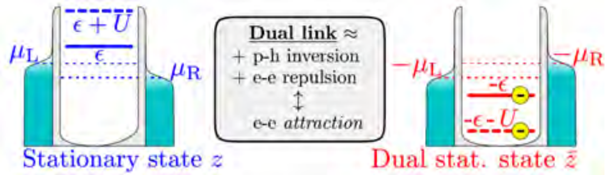
Fermion-parity duality for time-evolution Kernels

$$[W(H,\{\mu_\alpha\})]^\dagger = -\Gamma - (-1)^N W(-H,\{-\mu_\alpha\})(-1)^N$$



J. Schulenborg, R. B. Saptsov, F. Haupt, J. Splettstoesser, and M. R. Wegewijs, Phys. Rev. B **93**, 081411(R) (2016).

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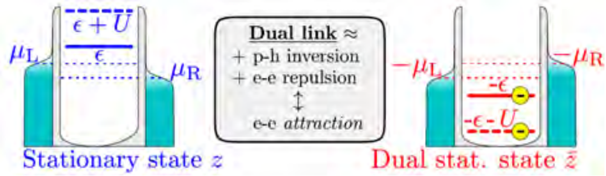

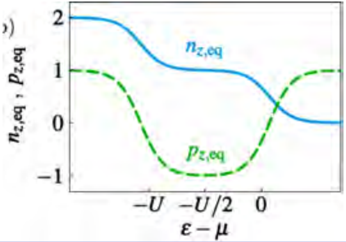

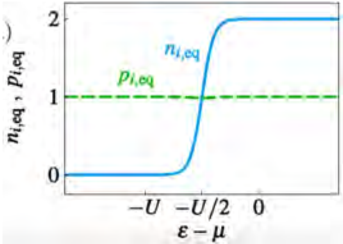

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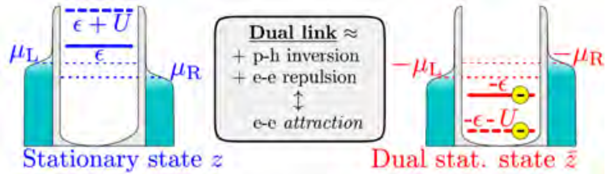

Probability conservation:

$(z'| = (\mathbf{1}|$ $\quad \gamma_z = 0$

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J. Schulenborg, R. B. Saptsov, F. Haupt, J. Splettstoesser, and M. R. Wegewijs, Phys. Rev. B **93**, 081411(R) (2016).

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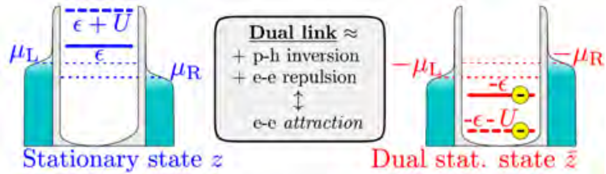

Probability conservation:

$(z'| = (\mathbf{1}| \qquad \gamma_z = 0$ ⟶ Duality: $\gamma_p = \Gamma - 0 \qquad |p) = |(-\mathbf{1})^{\hat{N}})$

$(p'| = ((-\mathbf{1})^{\hat{N}} z_i| \approx (z_i|$ ⟵ $\gamma_z = 0 \qquad |z)$

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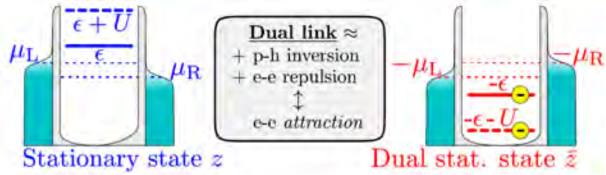

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$(c'| \qquad \gamma_c \qquad |c)$

J. Schulenborg, R. B. Saptsov, F. Haupt, J. Splettstoesser, and M. R. Wegewijs, Phys. Rev. B **93**, 081411(R) (2016).

(Nonlinear) charge and energy currents

$$I_N^\alpha = (N|W_\alpha|z)$$

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J. Vanherck, J. Schulenborg, R. B. Saptsov, J. Splettstoesser, and M. R. Wegewijs, Phys. Status solidi B **254**, 1600614 (2017).

(Nonlinear) charge and energy currents

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\begin{aligned}
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n_z stationary state occupation

$n_{z\alpha}$ **equilibrium** occupation wrt lead α.

J. Vanherck, J. Schulenborg, R. B. Saptsov, J. Splettstoesser, and M. R. Wegewijs, Phys. Status solidi B **254**, 1600614 (2017).

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tight-coupling parity mode

J. Vanherck, J. Schulenborg, R. B. Saptsov, J. Splettstoesser, and M. R. Wegewijs, Phys. Status solidi B **254**, 1600614 (2017).

Thermoelectric response

Linear response:

$$\begin{pmatrix} I \\ J \end{pmatrix} = \begin{pmatrix} L_{11} & L_{12} \\ L_{21} & L_{22} \end{pmatrix} \begin{pmatrix} V/T \\ \Delta T/T^2 \end{pmatrix}$$

and beyond...

- Thermoelectric effect – Seebeck coefficient/nonlinear thermopower

$$S = \frac{V\big|_{I=0}}{\Delta T} \xrightarrow{\text{linear response}} -\frac{1}{T}\frac{L_{11}}{L_{12}}$$

- Fourier heat – heat transfer in the absence of charge transfer

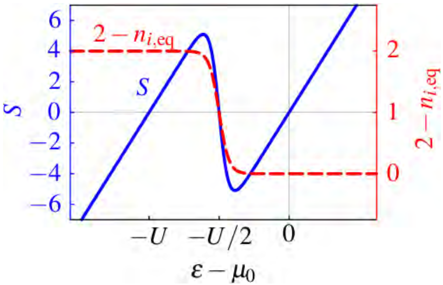
$$\kappa = \frac{\partial J\big|_{I=0}}{\partial \Delta T} \xrightarrow{\text{linear response}} L_{22} - \frac{L_{12}L_{21}}{L_{11}}$$

Seebeck coefficient

"Thermovoltage due to temperature gradient (in the absence of a charge current)"

Linear response Seebeck coefficient ⇔ characteristic energy

$$TS = \epsilon - \mu + \frac{U}{2}(2 - n_{\mathrm{i,eq}})$$



J. Schulenborg, A. Di Marco, J. Vanherck, M. R. Wegewijs, and J. Splettstoesser, Entropy **19**, 668 (2017).

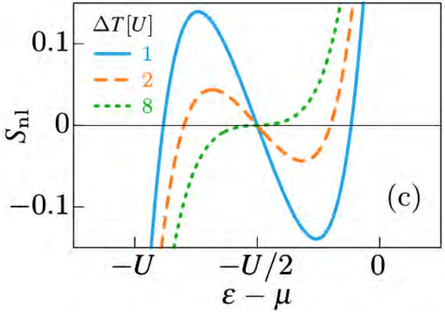
- Crossover at electron-hole symmetric point ⇔ resonance of the inverted (attractive) model
- Analyze feature using

$$n_{\mathrm{i,eq}} \approx 2\left[1 - f\left(\epsilon + \frac{U}{2}\right)\right]_{T \to T/2}$$

⇒ slope, maxima, temperature-halving (two-particle resonance)

Seebeck coefficient – nonlinear thermopower

$$S_{\mathrm{nl}} = \frac{V\big|_{I=0}}{\Delta T}$$



S. F. Svensson, E. A. Hoffmann, N. Nakpathomkun, P.M. Wu, H. Q. Xu,H. A. Nilsson, D. Sánchez, V. Kashcheyevs, and H. Linke, New J. Phys. **15**, 105011 (2013); A. Sierra, D. Sánchez: Phys. Rev. B **90**, 115313 (2014).

$$I_\alpha = \gamma_{c\alpha}\,(n_\alpha - n_z) \equiv 0 \quad \Rightarrow \quad n_{\mathrm{L}} = n_{\mathrm{R}}$$

- Only the "zero" at $-U/2$ is of fundamental nature!
- Temperature gradient at which other zeros vanish:

$$\frac{\Delta T_{\mathrm{crit}}}{U} \approx \frac{1}{2}\left[\frac{T}{U}\exp\left(\frac{U}{2T}\right) - \frac{T}{U} - \frac{1}{2}\right]$$

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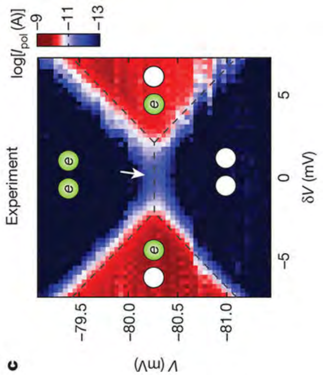
Recent realizations of **quantum dots with effective attractive electron interaction**:



Predict features in the Seebeck coefficient!

Hamo, *et al.*, Nature **535**, 395 (2016).
Prawiroatmodjo, *et al.*, Nat. Commun. **8**, 395 (2017).
G. Cheng, *et al.*, Nature **521**, 196 (2015).

Seebeck coefficient – quantum dots with attractive Coulomb interaction

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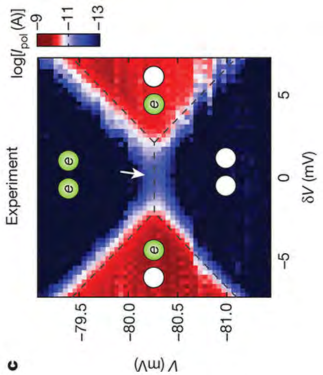

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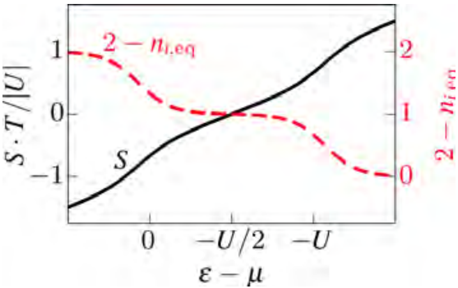

- Features at the resonances of the **inverted, repulsive** model!

J. Schulenborg, M.R. Wegewijs, J. Splettstoesser, *et al.*, unpublished.

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Fourier coefficient

"heat transfer in the absence of a charge current" (non tight-coupling)

Unexpected twist in the relation between Ohm's law and Fourier law

$$G = \frac{I}{V} \qquad \kappa = \frac{J|_{I=0}}{\Delta T}$$

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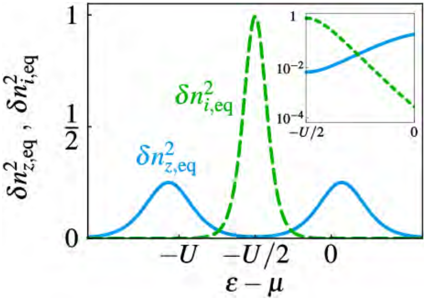

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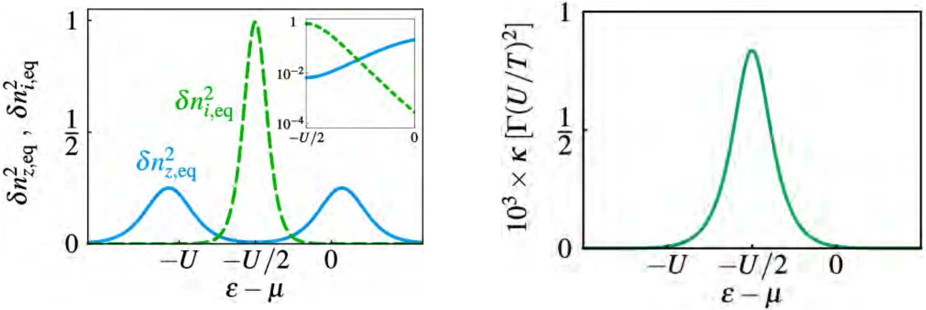

J. Schulenborg, A. Di Marco, J. Vanherck, M. R. Wegewijs, and J. Splettstoesser, Entropy **19**, 668 (2017).

Nonlinear Fourier heat

"Heat transfer in the absence of a charge current" (non tight-coupling ⇒ **parity mode!**)

$$\kappa_{\mathrm{nl}}^{\mathrm{L}} := \frac{J^{\mathrm{L}}|_{I=0}}{\Delta T} \quad = \quad -\gamma_{p\mathrm{L}} \frac{U}{\Delta T} \left(z_{\mathrm{iL}} (-1)^N | z \right) \Big|_{I=0}$$

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$$= \frac{1}{4} \frac{\Gamma_{\mathsf{L}} \Gamma_{\mathsf{R}}}{\Gamma^2} \frac{U}{\Delta T} \left(p_{z\mathsf{L}} - p_{z\mathsf{R}} \right) \Big|_{I=0}$$

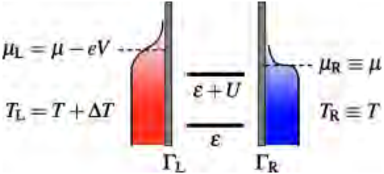
Compact **equilibrium** expressions!

$p_{z\mathsf{R}}$: (equilibrium) parity wrt right lead

at μ , T

$p_{z\mathsf{L}}$: (equilibrium) parity wrt left lead

at $\mu - S_{\mathsf{nl}}(\epsilon - \mu, U, T)\Delta T$, $T + \Delta T$.



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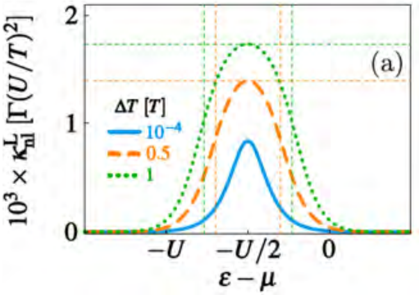
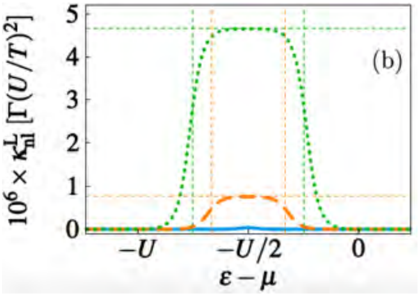
Nonlinear Fourier heat

Knowledge of the parity and the nonlinear Seebeck coefficient
$\rightarrow$ precise estimate of nonlinear Fourier heat

$$\kappa_{\mathrm{nl}}^{\mathrm{L}} = -\frac{1}{4}\frac{\Gamma_{\mathrm{L}}\Gamma_{\mathrm{R}}}{\Gamma^2}\frac{U}{4\Delta T}\left[\tanh\frac{U}{4(T+\Delta T)} - \tanh\frac{U}{4T}\right] \quad \text{for} \quad \left|\epsilon + \frac{U}{2} - \mu\right| \lesssim \frac{U}{2}\frac{\Delta T}{T+\Delta T}$$



U=10 T



U=30 T

J. Schulenborg, A. Di Marco, J. Vanherck, M. R. Wegewijs, and J. Splettstoesser, Entropy **19**, 668 (2017).

Conclusions and Outlook

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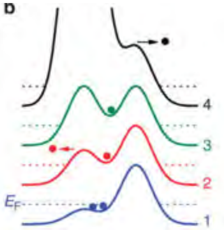
Can be extended to energy-dependent couplings

work in progress:

. . . ⇒ J. Schulenborg, J. Splettstoesser, and M. R. Wegewijs, to be submitted.
M. Kataoka, J. D. Fletcher, J. Schulenborg, J. Splettstoesser, *et al.*, in progress.



S. P. Giblin, M. Kataoka, J. D. Fletcher, P. See, T. J. B. M. Janssen, J. P. Griffiths, G. A. C. Jones, I. Farrer, D. A. Ritchie: Nat. Commun. **3**, 930 (2012)

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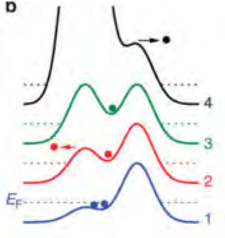

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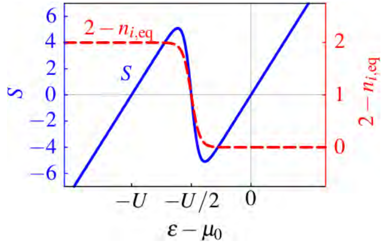
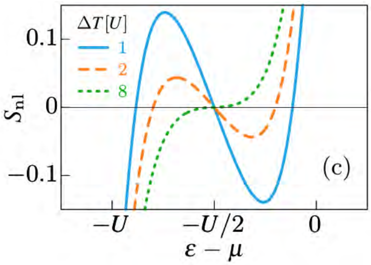
Seebeck coefficient

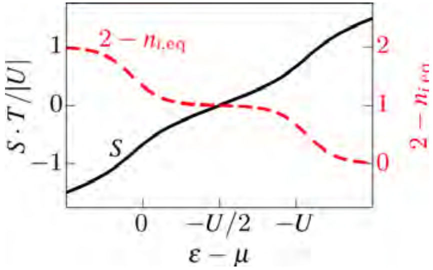
$$TS = \epsilon - \mu + \frac{U}{2}(2 - n_{\mathrm{i}})$$

- characteristic energy
- interpret feature otherwise

treated as “crossover"







Why is this particularly helpful for thermoelectrics?

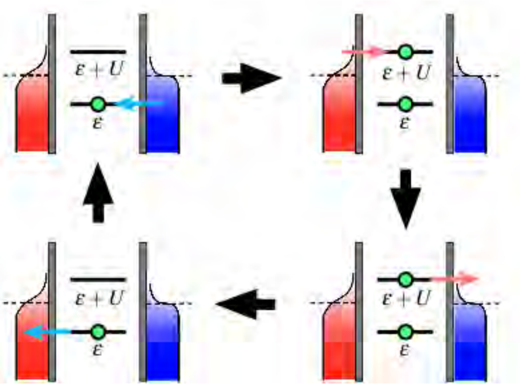
- In general: Fermion-parity duality imposes restrictions on open system dynamics
- **Important insight for Coulomb interaction physics**:

$$Un_\uparrow n_\downarrow = U - \frac{U}{2}(n_\uparrow + n_\downarrow) + \frac{U}{4}(-1)^{n_\uparrow + n_\downarrow}$$

- Thermoelectrics: energy stored on the dot in form of Coulomb interaction!

Fourier coefficient

"heat transfer in the absence of a charge current" (non tight-coupling)



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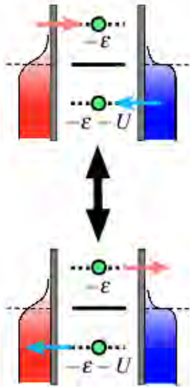
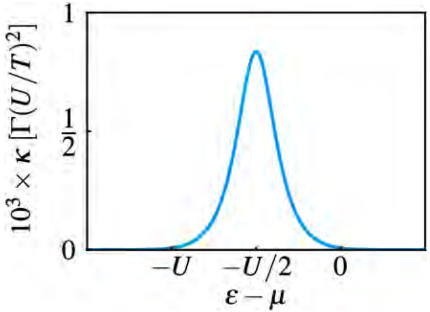


$$\kappa = \frac{J|_{I=0}}{\Delta T} = \frac{1}{T^2}\frac{\Gamma_\mathrm{L}\Gamma_\mathrm{R}}{\Gamma^2}\gamma_{p,\mathrm{eq}}\left(\frac{U}{2}\right)^2 \delta n^2_{z,\mathrm{eq}}\delta n^2_{\mathrm{i},\mathrm{eq}}$$



Derivation of the fermion parity duality

Derivation of the duality based on:

R. B. Saptsov, M. R. Wegewijs: Phys. Rev. B **86**, 235432 (2012); R. B. Saptsov, M. R. Wegewijs: Phys. Rev. B **90**, 045407 (2014).

- Take as convenient (exact) reference solution (in the wide-band limit), the solution for $T \to \infty$.
- Propagator $\Pi(t)$ of the time-evolution $\rho(t) = \Pi(t)\rho_0$ needs to be expanded around this reference solution only with respect to a part of the coupling (formally to all orders).

$$L^{\mathsf{T}} = L_+^{\mathsf{T}} + L_-^{\mathsf{T}} \quad , \quad L_q^{\mathsf{T}} = \sum_{12} T_{21} G_2^q J_1^{-q}$$

$$G_2^q \bullet = \frac{1}{\sqrt{2}} \left[d_2 \bullet + q(-\mathbf{1})^N \bullet (-\mathbf{1})^N d_2 \right] \quad , \quad J_1^q \bullet = \frac{1}{\sqrt{2}} \left[c_1 \bullet + q(-\mathbf{1})^{N^R} \bullet (-\mathbf{1})^{N^R} c_1 \right]$$

- For the extraction of this coupling part **heavily rely on the fermion-parity superselection principle**!
- Show duality based on propagator $\Pi(t)$ order by order in L_+.

For more details: see supplemental material of: J. Schulenborg, R. B. Saptsov, F. Haupt, J. Splettstoesser, and M. R. Wegewijs, Phys. Rev. B **93**, 081411(R) (2016).

Construction of eigenvectors and decay rates

Known mode

$|x) = x$

γ_x

Constructed co–vector

$(y'|$

$y' = (-\mathbf{1})^{\hat{N}} \mathcal{I} x$

$\gamma_y = \Gamma - \mathcal{I}\gamma_x$

Probability conservation:

$(z'| = (\mathbf{1}|$ $\quad \gamma_z = 0$

$(p'| = ((-\mathbf{1})^{\hat{N}} z_i| \approx (z_i|$

Duality:

$\gamma_p = \Gamma - 0 \quad |p) = |(-\mathbf{1})^{\hat{N}})$

$\gamma_z = 0 \quad |z)$

Charge mode is (known and) self-dual:

$(c'| \qquad \gamma_c \qquad |c)$

J. Schulenborg, R. B. Saptsov, F. Haupt, J. Splettstoesser, and M. R. Wegewijs, Phys. Rev. B **93**, 081411(R) (2016);
J. Vanherck, J. Schulenborg, R. B. Saptsov, J. Splettstoesser, and M. R. Wegewijs, Phys. Status solidi B **254**, 1600614 (2017).

Charge mode

Label	Amplitude	$-$ Eigenvalue $=$ decay rate	Mode
Zero (z)	$(z'_\alpha\| = (\mathbf{1}\|$ [trace]	$\gamma_{z\alpha} = 0$	$\|z_\alpha)$ [stationary state]
Charge (c)	$(c_\alpha{}'\| = (N\| - n_{z\alpha}(\mathbf{1}\|$ [$\sim$ charge operator]	$\gamma_{c\alpha} = \frac{\Gamma_\alpha}{2}\left[f_\alpha^+(\epsilon) + f_\alpha^-(\epsilon+U)\right]$	$\|c_\alpha) = \frac{1}{2}(-\mathbf{1})^{\hat{N}}\left[\|N) - n_{i\alpha}\|\mathbf{1})\right]$ [$\sim$ charge operator]
Parity (p)	$(p'_\alpha\| = (z_{i\alpha}(-\mathbf{1})^N\|$ [$\sim$ inverted stationary state]	$\gamma_{p\alpha} = \Gamma_\alpha$	$\|p_\alpha) = \|(-\mathbf{1})^N)$ [parity operator]

Estimates Seebeck coefficient

Linear Seebeck coefficient

$$T\,S = (\epsilon - \mu_{\text{eq}}) + \frac{U}{2}\left[2 - n_{\text{i,eq}}(\epsilon - \mu, U, T)\right]$$

Approximate occupation of the inverted stationary state

$$n_{\text{i,eq}} \approx 2f^{-}(2\epsilon + U) = 2\,f^{-}\left(\epsilon + \frac{U}{2}\right)\bigg|_{T\to T/2}$$

Find maxima

$$\frac{\partial n_{\text{i,eq}}}{\partial(\epsilon/T)} = \frac{2T}{U}$$

This gives

$$\frac{\epsilon_{\pm} - \mu_{\text{eq}}}{U} \approx -\frac{1}{2} \mp \frac{T/2}{U}\ln\left(\frac{U}{T/2}\right), \qquad S(\epsilon_{\pm}) \approx \pm\left[\frac{U}{2T} - \frac{1}{2}\left(1 + \ln\left(\frac{U}{T/2}\right)\right)\right]$$

Negative slope dominated by the interaction

$$\frac{dS}{d\epsilon}\bigg|_{\epsilon-\mu_{\text{eq}}=-U/2} \approx -\frac{1}{T}\left(\frac{U}{2T} - 1\right)$$