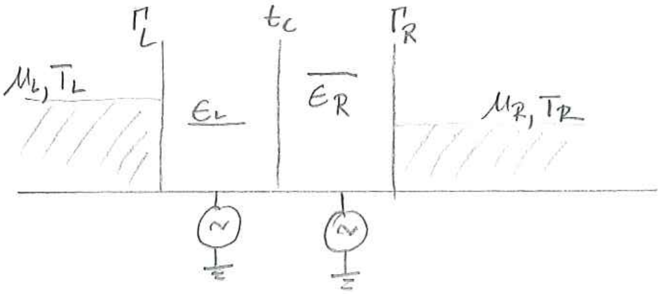
2. Operation and performance of a double-dot pump

we closely follow PRB 87, 245423 (2013)

2.1. System of interest



we have previously investigated the Hamiltonian and eigenstates of this system.

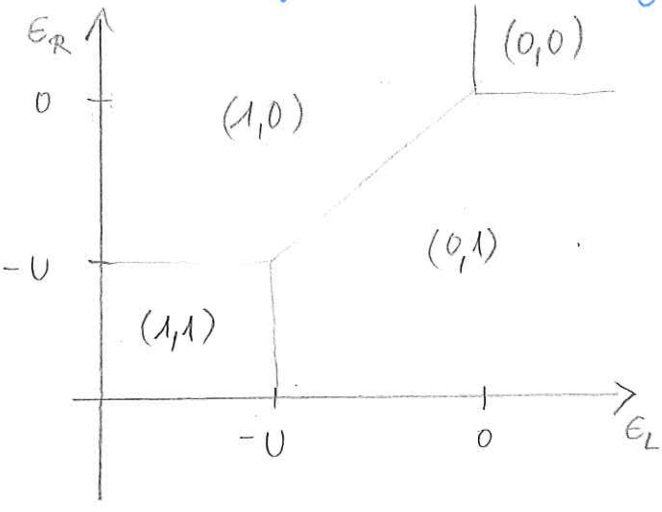
$$H_{tot} = \sum_{\alpha,k,\sigma} \epsilon_{\alpha k \sigma} c^\dagger_{\alpha k \sigma} c_{\alpha k \sigma} + \sum_{\alpha,k,\sigma} \left(t^{\alpha *}_{k\sigma} d^\dagger_{\alpha\sigma} c_{\alpha k \sigma} + h.c. \right)$$

$$+ \sum_\alpha \epsilon_\alpha \hat{n}_\alpha + U \hat{n}_L \hat{n}_R - \frac{t_c}{2} \sum_\sigma \left(d^\dagger_{L\sigma} d_{R\sigma} + h.c. \right)$$

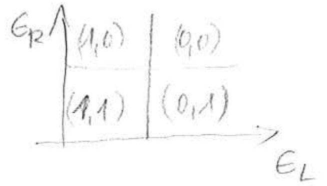
$$\epsilon_\alpha \equiv \epsilon_\alpha(t) = \bar{\epsilon}_\alpha + \delta\epsilon_\alpha(t)$$

$$= \bar{\epsilon}_\alpha + \delta\epsilon_\alpha \sin(\Omega t + \varphi_\alpha)$$ externally time-dependently driven parameters!

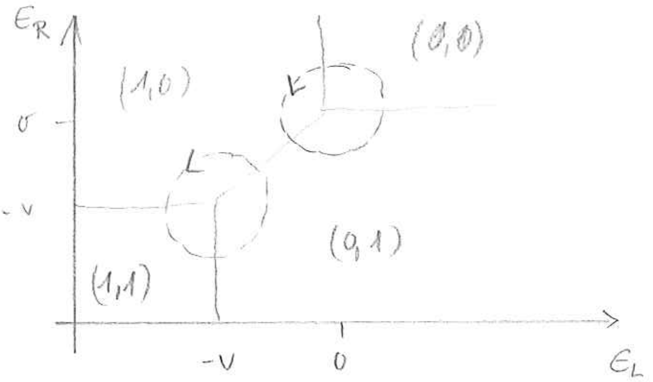
Stability diagram (stationary system, neglect interdot hopping)



to get this honeycomb shaped stability diagram interdot Coulomb is crucial! Otherwise, we would have:



Functioning of the pump

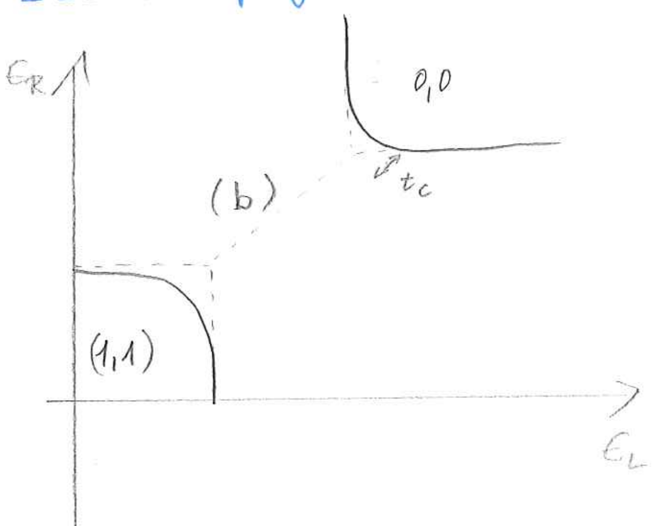


- pick a point $(\bar{\epsilon}_L, \bar{\epsilon}_R)$ around which parameters are driven
- choose amplitudes for the "size" of the cycle $\delta\epsilon, \delta\epsilon_R$
- choose a phase φ_α to fix the direction of the cycle

→ In a weakly coupled, slowly driven system, one charge after the other can be "squeezed" through the system.

- important condition: cycle needs to be large enough to enclose a triple point (one triple point, only)
- sign of the current depends on the triple point and the cycle direction
- quantization results from alternate coupling and decoupling to and from different reservoirs.

interdot coupling



relevant states (energy-eigenstates)

$$|s\rangle \in \{|0\rangle, |b\uparrow\rangle, |b\downarrow\rangle, |a\uparrow\rangle, |a\downarrow\rangle, |\uparrow\uparrow\rangle, |\downarrow\downarrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle\}$$

with $E_0 = 0$; $E_d = \epsilon_L + \epsilon_R + U$

$$E_{b/a} = E \mp \sqrt{\epsilon^2 + t_c^2}$$

with $E = \frac{1}{2}(\epsilon_L + \epsilon_R)$

$\epsilon = \epsilon_L - \epsilon_R$

Also the coupling constants to the energy eigenstates depend on the level positions!

$$\Gamma_{L,b/a} = \frac{\Gamma_L}{2}\left(1 \mp \frac{\epsilon}{\sqrt{\epsilon^2 + t_c^2}}\right)$$

$$\Gamma_{R,b/a} = \frac{\Gamma_R}{2}\left(1 \pm \frac{\epsilon}{\sqrt{\epsilon^2 + t_c^2}}\right)$$

$\Rightarrow$ far away from the (modified) triple points and the anticrossing, the situation is the same as when neglecting t_c

Further triple points get enlarged by

- voltage bias
- temperature smearing

$\rightarrow$ large cycles are required for (quantized) charge transport

$\rightarrow$ if $V_b > 0$ triple points merge and inhibit pumping

<u>Relevance of the double-dot pump for applications</u>

- source of single-particle current ($\rightarrow$ metrology)
- single-electron control
- pump charge <u>against</u> a bias

<u>Here</u>: - "battery charger"

in the presence of a temperature bias

- heat engine
- heat pump

2.2. Charge- and heat currents induced by time-dep. driving

To be calculated: $\quad I_\alpha^{(K)} = -e\, I_\alpha^{N(K)}$

with $\quad I_\alpha^{N(K)} = \sum\limits_{s,s'} (n_s - n_{s'})\, W^\alpha_{ss'}\, p_{s'}^{(K)} \qquad (*)$

and $\quad J_\alpha^{(K)} = I_\alpha^{E(K)} - \mu_\alpha I_\alpha^{N(K)}$

with $\quad I_\alpha^{E(K)} = \sum\limits_{s,s'} (E_s - E_{s'})\, W^\alpha_{ss'}\, p_{s'}^{(K)} \qquad (**)$

general properties of the charge current

$$I_L^{(K)}(t) + I_R^{(K)}(t) = -e \frac{d}{dt} \langle \hat{n} \rangle_t^{(K-1)}$$

with $\langle \hat{n} \rangle_t^{(K)} = \sum\limits_s n_s\, p_s^{(K)}$

E1 Exercise: show this relation using $(*)$ and the corresponding K-expansion of the master equation.

For time-averaged currents $\quad \bar{I} = \int\limits_0^{\mathcal{T}} \frac{dt}{\mathcal{T}}\, I(t)$

this yields: $\quad \bar{I}_L^{(K)} + \bar{I}_R^{(K)} = 0 \qquad$ (since driving is periodic)

general properties of the heat current

$$J_L^{(K)}(t) + J_R^{(K)}(t) = \sum_s E_s(t) \frac{d}{dt} p_s^{(K-1)} - V I^{(K)}(t)$$

with $I^{(K)}(t) = \frac{1}{2}\left(I_R^{(K)}(t) - I_L^{(K)}(t)\right)$

Exercise: show this relation using $(**)$ and the corresponding K-expansion of the master equation.

$\Rightarrow$ First principle of thermodynamics!!

Relates heat flow into the system to increase of energy and work done by (external) sources.

Even clearer when using

$$\sum_s E_s(t)\dot{p}_s(t) = \frac{d}{dt}\left(\sum_s E_s(t)p_s(t)\right) + \sum_s \dot{E}_s(t)p_s(t)$$

$$\Rightarrow \boxed{\begin{array}{ll} J_L^{(k)}(t) + J_R^{(k)}(t) = \frac{d}{dt}\langle E\rangle^{(k-1)} - \mathcal{P}_{ac}^{(k)} - \mathcal{P}_{dc}^{(k)} & \\ \text{with } \langle E\rangle^{(k)} = \sum_s E_s p_s^{(k)} & \text{internal energy} \\ \mathcal{P}_{ac}^{(k)} = \sum_s \dot{E}_s(t)\, p_s^{(k-1)}(t) & \text{work done by ac sources} \\ \mathcal{P}_{dc} = V I^{(k)}(t) & \text{work done by dc source (Joule's law)} \end{array}}$$

Note: we have derived the first law of thermodynamics (for a driven system) by doing a transport calculation!

we can clearly identify

- heat flow into the system
- change of internal energy
- work done by/on sources (depending on sign)

2.3. Results for the pumping current

slow driving : consider expansion up to $k = 1$

$k=0$: only yields a current inthe presence of a stationnary bias and in the vicinity of triple points.

→ can be excluded by choosing large cycles and limited external bias.

$k=1$: adiabatic-response. describes minimal delay that is needed to allow for a pumping current.

Charge current

Simple analytical solution from the Master equation calculation

$$I_\alpha^{(1)}(t) = -e \sum_{\eta=a,b} \frac{\Gamma_{\alpha,\eta}}{\Gamma_\eta} \left[\frac{d}{dt} p_\eta^{(0)} + \frac{d}{dt} p_d^{(0)} \right]$$

with $\Gamma_\eta = \Gamma_{\eta,L} + \Gamma_{\eta,R}$

$0 \leftrightarrow 1$ triple point : transport mostly via bonding state
$1 \leftrightarrow 2$ triple point : transport mostly via antibonding state

(contribute with opposite sign)

Next step: calculate the (experimentally) relevant time-average.

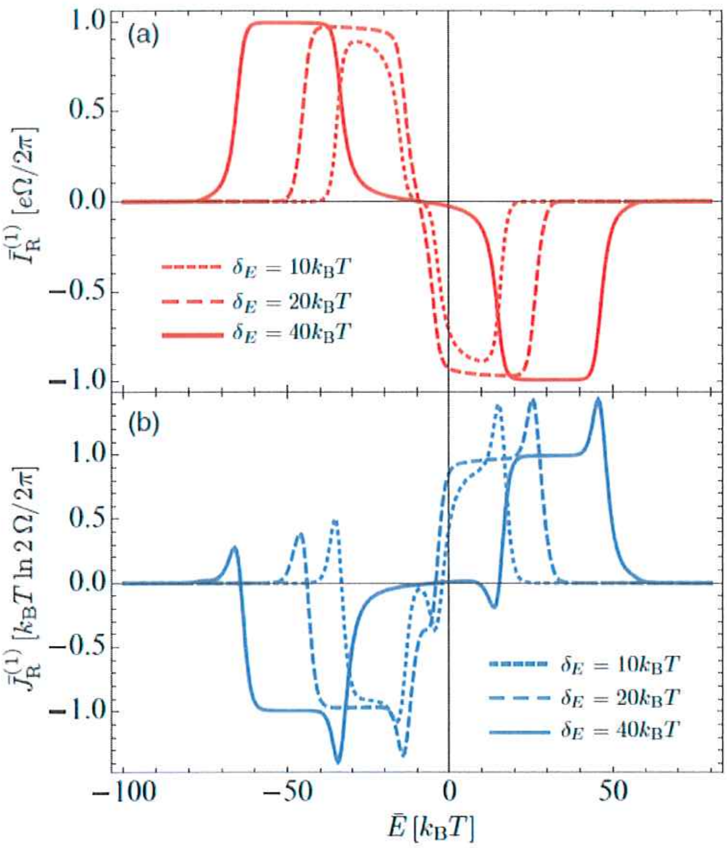


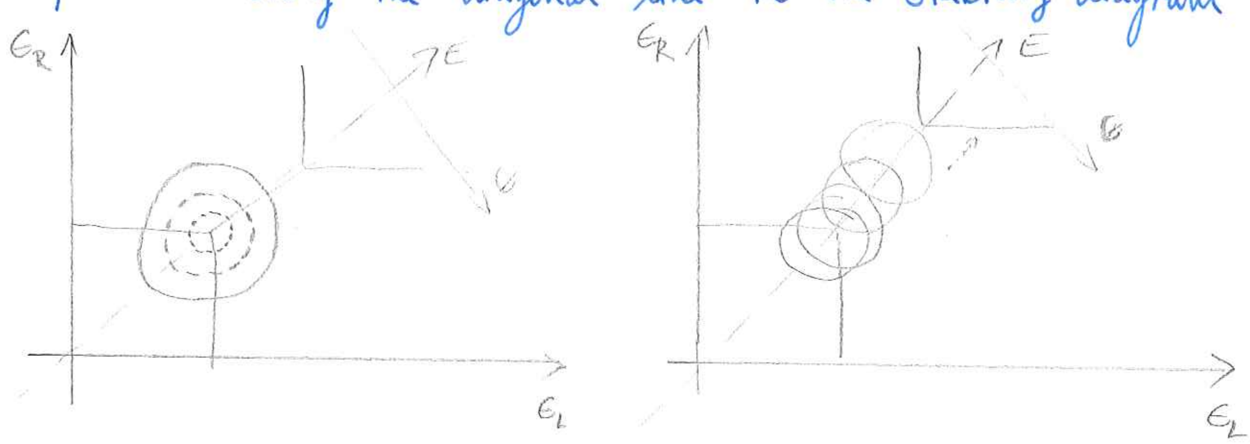
FIG. 2. (Color online) Contributions to first order in Ω to the average charge (a) and heat (b) currents plotted as a function of the mean energy $\bar{E}$. The pumping cycle is defined by $\delta_\varepsilon = 2\delta_E$, $\bar{\varepsilon} = 0$, $\phi = \pi/2$, and $\Omega = \Gamma/200$, and it corresponds to a circular orbit centered around zero detuning. In both panels, $T_L = T_R = T$, $V = 0$, $U = 20 k_BT$, $t_c = 10 k_BT$, $\Gamma_L = \Gamma_R = \Gamma/2$, and $\hbar\Gamma = k_BT/4$.

Result for the time averaged charge current, where we use the driving parameters

$$E(t) = \frac{1}{2}\left(\epsilon_L(t) + \epsilon_R(t)\right)$$

$$\epsilon(t) = \epsilon_L(t) - \epsilon_R(t)$$

→ plots are along the diagonal line in the stability diagram



→ depending on cycle size and position quantized charge can be transported in either direction.

- detuning has to be large enough to include the triple point
- U has to be large to separate triple points

→ maximum plateau size $\sim U + t_c$
[further reduced by applied bias and temperature smearing]

heat current

has in general a more complicated form
(we will address this issue in the next example study)

can be approximated by (if splitting between $|a\rangle$ and $|b\rangle$ is large)

$$J_\alpha^{(1)}(t) \approx -\epsilon_b(t)\frac{\Gamma_{\alpha,b}}{\Gamma_b}\frac{d}{dt}P_0^{(0)} + (\epsilon_a + U)\frac{\Gamma_{\alpha,a}}{\Gamma_a}\frac{d}{dt}P_d^{(0)} \qquad (0)$$

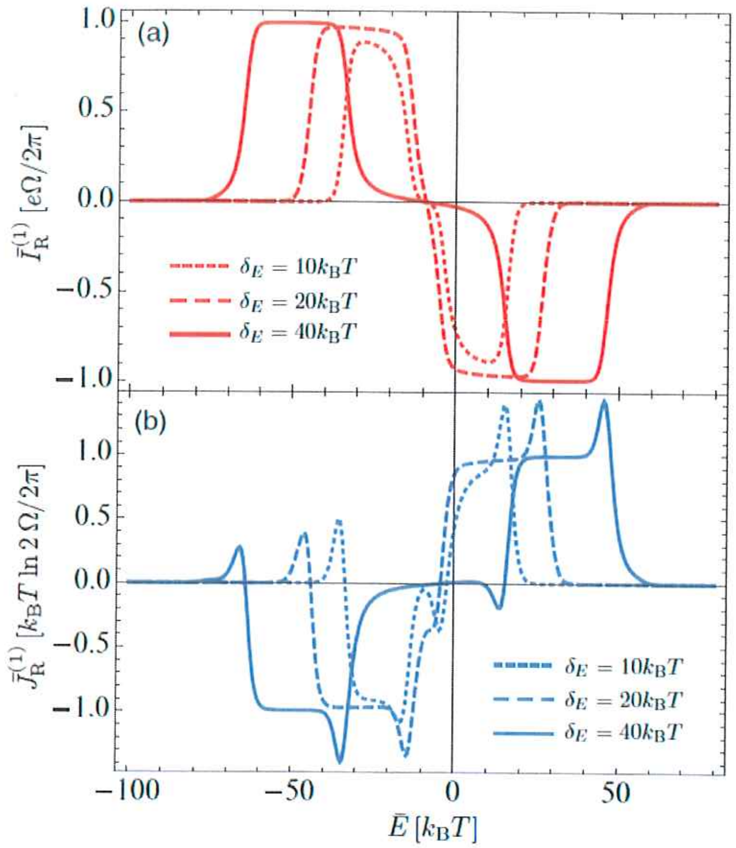
energy involved in the transition $0 \Leftrightarrow b$

energy involved in the transition $b \Leftrightarrow d$

time-averaged heat current

plateau-like features with side-peaks/dips

plateau height $\pm \frac{\Omega}{2\pi} k_B T \ln 2$



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What is the origin of this "quantized" value ?

For the time-averaged heat current for cycles fully enclosing a triple point, one can show

$$\frac{\bar{J}_\alpha^{(1)}}{k_B T} = \int_0^{\mathcal{T}} \frac{dt}{\mathcal{T}} \frac{\Gamma_{\alpha,\eta}}{\Gamma_\eta} \frac{d}{dt} S^{(0)} = \frac{1}{\mathcal{T}} \Delta S_\alpha^{(0)} \qquad (\bullet)$$

with the entropy difference due to the relevant tunneling event $\Delta S_\alpha^{(0)}$

Here $\Delta S_\alpha^{(0)} = \pm \ln 2$ due to spin-degeneracy of states.

E3 Exercise

Task: Show the agreement between Eqs. (0) and (⊛) with

$\Delta S_L^{(0)} = \pm \ln 2$.

Therefore take the following steps for the heat current into one specific lead (e.g. $\alpha = L$) and one specific triple point (e.g. $(\epsilon_L \epsilon_R) \approx (0,0)$).

a.) express the entropy $S^{(0)}$ together with $\dot{S}^{(0)}$ in terms of probabilities $p_s^{(0)}$ ($\dot{p}_s^{(0)}$). Which of these probabilities are nonzero (and possibly time-dependent) in the vicinity of the selected triple point?

b.) In the absence of a bias, the probabilities have the form

$$p_s^{(0)} = \frac{e^{-E_s/k_B T}}{\sum_s e^{-E_s/k_B T}}$$

Using this, show that $\frac{\Gamma_{\alpha,\eta}}{\Gamma_\eta} \frac{d}{dt} S^{(0)}$ equals the corresponding term of (0) for the selected triple point.

c.) Identify the contributing transitions for a large cycle around a triple point by investigating the prefactor $\frac{\Gamma_{\alpha,\eta}}{\Gamma_\eta}$.

d.) Evaluate the entropy change of the identified tunneling transition.

- $k_B T \ln 2$ is the minimum energy required to erase a bit of information (Landauer principle). Here encoded in the spin

→ see also Koski et al. PRL 113, 030601 (2014)
for a charge-state analogue in metallic islands.

- energy $k_B T \ln 2$ is provided by the external ac fields and flows with tunneling electrons.

lift spin degeneracy

apply a large magnetic field $B \gg k_B T$

⇒ $\Delta S = 0$ for all transitions between states along a cycle including a triple point

⇒ suppressed energy flow !!

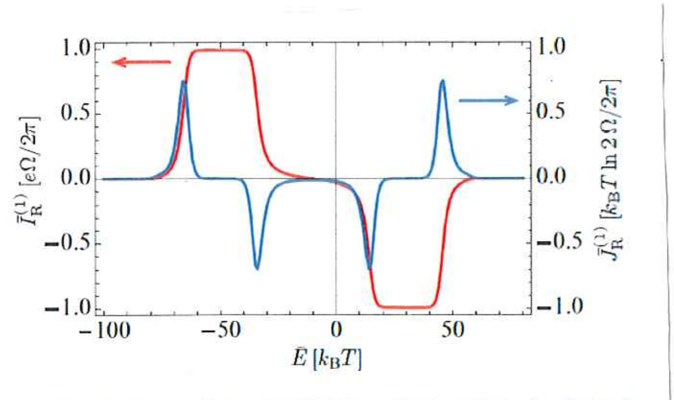


FIG. 3. (Color online) Contributions to first order in Ω to the average charge and heat currents for the case of a fully spin-polarized system. The pumping cycle is defined by $\delta_E = 40 k_B T$, $\delta_\varepsilon = 2\delta_E$, $\bar{\varepsilon} = 0$, $\phi = \pi/2$, and $\Omega = \Gamma/200$. Other parameters are $T_L = T_R = T$, $V = 0$, $U = 20 k_B T$, $t_c = 10 k_B T$, $\Gamma_L = \Gamma_R = \Gamma/2$, and $\hbar\Gamma = k_B T/4$.

Information-theoretical perspective:

no useful information is carried by a flow of fully spin-polarized electrons

Question: What is the origin of peaks and dips at the border of the (charge) plateaus ?

What determines their height ?

Reversible processes

* In the absence of a temperature gradient, Eqs. (●) and (○) allow us to write:

$$J_L^{(1)}(t) + J_R^{(1)}(t) = k_B T \cdot \frac{dS^{(0)}}{dt}$$

⇒ the process is reversible !

with $\bar{J}_L + \bar{J}_R = 0$ [heat is transported from one lead to the other]

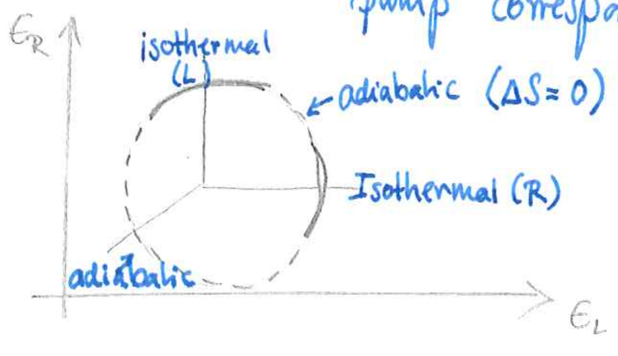
* for non-vanishing $\Delta T = T_L - T_R$, but large cycles (→ with full coupling / decoupling from reservoirs)

for each system-reservoir coupling: $\bar{J}_\alpha^{(1)} = \frac{1}{\mathcal{T}} k_B T_\alpha \Delta S_\alpha^{(0)}$

isothermal transitions!

different temperatures

⇒ cycle of the double-dot pump corresponds to a Carnot-cycle !



2.4. Performance of the 3 types of double-dot engines

charge pump / "battery charger"

$\Delta T = 0$, pump charge against a bias voltage V

→ possible for moderate bias, such that $|I^{(0)}| < |I^{(1)}|$

Efficiency: $\eta_{ch} = \dfrac{-\bar{I}V}{\bar{\mathcal{P}}_{ac}}$

← work done by pumping against bias $(-\bar{I}V > 0)$ on the dc source

← power provided by ac-sources

from 1st law: $\bar{\mathcal{P}}_{ac} = -\bar{J}_L - \bar{J}_R - \bar{\mathcal{P}}_{dc}$

↑ work done by the dc source

$$\Rightarrow \quad \eta_{ch} = \frac{+\bar{I}V}{\underbrace{\bar{J}_L + \bar{J}_R}_{\substack{=0 \text{ for } \Delta T = 0 \\ \text{and large cycles}}} + \bar{I}V} \longrightarrow 1$$

Heat pump / refrigerator

$V = 0 \quad \Delta T = T_{hot} - T_{cold}$ create a heat current out of the cold reservoir by pumping

coefficient of performance (efficiency of cooling)

$$COP = \frac{\bar{J}_{cold}}{\bar{\mathcal{P}}_{ac}}$$

← heat current out of cold reservoir

← work provided by ac-sources

with $V=0$, first law: $\bar{\mathcal{P}}_{ac} = -\bar{J}_{cold} - \bar{J}_{hot}$

for a large cycle $\bar{J}_{cold/hot} = \pm k_B T_{cold/hot} \ln 2 \frac{1}{\tau}$

$$\Rightarrow \quad COP \rightarrow \frac{T_{cold}}{T_{hot} - T_{cold}}$$ Carnot limit of cooling process!

Heat engine

$V=0$, use ΔT to do work on ac sources

$$\eta = \frac{-\bar{\mathcal{P}}_{ac}}{\bar{J}_{hot}}$$
$\leftarrow$ work done on the ac sources

$\leftarrow$ heat extracted from the hot reservoirs

with $V=0$, we have $-\bar{\mathcal{P}}_{ac} = \bar{J}_{hot} + \bar{J}_{cold} \underset{\uparrow}{=} \frac{1}{\tau} k_B (T_{hot} - T_{cold}) \ln 2$

large enough cycle

$$\Rightarrow \eta = \frac{T_{hot} - T_{cold}}{T_{hot}} = 1 - \frac{T_{cold}}{T_{hot}} = \eta_{carnot}$$

2.5. Limitations of the double-dot engines

ideal efficiencies are only obtained in specific cases !!

limitations occur due to

* <u>leakage currents</u> for - large voltage / temperature bias
  - small cycles
  - higher order tunnel coupling
* <u>Joule heating</u> due to faster driving $J \sim \Omega^2$

more details in PRB 87, 245423 (2013)