Role of work in matter exchange between finite quantum systems

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Acknowledgments

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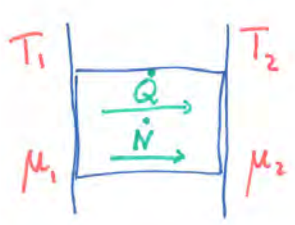
Overview

- Onsager relations
- Contacting two pieces of matter with different temperatures and chemical potentials
- Fluctuation relations for exchanged energy and particle numbers
- Work and heat
- Zero work: Onsager OK!
- Finite work: Onsager fails!
- Example
- Conclusions

E. Jeon, P. Talkner, J. Yi, Y.W. Kim, New J. Phys. **19**, 093006 (2017).

Onsager relations



$L_{Q,N} = L_{N,Q}$: reciprocity relation

$L = \begin{pmatrix} L_{Q,Q} & L_{Q,N} \\ L_{Q,N} & L_{N,N} \end{pmatrix}$: positive semi-definite, controls the flow direction

$$\dot{Q} = L_{Q,Q}\Delta\beta + L_{Q,N}\Delta(-\beta\mu)$$
$$\dot{N} = L_{N,Q}\Delta\beta + L_{N,N}\Delta(-\beta\mu)$$

Conditions: near equilibrium, i.e.

$|\Delta\beta| \equiv \; |\frac{1}{k_B T_1} - \frac{1}{k_B T_2}| \ll \bar{\beta} \equiv (\frac{1}{k_B T_1} + \frac{1}{k_B T_2})/2$

$|\Delta\beta\mu| \equiv |\frac{\mu_1}{k_B T_1} - \frac{\mu_2}{k_B T_2}| \ll (\frac{\mu_1}{k_B T_1} + \frac{\mu_2}{k_B T_2})/2$

The exchanged quantities (here Q and N) must undergo a Gauss-Markov process obeying the principle of detailed balance. For non-Markovian processes, as e.g. caused by the presence of other slow variables, deviations from the Onsager reciprocity relations may occur.[*]

Based on a fluctuation relation, Jarzynski and Wójcik investigated the statistics of transferred heat for classical systems.[†] Likewise, Andrieux et al. derived the Onsager relations for heat and particle transport between several quantum mechanical reservoirs.[‡] Both derivations rely on the assumption of very large but finite reservoirs.

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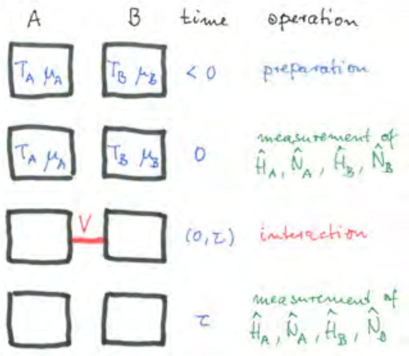
[*] G.F. Hubmer, U.M. Titulaer, J. Stat. Phys. **49**, 331 (1987).

[†] C. Jarzynski, D.K. Wóicik, Phys. Rev. Lett. **92**, 230602 (2004).

[‡] D. Andrieux, P. Gaspard, T. Monnai, S. Tasaki, New J. Phys. **11**, 043014 (2009).

Protocol



$$\hat{H}(t) = \hat{H}_A + \hat{H}_B + \hat{V}(t)$$
$$\hat{V}(t) = \Theta(t)\Theta(\tau - t)V$$
$$[\hat{H}_\alpha, \hat{N}_{\alpha'}] = 0, \; \alpha, \alpha' = A, B$$
$$[V, \hat{N}_A + \hat{N}_B] = 0$$

grand canonical initial state:

$$\hat{\rho}(0) = \prod_{\alpha=A,B} e^{-\beta_\alpha(\hat{H}_\alpha - \mu_\alpha \hat{N}_\alpha)} / \mathcal{Z}_\alpha$$
$$\mathcal{Z}_\alpha = \mathrm{Tr}_\alpha e^{-\beta_\alpha(\hat{H}_\alpha - \mu_\alpha \hat{N}_\alpha)}$$

Fluctuation relation

Potential measurement results: Eigenvalues $E_j^A, N_j^A, E_j^B, N_j^B$ of the respective operators; $j = i, f$: complete set of quantum numbers. From the two measurements the exchanged energies, $\Delta E_\alpha = E_f^\alpha - E_i^\alpha$, and particle numbers, $\Delta N = N_f^A - N_i^A = -N_f^B + N_i^B$, follow with probability[§]

$$P_{\Delta E}(\Delta E_A, \Delta E_B, \Delta N) = \sum_{f,i} p(f,i)\delta(\Delta N - N_f^A + N_i^A) \times \prod_{\alpha=A,B} \delta(\Delta E_\alpha - E_f^\alpha + E_i^\alpha)$$

$$p(f,i) = T_{f|i} P_i, \quad T_{f|i} = |\langle f|\hat{U}|i\rangle|^2 = T_{i|f}, \quad \hat{U} = e^{-i(\hat{H}_A + \hat{H}_B + V)\tau/\hbar}$$

$$P_i = \prod_{\alpha=A,B} e^{-\beta_\alpha(E_i^\alpha - \mu_\alpha N_i^\alpha)}/\mathcal{Z}_\alpha, \quad P_i = e^{M_{f,i}} P_f$$

$$M_{f,i} = \sum_\alpha \beta_\alpha \left[(E_f^\alpha - E_i^\alpha) - \mu_\alpha (N_f^\alpha - N_i^\alpha)\right]$$

[§] M. Campisi, P. Hänggi, P. Talkner, Rev. Mod. Phys. **83**, 771 (2011).

$$\frac{P_{\Delta E}(\Delta E_A, \Delta E_B, \Delta N)}{P_{\Delta E}(-\Delta E_A, -\Delta E_B, -\Delta N)} = e^{\sum_\alpha \beta_\alpha(\Delta E_\alpha - \mu_\alpha \Delta N_\alpha)}$$

Introducing work and heat as

$$W = \Delta E_A + \Delta E_B, \quad Q = (\Delta E_A - \Delta E_B)/2 - \bar{\mu}\Delta N, \quad \bar{\mu} = (\mu_A + \mu_B)/2$$

one obtains a fluctuation relation for work, heat and exchanged particle number:

$$\boxed{\frac{P_{WQ}(W, Q, \Delta N)}{P_{WQ}(-W, -Q, -\Delta N)} = e^{\bar{\beta} W + \Delta\beta Q - \bar{\beta}\Delta\mu\Delta N}}$$

$$P_{WQ}(W, Q, \Delta N) = P_{\Delta E}(W/2 + Q + \bar{\mu}\Delta N, W/2 - Q - \bar{\mu}\Delta N, \Delta N)$$

Vanishing Work

Assume $W = 0$ is the only possible outcome:

$$P_{WQ}(W, Q, \Delta N) = \delta(W) P_Q(Q, \Delta N)$$

$$\Longrightarrow$$

$$P_Q(Q, \Delta N) = e^{Q\Delta\beta - \Delta N \bar{\beta}\Delta\mu} P_Q(-Q, -\Delta N)$$

$$\xRightarrow{\int dQ d\Delta N}$$

$$\langle e^{Q\Delta\beta - \Delta N \bar{\beta}\Delta\mu} \rangle = 1$$

$$\xRightarrow{\text{Jensen}}$$

$$\Delta\beta \langle Q \rangle - \bar{\beta}\Delta\mu \langle \Delta N \rangle \geq 0$$

Usual directionality of average heat and particle flow not only close to equilibrium.

$W = 0$, close to equilibrium

$|\Delta\beta Q|, |\bar{\beta}\Delta\mu\Delta N| \ll 1$:

$$P_Q(Q,\Delta N) = \underbrace{e^{Q\Delta\beta - \Delta N\bar{\beta}\Delta\mu}}_{\approx 1+\Delta\beta Q - \bar{\beta}\Delta\mu\Delta N} P_Q(-Q,-\Delta N)$$

$\int dQd\Delta NQ\times\ldots, \int dQd\Delta N\Delta N\times\ldots$:

$$\langle Q\rangle = \frac{1}{2}\left[\langle Q^2\rangle_0^0\Delta\beta - \langle Q\Delta N\rangle_0^0\bar{\beta}\Delta\mu\right]$$

$$\langle \Delta N\rangle = \frac{1}{2}\left[\langle Q\Delta N\rangle_0^0\Delta\beta - \langle \Delta N^2\rangle_0^0\bar{\beta}\Delta\mu\right]$$

$$\langle\cdot\rangle_0^0 = \int dQd\Delta N \cdot P_Q^{\Delta\beta=\Delta\mu=0}(Q,\Delta N)$$

If one can assume that after a short time $t \ll \tau$ a quasi-stationary state establishes extending up to τ, $Q \approx \dot{q}\tau$ and $\Delta N \approx \dot{n}\tau$ with constant heat and particle fluxes $\dot{q}$ and $\dot{n}$. These fluxes are related by a symmetric and non-negative matrix to the affinity differences $\Delta\beta$ and $-\bar{\beta}\Delta\mu$ and hence comply with the Onsager relations.

Finite work, close to equilibrium

$\Delta\beta \ll \bar{b}$, $\Delta\mu \ll \bar{\mu}$, $W \neq 0$:

$$\langle Q\rangle = \langle X^{\beta}(\tau) - X^{\beta}(0)\rangle_0 + C_{\beta,\beta}\Delta\beta + C_{\beta,\mu}(-\bar{\beta}\Delta\mu)$$
$$\langle \Delta N\rangle = \langle X^{\mu}(\tau) - X^{\mu}(0)\rangle_0 + C_{\mu,\beta}\Delta\beta + C_{\mu,\mu}(-\bar{\beta}\Delta\mu)$$

$$X_j^{\beta} = \tfrac{1}{2}\left[\delta E_j^A - \delta E_j^B - \bar{\mu}(\delta N_j^A - \delta N_j^B)\right], \quad C_{\chi,\eta} = -\langle [X^{\chi}(\tau) - X^{\chi}(0)] X^{\eta}(0)\rangle_0$$
$$X_j^{\mu} = \tfrac{1}{2}\left(\delta N_j^A - \delta N_j^B\right), \quad \delta Y_j^{\alpha} = Y_j^{\alpha} - \textstyle\sum_j Y_j^{\alpha} P_j^0, \quad Y_j^{\alpha} = E_j^{\alpha}, N_j^{\alpha}$$
$$\langle\cdot\rangle_0 = \textstyle\sum_{i,f} \cdot\, T_{f|i} P_i^0, \quad P_i^0 = \prod_{\alpha=A,B} e^{-\bar{\beta}(E_i^{\alpha} - \bar{\mu} N_i^{\alpha})}/Z_{\alpha}^0$$

Deviations from Onsager:
(i) Offset $\langle X^{\chi}(\tau) - X^{\chi}(0)\rangle_0$ independent of affinity differences $\Delta\beta$ and $\Delta\mu$, leading to spontaneous transport and possibly to transport opposite to the "normal" direction.
(ii) Reciprocity relations are violated: $C_{\chi,\eta} \neq C_{\eta,\chi}$.

Both deviations are a consequence of contacting and separating the two parts, an operation that performs work on the total system and breaks the time translational symmetry.

Modified heat and particle number

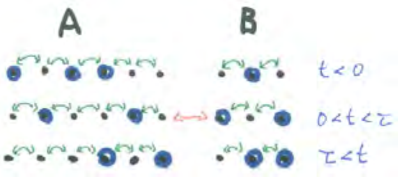
$$\langle Q(e^{-\bar{\beta}W}+1)\rangle = 2\left(L_{\beta,\beta}\Delta\beta + L_{\beta,\mu}(-\bar{\beta}\Delta\mu)\right)$$
$$\langle \Delta N(e^{-\bar{\beta}W}+1)\rangle = 2\left(L_{\mu,\beta}\Delta\beta + L_{\mu,\mu}(-\bar{\beta}\Delta\mu)\right)$$

$$2L_{\chi,\eta} = \langle (X^{\chi}(\tau) - X^{\chi}(0))\,(X^{\eta}(\tau) - X^{\eta}(0))\rangle_0$$

L: symmetric and non-negative definite.
$D = L - C$: deviation from the transport matrix governing Q and Δn.

$$2D_{\chi,\eta} = \langle (X^{\chi}(\tau) - X^{\chi}(0))\,(X^{\eta}(\tau) + X^{\eta}(0))\rangle_0$$

Example



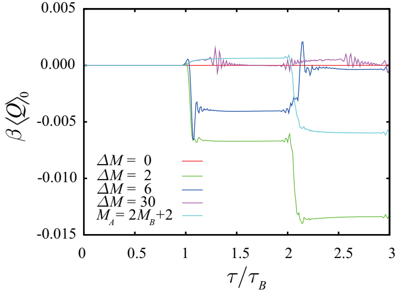
$$\hat{H}_\alpha = -\gamma \sum_{x_\alpha=1}^{M_\alpha-2} \left[\hat{c}^\dagger_{x_\alpha} \hat{c}_{x_\alpha+1} + \hat{c}^\dagger_{x_\alpha+1} \hat{c}_{x_\alpha} \right], \quad \alpha = A, B$$

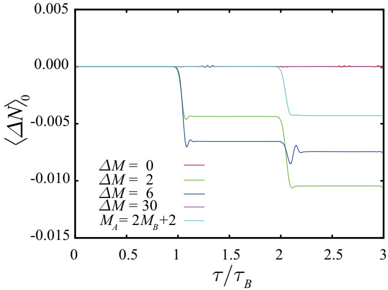
$$V = -\gamma_C \left(\hat{c}^\dagger_{1_A} \hat{c}_{1_B} + \hat{c}^\dagger_{1_B} \hat{c}_{1_A} \right)$$

$$\hat{N}_\alpha = \sum_{x_\alpha=1}^{M_\alpha-1} \hat{c}^\dagger_{x_\alpha} \hat{c}_{x_\alpha}$$

$\hat{c}^\dagger_{x_\alpha}$ ($\hat{c}_{x_\alpha}$): Fermion creation (annihilation) operator of a particle at site x_α.

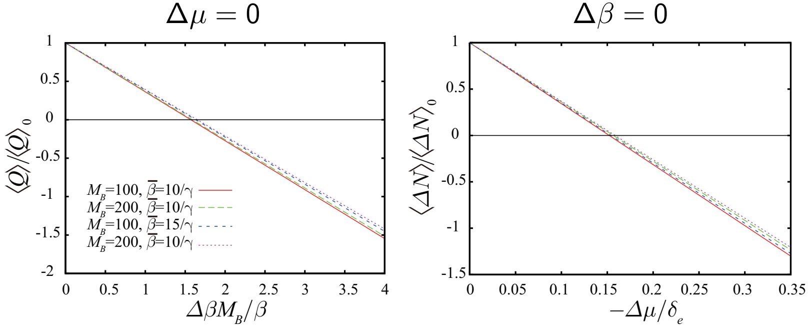
Spontaneous transport



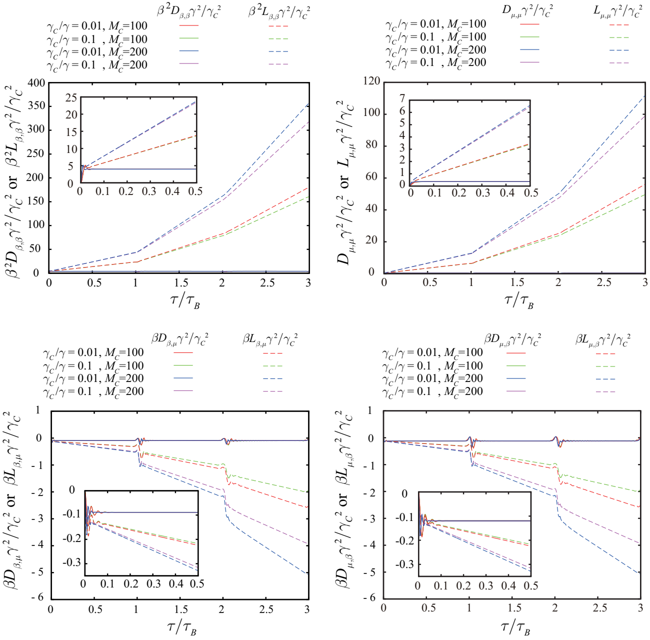


$\Delta M = M_A - M_B$, $\beta_A = \beta_B = 10/\gamma$, $\mu_A = \mu_B = 0.2\gamma$, $\gamma_C = 0.1\gamma$.
$\tau_B = M_B\hbar/\gamma$: round trip time in B.

Inversion of transport direction

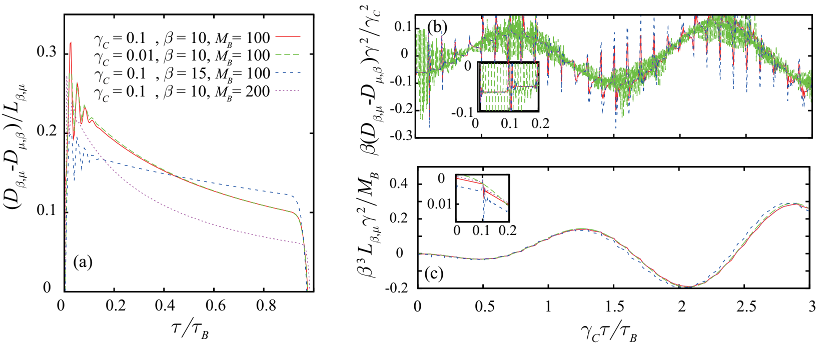


Amount of heat (left) and particles (right) transported at $1.5\tau_B$. At small affinity biases the transport goes into the "wrong" direction. $\delta_e = 2\gamma/M_B$ denotes the level splitting near the band center. $\Delta M = 2$.



β²D_{β,β}γ²/γ_C²
β²L_{β,β}γ²/γ_C²
γ_C/γ = 0.01, M_C=100
γ_C/γ = 0.1 , M_C=100
γ_C/γ = 0.01, M_C=200
γ_C/γ = 0.1 , M_C=200
β²D_{β,β}γ²/γ_C² or β²L_{β,β}γ²/γ_C²
τ/τ_B
D_{μ,μ}γ²/γ_C²
L_{μ,μ}γ²/γ_C²
D_{μ,μ}γ²/γ_C² or L_{μ,μ}γ²/γ_C²
βD_{β,μ}γ²/γ_C²
βL_{β,μ}γ²/γ_C²
βD_{β,μ}γ²/γ_C² or βL_{β,μ}γ²/γ_C²
βD_{μ,β}γ²/γ_C²
βL_{μ,β}γ²/γ_C²
βD_{μ,β}γ²/γ_C² or βL_{μ,β}γ²/γ_C²

Transport asymmetry



Conclusions

- Contacting and separating two systems changes the total energy and breaks the time-translation symmetry.
- This may lead to spontaneous transport in the absence of any affinity bias and to deviations of the transport matrix from the Onsager symmetry.
- While the deviation D of the actual transport-matrix C from the symmetric and positive matrix L initially changes jump-like, it stays almost constant, and C itself changes piece-wise linearly with breaks at multiples of the signal propagation time in the smaller system.
- In the limit of two large systems, the work done by contacting and separating them can be neglected and the Onsager symmetries are recovered. Spontaneous transport may be seen only after a large time.

For more details see:

E. Jeon, P. Talkner, J.Yi, Y.W. Kim, New J. Phys. **19**, 093006, (2017).