Local Equilibrium Aspects of Small Quantum Systems

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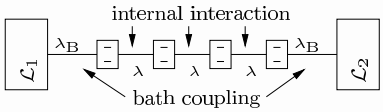
Introduction

We have been considering small quantum systems built up of several weakly coupled subsystems. Despite the fact that the total system is described by pure unitary Schrödinger dynamics, we find any single subsystem to be in a thermal equilibrium state as theoretically predicted [1]. If we couple such low-level systems additionally to an environment (many level systems under full system Schrödinger dynamics or modeled by the Lindblad formalism) the system is globally as well as locally at the same temperature, dependent on the type and strength of the internal couplings. Within such a diminutive system also non-equilibrium properties like quantum heat conduction [2] can be studied. Indeed, we have found a normal heat conductance for many different internal coupling types, but also ballistic transport scenarios.

[1] J. Gemmer, M. Michel and G. Mahler, *Quantum Thermodynamics*, in press, Springer (2004)
[2] M. Michel, M. Hartmann, J. Gemmer and G. Mahler, Eur. Phys. J. B **34**, 325 (2003)

Local Equilibrium Model

Here we investigate a chain of N weakly interacting subsystems with next neighbor Heisenberg interaction, Förster (only energy exchange) coupling or a totally random interaction, according to the Hamiltonian $\hat{H} = \hat{H}_{\rm loc} + \hat{H}_{\rm int}$. Additionally, the system is coupled at both ends to separate heat baths with temperature $T_{\rm mean} \pm \Delta T$. The Liouville-von-Neumann equation for the density operator of the system reads



$$\frac{\partial\hat{\rho}}{\partial t} = \mathcal{L}\hat{\rho} = \Big(\mathcal{L}_{\rm sys} + \mathcal{L}_1(T_{\rm mean}+\Delta T) + \mathcal{L}_2(T_{\rm mean}-\Delta T)\Big)\hat{\rho}\,, \qquad (1)$$

with the coherent part

$$\mathcal{L}_{\rm sys}\hat{\rho} = -\frac{\rm i}{\hbar}\,[\hat{H},\hat{\rho}]$$

and two incoherent Lindblad super-operators $\mathcal{L}_{1/2}$ at the respective temperature $T_{\rm mean} \pm \Delta T$, modeling two heat baths. After a relaxation time the system reaches a stationary local equilibrium state $\hat{\rho}_{\rm stat}$ with a constant temperature profile and heat current. Taking the local energy expectation value as a measure for temperature, the temperature difference between two adjacent subsystems is given by (in units of ΔE)

$$\Delta T^{(\mu,\mu+1)} = {\rm Tr}\left\{\Big(\hat{H}^{(\mu)}_{\rm loc} - \hat{H}^{(\mu+1)}_{\rm loc}\Big)\hat{\rho}_{\rm stat}\right\}.$$

The respective current operator can be derived from the equation of continuity

$$\dot{\rm i}[\hat{H},\hat{H}^{(\mu)}_{\rm loc}] = \hat{j}^{(\mu-1,\mu)} - \hat{j}^{(\mu,\mu+1)}\,,$$

finding in case of Heisenberg as well as Förster (only energy exchange) interaction

$$\hat{j}^{(\mu,\mu+1)} = {\rm i}\,C_{\rm F}(\hat{\sigma}^{(\mu)}_{-}\hat{\sigma}^{(\mu+1)}_{+} - \hat{\sigma}^{(\mu)}_{+}\hat{\sigma}^{(\mu+1)}_{-})\,.$$

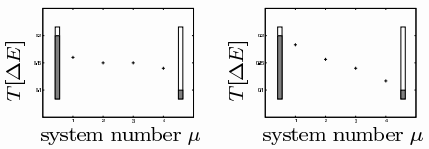
In case of normal heat conduction the famous Fourier's Law should hold connecting local temperature difference and the current by

$${\rm Tr}\left\{\hat{j}^{(\mu,\mu+1)}\hat{\rho}_{\rm stat}\right\} = -\kappa\Delta T^{(\mu,\mu+1)}\,,$$

where κ denotes the heat conductivity.

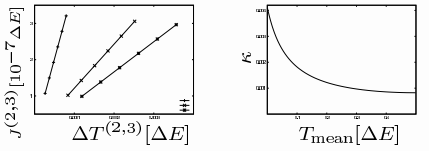
Numerical Investigation

We show results for a numerical integration of the Liouville-von-Neumann equation (1) of the system. Local temperature profile for different internal couplings:



Ballistic transport in a Förster coupled spin chain (left) and normal transport in a Heisenberg coupled chain (right).

Fourier's Law and conductivity κ:



Fourier's Law for different mean temperatures in a Heisenberg chain (left). Conductivity κ for a Heisenberg chain (right).

Perturbation Theory in Liouville Space

We consider as the unperturbed system the Liouville operator $\mathcal{L}_0 = \mathcal{L}_{\rm sys} + \mathcal{L}_1(T_{\rm mean}) + \mathcal{L}_2(T_{\rm mean})$ with the two bath super-operators at the same temperature. After relaxation the system is to be found in the stationary global equilibrium state $\hat{\rho}_0$. The eigensystem of $\mathcal{L}_0$ is given by $\mathcal{L}_0|\hat{\rho}_j) = l_j|\hat{\rho}_j)$ for $j = 0,\ldots,n^{2N}-1$ with $l_j \le 0$. Note that $\hat{\rho}_0$ has to be the only eigenstate with $l_0 = 0$ and therefore represents a stable fixed point of the dynamics. Since this basis is not orthogonal we need a dual basis finding $\sum_j|\hat{\rho}_j)(\hat{\rho}^j| = \mathbb{1}$.

As a perturbation we consider the activation of different bath temperatures given by the Liouville operator

$$\begin{aligned}\mathcal{L}'(\Delta T,t) &= \mathcal{L}_1(T+\frac{\Delta T}{2}f(t)) + \mathcal{L}_2(T-\frac{\Delta T}{2}f(t))\\ &= \mathcal{L}_1(T) + \mathcal{L}_2(T) + \frac{\Delta T\lambda_{\rm B}}{2}f(t)\mathcal{E}\,,\end{aligned}$$

with the switch on function

$$f(t) = \Theta(-t){\rm e}^t + \Theta(t)\,, \quad \text{with} \quad \Theta(t) = \begin{cases}0 & t<0\\ 1 & t>0\end{cases}.$$

Perturbed Density Operator

Starting from the past in a thermal equilibrium state $\hat{\rho}_0$, we assume the time dependent state of the whole system to be

$$\hat{\rho} = \hat{\rho}_0 + \Delta\hat{\rho}(t)\,.$$

Introducing this into the complete Liouville equation, supressing terms of higher order in the perturbation, one finds the time evolution equation for $\Delta\hat{\rho}(t)$,

$$\frac{\partial}{\partial t}\Delta\hat{\rho}(t) - \mathcal{L}_0\Delta\hat{\rho}(t) = \mathcal{L}'(\Delta T,t)\hat{\rho}_0\,.$$

With a transformation similar to the one introduced by Kubo in Hilbert space,

$${\rm e}^{\mathcal{L}_0 t}\Big(\frac{\partial}{\partial t}({\rm e}^{-\mathcal{L}_0 t}\Delta\hat{\rho}(t))\Big) = \frac{\partial}{\partial t}\Delta\hat{\rho}(t) - \mathcal{L}_0\Delta\hat{\rho}(t)\,,$$

one can integrate the differential equation using the special form of $\mathcal{L}'$, to find the formal solution

$$\Delta\hat{\rho}(t) = \frac{\Delta T\lambda_{\rm B}}{2}\int_{-\infty}^{t}{\rm d}t'{\rm e}^{\mathcal{L}_0(t-t')}f(t')\mathcal{E}\hat{\rho}_0\,.$$

Plugging in the unit operator of Liouville space

$$\Delta\hat{\rho}(t) = \frac{\Delta T\lambda_{\rm B}}{2}\int_{-\infty}^{t}{\rm d}t'{\rm e}^{\mathcal{L}_0(t-t')}\sum_j|\hat{\rho}_j)(\hat{\rho}^j|f(t')\mathcal{E}\hat{\rho}_0$$

and carrying out integration over t, we find

$$\Delta\hat{\rho}(t) = \frac{\Delta T\lambda_{\rm B}}{2}\sum_{j=1}^{n^{2N}-1}\Big(\frac{{\rm e}^{l_j t}}{1-l_j} + \frac{{\rm e}^{l_j t}-1}{l_j}\Big)(\hat{\rho}^j|\mathcal{E}|\hat{\rho}_0)|\hat{\rho}_j)\,.$$

Since we are interested in a local equilibrium state – a stationary state with a constant current and temperature profile, which is reached after a certain relaxation time – we consider the limit of $t\to\infty$

$$\Delta\hat{\rho} = \frac{\Delta T\lambda_{\rm B}}{2}\sum_{j=1}^{n^{2N}-1}\frac{(\hat{\rho}^j|\mathcal{E}|\hat{\rho}_0)}{l_j}|\hat{\rho}_j)\,.$$

Temperature Profile and Current

From the perturbed part of the stationary equilibrium state of the system we derived the actual temperature profile and the respective current using

$$J = {\rm Tr}\left\{\hat{J}\hat{\rho}\right\} = {\rm Tr}\left\{\hat{J}(\hat{\rho}_0+\Delta\hat{\rho})\right\} = {\rm Tr}\left\{\hat{J}\Delta\hat{\rho}\right\}$$
$$\Delta T^{(\mu,\mu+1)} = {\rm Tr}\left\{\Delta\hat{H}^{(\mu,\mu+1)}_{\rm loc}\Delta\hat{\rho}\right\}$$

in perfect agreement with the numerical results for the concrete situations above.

The most remarkable point here is the fact that the global temperature difference ΔT is a parameter only. Numerically this is an attractive feature, since a repeated diagonalization for different external gradients is not necessary any more. The current here is

$$J = \left(\frac{\lambda_{\rm B}}{2}\sum_{j=1}^{n^{2N}-1}\frac{(\hat{\rho}^j|\mathcal{E}|\hat{\rho}_0)}{l_j}|\hat{\rho}_j)\right)\Delta T\,.$$

Without the need of any further consideration of the behavior within the chain (linear temperature gradient, flat profile etc.) Fourier's Law combining the current and the external temperature gradient is shown to hold.