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Physica E 29 (2005) 129–135
PHYSICA E
www.elsevier.com/locate/physe

Quantum heat transport: Perturbation theory in Liouville space

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Available online 27 June 2005

Abstract

We consider chains consisting of several identical subsystems weakly coupled by various types of next-neighbor interactions. At both ends the chain is coupled to a respective heat bath with different temperature modeled by a Lindblad formalism. The temperature gradient introduced by this environment is then treated as an external perturbation. We propose a method to calculate the heat current and the local temperature profile of the resulting stationary state as well as the heat conductivity in such systems. This method is similar to Kubo techniques used, e.g., for electrical transport but extended here to the Liouville space.

PACS: 05.60.Gg; 05.30.−d; 05.70.Ln

Keywords: Quantum transport; Quantum statistical mechanics; Non-equilibrium and irreversible thermodynamics

1. Introduction

As a specific topic of non-equilibrium thermodynamics, heat conduction has long since been of central interest. Instead of reaching a complete equilibrium state, the composite system under some appropriate perturbation enters a local equilibrium state—small parts of the system approach equilibrium but not the whole system.

Within non-equilibrium statistical mechanics the theory of linear response, originally developed to account for electric conductivity, is a very important method to investigate dynamical as well as static properties of materials [1–4]. In this context the famous Kubo formulas [5] have led to a rapid development in the theoretical understanding of processes induced by an external perturbation of the system. However, a direct mapping of these ideas on pure thermal transport phenomena (perturbations due to thermal gradients [6]) faces serious problems: Contrary to the case of external perturbations by an electric field,

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1386-9477/$ - see front matter
doi:10.1016/j.physe.2005.05.010

thermal perturbations cannot directly be described by a potential term in the Hamiltonian of the system. Rather, the thermal perturbation is introduced by heat baths with different temperatures coupled to the system, thus calling for a more detailed description than is needed for electric transport. Nevertheless, those methods are often used, eventually because of their immediate success in describing non-equilibrium processes [1,7–9].

Recently, the main focus of considerations on heat conduction and Fourier's law has shifted toward small (one-dimensional) quantum systems [10,11]. Typically, these systems are chains of identical subsystems weakly coupled by some next-neighbor interaction. Based on the Lindblad formalism [12] or on techniques of quantum master equations [13], heat baths are then weakly coupled to the chain at both ends. It has been found that in such systems the appearance of a normal heat conduction depends on the type of the interaction between these elementary subsystems [14]. Most quantum-mechanical interaction types show a normal heat conduction behavior (constant non-vanishing local temperature gradients), whereas for some special coupling the local gradient within the chain vanishes (divergence of the conductivity, non-normal scenario).

Let us now introduce the model system, which we are going to investigate in the following based on the full numerical integration of Liouville–von Neumann (LvN) equation as well as on a perturbation theory in Liouville space.

2. Model system

The dynamics of the quantum model for heat transport is given by the LvN for open systems

$$\frac{\partial}{\partial t}\hat{\rho} = \mathscr{L}\hat{\rho}. \tag{1}$$

Thus we have to consider super operators—here $\mathscr{L}$—acting on operators in Hilbert space, e.g. the density operator of the system (see Refs. [15–17]). The complete Liouville operator of the open system under consideration is given by

$$\mathscr{L} = \mathscr{L}_{\mathrm{sys}} + \mathscr{L}_1(T_1) + \mathscr{L}_2(T_2). \tag{2}$$

The first term controls the coherent evolution of the quantum system defined by the Hamiltonian $\hat{H}$: it is defined by its action on the density operator $\hat{\rho}$ according to

$$\mathscr{L}_{\mathrm{sys}}\hat{\rho} = -\frac{\mathrm{i}}{\hbar}[\hat{H},\hat{\rho}], \tag{3}$$

like for closed quantum systems. The system $\hat{H}$ is here a chain of N identical subunits with n levels each, coupled weakly by a next-neighbor interaction, thus living in a Liouville space of dimension n^{2N}. One could think of several concrete model systems, for example spin models ($n=2$), for which the Hamiltonian would read

$$\hat{H} = \sum_{\mu=1}^{N}\hat{\sigma}_3^{(\mu)} + \sum_{\mu=1}^{N-1}\Big(J_x\hat{\sigma}_1^{(\mu)}\hat{\sigma}_1^{(\mu+1)} + J_y\hat{\sigma}_2^{(\mu)}\hat{\sigma}_2^{(\mu+1)} + J_z\hat{\sigma}_3^{(\mu)}\hat{\sigma}_3^{(\mu+1)}\Big). \tag{4}$$

The first term is the local part of the Hamiltonian, whereas the second defines the interaction between the subsystems ($\hat{\sigma}_i^{(\mu)}$ denote the Pauli operators of the μth spin). Choosing $J_x = J_y = J_z$ we get the Heisenberg interaction and for $J_z = 0$, $J_x = J_y$ an energy transfer coupling only (XY model). Furthermore, to avoid any bias we will often use a random next-neighbor interaction but without disorder (the same random interaction between different subsystems).

The chain is weakly coupled to two heat baths, one at each end of the system, given by the super operators $\mathscr{L}_1(T_1)$ and $\mathscr{L}_2(T_2)$ in Eq. (2). This bath coupling could be realized by standard Lindblad operators [12,14], well known from the theory of open systems in quantum optics. Another equivalent possibility is to derive a quantum master equation for the model system leading to a special bath coupling like e.g. in Ref. [13].

3. Current and local temperature profile

We are interested in the stationary state of the above-described system, namely of the LvN