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The Stationary State and the Heat Equation for a Variant of Davies' Model of Heat Conduction

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We study a variant of Davies' model of heat conduction, consisting of a chain of (classical or quantum) harmonic oscillators, whose ends are coupled to thermal reservoirs at different temperatures, and where neighboring oscillators interact via intermediate reservoirs. In the weak coupling limit, we show that a unique stationary state exists, and that a discretized heat equation holds. We give an explicit expression of the stationary state in the case of two classical oscillators. The heat equation is obtained in the hydrodynamic limit, and it is proved that it completely describes the macroscopic behavior of the model.

KEY WORDS: Weak coupling limit; stationary state supporting a temperature gradient; local equilibrium; heat equation.

1. INTRODUCTION

In this paper we study the stationary state and the transport properties of a variant of Davies' model of heat conduction,[1] consisting of a chain S of N harmonic oscillators, where the ends are coupled to thermal reservoirs R_- and R_+ at inverse temperatures β_- and β_+, and where neighboring oscillators exchange energy via intermediate reservoirs $R_{j,j+1}$, which, at least up to second order in their coupling constants with S, do neither absorb nor give energy to the system S. The reduced dynamics is studied in the weak coupling (van Hove) limit,[2,3] which consists in considering only the lowest-order nonvanishing effects in the coupling constant λ of S to $R=(R_-, \{R_{j,j+1}\}, R_+)$, for times of the order of λ^{-2}. The model can be studied both classically and quantum mechanically, without great modifications.

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It is not too hard to prove that the expectation values of the local Hamiltonians H_j: $j=1,...,N$ satisfy a discretized heat equation, whose stationary solution exhibits a linear profile (in the case of a homogeneous chain), as in Ref. 1; and that a stationary state exists (cf. Ref. 4). On the other hand, an explicit determination of the stationary state is exceedingly difficult. There are general methods of solution, which are based on an assumption of detailed balance; see Ref. 5 for Fokker–Planck equations, and Ref. 6 for Markov population processes. However, these methods are not applicable in the present case, since the detailed balance condition does not hold. As a matter of fact, the validity of this condition is the exception rather than the rule in nonequilibrium situations. Nevertheless, for the classical version of the model and in the simplest case $N=2$, we have been able to construct the stationary state ρ_∞ explicitly, as a uniformly convergent power series expansion in the difference of the inverse temperatures β_- and β_+ of the end resevoirs. As should be expected, ρ_∞ is not a local equilbrium state; deviations from local equilibrium manifest themselves starting from second order in $\beta_- - \beta_+$. For general N, we can only say that the stationary state differs from the local equilibrium state corresponding to the stationary temperature distribution by terms of the order of $(\beta_- - \beta_+)^2$; however, those terms become negligibly small on the macroscopic scale in the hydrodynamic limit ($N \to \infty$, keeping the length L of the chain fixed). There are hopes that the results of Refs. 4 and 7 concerning the hydrodynamic behavior of stochastic lattice systems can be somehow extended to the present model.

We spend a few words on the motivations for studying models involving intermediate reservoirs. In all attempts to understand heat conduction from an underlying Hamiltonian dynamics, the main difficulty has been to construct tractable microscopic models exhibiting some local dissipation properties, leading to a stationary state supporting a temperature gradient. The harmonic approximation for a crystal leads to an infinite heat conductivity, and anharmonic systems are, with a few exception, not exactly solvable. Also numerical investigations (see Ref. 8 for a review) have not given very encouraging results, with few exceptions (see, e.g., Ref. 9). Models based on the replacement of the Hamiltonian description by a kinetic equation such as the Boltzmann equation have been studied since 1929 in a nonrigorous way[10]; in recent times, Fourier's law of heat conduction has been rigorously derived, via Grad limit and Boltzmann equation, for the Lorentz gas (Lebowitz and Spohn[11]).

For models of solids, an appropriate idealization, following an idea of van Hove,[2] could be that of dividing the conducting bar into macroscopically small cells and splitting the Hamiltonian as the sum of single-cell terms plus a cell–cell interaction: the latter term should be small

compared to the former, thus justifying a weak coupling limit with rescaled time, which leads to a Pauli-type master equation for the occupation probabilities of the various levels of the unperturbed energy. However, it seems hardly possible to perform such a program with full mathematical rigor, since it involves a limit of weak cell–cell coupling and a thermodynamic limit for each cell simultaneously.

A simplified version of this idea is that of describing the heat conducting bar as consisting of simple systems and reservoirs, corresponding roughly to the observed and to the unobserved degrees of freedom of the macroscopic system, respectively. The thermodynamic limit for the reservoirs can be taken first, and then the limit of weak coupling between systems and reservoirs can be taken more easily. Since the weak coupling limit *á la* van Hove leads to an energy conserving evolution, the reservoirs which are responsible for local dissipation must not exchange energy with the observed systems. A model constructed by Bolsterli, Rich, and Visscher[12] satisfies this condition if the temperatures of the intermediate reservoirs are adjusted self-consistently, given the temperatures of the end reservoirs. The substantial advantage of the model of Davies,[1] studied also by Alicki,[13] is that the absence of energy transfer between the system and the intermediate reservoirs holds irrespective of their states, which need not be specified. In the variant we study here, the energy spectrum of each system S_j representing a macroscopic cell is unbounded from above, which seems to be a better simulation of van Hove's scheme.

The final step toward a derivation of the heat equation from lattice models should be the hydrodynamic limit (lattice spacing $\varepsilon \to 0$, macroscopic length fixed and macroscopic time of the order of ε^{-2}). This has formed the object of several investigations[4,7] of various authors (De Masi, Ferrari, Ianiro, Galves, Kipnis, Marchioro, Pellegrinotti, Presutti, Rost, Spohn,...) for classical lattice models with stochastic interactions. Davies' model is covered by the results of Refs. 4 and 7; the present variant is not, but it should be possible to adapt those methods to this situation. In the present paper we only study the macroscopic behavior of the model in the hydrodynamic limit, leaving aside the problem of fluctuations.

The paper is organized as follows. In Section 2, we discuss the general features of the model for arbitrary N. In Section 3, we construct the stationary states for the classical version with $N=2$. Section 4 contains our results on the hydrodynamic limit.

2. THE MODEL: EQUATIONS OF MOTION

Our variant of the model of Davies [see Remark (v) of Section 2 in Ref. 1] is as follows. We have a chain S of N quantum mechanical har-

monic oscillators (with unit mass) S_j: $j=1,...,N$, where S_1 and S_N are weakly coupled to thermal reservoirs R_- and R_+ respectively, and where neighboring oscillators exchange energy via weak coupling to intermediate reservoirs $R_{j,j+1}$: $j=1,...,N-1$. All the reservoirs may be assumed to be infinitely extended quasifree boson systems. There is a corresponding classical version of the model, which can be obtained from the quantum one by taking the formal classical limit ($\hbar \to 0$, $(i\hbar)^{-1}[A, B] \to \{A, B\}$), or also studied directly, on the same lines as for the quantum model.[14]

The initial state of the system plus reservoirs is assumed to be of the form

$$W = \rho \otimes \omega_- \otimes \left[\bigotimes_{j=1}^{N-1} \omega_{j,j+1} \right] \otimes \omega_+ \tag{2.1}$$

where ρ is an arbitrary density operator for S, and where ω_-, $\omega_{j,j+1}$, ω_+ are fixed reference states for R_-, $R_{j,j+1}$, R_+, respectively.

The Hamiltonian is chosen as

$$H_\lambda = H_S + H_R + \lambda H_{SR} \tag{2.2}$$

where

$$H_S = \hbar\omega \sum_{j=1}^{N} a_j^* a_j = \sum_{j=1}^{N} H_j \tag{2.3}$$

$$H_{SR} = \hbar^{1/2} a_1 \otimes b_-^* + \hbar \sum_{j=1}^{N-1} a_j a_{j+1}^* \otimes b_{j,j+1}^* + \hbar^{1/2} a_N \otimes b_+^* + \text{conj} \tag{2.4}$$

Here

$$a_j = (2\hbar)^{-1/2}(\omega^{1/2} q_j + i\omega^{-1/2} p_j) \tag{2.5}$$

and b_-^*, $b_{j,j+1}^*$, b_+^* are suitable linear combinations of creation operators for the reservoirs R_-, $R_{j,j+1}$, R_+, respectively. H_R is the sum of the Hamiltonians implementing the quasifree evolutions of the reservoirs in the GNS representations determined by their reference states, which we assume to be stationary for the quasifree evolution and invariant under the gauge transformation $b \mapsto e^{-i\theta} b$.

In the weak coupling limit $\lambda \to 0$, $\tau = \lambda^2 t$ const, the effect of the reservoirs on the reduced evolution of the density operator of S is determined by the two-point correlation functions

$$h_{(\cdots)}(\alpha) = \int_{-\infty}^{+\infty} e^{-i\alpha t} \omega_{(\cdots)}(b_{(\cdots)} e^{iH_R t/\hbar} b_{(\cdots)}^* e^{-iH_R t/\hbar})\, dt \tag{2.6a}$$

$$\tilde{h}_{(\cdots)}(\alpha) = \int_{-\infty}^{+\infty} e^{-i\alpha t} \omega_{(\cdots)}(b_{(\cdots)}^* e^{iH_R t/\hbar} b_{(\cdots)} e^{-iH_R t/\hbar})\, dt \tag{2.6b}$$

where $(\cdots)$ stands for any reservoir index: $-, j, j+1, +$. We assume that the integrals (2.6) are convergent, and tend to finite limits in the classical limit $\hbar \to 0$, whereas the difference $h_{(\cdots)}(\alpha) - \tilde{h}_{(\cdots)}(-\alpha)$ is of the order of $\hbar$. The assumption that R_- and R_+ are thermal reservoirs, at inverse temperatures β_- and β_+, respectively, is expressed by

$$\tilde{h}_-(-\alpha) = e^{-\beta_- \hbar\alpha} h_-(\alpha), \qquad \tilde{h}_+(-\alpha) = e^{-\beta_+ \hbar\alpha} h_+(\alpha) \tag{2.7}$$

Concerning the intermediate reservoirs, we only assume that

$$\tilde{h}_{j,j+1}(0) = h_{j,j+1}(0), \qquad j = 1, \ldots, N-1 \tag{2.8}$$

If we ignore the technical difficulties stemming from the fact that H_{SR} is unbounded, and perform the weak coupling limit as in Ref. 3, we find that the time evolution of the density matrix ρ of S, in the interaction picture, is asymptotically given by a dynamical semigroup

$$\exp[K\tau](\rho) = \lim_{\substack{\lambda \to 0 \\ \lambda^2 t = \tau}} e^{iH_S t/\hbar} \operatorname{Tr}_R [e^{-iH_\lambda t/\hbar} W e^{iH_\lambda t/\hbar}] e^{-iH_S t/\hbar} \tag{2.9}$$

The explicit form of K (cf. Refs. 1 and 3) is the following:

$$K = K_- + \sum_{j=1}^{N-1} K_{j,j+1} + K_+ \tag{2.10}$$

where

$$K_-(\rho) = -i[X_-, \rho] + \frac{1}{2\hbar} h_-(\omega)\{([a_1\rho, a_1^*] + [a_1, \rho a_1^*]) + e^{-\beta_- \hbar\omega}([a_1^*\rho, a_1] + [a_1^*, \rho a_1])\} \tag{2.11a}$$

$$K_{j,j+1}(\rho) = -i[X_{j,j+1}, \rho] - \frac{1}{2} h_{j,j+1}(0)\{[a_j a_{j+1}^*, [a_j^* a_{j+1}, \rho]] + [a_j^* a_{j+1}, [a_j a_{j+1}^*, \rho]]\} \tag{2.11b}$$

$$K_+(\rho) = -i[X_+, \rho] + \frac{1}{2\hbar} h_+(\omega)\{([a_N\rho, a_N^*] + [a_N, \rho a_N^*]) + e^{-\beta_+ \hbar\omega}([a_N^*\rho, a_N] + [a_N^*, \rho a_N])\} \tag{2.11c}$$

with

$$X_- = \frac{1}{2\pi\hbar} \mathscr{P} \int_{-\infty}^{+\infty} \{(\alpha - \omega)^{-1} h_-(\alpha) a_1^* a_1 + (\alpha + \omega)^{-1} \tilde{h}_-(\alpha) a_1 a_1^*\}\, d\alpha \tag{2.12a}$$

$$X_{j,j+1}=\frac{1}{2\pi}\mathscr{P}\int_{-\infty}^{+\infty}\{\alpha^{-1}h_{j,j+1}(\alpha)a_j^*a_ja_{j+1}a_{j+1}^* + \alpha^{-1}\tilde{h}_{j,j+1}(\alpha)a_ja_j^*a_{j+1}^*a_{j+1}\}\,d\alpha \tag{2.12b}$$

$$X_+=\frac{1}{2\pi\hbar}\mathscr{P}\int_{-\infty}^{+\infty}\{(\alpha-\omega)^{-1}h_+(\alpha)a_N^*a_N+(\alpha+\omega)^{-1}\tilde{h}_+(\alpha)\,a_N^*a_N\}\,d\alpha \tag{2.12c}$$

We shall assume without further mention that the nonnegative constants $h_-(\omega)$, $h_{j,j+1}(0)$, $j=1,\ldots,N-1$, $h_+(\omega)$ are strictly positive.

In spite of the formal nature of the above derivation, we have the following:

Proposition 2.1. The unbounded operator K, defined by Eqs. (2.10), (2.11), (2.12) on a suitable domain, determines a dynamical semigroup via the method of the minimal solution.[15]

The proof is an application of Theorem 4.1 of Ref. 15.

We now turn to the investigation of the existence of a stationary state and of the transport properties of the model. If a normal stationary states exists, it should be expected that it is unique and that all normal states approach it in the limit as $t\to\infty$ under the action of $\exp[Kt]$ (this "follows," up to technicalities, from Ref. 16; see also Ref. 14 for the classical case). By the invariance of K under the gauge transformations $a_j\mapsto e^{-i\theta_j}a_j$, the set $\mathscr{E}$ of states which are functions of the local Hamiltonians H_j: $j=1,\ldots,N$ is globally invariant under $\exp[Kt]$: $t\geqslant 0$, and the stationary state, if it exists (and if it is indeed unique, as expected) belongs to $\mathscr{E}$. From now on, we restrict our consideration to states ρ in $\mathscr{E}$; for them we shall be able to prove rigorous results.

In the classical case, the natural method for finding the stationary state is to try to solve the stationary Fokker–Planck equation. A state $\exp[Kt](\rho)$ in $\mathscr{E}$ can be expressed by a function $\rho(\boldsymbol{\mu};t)$, $\boldsymbol{\mu}=(\mu_1,\ldots,\mu_N)$, $\mu_j=\omega^{-1}H_j=\frac{1}{2}|\omega^{1/2}q_j+i\omega^{-1/2}p_j|^2$, $j=1,\ldots,N$. Upon replacing a_j by $(2\hbar)^{-1/2}(\omega^{1/2}q_j+i\omega^{-1/2}p_j)$ in (2.11), (2.12) and taking the classical limit

$$\hbar\to 0,\qquad (i\hbar)^{-1}[A,B]\to\{A,B\},\qquad \tfrac{1}{2}[A,B]_+\to AB=BA \tag{2.13}$$

(cf. Ref. 14), we can obtain the Fokker–Planck equation for $\rho(\boldsymbol{\mu};t)$. After a lengthy but straightforward calculation, we find

$$\frac{\partial}{\partial t}\rho(\boldsymbol{\mu};t)=\left(L_-+\sum_{j=1}^{N-1}L_{j,j+1}+L_+\right)\rho(\boldsymbol{\mu};t) \tag{2.14}$$

where

$$L_- = h_-(\omega)\left[\mu_1 \frac{\partial^2}{\partial \mu_1^2} + (\beta_- \omega \mu_1 + 1)\frac{\partial}{\partial \mu_1} + \beta_- \omega\right] \tag{2.15a}$$

$$L_{j,j+1} = h_{j,j+1}(0)\left[\mu_j \mu_{j+1}\left(\frac{\partial^2}{\partial \mu_j^2} + \frac{\partial^2}{\partial \mu_{j+1}^2} - 2\frac{\partial^2}{\partial \mu_j\, \partial \mu_{j+1}}\right) + (\mu_j - \mu_{j+1})\left(\frac{\partial}{\partial \mu_{j+1}} - \frac{\partial}{\partial \mu_j}\right)\right] \tag{2.15b}$$

$$L_+ = h_+(\omega)\left[\mu_N \frac{\partial^2}{\partial \mu_N^2} + (\beta_+ \omega \mu_N + 1)\frac{\partial}{\partial \mu_N} + \beta_+ \omega\right] \tag{2.15c}$$

The stationary solution of (2.14), (2.15) is constructed in Section 3, for the simplest case $N=2$, as a uniformly convergent power series expansion in $\delta \equiv \frac{1}{2}(\beta_- - \beta_+)$.

For the quantum version of the model, one could try to solve the corresponding Fokker–Planck equation for the Glauber–Sudarshan quasiprobability function P, which is of the same form as (2.14), but with different expressions for L_- and L_+. However, we have not been able to go very far along this approach.

There is an alternative way of studying the time evolution of a state ρ in $\mathscr{E}$, which is applicable both in the classical and in the quantum version of the model, and which allows to prove that there exists a unique state ρ_∞ such that

$$\lim_{t \to \infty} \exp[Kt](\rho) = \rho_\infty \qquad \text{for all } \rho \text{ in } \mathscr{E} \tag{2.16}$$

The expression of ρ_∞ is given in a rather implicit fashion, but more concrete results can be obtained in the limit as $N \to \infty$ (see Section 4 below). We dedicate the remaining of the Section to this approach to the problem.

We introduce the notation $\langle \rho; A \rangle$ for the expectation value of an observable A in a state ρ, both classically and quantum mechanically. Explicitly, we have

$$\langle \rho; A \rangle = \begin{cases} \mathrm{Tr}[\rho A] & \text{(quantum)} \quad (2.17a) \\ \int \cdots \int_{\mathbb{R}^{2N}} \rho A \, dq_1 \, dp_1 \cdots dq_N \, dp_N & \text{(classical)} \quad (2.17b) \end{cases}$$

A state $\exp[Kt](\rho)$ in $\mathscr{E}$ is completely determined by the correlation function $G(\mathbf{k}; t)$: $\mathbf{k} = (k_-, k_1, \ldots, k_N, k_+)$; $k_r = 0, 1, 2, \ldots$; $r = -, 1, \ldots, N, +$; $t \in \mathbb{R}^+$, defined by

$$G(\mathbf{k};t)=T_-^{k_-}T_+^{k_+}\left\langle \exp[Kt](\rho);\prod_{j=1}^{N}(k_j!)^{-1}:H_j^{k_j}:\right\rangle \tag{2.18}$$

$$T_\pm=\hbar\omega(e^{\beta_\pm\hbar\omega}-1)^{-1} \qquad \text{(quantum)} \tag{2.19a}$$

$$T_\pm=\beta_\pm^{-1} \qquad \text{(classical)} \tag{2.19b}$$

As we shall see presently, the time evolution of the $G(\mathbf{k};t)$ admits of an alternative interpretation in terms of a Markov jump process describing fictitious "particles" on the sites $(-, 1,..., N, +)$, jumping to neighboring sites and being eventually absorbed by the boundaries $\{-, +\}$. As in Ref. 4, this Markov jump process can be used to show that (2.16) holds. We are indebted to C. Kipnis for this observation.

Proposition 2.2. The correlation functions $G(\mathbf{k};t)$ satisfy

$$\begin{aligned}\frac{d}{dt}G(\mathbf{k};t)&=\gamma_-k_1[G(k_-+1,k_1-1,...;t)-G(\mathbf{k};t)]\\&+\sum_{j=1}^{N-1}\gamma_{j,j+1}\{k_j(k_{j+1}+1)[G(...,k_j-1,k_{j+1}+1,...;t)-G(\mathbf{k};t)]\\&+k_{j+1}(k_j+1)[G(...,k_j+1,k_{j+1}-1,...;t)-G(\mathbf{k};t)]\}\\&+\gamma_+k_N[G(...,k_N-1,k_++1;t)-G(\mathbf{k};t)]\end{aligned} \tag{2.20}$$

where

$$\gamma_\pm=\hbar^{-1}(1-e^{-\beta_\pm\hbar\omega})\,h_\pm(\omega) \qquad \text{(quantum)} \tag{2.21a}$$

$$\gamma_\pm=\beta_\pm\omega h_\pm(\omega) \qquad \text{(classical)} \tag{2.21b}$$

$$\gamma_{j,j+1}=h_{j,j+1}(0),\ j=1,...,N-1 \qquad \text{(quantum and classical)} \tag{2.21c}$$

Proof. We consider the quantum case; the classical case may be studied along the same lines, or also by taking the classical limit on the final result of the calculations. The $G(\mathbf{k};t)$ can be obtained as derivatives of a generating functional $f(\mathbf{u};t)$, $\mathbf{u}=(u_1,...,u_N)$, $u_j\in\mathbb{R}^+$, $j=1,...,N$; $t\in\mathbb{R}^+$, as

$$G(\mathbf{k};t)=T_-^{k_-}T_+^{k_+}\left(\prod_{j=1}^{N}(-1)^{k_j}\frac{\partial^{k_j}}{\partial u_j^{k_j}}\right)f(\mathbf{u};t)\Big|_{\mathbf{u}=0} \tag{2.22}$$

where

$$f(\mathbf{u};t)=\left\langle \exp[Kt](\rho);\exp\left[i(\hbar\omega)^{1/2}\sum_{j=1}^{N}z_ja_j^*\right]\exp\left[i(\hbar\omega)^{1/2}\sum_{j=1}^{N}\bar{z}_ja_j\right]\right\rangle \tag{2.23}$$

with $u_j = |z_j|^2$, $z_j \in \mathbb{C}$, $j = 1,...,N$, and where ρ is in $\mathscr{E}$. A lengthy but straightforward computation, starting from (2.11), leads to

$$\frac{\partial}{\partial t} f(\mathbf{u}; t) = \left[D_- + \sum_{j=1}^{N-1} D_{j,j+1} + D_+ \right] f(\mathbf{u}; t) \tag{2.24}$$

where

$$D_- = -\gamma_- u_1 \left(\frac{\partial}{\partial u_1} + T_- \right) \tag{2.25a}$$

$$D_{j,j+1} = \gamma_{j,j+1} \left[(u_{j+1} - u_j) \left(\frac{\partial}{\partial u_j} - \frac{\partial}{\partial u_{j+1}} \right) + u_j u_{j+1} \left(\frac{\partial}{\partial u_j} - \frac{\partial}{\partial u_{j+1}} \right)^2 \right], \quad j = 1,..., N-1 \tag{2.25b}$$

$$D_+ = -\gamma_+ u_N \left(\frac{\partial}{\partial u_N} + T_+ \right) \tag{2.25c}$$

and where $T_\pm$ and the γs are defined by (2.19) and (2.21), respectively. Differentiating (2.24) as in (2.22) yields (2.20). ∎

Remark 2.3. Equation (2.20) defines the generator of the Markov semigroup associated with the Markov jump process mentioned above. It should be compared with the similar equations of Refs. 4 and 7a.

It is clear that each "particle" will be absorbed, in the limit as $t \to \infty$, by one of the boundaries. We denote by $\mathbb{P}_\infty(k_-, k_+ | k_1,..., k_N)$ the probability that, starting at $t = 0$ with k_j "particles" at site j, $j = 1,..., N$, k_- (resp. k_+) of them will be eventually absorbed by the left (resp. right) boundary. The problem of determining $\mathbb{P}_\infty(k_-, k_+ | k_1,..., k_N)$ explicitly appears to be a hard one, and we have no answers so far; nevertheless, the fact that the $\mathbb{P}_\infty$s exist is sufficient to conclude that (2.16) holds. Indeed, we have the following:

Proposition 2.4. For all ρ in $\mathscr{E}$, we have

$$\begin{aligned} \lim_{t \to \infty} \left\langle \exp[Kt](\rho); \prod_{j=1}^{N} (k_j!)^{-1} : H_j^{k_j} : \right\rangle \\ = \sum_{k_-, k_+ : k_- + k_+ = \sum_{j=1}^N k_j} T_-^{k_-} T_+^{k_+} \mathbb{P}_\infty(k_-, k_+ | k_1,..., k_N) \\ \equiv \left\langle \rho_\infty; \prod_{j=1}^{N} (k_j!)^{-1} : H_j^{k_j} : \right\rangle \end{aligned} \tag{2.26}$$

Proof (cf. Ref. 4). Just follow the time evolution of $G(\mathbf{k}; t)$ for large t. ∎

The transport properties of the model are described in the following proposition, which is the special case of Proposition 2.2 corresponding to $\sum k_j = 1$.

Proposition 2.5. The internal energy density

$$T_j(t) = \langle \exp[Kt](\rho); H_j \rangle, \qquad j = 1,..., N,\ t \in \mathbb{R}^+ \tag{2.27}$$

satisfies the discretized heat equation

$$\frac{d}{dt} T_j(t) = \gamma_{j-1,j}[T_{j-1}(t) - T_j(t)] + \gamma_{j,j+1}[T_{j+1}(t) - T_j(t)], \qquad j = 1,..., N \tag{2.28}$$

where $\gamma_{0,1} = \gamma_-$, $\gamma_{N,N+1} = \gamma_+$, and where

$$T_0(t) \equiv T_-, \qquad T_{N+1}(t) \equiv T_+, \qquad \text{for all } t \tag{2.29}$$

In particular, the stationary energy distribution T_j^{st}: $j = 1,..., N$, in the special case of a homogeneous chain, $\gamma_{j,j+1} = \gamma$ for all j, is given by

$$T_j^{\text{st}} = T_- + j(N+1)^{-1}(T_+ - T_-) \tag{2.30}$$

and the heat flux in the stationary state[13,17] is given by

$$J_{\text{st}} = \gamma(N+1)^{-1}(T_+ - T_-) \tag{2.31}$$

We can also consider the special case of Proposition 2.2 corresponding to $\sum k_j = 2$. Define the truncated energy–energy correlations $V_{r,s}(t)$: r, $s = 1,..., N$ by

$$V_{r,s}(t) = G(\mathbf{k}(r, s); t) - T_r(t)\, T_s(t) \tag{2.32}$$

where

$$k_j(r, s) = \delta_{j,r} + \delta_{j,s}: \qquad j = -, 1,..., N, +. \tag{2.33}$$

Then we have the following:

Proposition 2.6. The truncated energy–energy correlations $V_{r,s}(t)$ are given by

$$V_{r,s}(t) = \left(\exp[\mathscr{L}t]\ V(0) + \int_0^t \exp[\mathscr{L}(t-t')]\ C(t')\, dt' \right)_{r,s} \tag{2.34}$$

where the linear operator $\mathscr{L}$ on $\mathbb{R}^{N^2}$ is defined by

$$(\mathscr{L}V)_{r,s} = (1+\delta_{r+1,s})[\gamma_{r,r+1}(V_{r+1,s}-V_{r,s})+\gamma_{s-1,s}(V_{r,s-1}-V_{r,s})] + (1+\delta_{r-1,s})[\gamma_{r-1,r}(V_{r-1,s}-V_{r,s})+\gamma_{s,s+1}(V_{r,s+1}-V_{r,s})] \tag{2.35}$$

with the boundary conditions

$$V_{r,0} = V_{0,s} = V_{r,N+1} = V_{N+1,s} = 0 \tag{2.36}$$

and where $C(t) = \{C_{r,s}(t)\colon r, s = 1,...,N\}$ is defined by

$$C_{r,s}(t) = \delta_{r+1,s}\gamma_{r,r+1}[T_{r+1}(t)-T_r(t)]^2 + \delta_{r-1,s}\gamma_{r-1,r}[T_{r-1}(t)-T_r(t)]^2 \tag{2.37}$$

Proof (Sketch). A straightforward calculation, starting from Proposition 2.2, shows that

$$\frac{d}{dt}V_{r,s}(t) = (\mathscr{L}V(t))_{r,s} + C_{r,s}(t) \tag{2.38}$$

whence (2.34) follows. ∎

Remark 2.7. Equation (2.34) shows that the energy–energy correlations that are initially present are damped away by $\exp[\mathscr{L}t]$ as $t \to \infty$, but new correlations are built up by the presence of the source term $C(t)$; for fixed N, these correlations are of the order of $(T_+ - T_-)^2$. A comparison of (2.37) with Ref. 13 shows that $C(t)$ is related to the entropy production. In particular, the local equilibrium state

$$\rho_{\text{loc}} = Z^{-1}\exp\left[-\sum_{j=1}^{N}\beta_j H_j\right] \tag{2.39}$$

with β_j such that $\hbar\omega(e^{\beta_j\hbar\omega}-1)^{-1} = T_j^{\text{st}}$ (or $\beta_j^{-1} = T_j^{\text{st}}$ in the classical case) satisfies $\langle\rho_{\text{loc}}; H_j\rangle = T_j^{\text{st}} = \langle\rho_\infty; H_j\rangle$ for all j, but does not coincide with ρ_∞, since $V_{r,s}$ vanishes identically in ρ_{loc}. Nevertheless, the correlations in the stationary state are small on the macroscopic scale in the limit as $N \to \infty$, as we shall see in Section 4.

Remark 2.8. The fact that the (discretized) heat equation holds exactly, with temperature independent conductivity γ, is related to the highly idealized nature of the model, whose stochastic properties, embodied in the intermediate reservoirs, are independent of the temperature.

3. THE STATIONARY STATE FOR $N=2$

For the classical version of the model, with $N=2$, we determine the stationary state by finding the stationary solution of Equation (2.14). We introduce new variables and new temperature parameters

$$\xi=\mu_1+\mu_2, \qquad \eta=\mu_1-\mu_2 \tag{3.1a}$$

$$\beta=\tfrac{1}{2}(\beta_-+\beta_+), \qquad \delta=\tfrac{1}{2}(\beta_--\beta_+) \tag{3.1b}$$

and choose $\omega=1$ and

$$h_-(1)=h_{1,2}(0)=h_+(1)=1 \tag{3.2}$$

The stationary Fokker–Planck equation becomes

$$\left[\xi\frac{\partial^2}{\partial\xi^2}-(\xi+\xi^2-\eta^2)\frac{\partial^2}{\partial\eta^2}+2\eta\frac{\partial^2}{\partial\xi\,\partial\eta}+(2+\beta\xi+\delta\eta)\frac{\partial}{\partial\xi}\right.$$
$$\left.+(\delta\xi+(\beta-2)\eta)\frac{\partial}{\partial\eta}+2\beta\right]\rho=0 \tag{3.3}$$

When $\delta=0$ (equal temperatures), the stationary state is the canonical distribution $Z^{-1}e^{-\beta\xi}$. This suggests the Ansatz

$$\rho(\xi,\eta)=e^{-\beta\xi}g(\xi,\eta) \tag{3.4}$$

Inserting (3.4) into (3.3) gives

$$\xi\frac{\partial^2 g}{\partial\xi^2}+(\xi+\xi^2-\eta^2)\frac{\partial^2 g}{\partial\eta^2}+2\eta\frac{\partial^2 g}{\partial\xi\,\partial\eta}$$
$$+(2+\delta\eta-\beta\xi)\frac{\partial g}{\partial\xi}+[\delta\xi-(\beta+2)\eta]\frac{\partial g}{\partial\eta}-\beta\delta\eta g=0 \tag{3.5}$$

Note that, when $\delta=0$, a constant solves (3.5).

The differential operator in (3.5) may be written as a sum $T_{(\xi,\eta)}+T_{(\eta)}$, where

$$T_{(\eta)}=-\eta^2\frac{\partial^2}{\partial\eta^2}-(\beta+2)\eta\frac{\partial}{\partial\eta}-\beta\delta\eta \tag{3.6}$$

involves only the variable η. The kernel of $T_{(\eta)}$ contains the function

$$\phi(\eta)=\Gamma(\beta+2)(\beta\delta\eta)^{-(1/2)(\beta+1)}J_{\beta+1}(2(\beta\delta\eta)^{1/2})$$
$$=\Gamma(\beta+2)\sum_{n=0}^{\infty}\frac{(-\beta\delta\eta)^n}{n!\,\Gamma(\beta+n+2)} \tag{3.7}$$

where $J_{\beta+1}$ is a Bessel function of the first kind. The normalization constant in (3.7) has been chosen in such a way that $\phi(\eta)=1$ when $\delta=0$. This suggests to us that we look for a solution of (3.5) in the form

$$g(\xi,\eta)=\phi(\eta)+\psi(\xi,\eta) \tag{3.8}$$

Then $\psi(\xi,\eta)$ must satisfy

$$\begin{aligned}[T_{(\xi,\eta)}+T_{(\eta)}]\,\psi(\xi,\eta) &= -T_{(\xi,\eta)}\phi(\eta)\\ &=\frac{\delta^2\beta\xi}{(\beta+2)(\beta+3)}\sum_{r=0}^{\infty}\frac{(r+3-\beta\xi)(-\beta\delta\eta)^r}{r!(\beta+4)_r}\end{aligned} \tag{3.9}$$

where $(x)_y\equiv\Gamma(x+y)/\Gamma(x)$ is the Pochhammer symbol.

The right-hand side of (3.9) is independent of η up to order δ^2, so that we can write

$$\psi(\xi,\eta)=\psi_0(\xi)+\psi_1(\xi,\eta) \tag{3.10}$$

where

$$\psi_0(\xi)=O(\delta^2),\qquad \psi_1(\xi,\eta)=o(\delta^2) \tag{3.11}$$

The equation for $\psi_0(\xi)$ is obtained from (3.9) by suppressing all the terms with $r\geqslant 1$ in the right-hand side, and we observe that it admits the simple particular solution

$$\psi_0(\xi)=\frac{\delta^2\beta}{2(\beta+2)(\beta+3)}\xi^2 \tag{3.12}$$

This observation is crucial for the construction of the stationary state, in that it allows us to set up a hierarchy of ordinary differential equations admitting polynomial solutions. Indeed, Eqs. (3.9), (3.12) suggest the Ansatz

$$\psi(\xi,\eta)=\frac{\delta^2\beta}{(\beta+2)(\beta+3)}\sum_{r=0}^{\infty}\frac{(-\beta\delta\eta)^r}{r!(\beta+4)_r}\sum_{k=0}^{r}\eta^k B_{k,r}(\xi) \tag{3.13}$$

where $B_{0,0}(\xi)=\xi^2/2$, and where

$$B_{k,r}(\xi)=\sum_{l=0}^{n(k,r)}C_{k,r}^{l}\xi^l,\qquad k\leqslant r=0,\,1,\,2,\ldots \tag{3.14}$$

Now we have the following:

Lemma 3.1. Equation (3.9) admits a solution in the form (3.13), provided the $B_{k,r}(\xi)$ satisfy the following hierarchy of ordinary linear differential equations:

$$\xi B''_{k,r} + [2(k+1) - \beta\xi] B'_{k,r} - k(\beta + k + 1) B_{k,r}$$
$$= r(r+\beta+3)[\beta^{-1} B'_{k-1,r-1} - B_{k-1,r-1}] + \xi(r+3-\beta\xi)\delta_{k,r}$$
$$+ \beta^{-1} r(r+\beta+3)(k+1)\xi B_{k+1,r-1} - (k+2)(k+1)\,\xi(1+\xi) B_{k+2,r} \tag{3.15}$$

Lemma 3.2. The hierarchy (3.15) admits a polynomial solutions in the form (3.14), where

$$n(k, r) = r - k + 2 \tag{3.16a}$$

$$C^l_{k,r} = 0 \qquad \text{for } r-k \text{ odd} \tag{3.16b}$$

The remaining $C^l_{k,r}$ are determined by a set of recursion relations, starting from

$$C^0_{0,0} = C^1_{0,0} = 0, \qquad C^2_{0,0} = \tfrac{1}{2}, \qquad C^0_{0,2j} = 0 \tag{3.17}$$

Lemma 3.1 is proved by a straightforward verification. The proof of Lemma 3.2 was obtained in Ref. 18; it is too long for inclusion here.

Now we are ready to state then main result of the present Section.

Theorem 3.3. For sufficiently small δ, the stationary state $\rho_\infty(\xi, \eta)$ is given by

$$\rho_\infty(\xi,\eta) = Z^{-1} e^{-\beta\xi} \left[\Gamma(\beta+2)(\beta\delta\eta)^{-(1/2)(\beta+1)} J_{\beta+1}(2(\beta\rho\eta)^{1/2}) \right.$$
$$\left. + \frac{\beta\delta^2}{(\beta+2)(\beta+3)} \sum_{r=0}^{\infty} \frac{(-\beta\delta)^r}{r!(\beta+4)_r} \sum_{k=0}^{r} \eta^k B_{k,r}(\xi) \right] \tag{3.18}$$
$$= Z^{-1} e^{-\beta\xi} \left\{ 1 - \frac{\beta}{\beta+2}\delta\eta + \sum_{n=2}^{\infty} \frac{(-\beta\delta)^n}{n!(\beta+2)_n} \right.$$
$$\left. \times \left[\eta^n + \frac{n(n-1)}{\beta} \sum_{k=0}^{n-2} \eta^k B_{k,n-2}(\xi) \right] \right\} \tag{3.19}$$

where Z^{-1} is a positive normalization constant, and where $B_{k,r}(\xi)$ is the solution of the hierarchy (3.15). The series expansion (3.19) converges uniformly in ξ, η.

Proof (Sketch). It can be shown[18] that the series

$$\sum_{r=0}^{\infty} \frac{(\beta|\delta|)^r}{r!(\beta+4)_r} \sup_{0 \leqslant |\eta| \leqslant \xi < +\infty} \left\{ \left| \sum_{k=0}^{r} e^{-\beta\xi} \eta^k B_{k,r}(\xi) \right| \right\} \tag{3.20}$$

and

$$\sum_{r=0}^{\infty} \frac{(\beta|\delta|)^r}{r!(\beta+4)_r} \int_{\xi=0}^{\infty} \int_{\eta=-\xi}^{\xi} \left| \sum_{k=0}^{r} e^{-\beta\xi} \eta^k B_{k,r}(\xi) \right| d\eta \, d\xi \tag{3.21}$$

are convergent for sufficiently small δ. From this result and from known properties of the Bessel functions, it follows that the series expansion (3.19) is uniformly convergent and defines an absolutely integrable function $\rho^0(\xi, \eta)$, which is a solution of the stationary Fokker–Planck equation (3.3) by construction. Now we prove that ρ^0 gives the stationary state ρ_∞, when correctly normalized. We can write

$$\rho^0(\xi, \eta) = \alpha_+ \rho^+(\xi, \eta) - \alpha_- \rho^-(\xi, \eta)$$

where α_+, α_- are nonnegative real numbers, and where ρ^+, ρ^- are states in $\mathscr{E}$. Then, for all observables A, we have

$$\begin{aligned} \langle \rho^0; A \rangle &= \langle \exp[Kt](\rho^0); A \rangle \\ &= \alpha_+ \langle \exp[Kt](\rho^+); A \rangle - \alpha_- \langle \exp[Kt](\rho^-); A \rangle \\ &\xrightarrow[t \to \infty]{} (\alpha_+ - \alpha_-) \langle \rho_\infty; A \rangle \end{aligned} \tag{3.22}$$

by Proposition 2.4. Then ρ_∞ is a normal state, given by a distribution function $\rho_\infty(\xi, \eta)$, which is proportional to $\rho^0(\xi, \eta)$. The normalization constant Z^{-1} is positive by continuity for sufficiently small δ, since $\rho^0(\xi, \eta)$ is proportional to $e^{-\beta\xi}$ for $\delta = 0$. ∎

Remark 3.4. The stationary expectation values of μ_1 and μ_2 can be computed exactly from Eq. 3.3, as in Proposition 2.5: they are

$$\langle \mu_1 \rangle_{\text{st}} = \frac{\beta + 2 - \delta}{\beta(\beta+2) - \delta^2}, \qquad \langle \mu_2 \rangle_{\text{st}} = \frac{\beta + 2 + \delta}{\beta(\beta+2) - \delta^2} \tag{3.23}$$

It is interesting to compare the stationary state ρ_∞ with the local equilibrium state ρ_{loc} with inverse temperatures $\beta_1 = \langle \mu_1 \rangle_{\text{st}}^{-1}$ and $\beta_2 = \langle \mu_2 \rangle_{\text{st}}^{-1}$, and with the product state $\rho_\otimes$ defined by

$$\rho_\otimes = \left(\int_{\mathbf{R}^2} \rho_\infty \, dq_2 \, dp_2 \right) \left(\int_{\mathbf{R}^2} \rho_\infty \, dq_1 \, dp_1 \right) \tag{3.24}$$

Up to second order in δ, we have

$$\rho_\infty = \frac{\beta^2}{4\pi^2} e^{-\beta\xi} \left\{ 1 - \frac{\delta\beta\eta}{\beta+2} + \frac{\delta^2}{(\beta+2)(\beta+3)} \left[\frac{1}{2} (\beta^2\eta^2 + \beta\xi^2) - \left(1 + \frac{3}{\beta} \right) \right] + \cdots \right\} \tag{3.25a}$$

$$\rho_{\mathrm{loc}}=\frac{\beta^2}{4\pi^2}e^{-\beta\xi}\left\{1-\frac{\delta\beta\eta}{\beta+2}+\frac{\delta^2}{(\beta+2)^2}\left[\frac{1}{2}\beta^2\eta^2+2\xi-\left(1+\frac{4}{\beta}\right)\right]+\cdots\right\} \tag{3.25b}$$

$$\rho_{\otimes}=\frac{\beta^2}{4\pi^2}e^{-\beta\xi}\left\{1-\frac{\delta\beta\eta}{\beta+2}+\frac{\delta^2}{(\beta+2)^2(\beta+3)}\left[\frac{\beta^3+3\beta^2+\beta}{2}\eta^2-\frac{\beta}{2}\xi^2\right.\right.$$
$$\left.\left.+(5-\beta^2)\xi-\frac{(\beta+8)(\beta-1)}{\beta}\right]+\cdots\right\} \tag{3.25c}$$

whence we see that deviations from local equilibrium and correlations between the sites appear starting from order δ^2.

4. MACROSCROPIC BEHAVIOR IN THE HYDRODYNAMIC LIMIT

In this section, we assume that the oscillators $S_j: j=1,\ldots, N$, are placed on the interval $(0, L)$, at coordinates $x_j=\varepsilon j$, with $\varepsilon=L(N+1)^{-1}$, and we let $\varepsilon\to 0$, keeping the macroscopic length L fixed and viewing the system as a continuum. For the sake of simplicity, we take a homogeneous chain, with $\gamma_{j,j+1}=\gamma$ for all j.

Let $T(x)$ be a strictly positive smooth function, with $T(0)=T_-$ and $T(L)=T_+$. It is not hard to prove that the solution of the discretized heat equation (2.28), with initial condition $T_j(0)=T(\varepsilon j)$ and with the boundary conditions (2.29), is an approximation to the solution of the heat equation

$$\frac{\partial}{\partial t}T(x,t)=\gamma\frac{\partial^2}{\partial x^2}T(x,t): \qquad x\in(0,L),\ t\in\mathbb{R}^+ \tag{4.1}$$

with initial condition $T(x,0)=T(x)$ and with the boundary conditions

$$T(0,t)=T_-, \quad T(L,t)=T_+, \qquad \text{for all } t \tag{4.2}$$

in the sense that

$$\lim_{\varepsilon\to 0}\sup_{j=1,\ldots,N}|T_j(t/\varepsilon^2)-T(\varepsilon j,t)|=0, \qquad \varepsilon=L(N+1)^{-1} \tag{4.3}$$

uniformly on compact intervals in t. The result can be obtained by an application of the theory of approximation of contraction semigroups, as found, for instance, in Chapter 9 of Kato's book[19].

Now we prove that the macroscopic behavior of the model in the hydrodynamic limit is completely determined by the heat equation. In other words, starting from a local equilibrium state

$$\rho^{\varepsilon} = Z^{-1} \exp\left[- \sum_{j=1}^{N} \beta(\varepsilon j) H_j \right] \tag{4.4}$$

and letting the system evolve for a time of the order of ε^{-2}, the expectation values of macroscopic observables in the state $\exp[Kt/\varepsilon^2](\rho^{\varepsilon})$ are close (for small ε) to the expectation values in the local equilibrium state

$$\rho^{\varepsilon}(t) = Z^{-1} \exp\left[- \sum_{j=1}^{N} \beta(\varepsilon j, t) H_j \right]$$

where $T(x, t) = \hbar\omega(e^{\beta(x,t)\hbar\omega} - 1)^{-1}$ (or $T(x, t) = \beta(x, t)^{-1}$ in the classical case) satisfies the heat equation (4.1), with the boundary conditions (4.2). However, small deviations from local equilibrium should appear when considering the time evolution of fluctuation observables.[7]

Macroscopic obsevables are defined as (Wick-ordered) polynomials in the smeared energies $H^{\varepsilon}(g)$: $g \in C^{\infty}[0, L]$ given by

$$H^{\varepsilon}(g) = \varepsilon \sum_{j=1}^{N} g(\varepsilon j) H_j \colon \varepsilon = L(N+1)^{-1},\ g \in C^{\infty}[0, L] \tag{4.5}$$

This corresponds to the idea that a "macroscopic point" is indeed a macroscopically small region, containing a very large number of atoms. As initial state, we take a local equilibrium state of the form (4.4), where $T(x) = \hbar\omega(e^{\beta(x)\hbar\omega} - 1)^{-1}$ (or $T(x) = \beta(x)^{-1}$ in the classical case) is a smooth function, with $T(0) = T_-$, $T(L) = T_+$. We define

$$K^{\varepsilon} = \varepsilon^{-2}\left(K_- + \sum_{j=1}^{N-1} K_{j,j+1} + K_+ \right), \qquad \varepsilon = L(B+1)^{-1} \tag{4.6}$$

and we have the following:

Theorem 4.1. The smeared energy correlations

$$\langle \exp[K^{\varepsilon} t](\rho^{\varepsilon}); :H^{\varepsilon}(g_1) \cdots H^{\varepsilon}(g_n): \rangle \colon g_1, \ldots, g_n \in C^{\infty}[0, L] \tag{4.7}$$

factorize, in the limit as $\varepsilon \to 0$, to

$$\prod_{r=1}^{n} \int_0^L g_r(x)\, T(x, t)\, dx \tag{4.8}$$

Proof. It is convenient to view the expressions (4.7) as defining the joint distributions of random variables $X_t^\varepsilon(g)$: $g \in C^\infty[0, L]$ with respect to probability measures $\mathbb{P}_t^\varepsilon$, defined on a measurable space $(\Omega, \mathscr{F})$ which we need not specify, as

$$\int_\Omega X_t^\varepsilon(g_1) \cdots X_t^\varepsilon(g_n)\, d\mathbb{P}_t^\varepsilon = \langle \exp[K^\varepsilon t](\rho^\varepsilon); :H^\varepsilon(g_1) \cdots H^\varepsilon(g_n):\rangle \quad (4.9)$$

We have, from (2.27) and (4.3),

$$\langle \exp[K^\varepsilon t](\rho^\varepsilon); H^\varepsilon(g)\rangle = \varepsilon \sum_{j=1}^{N} g(\varepsilon j)\, T_j(t/\varepsilon^2)$$

$$\xrightarrow[\varepsilon \to 0]{} \int_0^L g(x)\, T(x, t)\, dx \quad (4.10)$$

where $T_j(t)$ [resp., $T(x, t)$] is the solution of the discretized heat equation (2.28) [resp., of the heat equation (4.1)] with the appropriate initial and boundary conditions.

Taking into account (4.10), it suffices to prove that the variance

$$\int_\Omega \left| X_t^\varepsilon(g) - \varepsilon \sum_{j=1}^{N} g(\varepsilon j)\, T_j(t/\varepsilon^2) \right|^2 d\mathbb{P}_t^\varepsilon \quad (4.11)$$

$$= \varepsilon^2 \sum_{r,s=1}^{N} g(\varepsilon r)\, g(\varepsilon s)(1 + \delta_{r,s})\, V_{r,s}(t/\varepsilon^2) + \varepsilon^2 \sum_{r=1}^{N} g(\varepsilon r)^2\, T_r(t/\varepsilon^2)^2$$

[where $V_{r,s}(t)$ has been defined in Equation (2.32)] vanishes in the limit as $\varepsilon \to 0$. Define a scalar product $\langle \cdot, \cdot \rangle_\varepsilon$ on $\mathbb{R}^{N^2}$ [$\varepsilon = L(N+1)^{-1}$] by

$$\langle a, b\rangle_\varepsilon = \varepsilon^2 \sum_{r,s=1}^{N} a_{r,s}(1 + \delta_{r,s}) b_{r,s} \colon a = \{a_{r,s}\},\ b = \{b_{r,s}\} \quad (4.12)$$

and denote by $\| \cdot \|_\varepsilon$ the corresponding norm. Then (4.11) is majorized by

$$\| V(t/\varepsilon^2) \|_\varepsilon \left[\varepsilon^2 \sum_{r,s=1}^{N} |g(\varepsilon r)\, g(\varepsilon s)|^2 (1 + \delta_{r,s}) \right]^{1/2} + O(\varepsilon)$$

$$\underset{\varepsilon \to 0}{\sim} \| V(t/\varepsilon^2) \|_\varepsilon \left[\int_0^L |g(x)|^2\, dx + O(\varepsilon) \right] \quad (4.13)$$

Now we estimate $\| V(t/\varepsilon^2) \|_\varepsilon$. It can be easily seen that $\mathscr{L}$ defined by (2.35), (2.36) is a negative self-adjoint operator with respect to the scalar product $\langle \cdot, \cdot \rangle_\varepsilon$, so that $\exp[\mathscr{L} t]$ is a contraction in the norm $\| \cdot \|_\varepsilon$. With the initial

state of the form (4.4), we have $V_{r,s}(0)=0$, so that, by Proposition 2.6, we obtain

$$\begin{aligned}\|V(t/\varepsilon^2)\|_\varepsilon &= \left\| \int_0^{t/\varepsilon^2} \exp[\mathscr{L}(t/\varepsilon^2 - t')]\, C(t')\, dt' \right\|_\varepsilon \\ &\leqslant (t/\varepsilon^2) \sup_{0\leqslant t'\leqslant t/\varepsilon^2} \|C(t')\|_\varepsilon \\ &= (t/\varepsilon^2)\gamma \sup_{0\leqslant t'\leqslant t/\varepsilon^2} \left[\varepsilon^2 \sum_{r,s=1}^{N} (1+\delta_{r,s})\{\delta_{r+1,s}[T_{r+1}(t') - T_r(t')]^4 \right. \\ &\quad \left. + \delta_{r-1,s}[T_{r-1}(t') - T_r(t')]^4\} \right]^{1/2} \end{aligned} \tag{4.14}$$

The summation in the right-hand side of (4.14) contains $2(N-1)=O(\varepsilon^{-1})$ terms, and for reasonably smooth initial conditions we have $|T_{r\pm1}(t) - T_r(t)| = O(\varepsilon|T_+ - T_-|)$ uniformly in $t\in\mathbb{R}^+$ [this follows from (4.3) and from known properties of the solution to the heat equation]. So we conclude that

$$\|V(t/\varepsilon^2)\|_\varepsilon = t\gamma O(|T_+ - T_-|^2)\, O(\varepsilon^{1/2}) \to 0 \qquad \text{as} \quad \varepsilon \to 0 \tag{4.15}$$

thus proving the theorem. ∎

Remark 4.2. The estimate (4.15) allows only to prove that the variance (4.11) vanishes at least as fast as $\varepsilon^{1/2}$ in the limit as $\varepsilon \to 0$. This is probably too crude; it should be possible to prove that (4.11) is of the order of ε and to find the limiting expression of the covariance of the fluctuation observables

$$\mathscr{F}_t^\varepsilon(g) = \varepsilon^{1/2} \sum_{j=1}^{N} g(\varepsilon j)[H_j - T_j(t/\varepsilon^2)] \tag{4.16}$$

explicitly [cf. Refs. 7(c), (d), (e)].

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