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Heat Conduction and Entropy Production in Anharmonic Crystals with Self-Consistent Stochastic Reservoirs

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Abstract We investigate a class of anharmonic crystals in d dimensions, $d \geq 1$, coupled to both external and internal heat baths of the Ornstein-Uhlenbeck type. The external heat baths, applied at the boundaries in the 1-direction, are at specified, unequal, temperatures T_{L} and T_{R}. The temperatures of the internal baths are determined in a self-consistent way by the requirement that there be no net energy exchange with the system in the non-equilibrium stationary state (NESS). We prove the existence of such a stationary self-consistent profile of temperatures for a finite system and show that it minimizes the entropy production to leading order in $(T_{\mathrm{L}} - T_{\mathrm{R}})$. In the NESS the heat conductivity κ is defined as the heat flux per unit area divided by the length of the system and $(T_{\mathrm{L}} - T_{\mathrm{R}})$. In the limit when the temperatures of the external reservoirs go to the same temperature T, $\kappa(T)$ is given by the Green-Kubo formula, evaluated in an equilibrium system coupled to reservoirs all having the temperature T. This $\kappa(T)$ remains bounded as the size of the system goes to infinity. We also show that the

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corresponding infinite system Green-Kubo formula yields a finite result. Stronger results are obtained under the assumption that the self-consistent profile remains bounded.

Keywords Thermal conductivity · Green-Kubo formula · Self-consistent thermostats · Entropy production · Nonequilibrium stationary states

1 Introduction

The rigorous derivation of Fourier's law of heat conduction for classical systems with Hamiltonian bulk dynamics (or for quantum systems with Schrödinger evolution) with boundaries kept at different temperatures is an open problem in mathematical physics [9]. The situation is different for systems with purely stochastic dynamics, e.g. for the Kipnis, Marchioro, Presutti (KMP) model [14], where such results can be readily derived [13, 19]. An interesting area of current research are hybrid models in which the time evolution is governed by a combination of deterministic and stochastic dynamics. The deterministic part of the dynamics is given by the usual Hamiltonian evolution. The stochastic part can be of two different types. In the first type, the stochastic part is constructed to strictly conserve the energy, as studied in [5], or conserve also momentum, as in [1, 2]. In the second type, studied in [7] and [8], the stochastic part is implemented by coupling the particles of the system to "internal" heat baths with which they can exchange energy. To obtain a heat flow between external reservoirs at specified temperatures T_{L}, T_{R}, acting at the left and right boundaries of the system, the temperatures of the internal heat baths are chosen in a self-consistent manner by the requirement that in the nonequilibrium stationary state (NESS) there be no net energy flux between these baths and the system [7, 8]. Because of this self-consistency condition, there is an average constant energy flux across the system in the NESS, supplied by the external reservoirs at specified, unequal, temperatures coupled to the boundaries of the system, and then carried by the Hamiltonian dynamics. A proof of Fourier's law for both types of hybrid models has been obtained for the case when the Hamiltonian dynamics is linear [5, 8], i.e., for a system of coupled harmonic oscillators.

In the present work we investigate the self-consistent model for anharmonic crystals. Unlike the case of the harmonic system, where it is known that Fourier's law does not hold when the "noise" is turned off (the heat conductivity then becoming infinite), one expects that in the anharmonic system with a pinning self-potential the conductivity will stay finite, i.e., it will satisfy Fourier's law, even when the strength of the noise goes to zero. We are quite far from proving this, however. What we do show here is that, for these anharmonic systems, conductivity for the finite system, defined by first letting both T_{L} and T_{R} approach the same value, is given by a Green-Kubo formula. We also prove that this Green-Kubo conductivity is bounded in the system size, whenever the noise is finite.

These results are obtained by studying the entropy production in the reservoirs in the NESS specified by the temperatures of all the reservoirs. We prove that the self-consistent profile minimizes, among all possible temperature profiles, the entropy production to the leading order in the difference of the boundary temperatures $T_{\mathrm{L}} - T_{\mathrm{R}}$. We then prove a uniform bound for the entropy production of a stationary state with a profile linear in the inverse temperatures. This leads to a bound on the leading term of the conductivity of the self-consistent system, given by the Green-Kubo formula for the finite system with all reservoirs at the same temperature T.

Furthermore, we show that the corresponding Green-Kubo formula for the infinite system, giving the conductivity of the infinite system as a space-time integral of the energy-current correlations, is convergent. The bound we derive implies that the conductivity vanishes in the limit of infinitely strong coupling to the reservoirs. This behavior is also apparent in the explicit expression of the conductivity of the corresponding harmonic system (see (7.10) in [8]). The violent contact with the reservoirs most likely makes local equilibrium so strong that eventually no transmission is possible.

There are no comparable results for anharmonic crystals with the first type of hybrid dynamics, but only some bounds on the conductivity [2]. Under the assumption that the self-consistent temperature profile remains bounded, we show that the conductivity of the finite systems with a fixed $T_{\mathrm{L}} - T_{\mathrm{R}} > 0$ is uniformly bounded in the size of the system. (This assumption is "clearly" correct but we are unable to prove it, see Sect. 9.)

The model considered is described in Sect. 2 while Sect. 3 contains a summary of the results proven in this paper. The existence of a NESS with a self-consistent temperature profile is proven in Sect. 4. Entropy production in the NESS is discussed in Sect. 5, and in Sect. 6 we prove that the stationary state corresponding to the self-consistent profile minimizes, at the leading order in the temperature difference $(T_{\mathrm{L}} - T_{\mathrm{R}})$, the entropy production. Thermal conductivity in the NESS is discussed in Sect. 7 and for the infinite homogeneous system in Sect. 8. Finally, in Sect. 9 we present some concluding remarks.

2 Time Evolution

Atoms are labeled by $x = (x_1, \ldots, x_d) \in \{-N, \ldots, N\}^d = \Lambda_N$, $N \geq 1$. Each atom is in contact with a heat reservoir at temperature T_x. The interactions with the reservoirs are modeled by Ornstein-Uhlenbeck processes at corresponding temperatures. The atoms have all the same mass $m = 1$. Their velocities are denoted by p_x and the "positions" by q_x, with $q_x, p_x \in \mathbb{R}$. We consider a mixture of fixed and periodic boundary conditions. The fixed boundary conditions are applied in the 1-direction, and the corresponding boundary sites will be used to make contact with external heat reservoirs. In the remaining directions, we apply periodic boundary conditions. Explicitly, let $\overline{\partial}\Lambda_N$ denote the set with $|x_1| = N + 1$ and let $[x]_i = -N + (x_i + N) \bmod (2N + 1)$, for $i \geq 2$. The boundary conditions are then $q_x = 0$, for $x \in \overline{\partial}\Lambda_N$. In addition, we let the inner boundary of Λ_N consist of those x with $|x_1| = N$, and we denote it by $\partial\Lambda_N$.

As we will show, the heat flux in the stationary state will be entirely in the 1-direction and the properties of the system will be uniform in the $d - 1$ periodic directions. We define $\Lambda'_N = \{x \in \Lambda_N : -N \leq x_1 < N\}$ to label the bonds in the 1-direction.

The Hamiltonian of the system is given by

$$\begin{aligned} \mathcal{H}_N &= \sum_{x\in\Lambda_N} \mathcal{E}_x, \\ \mathcal{E}_x &= \frac{p_x^2}{2} + \sum_{j=1}^{d} \frac{V(q_x - q_{x-e_j}) + V(q_{x+e_j} - q_x)}{2} + W(q_x), \quad x \in \Lambda_N, \end{aligned} \tag{2.1}$$

where the e_i, $i = 1, \ldots, d$, denote the Cartesian basis vectors. We assume that V and W are smooth positive symmetric functions on $\mathbb{R}$ with quadratic growth at infinity:

$$\lim_{\lambda\to\infty} W''(\pm\lambda) = W''_\infty > 0, \qquad \lim_{\lambda\to\infty} V''(\pm\lambda) = V''_\infty > 0. \tag{2.2}$$

Clearly then, there are $C_1, C_2 > 0$ such that

$$C_1(q^2 - 1) \leq V(q) \leq C_2(q^2 + 1), \qquad C_1(q^2 - 1) \leq W(q) \leq C_2(q^2 + 1). \tag{2.3}$$

The dynamics is described by the following system of stochastic differential equations:

$$\begin{aligned} dq_x &= p_x dt, \\ dp_x &= -\partial_{q_x}\mathcal{H}_N\, dt - \gamma_x p_x\, dt + \sqrt{2\gamma_x T_x}\, dw_x(t), \end{aligned} \tag{2.4}$$

with $\gamma_x > 0$ for all $x \in \Lambda_N$. Here $w_x(t), x \in \Lambda_N$, are independent standard Brownian motions (with 0 average and diffusion equal to 1). The generator of this process has the form

$$\begin{aligned} L_N &= \sum_{x\in\Lambda_N} (\partial_{p_x}\mathcal{H}_N \partial_{q_x} - \partial_{q_x}\mathcal{H}_N \partial_{p_x}) + \sum_{x\in\Lambda_N} \gamma_x (T_x \partial^2_{p_x} - p_x \partial_{p_x}) \\ &= A + S, \end{aligned} \tag{2.5}$$

where A is the Hamiltonian part, anti-symmetric in the momentum variables, and S is the symmetric part corresponding to the action of the reservoirs. Then

$$L_N \mathcal{E}_x = \sum_{i=1}^{d} (j_{x-e_i,x} - j_{x,x+e_i}) + J_x, \quad x \in \Lambda_N \tag{2.6}$$

with $J_x = \gamma_x (T_x - p_x^2)$ and

$$j_{x,x+e_i} = 0, \quad \text{if } [x] \notin \Lambda_N \text{ or } [x+e_i] \notin \Lambda_N, \tag{2.7}$$

$$j_{x,x+e_i} = -\frac{1}{2}(p_{[x]} + p_{[x+e_i]}) V'(q_{[x+e_i]} - q_{[x]}), \quad \text{otherwise.} \tag{2.8}$$

In particular, then $j_{x,x+e_1}$ can be non-zero only if $x \in \Lambda'_N$.

In Sect. 3 of [16] it is shown that, for any choice of the temperatures $\mathbf{T} = \{T_x \geq 0\}$, there exists an explicit Lyapunov function for the corresponding stochastic evolution, as long as $\gamma_x > 0$ for all x. This implies the existence of the corresponding stationary measure that we will denote by $\mu(\mathbf{T})$.

If at least one $T_x > 0$, then the generator L_N defined in (2.5) is (weakly)-hypoelliptic, in the sense that the Lie algebra generated by the *vector fields* $\{A, \partial_{p_x}, x \in \Lambda_N\}$ has full range in the tangent space of the phase space $(\mathbb{R}^{2d})^{\Lambda_N}$. In particular, the dynamics has probability transitions with smooth densities with respect to the Lebesgue measure on the phase space. If all $T_x > 0$, also the corresponding control problem has a strong solution (cf. Sect. 3 in [16], or [11]) and uniqueness of the stationary measure follows from these properties. These methods could be extended to the case $T_x \geq 0$, at least if $\mathcal{H}_N(p,q)$ is strictly convex [17]. The investigation of the uniqueness of the stationary measure goes beyond the purposes of the present paper, in particular, since zero temperatures will be relevant only in the general proof of existence of a self-consistent temperature profile in Sect. 4. So we will assume the uniqueness even in the case of temperatures not strictly positive.

The spatial periodicity will be exploited in the following to remove (most likely irrelevant) technical difficulties associated with irregular boundary behavior. To this end, we will assume that also the heat bath couplings respect this periodicity, i.e., *we will always assume that γ_x depends only on x_1*. Then in the case where also T_x depends only on x_1, the stochastic dynamics is fully invariant under periodic translations. Since the stationary measure $\mu(\mathbf{T})$ is unique, then also any of the corresponding expectation values must be invariant.

We denote the constant temperature profile, $T_x = T_o$ for all $x \in \Lambda_N$, as $\mathbf{T}_o$. Then $\mu(\mathbf{T}_o) = \mu_{T_o}$, the Gibbs measure at temperature T_o, defined by

$$\mu_{T_o} = Z_{T_o}^{-1} \exp(-\mathcal{H}_N(p,q)/T_o) dp\, dq = G_{T_o}(p,q) dp\, dq. \tag{2.9}$$

We use μ_{T_o} as a reference measure and denote the related expectation by $\langle\cdot\rangle_0$.

Computing the adjoint of L_N with respect to the Lebesgue measure we have[1]

$$L_N^{*(1)} = -A + \sum_{x\in\Lambda_N} S_x^{*(1)} \tag{2.10}$$

where $S_x^{*(1)} = \gamma_x(T_x\partial_{p_x}^2 + 1 + p_x\partial_{p_x})$. We denote by $f_N = f_N(\mathbf{T})$ the density of the stationary state $\mu(\mathbf{T})$ with respect to Lebesgue measure. This is the solution of $L_N^{*(1)} f_N = 0$. Due to hypoellipticity, f_N is a smooth function of (p,q), and this implies also smoothness in $\mathbf{T}$. To see this, note that $\partial_{T_y} f_N$ is the solution of the equation

$$L_N^{*(1)}\partial_{T_y} f_N = -\gamma_y\partial_{p_y}^2 f_N. \tag{2.11}$$

Since the right hand side is smooth in (p,q), this equation has a smooth solution, and smoothness in $\mathbf{T}$ follows by a standard iteration of the argument.

3 Summary of Results

Given the temperatures $\mathbf{\Theta}_R = \{\Theta_y\}_{y\in R}$ in a set $R\subset\Lambda_N$, we say that a temperature profile $\mathbf{T} = \{T_x\}_{x\in\Lambda_N}$ is *self-consistent*, if $T_x = \Theta_x$ for all $x\in R$, and the corresponding stationary state has the property

$$\langle p_x^2\rangle = T_x, \quad \text{for all } x\in\Lambda_N\setminus R, \tag{3.1}$$

where $\langle\cdot\rangle$ denotes expectation with respect to the NESS, $\mu(\mathbf{T})$, assumed to be unique. Eventually we may choose $R = \partial\Lambda_N$ or part of it. But the following result is independent from the geometry.

Theorem 1 *For any choice of a non-empty $R\subset\Lambda_N$, and for any choice of temperatures $\mathbf{\Theta}_R = \{\Theta_y\}_{y\in R}$ not all equal to 0, there exists a self-consistent temperature profile $\mathbf{T} = \{T_x\}_{x\in\Lambda_N\setminus R}$. In addition, if R and $\mathbf{\Theta}_R$ are invariant under translations in all of the $d-1$ periodic directions of Λ_N, then a self-consistent profile invariant under these translations can be found.*

The main body of our results concerns the case where the reservoirs on the two sides in the non-periodic direction are fixed to constant but unequal temperatures. We call this case the *boundary layer setup*. More explicitly, we then define $R = \partial\Lambda_N = \partial_L\Lambda_N\cup\partial_R\Lambda_N$, where $\partial_L\Lambda_N = \{x : x_1 = -N\}$ and $\partial_R\Lambda_N = \{x : x_1 = N\}$, and we fix on the left the temperatures $T_x = T_L$ for $x\in\partial_L\Lambda_N$, and on the right $T_x = T_R$ for $x\in\partial_R\Lambda_N$, $T_R < T_L$. We also set $\beta_L = T_L^{-1}$, and $\beta_R = T_R^{-1}$. Uniqueness of the self-consistent profile is not claimed in Theorem 1, and this remains an open problem in the generality of the theorem. However, by restricting to small temperature differences and then relying on the implicit function theorem, we can get a self-consistent profile which is essentially unique.

[1] We wish to reserve the standard notation for adjoint for certain weighted L^2-spaces, to be introduced later. Hence the notation $L_N^{*(1)}$ for the adjoint here.

Theorem 2 *For any given $T_o > 0$ and N, there are $\varepsilon_0, \delta > 0$ with the following property: In the boundary layer setup with T_L, T_R such that $|T_L - T_o|, |T_R - T_o| < \frac{1}{2}\varepsilon_0$ there is a self-consistent extension of the temperature profile, $\mathbf{T}^{sc}(T_L, T_R)$, and the extension is unique in the sense that no other profile $\mathbf{T}$ with $\max_x |T_x - T_o| < \delta$ is self-consistent. In addition, $\mathbf{T}^{sc}$ is invariant under translations in all of the $d-1$ periodic directions of Λ_N, and the map $(T_L, T_R) \mapsto \mathbf{T}^{sc}(T_L, T_R)$ is smooth.*

As an aside, let us remark that a careful inspection of the proof of Theorem 2 shows that its assumptions could be greatly relaxed, allowing for more general sets R and almost arbitrary potentials V and W. However, since the range of its applicability, determined by ε_0, can depend on N and might go to zero as $N \to \infty$, we have included the proof of the more general result in Theorem 1. Furthermore, the assumptions about the asymptotic quadratic behavior of V and W will be used in latter proofs, and thus cannot be neglected. From now on, we assume that $T_L - T_R$ is sufficiently small for applying Theorem 2, and let $\mathbf{T}^{sc}$ denote the corresponding self-consistent extension of the temperature profile, which is thus invariant under periodic translations and leads to a unique, periodically invariant, stationary state.

For a generic profile $\mathbf{T}$, we define the entropy production in a reservoir in the steady state $\mu(\mathbf{T})$ as the energy flux entering that reservoir divided by its temperature [4]. The total steady state entropy production is then given by

$$\sigma(\mathbf{T}) = \sum_{x\in\Lambda_N} \frac{\langle -J_x\rangle}{T_x} = \sum_{x\in\Lambda_N} \gamma_x \left(\frac{\langle p_x^2\rangle}{T_x} - 1 \right). \tag{3.2}$$

By using the local energy conservation (2.6) and denoting $\beta_x = T_x^{-1}$, we can write this as

$$\sigma(\mathbf{T}) = \sum_{i=1}^{d} \sum_{x\in\Lambda'_N} (\beta_{x+e_i} - \beta_x)\langle j_{x,x+e_i}\rangle. \tag{3.3}$$

It is well known [4] that $\sigma(\mathbf{T}) \geq 0$.

For the self-consistent profile $\mathbf{T}^{sc}$, there are no fluxes to the reservoirs for $x \notin \partial\Lambda_N$ and consequently, as will be shown below, $\langle j_{x,x+e_1}\rangle = \bar{j}_N$ for all $x \in \Lambda'_N$. The entropy production (3.3) is then equal to

$$\sigma(\mathbf{T}^{sc}) = (2N+1)^{d-1}(\beta_R - \beta_L)\bar{j}_N. \tag{3.4}$$

Thus we can estimate the magnitude of the self-consistent current by estimating the entropy production.

Theorem 3

$$\sigma(\mathbf{T}^{sc}) \leq (2N+1)^{d-2}(\beta_R - \beta_L)^2 C(\mathbf{T}^{sc}, \gamma) \tag{3.5}$$

where, up to a constant c depending only on the potentials V and W,

$$C(\mathbf{T}^{sc}, \gamma) = c\frac{\max_x \gamma_x T_x^{sc}}{\min_x \gamma_x^2}\left(1 + \max_x T_x^{sc}\right). \tag{3.6}$$

Consequently, the average self-consistent current is bounded by

$$0 \leq \bar{j}_N \leq C(\mathbf{T}^{sc}, \gamma)\frac{\beta_R - \beta_L}{2N+1}. \tag{3.7}$$

We expect, but are not able to prove, that the self-consistent profiles remain uniformly bounded in N. From such a bound it would follow that $\bar{j}_N = \mathcal{O}(N^{-1})$. We expect in fact that $T_x \in [T_{\mathrm{R}}, T_{\mathrm{L}}]$, as in the harmonic case [8], c.f., Sect. 9. What we can prove is that the first order term of $\bar{j}_N$ in an expansion in the imposed temperature gradient is $\mathcal{O}(N^{-1})$. This is possible even without explicit knowledge about the asymptotics of the self-consistent profile. To this end, we consider also profiles $\mathbf{T}^{\beta\mathrm{lin}}$ which are extensions in the boundary layer setup to a profile with linear β_x; we define

$$(T_x^{\beta\mathrm{lin}})^{-1} = \frac{1}{2}\left(\frac{\beta_{\mathrm{R}} - \beta_{\mathrm{L}}}{N} x_1 + \beta_{\mathrm{R}} + \beta_{\mathrm{L}}\right), \quad x \in \Lambda_N. \tag{3.8}$$

For these profiles, the entropy production satisfies

$$\sigma(\mathbf{T}^{\beta\mathrm{lin}}) = \frac{\beta_{\mathrm{R}} - \beta_{\mathrm{L}}}{2N} \sum_{x \in \Lambda'_N} \langle j_{x,x+e_i} \rangle_{\mathbf{T}^{\beta\mathrm{lin}}}, \tag{3.9}$$

and we can derive a more precise bound for it.

Theorem 4 *Given $b > 0$, there exists a constant $C_2(\gamma; b)$, depending only on γ, V, W, and b, such that for all $T_{\mathrm{R}} \le T_{\mathrm{L}} \le b$,*

$$\sigma(\mathbf{T}^{\beta\mathrm{lin}}) \le (2N+1)^{d-2} (\beta_{\mathrm{R}} - \beta_{\mathrm{L}})^2 C_2(\gamma; b). \tag{3.10}$$

Obviously, if $\mathbf{T}_{\mathrm{o}}$ is any constant temperature profile, we have $\sigma(\mathbf{T}_{\mathrm{o}}) = 0$. Furthermore, $\frac{\partial \sigma}{\partial T_x}(\mathbf{T}_{\mathrm{o}}) = 0$, and the second order derivatives can also be computed, yielding the following theorem.

Theorem 5 *The Taylor expansion of σ around a constant profile $\mathbf{T}_{\mathrm{o}}$ at the second order gives*

$$\sigma(\mathbf{T}_{\mathrm{o}} + \varepsilon \mathbf{v}) = \frac{\varepsilon^2}{T_{\mathrm{o}}^2} Q(\mathbf{v}; T_{\mathrm{o}}) + \mathcal{O}(\varepsilon^3), \quad Q(\mathbf{v}; T_{\mathrm{o}}) = \sum_{x,y \in \Lambda_N} \mathcal{J}_{y,x} v_y v_x, \tag{3.11}$$

where, with $\langle\cdot\rangle_0$ denoting the expectation in $\mu(\mathbf{T}_{\mathrm{o}})$,

$$\mathcal{J}_{y,x} = \gamma_x \delta_{y,x} - \gamma_x \gamma_y \langle h_x (-L_N(\mathbf{T}_{\mathrm{o}}))^{-1} h_y \rangle_0, \quad h_x = \frac{p_x^2}{T_{\mathrm{o}}} - 1. \tag{3.12}$$

The matrix $\mathcal{J}$ is positive, and if $\mathcal{J}_{y,x}$ is restricted to $x, y \in \Lambda_N \setminus \partial\Lambda_N$, it becomes strictly positive.

We now denote $\delta T = T_{\mathrm{L}} - T_{\mathrm{R}}$ and $T_{\mathrm{o}} = (T_{\mathrm{L}} + T_{\mathrm{R}})/2$. The next result says that the self-consistent profile minimizes entropy production, at least up to the leading order in the gradient of the imposed temperature difference, δT.

Theorem 6 *The self-consistent profile $\mathbf{T}^{\mathrm{sc}}$ is a smooth function of T_{L} and T_{R}. For a fixed T_{o}, its first order Taylor expansion*

$$T_x^{\mathrm{sc}} = T_{\mathrm{o}} + \mathrm{g}^{\mathrm{sc}}(x) \delta T + \mathcal{O}(\delta T^2), \quad x \in \Lambda_N, \tag{3.13}$$

is such that $\mathbf{v} = \mathbf{g}^{\mathrm{sc}}$ is the unique minimizer of $Q(\mathbf{v}; T_{\mathrm{o}})$ for fixed $v(x) = \pm\frac{1}{2}$, $x \in \partial\Lambda_N$, where we choose the $+$-sign for $x \in \partial_{\mathrm{L}}\Lambda_N$, and $-$ for $x \in \partial_{\mathrm{R}}\Lambda_N$.

Consequently, the self-consistent profile minimizes the entropy production up to errors of the order of δT^3. In particular, the leading term of the self-consistent profile can be obtained by minimization of the entropy production. This is consistent with the general belief that for small deviations from the equilibrium state imposed by external constraints, the stationary state will be such that it minimizes the entropy production with respect to variation in the unconstrained parameters [12]. The entropy production has also been studied by Bodineau and Lefevere [6] in this model, and originally by Maes, et al., [15] in the context of heat conduction networks.

We define the thermal conductivity in the self-consistent stationary state (of the finite system) as

$$\kappa_N^{\mathrm{sc}}(T_{\mathrm{o}}) = \lim_{\delta T\to 0} \frac{2N+1}{\delta T}\, \bar{j}_N. \tag{3.14}$$

This is related to the entropy production by (3.4), yielding

$$\kappa_N^{\mathrm{sc}}(T_{\mathrm{o}}) = Q(\mathbf{g}^{\mathrm{sc}}; T_{\mathrm{o}})/(2N+1)^{d-2}, \tag{3.15}$$

where, as in Theorem 5, we have defined

$$Q(\mathbf{v}; T_{\mathrm{o}}) = \mathbf{v}\cdot \mathcal{J}(T_{\mathrm{o}})\mathbf{v} = T_{\mathrm{o}}^2 \lim_{\varepsilon\to 0} \frac{\sigma(\mathbf{T}_{\mathrm{o}} + \varepsilon \mathbf{v})}{\varepsilon^2}. \tag{3.16}$$

Since $\mathbf{g}^{\mathrm{sc}}$ minimizes $Q(\cdot)$, we find using (3.10)

$$\kappa_N^{\mathrm{sc}}(T_{\mathrm{o}}) \le (2N+1)^{2-d} T_{\mathrm{o}}^2 \lim_{\delta T\to 0} \frac{\sigma(\mathbf{T}^{\beta\mathrm{lin}})}{\delta T^2} \le T_{\mathrm{o}}^{-2} C_2(\gamma; 2T_{\mathrm{o}}). \tag{3.17}$$

In particular, since the bound does not depend on N, this proves that the self-consistent conductivity defined by (3.14) is uniformly bounded in N. It also has a Green-Kubo type of representation, as summarized in the following theorem.

Theorem 7 *The self-consistent conductivity is uniformly bounded in N and satisfies*

$$\kappa_N^{\mathrm{sc}}(T_{\mathrm{o}}) = \frac{1}{T_{\mathrm{o}}^2} \int_0^\infty \sum_{x\in\Lambda_N'} (-(2N+1)\nabla_{e_1} \mathrm{g}^{\mathrm{sc}}(x)) \langle j_{x,x+e_1}(t) j_{0,e_1}(0)\rangle_0 \, dt \tag{3.18}$$

where $\langle\cdot\rangle_0$ denotes the mean over the initial conditions distributed according to the equilibrium measure at the temperature T_{o} with the time evolution given by the dynamics corresponding to $\mathbf{T}_{\mathrm{o}}$, i.e., all the reservoirs are at temperature T_{o}. Here $\nabla_{e_1} \mathrm{g}^{\mathrm{sc}}(x) = \mathrm{g}^{\mathrm{sc}}(x+e_1) - \mathrm{g}^{\mathrm{sc}}(x)$ denotes a discrete gradient.

A similar Green-Kubo formula can be obtained for the entropy production in the stationary state of the profile $\mathbf{T}^{\beta\mathrm{lin}}$. We will prove that

$$\begin{aligned}(2N+1)^{2-d} T_{\mathrm{o}}^2 \lim_{\delta T\to 0} \frac{\sigma(\mathbf{T}^{\beta\mathrm{lin}})}{\delta T^2} &= \lim_{\delta T\to 0} \frac{2N+1}{\delta T} \frac{1}{|\Lambda_N'|} \sum_{x\in\Lambda_N'} \langle j_{x,x+e_1}\rangle_{\mu(\mathbf{T}^{\beta\mathrm{lin}})} \\ &= \left(1+\frac{1}{2N}\right) \frac{1}{T_{\mathrm{o}}^2} \int_0^\infty \frac{1}{|\Lambda_N'|} \sum_{x,y\in\Lambda_N'} \langle j_{y,y+e_1}(t) j_{x,x+e_1}(0)\rangle_0 \, dt. \end{aligned}\tag{3.19}$$

By (3.17), this is always an upper bound for $\kappa_N^{\mathrm{sc}}(T_{\mathrm{o}})$. We expect the self-consistent profile to become linear away from the boundaries in the limit $\varepsilon \to 0$, and to find $\nabla_{e_1} g^{\mathrm{sc}}(x) \approx -\frac{1}{2N}$, whenever x_1 is not too close to $\pm N$. Although a proof of this property is still missing, we conjecture accordingly that both $\kappa_N^{\mathrm{sc}}(T_{\mathrm{o}})$ and the right hand side of (3.19) have the same limit as $N \to \infty$.

The last result concerns the Green-Kubo representation of the conductivity in the *infinite system*. Consider the infinite system on $\mathbb{Z}^d$ with all $\gamma_x = \gamma$ and all thermostats at temperature T_{o}. This infinite dynamics has a unique invariant measure given by the Gibbs measure on $(\mathbb{R}^{2d})^{\mathbb{Z}^d}$ at temperature T_{o}, defined by the usual DLR relations. We denote also the infinite volume Gibbs measure by $\mu_{T_{\mathrm{o}}}$. The existence of the dynamics of this infinite system in equilibrium at any given temperature can be proven by standard techniques (cf. [18], where a similar result is proven for an analogous system in continuous space). A proof of the existence of the dynamics in dimension 2 for a certain set of non-equilibrium initial configurations is proven in [10]. Consequently, we look at the dynamics starting from this equilibrium distribution, and let $\mathbb{E}$ denote the expectation over the corresponding stochastic process.

Theorem 8 *There is a unique limit for*

$$\frac{1}{T_{\mathrm{o}}^2} \lim_{\lambda \to 0} \sum_{x \in \mathbb{Z}^d} \int_0^\infty e^{-\lambda t} \mathbb{E}[j_{x,x+e_1}(t) j_{0,e_1}(0)]\, dt = \kappa(T_{\mathrm{o}}) \le \frac{C}{\gamma}, \tag{3.20}$$

where $C = \mathbb{E}[(V'(q_{e_1}(0) - q_0(0)))^2]/T_{\mathrm{o}}$ *is finite and depends only on* T_{o}.

As we have mentioned in the introduction, the above bound for the conductivity goes to zero when $\gamma \to \infty$.

As argued earlier, we expect the self-consistent conductivity and the Green-Kubo formula for the linear profile to have the same limit as $N \to \infty$. However, inspecting the definition of the latter quantity in (3.19) shows that this limit should be given by (3.20), provided the current-current correlations $\langle j_{x,x+e_1}(t) j_{y,y+e_1}(0)\rangle_0$ have a sufficiently fast uniform decay both in t and in the spatial separation $|x - y|$ (the limiting infinite system dynamics are translation invariant also in the first direction, which should be employed to cancel the sum over y in (3.19)). Therefore, we also conjecture that $\kappa_N^{\mathrm{sc}}(T_{\mathrm{o}}) \to \kappa(T_{\mathrm{o}})$, at least along some subsequence of $N \to \infty$.

4 Self-consistent Profiles: Existence

The following Lemma shows that zero temperatures cannot appear in self-consistent temperature profiles. (We will also give a second proof of local existence of self-consistent profiles in Sect. 6 which does not rely on the assumptions made about profiles containing zero temperatures.)

Lemma 1 *If* $\{T_x, x \in \Lambda_N\}$ *are not all identically zero, then* $\langle p_y^2 \rangle > 0$ *for all* $y \in \Lambda_N$.

Proof This is a consequence of the smoothness of the density of the transition probability $P_t(q', p'; q, p)$ of the process. Since $\int P_t(q', p'; q, p) dq\, dp = 1$, for any (q', p') there exists an open set of positive Lebesgue measure $A = A(q', p', t)$ such that

$$\int_A P_t(q', p'; q, p) dq\, dp > 0. \tag{4.1}$$

If there exists x such that $\langle p_x^2\rangle = 0$, then

$$0 = \int \mu(\mathbf{T}; dq', dp') \int p_x^2 P_t(q', p'; q, p) dq\, dp \tag{4.2}$$

which clearly is in contradiction with (4.1). □

Proof of Theorem 1 Given any collection of parameters $u \in [0,\infty)^{R^c}$, $x \in R^c$, let us define the corresponding temperature profile $\mathbf{T}(u)$ by

$$T(u)_x = T(u;\Theta)_x = \begin{cases} u_x, & \text{if } x \in R^c, \\ \Theta_x, & \text{if } x \in R. \end{cases} \tag{4.3}$$

As before, we denote the density of the corresponding stationary measure by $f_N(q, p; \mathbf{T}(u), V, W)$. We have seen in Sect. 2 that, by the hypoelliptic properties of the dynamics (cf. [16]), f_N is a smooth function of (q, p) and consequently of $\mathbf{T}$. By a straightforward scaling argument, we then have for any u and $\lambda > 0$,

$$\lambda^M f_N(\sqrt{\lambda} q, \sqrt{\lambda} p; \mathbf{T}(u), V, W) = f_N(q, p; \mathbf{T}(u)/\lambda, V_\lambda, W_\lambda) \tag{4.4}$$

where $V_\lambda(q) = \lambda^{-1} V(\sqrt{\lambda} q)$ and $W_\lambda(q) = \lambda^{-1} W(\sqrt{\lambda} q)$. An argument similar to that used at the end of Sect. 2 to prove regularity in $\mathbf{T}$ shows that $f_N(q, p; \mathbf{T}(u)/\lambda, V_\lambda, W_\lambda)$ is smooth in λ. Under the conditions assumed on V and W, we have $\lim_{\lambda\to\infty} V_\lambda(q) = V_\infty(q)$ and $\lim_{\lambda\to\infty} W_\lambda(q) = W_\infty(q)$ with $V_\infty(q) = \frac{1}{2} V''_\infty q^2$ and $W_\infty(q) = \frac{1}{2} W''_\infty q^2$.

We apply the scaling relation to prove that for high enough temperatures the system behaves essentially like a Gaussian. More precisely, consider arbitrary sequences $\lambda_n \to \infty$ and $\mathbf{b}^{(n)} \in [0,\infty)^{\Lambda_N}$, such that $\mathbf{b}^{(n)}$ converges to $\mathbf{b} \in [0,\infty)^{\Lambda_N}$. Define further $T_x^{(n)} = \lambda_n b_x^{(n)}$, $x \in \Lambda_N$. Then by the scaling relation (4.4), for any x',

$$\frac{1}{\lambda_n}\langle p_{x'}^2\rangle(\mathbf{T}^{(n)}, V, W) = \langle p_{x'}^2\rangle(\mathbf{b}^{(n)}, V_{\lambda_n}, W_{\lambda_n}) \underset{n\to\infty}{\longrightarrow} \langle p_{x'}^2\rangle(\mathbf{b}, V_\infty, W_\infty). \tag{4.5}$$

The last expectation is with respect to the stationary state of a purely harmonic system. This system was studied in [8], where it was proved, in Sects. 3 and 7, that there is a doubly stochastic matrix M, with strictly positive entries, such that for any profile of temperatures $\mathbf{b}$ and for all x',

$$\langle p_{x'}^2\rangle(\mathbf{b}, V_\infty, W_\infty) = \sum_{y\in\Lambda_N} M_{x'y} b_y.$$

(Strictly speaking, the result was proven only for periodic profiles in [8]. However, the above properties, linearity in $\mathbf{b}$, as well as positivity and double stochasticity of M, are easily generalized for non-periodic profiles, although we do not go into details here.) Since $\sum_y M_{xy} = 1$ for all x, this implies

$$\langle p_{x'}^2\rangle(\mathbf{b}, V_\infty, W_\infty) \le \max_y b_y = \|\mathbf{b}\|_\infty, \tag{4.6}$$

and the equality holds if and only if $\mathbf{b}$ is a constant vector, i.e., b_x is independent of x.

We can now prove the existence of a self-consistent profile. Let $R^c = \Lambda_N \setminus R$, and consider the mapping $F : X \to X$, $X = [0,\infty)^{R^c}$ defined for $u \in [0,\infty)^{R^c}$, $x \in R^c$, by

$$F(u)_x = \langle p_x^2\rangle(\mathbf{T}(u), V, W). \tag{4.7}$$

Since some of the temperatures are kept fixed to non-zero values, the hypoelliptic properties of $L_N^{*(1)}$ imply that F is everywhere continuous. For any $L > 0$ define $X_L = [0, L]^{R^c} \subset X$. We will soon prove that there is an $L > 0$ such that $F(X_L) \subset X_L$. Since X_L is homeomorphic to the unit ball of $\mathbb{R}^{|R^c|}$ and F is continuous on X_L, we can conclude from the Brouwer fixed point theorem that there is at least one $u \in X_L$ such that $F(u) = u$. By Lemma 1, if there is x such that $u_x = 0$, then $F(u)_x > 0$, and such u cannot be fixed points. Thus for any fixed point $0 < u_x \le L < \infty$ for all x, and $\mathbf{T}(u)$ is then a proper self-consistent temperature profile.

We prove the existence of a constant L, for which $F(X_L) \subset X_L$, by contradiction. If no such L exists, then for all $L > 0$ there is $u^{(L)} \in X_L$ such that $\|F(u^{(L)})\|_\infty > L$. Then necessarily $\|u^{(L)}\|_\infty \to \infty$, since otherwise there would exists a convergent subsequence, which is incompatible with $\|F(u^{(L)})\|_\infty \to \infty$. Let $\lambda_L = \|u^{(L)}\|_\infty$ and $v^{(L)} = \lambda_L^{-1} u^{(L)}$, so that $\lambda_L \to \infty$ and $\|v^{(L)}\|_\infty = 1$. The sequence $(v^{(L)})$ belongs to a compact subset of X, and we can find a subsequence such that $v^{(L)} \to v$ in X. For this final subsequence we can apply (4.5) and (4.6), which shows that for all x

$$\limsup_{L} \lambda_L^{-1} F(\lambda_L v^{(L)})_x < \|v\|_\infty = 1. \tag{4.8}$$

Equality is not possible here, as the limit $\mathbf{b}$ of $\lambda_L^{-1}\mathbf{T}(\lambda_L v^{(L)})$ has at least one component equal to one, but $b_x = 0$ for all $x \in R$, and thus $\mathbf{b}$ cannot be a constant vector. However, by construction, for every L there is $x(L)$ such that $F(\lambda_L v^{(L)})_{x(L)} > L \ge \|u(L)\|_\infty = \lambda_L$, which leads to contradiction. This proves the existence of $L > 0$ with the required properties and concludes the proof of the first part of the theorem.

For the second part, let us first point out that, if R is invariant under all periodic translations of Λ_N, it must be of the form $R = R_1 \times I_N^{d-1}$, where $I_N = \{-N, \ldots, N\}$ and $R_1 \subset I_N$ is non-empty. Similarly, Θ_x can only depend on x_1. Let $R_1^c = I_N \setminus R_1$, let P_1 denote the projection on the first axis in $\mathbb{Z}^d$, and define $R' = P_1 R^c = R_1^c \times \{\mathbf{0}\}$, which is a subset of $R^c = \Lambda_N \setminus R$. If R' is empty, $R = \Lambda_N$ and there is nothing to prove. Otherwise, let us consider the map $F' : X' \to X'$, $X' = [0, \infty)^{R'}$, defined by $F'(u)_x = \langle p_x^2 \rangle(\mathbf{T}'(u), V, W)$, where

$$T'(u)_x = \begin{cases} u_{P_1 x}, & \text{if } x \in R^c, \\ \Theta_x, & \text{otherwise.} \end{cases} \tag{4.9}$$

Every such $T'(u)$ is clearly invariant under all periodic translations. We can then repeat the analysis made above for F' and conclude that it has a fixed point $\bar{u}$ with $0 < \bar{u}_x < \infty$. Since $\bar{T} = T'(\bar{u})$ is periodic, the dynamics is completely invariant under periodic translations, implying that also expectation values in the unique stationary state are invariant. Therefore, for any $x \in R^c$, we have $\langle p_x^2 \rangle(\bar{T}) = \langle p_{P_1 x}^2 \rangle(\bar{T}) = u_{P_1 x} = \bar{T}_x$. This proves that $\bar{T}$ is an invariant, self-consistent profile. □

5 Entropy Production Bound

In this section we prove the entropy production bounds stated in Theorems 3 and 4. Given a generic profile of temperatures $\mathbf{T}$, we recall the notation $f_N = f_N(\mathbf{T})$ for the density of the stationary measure $\mu(\mathbf{T})$ with respect to Lebesgue measure, and let $\langle \cdot \rangle$ denote expectation with respect to $\mu(\mathbf{T})$. A simple computation shows that $\langle A \ln f_N \rangle = 0$ for A defined in (2.5). Therefore, by stationarity we have

$$0 = -\langle L_N \ln f_N \rangle = -\sum_x \langle S_x \ln f_N \rangle \tag{5.1}$$

where $S_x = \gamma_x(T_x \partial_{p_x}^2 - p_x \partial_{p_x})$. Let $\psi_x = f_N/G_{T_x}$, where $G_T = Z_T^{-1} \mathrm{e}^{-\mathcal{H}_N/T}$, as in (2.9). Then we can rewrite the last term as

$$-\langle S_x \ln f_N \rangle = -\int (S_x \ln \psi_x)\psi_x G_{T_x} dp\, dq - \int S_x(\ln G_{T_x}) f_N dp\, dq. \tag{5.2}$$

Since $p_x G_{T_x} = -T_x \partial_{p_x} G_{T_x}$ and $S_x(\ln G_{T_x}) = -\gamma_x(T_x - p_x^2)/T_x = -J_x/T_x$, we find by integration by parts that

$$-\langle S_x \ln f_N \rangle = T_x \gamma_x \int \frac{(\partial_{p_x}\psi_x)^2}{\psi_x} G_{T_x} dp\, dq + \frac{\langle J_x \rangle}{T_x}. \tag{5.3}$$

So by (5.1), the entropy production satisfies

$$\sigma(\mathbf{T}) = -\sum_{x\in\Lambda_N} \frac{\langle J_x \rangle}{T_x} = \sum_{x\in\Lambda_N} \mathcal{D}_x, \tag{5.4}$$

where

$$\mathcal{D}_x = \gamma_x T_x \int \frac{(\partial_{p_x}\psi_x)^2}{\psi_x} G_{T_x} dp\, dq. \tag{5.5}$$

In particular, $\sigma(\mathbf{T}) \geq 0$, and by using the local conservation of energy, (2.6), (3.3) holds.

Let us for the remainder of this section assume that $\mathbf{T}$ is a temperature profile which is invariant under the periodic translations. The results then hold for both $\mathbf{T}^{\mathrm{sc}}$ and $\mathbf{T}^{\beta \mathrm{lin}}$. Obviously, then by (3.3)

$$\sigma(\mathbf{T}) = \sum_{x\in\Lambda_N'} (\beta_{x+e_1} - \beta_x)\langle j_{x,x+e_1} \rangle. \tag{5.6}$$

Therefore, it will suffice to find a bound for $|\langle j_{x,x+e_1}\rangle|$.

Applying the definition of the current observable, (2.7) and (2.8), and then integration by parts, shows that

$$\begin{aligned} \langle j_{x,x+e_1} \rangle &= -\frac{1}{2}\int V'(r_x) \sum_{n=0}^{1} \cdot \psi_{x'} p_{x'} G_{T_{x'}}|_{x'=x+ne_1} dp\, dq \\ &= -\sum_{n=0}^{1} \frac{T_{x'}}{2} \int V'(r_x) G_{T_{x'}} \partial_{p_{x'}} \psi_{x'} dp\, dq \Big|_{x'=x+ne_1} \end{aligned} \tag{5.7}$$

where $r_x = q_{x+e_1} - q_x$. We use that $1 = \psi_{x'}^{1/2}/\psi_{x'}^{1/2}$ whenever $\psi_{x'} \neq 0$, and then apply the Schwarz inequality. This shows that

$$|\langle j_{x,x+e_1} \rangle|^2 \leq \max_{y\in\Lambda_N} \frac{T_y}{\gamma_y} \langle V'(r_x)^2 \rangle \frac{1}{2} \sum_{n=0}^{1} \mathcal{D}_{x+ne_1}. \tag{5.8}$$

Therefore, we have obtained the following relation between the total sum of currents and the entropy production

$$\left(\sum_{x\in\Lambda_N'} |\langle j_{x,x+e_1}\rangle|\right)^2 \leq \max_{y\in\Lambda_N} \frac{T_y}{\gamma_y} \sum_{x\in\Lambda_N'} \langle V'(r_x)^2 \rangle \sum_{x\in\Lambda_N'} \frac{1}{2} \sum_{n=0}^{1} \mathcal{D}_{x+ne_1}$$

$$\leq \sigma(\mathbf{T}) \max_{y\in\Lambda_N} \frac{T_y}{\gamma_y} \sum_{x\in\Lambda'_N} \langle V'(r_x)^2\rangle. \tag{5.9}$$

For this bound to be useful, we still need to consider $\sum_{x\in\Lambda'_N}\langle V'(r_x)^2\rangle$. Since $L_N(q_x^2) = 2q_x p_x$, we have $\langle q_x p_x\rangle = 0$ for all x. Similarly, $L_N\mathcal{H} = \sum_{x\in\Lambda_N}\gamma_x(T_x - p_x^2)$ implies $\sum_x \gamma_x T_x = \sum_x \gamma_x\langle p_x^2\rangle$. Now

$$L_N\Bigg(\sum_{x\in\Lambda_N} p_x q_x\Bigg) = \sum_{x\in\Lambda_N} p_x^2 - \sum_{x\in\Lambda_N} q_x\partial_{q_x}\mathcal{H} - \sum_{x\in\Lambda_N}\gamma_x p_x q_x, \tag{5.10}$$

and thus

$$\sum_{x\in\Lambda_N}\gamma_x T_x \geq \min_y \gamma_y \sum_{x\in\Lambda_N}\langle p_x^2\rangle = \min_y \gamma_y \Bigg\langle \sum_{x\in\Lambda_N} q_x\partial_{q_x}\mathcal{H}\Bigg\rangle. \tag{5.11}$$

From the asymptotics of V and W we can conclude that there are $C > 0$ and $C' \geq 0$ such that

$$V'(r)^2 \leq C(rV'(r) + C') \quad \text{and} \quad rW'(r) \geq -C'. \tag{5.12}$$

But since

$$\partial_{q_x}\mathcal{H} = W'(q_x) + \sum_{j=1}^{d}(V'(q_x - q_{x-e_j}) - V'(q_{x+e_j} - q_x))$$
$$+ \frac{1}{2}(\mathbb{1}(x\in\partial_{\mathrm{R}}\Lambda_N)V'(-q_x) - \mathbb{1}(x\in\partial_{\mathrm{L}}\Lambda_N)V'(q_x)), \tag{5.13}$$

with $\mathbb{1}$ denoting the characteristic function, we have

$$\sum_{x\in\Lambda_N} q_x\partial_{q_x}\mathcal{H} = \sum_{x\in\Lambda_N}\Bigg[q_x W'(q_x) + \sum_{j=2}^{d} rV'(r)|_{r=q_{x+e_j}-q_x}\Bigg]$$
$$+ \sum_{x\in\Lambda'_N} r_x V'(r_x) + \frac{1}{2}\sum_{x\in\partial_{\mathrm{R}}\Lambda} q_x V'(q_x) + \frac{1}{2}\sum_{x\in\partial_{\mathrm{L}}\Lambda}(-q_x)V'(-q_x).$$
$$\geq \sum_{x\in\Lambda'_N} r_x V'(r_x) - |\Lambda_N|C'(d+1). \tag{5.14}$$

Combining this with (5.11) shows that

$$\sum_{x\in\Lambda'_N}\langle V'(r_x)^2\rangle \leq C|\Lambda_N|\Bigg(C'(d+2) + \frac{\max_y \gamma_y T_y}{\min_y \gamma_y}\Bigg). \tag{5.15}$$

Consequently, there is $c > 0$, which depends only on V and W, such that

$$\Bigg(\sum_{x\in\Lambda'_N} |\langle j_{x,x+e_1}\rangle|\Bigg)^2 \leq c\sigma(\mathbf{T})|\Lambda_N|\frac{\max_x \gamma_x T_x}{\min_x \gamma_x^2}(1 + \max_x T_x). \tag{5.16}$$

Let us next consider the case $\mathbf{T} = \mathbf{T}^{\beta\text{lin}}$. Applying the definition of $\mathbf{T}^{\beta\text{lin}}$ to (5.6) shows that then (3.9) holds, i.e., $\sigma(\mathbf{T}^{\beta\text{lin}}) = \frac{\beta_{\text{R}}-\beta_{\text{L}}}{2N}\sum_{x\in\Lambda'_N}\langle j_{x,x+e_i}\rangle$. Then by (5.16) and using the fact that $T_x^{\beta\text{lin}} \le T_{\text{L}}$

$$\sigma(\mathbf{T}^{\beta\text{lin}}) \le c'|\beta_{\text{R}}-\beta_{\text{L}}|^2(2N+1)^{d-2}(1+T_{\text{L}})^2, \tag{5.17}$$

where c' is a constant depending only on γ, V, and W. Therefore, we have now proven Theorem 4.

Finally, let us consider the self-consistent case, $\mathbf{T} = \mathbf{T}^{\text{sc}}$. For the corresponding stationary measure we find from (2.6),

$$\sum_{j=1}^{d}(\langle j_{x,x+e_j}\rangle - \langle j_{x-e_j,x}\rangle) = 0, \quad x \notin \partial\Lambda_N. \tag{5.18}$$

Since the system, including the self-consistent profile, is periodic in any of the Cartesian directions e_i, $i \ge 2$, also the unique stationary measures are invariant under translations in these directions. Therefore,

$$\langle j_{x,x+e_i}\rangle = \langle j_{x-e_i,x}\rangle, \quad i \ne 1,\ x \in \Lambda_N. \tag{5.19}$$

Consequently, by (5.18) and (2.6),

$$\begin{aligned}
&\langle j_{x,x+e_1}\rangle = \langle j_{x-e_1,x}\rangle, \quad x \notin \partial\Lambda_N,\\
&\langle j_{x,x+e_1}\rangle = \langle J_x\rangle = \gamma_x(T_{\text{L}} - \langle p_x^2\rangle), \quad x \in \partial_{\text{L}}\Lambda_N,\\
&\langle j_{x-e_1,x}\rangle = -\langle J_x\rangle = \gamma_x(\langle p_x^2\rangle - T_{\text{R}}), \quad x \in \partial_{\text{R}}\Lambda_N.
\end{aligned} \tag{5.20}$$

We denote the constant current by $\bar{j}_N$, i.e., now we have $\langle j_{x,x+e_1}\rangle = \bar{j}_N$, for all $x \in \Lambda'_N$. Therefore, by (5.6),

$$\sigma(\mathbf{T}^{\text{sc}}) = \bar{j}_N \sum_{x\in\Lambda'_N}(\beta_{x+e_1} - \beta_x) = \bar{j}_N(\beta_{\text{R}} - \beta_{\text{L}})(2N+1)^{d-1}, \tag{5.21}$$

which proves (3.4). This immediately implies that $\text{sign}(T_{\text{L}} - T_{\text{R}})\bar{j}_N \ge 0$. But on the other hand, $\bar{j}_N = \frac{1}{|\Lambda'_N|}\sum_{x\in\Lambda'_N}\langle j_{x,x+e_1}\rangle$, and thus also for the self-consistent profile $\sigma(\mathbf{T}^{\text{sc}}) = \frac{\beta_{\text{R}}-\beta_{\text{L}}}{2N}\sum_{x\in\Lambda'_N}\langle j_{x,x+e_i}\rangle$. Applying (5.16) then completes the proof of Theorem 3.

6 Minimization of Entropy Production

For a given $T_{\text{o}} > 0$, we use the Gibbs measure $\mu_{T_{\text{o}}} = G_{T_{\text{o}}}dp\,dq$ as a reference measure and we denote the related expectation by $\langle\cdot\rangle_0$. We consider the generator L on the Hilbert space $L^2(\mu_{T_{\text{o}}})$. Recall that for any temperature profile $\mathbf{T} = \{T_x, x \in \Lambda_N\}$ we have $L = L(\mathbf{T}) = A + S(\mathbf{T})$. Its adjoint is

$$L^* = -A + \sum_{x\in\Lambda_N} S_x^* \tag{6.1}$$

where $S_x = \gamma_x(T_x \partial_{p_x}^2 - p_x \partial_{p_x})$, and thus

$$S_x^* = S_x + \gamma_x \frac{\Delta T_x}{T_o}(-2p_x \partial_{p_x} + h_x) \tag{6.2}$$

with $\Delta T_x = T_x - T_o$ and

$$h_x = \frac{p_x^2}{T_o} - 1. \tag{6.3}$$

Observe that $\langle h_x h_{x'} \rangle_0 = 2\delta_{x,x'}$ and $-S_{x,T_o} h_x = 2\gamma_x h_x$.

Set $L_0 = L(\mathbf{T}_o)$ and consequently $L_0^* = -A + S(\mathbf{T}_o)^* = -A + S(\mathbf{T}_o)$.

Lemma 2 *For all* y, x

$$\partial_{T_y} \langle p_x^2 \rangle_{\mu(\mathbf{T})}|_{\mathbf{T}=\mathbf{T}_o} = \gamma_y \langle h_y (-L_0)^{-1} h_x \rangle_0 = \gamma_y \langle h_x (-L_0)^{-1} h_y \rangle_0. \tag{6.4}$$

Proof Let us denote by $f = f(\mathbf{T})$ the density of $\mu(\mathbf{T})$ with respect to μ_{T_o}. Then f is solution of the equation $L^*(\mathbf{T}) f(\mathbf{T}) = 0$. Since the coefficients in $L^*(\mathbf{T})$ are smooth in $\mathbf{T}$, f is smooth in $\mathbf{T}$ and $f_y = \partial_{T_y} f(\mathbf{T})$ solves the equation

$$L^*(\mathbf{T}) f_y(\mathbf{T}) = -(\partial_{T_y} L^*)(\mathbf{T}) f(\mathbf{T}) = -\frac{\gamma_y}{T_o}(T_o \partial_{p_y}^2 - 2p_y \partial_{p_y} + h_y) f(\mathbf{T}). \tag{6.5}$$

Since $f(\mathbf{T}_o) = 1$, we have found that $f_y(\mathbf{T}_o)$ is solution of

$$-L_0^* f_y(\mathbf{T}_o) = \frac{\gamma_y}{T_o} h_y. \tag{6.6}$$

Notice that f_y has a bounded $L^2(\mu_{T_o})$ norm (cf. [20]), and by a standard argument (multiply equation (6.6) by f_y and integrate with respect to μ_{T_o}) we obtain a bound

$$\sum_x \gamma_x \langle (\partial_{p_x} f_y)^2 \rangle_0 \le \gamma_y T_o^{-1}. \tag{6.7}$$

Now, since $h_x G_{T_o} = -\partial_{p_x}(p_x G_{T_o})$,

$$\langle h_x \rangle_{\mu(\mathbf{T})} = \langle p_x \partial_{p_x} f(\mathbf{T}) \rangle_0. \tag{6.8}$$

Then differentiating with respect to T_y we have

$$\partial_{T_y} \langle h_x \rangle_{\mu(\mathbf{T})} = \langle p_x \partial_{p_x} f_y(\mathbf{T}) \rangle_0 \tag{6.9}$$

and taking the limit $\mathbf{T} \to \mathbf{T}_o$

$$\partial_{T_y} \langle h_x \rangle_{\mu(\mathbf{T})}|_{\mathbf{T}=\mathbf{T}_o} = \langle p_x \partial_{p_x} f_y(\mathbf{T}_o) \rangle_0 = \langle h_x f_y(\mathbf{T}_o) \rangle_0 = \frac{\gamma_y}{T_o} \langle h_x (-L_0^*)^{-1} h_y \rangle_0. \tag{6.10}$$

Observe that, since h is an even function of p, one can, by a change of variables $p \to -p$, replace L_0^* with L_0 in (6.10). This proves (6.4). □

Define $F : \mathbb{R}_+^{\Lambda_N} \to \mathbb{R}^{\Lambda_N}$ as

$$F_x(\mathbf{T}) = \langle J_x \rangle_{\mu(\mathbf{T})} = \gamma_x (T_x - \langle p_x^2 \rangle_{\mu(\mathbf{T})}). \tag{6.11}$$

Its Jacobian at $\mathbf{T} = \mathbf{T}_o$ is given by

$$\mathcal{J}_{y,x} = \gamma_x \delta_{y,x} - \gamma_x \partial_{T_y} \langle p_x^2 \rangle_{\mu(\mathbf{T})}|_{\mathbf{T}=T_o} = \gamma_x \delta_{y,x} - \gamma_x \gamma_y \langle h_x (-L_0)^{-1} h_y \rangle_0. \tag{6.12}$$

Observe that $\mathcal{J}$ is symmetric and that $F(\mathbf{T}_o) = 0$ for any value of T_o. It follows that 0 is an eigenvalue of $\mathcal{J}$, and we will show shortly that $\mathcal{J} \geq 0$, and the eigenspace corresponding to 0 is one-dimensional and generated by the constant vector. Then the matrix $M = (\mathcal{J}_{x,y})_{x,y \in R^c}$ is invertible, and thus there is a neighborhood in (T_L, T_R) containing (T_o, T_o) such that the implicit function theorem can be applied to obtain a self-consistent profile. This implies that constants ε_0 and δ for the first part of Theorem 2 can be found. It also follows that $\mathbf{T}^{sc}(T_L, T_R)$ is smooth. To see that it must also be invariant under the periodic translations, we first point out that in the boundary layer setup clearly any translate of a self-consistent profile is also self-consistent. Since the translations correspond to a permutation of indices, they remain in the neighborhood determined by δ, and thus by the uniqueness of the self-consistent profile in this neighborhood, $T^{sc}(T_L, T_R)$ must itself be invariant.

Therefore, to complete the proof of Theorem 2 we only need to prove the following Lemma.

Lemma 3 $\mathcal{J} \geq 0$, *and* $\mathcal{J}a = 0$ *implies* a_x *is a constant in* x.

Proof Let $a \in \mathbb{R}^{\Lambda_N}$, and define $h = \sum_{x \in \Lambda_N} a_x h_x$. It follows from the antisymmetry of A and the symmetry of S_0:

$$\langle (Ah)(-L_0)^{-1}(Ah) \rangle_0 = \langle h(-S_0)h \rangle_0 - \langle (S_0 h)(-L_0)^{-1}(S_0 h) \rangle_0. \tag{6.13}$$

Since $S_0 h = -2 \sum_x a_x \gamma_x h_x$, we obtain

$$\begin{aligned} \langle (Ah)(-L_0)^{-1}(Ah) \rangle_0 &= \langle h(-S_0)h \rangle_0 - 4 \sum_{x,y} a_x a_y \gamma_x \gamma_y \langle h_x (-L_0)^{-1} h_y \rangle_0 \\ &= 4 \sum_x \gamma_x a_x^2 - 4 \sum_{x,y} a_x a_y \gamma_x \gamma_y \langle h_x (-L_0)^{-1} h_y \rangle_0 \\ &= 4 \sum_{x,y} a_x a_y \mathcal{J}_{x,y}. \end{aligned} \tag{6.14}$$

Therefore, to prove that $\mathcal{J}$ has the properties stated above, it suffices to study the left hand side of (6.13), and to prove that it is always positive, and equal to zero if and only if a is a constant vector. (Studying real vectors a suffices here, as $\mathcal{J}$ is a symmetric matrix.)

In fact, define $u = (-L_0)^{-1}(Ah)$. Since for any observable F belonging to the domain of A, $\langle F(AF) \rangle_0 = 0$, we have then

$$\langle (Ah)(-L_0)^{-1}(Ah) \rangle_0 = \langle u(-S_0)u \rangle_0 = \sum_x \gamma_x T_o \langle (\partial_{p_x} u)^2 \rangle_0 \geq 0. \tag{6.15}$$

This proves the required positivity. In addition, if the left hand side is zero, then $u(p,q)$ cannot depend on p, and thus

$$-L_0 u = -Au = -\sum_x p_x \partial_{q_x} u(q) = Ah = -\frac{2}{T_0} \sum_x a_x p_x \partial_{q_x} \mathcal{H}. \tag{6.16}$$

It follows, for all x,

$$\frac{2}{T_{\mathrm{o}}} a_x \partial_{q_x} \mathcal{H} = \partial_{q_x} u(q). \tag{6.17}$$

Thus the function

$$\mathcal{G}(q) = \frac{T_{\mathrm{o}}}{2} u(q) - \sum_{x \in \Lambda_N} a_x W(q_x) \tag{6.18}$$

satisfies, by (5.13),

$$\begin{aligned} \partial_{q_x} \mathcal{G}(q) = a_x \Bigg[& \sum_{j=1}^{d} (V'(q_x - q_{x-e_j}) - V'(q_{x+e_j} - q_x)) \\ & + \frac{1}{2} \mathbb{1}(x \in \partial_{\mathrm{R}} \Lambda_N) V'(-q_x) - \frac{1}{2} \mathbb{1}(x \in \partial_{\mathrm{L}} \Lambda_N) V'(q_x) \Bigg]. \end{aligned} \tag{6.19}$$

For $x \in \Lambda'_N$ and $k = 1, 2, \ldots$ we differentiate (6.19) with respect to q_{x+e_k} and obtain

$$-a_x V''(q_{x+e_k} - q_x) = \partial^2_{q_x, q_{x+e_k}} \mathcal{G}(q) = -a_{x+e_k} V''(q_{x+e_k} - q_x). \tag{6.20}$$

Since there exists an r_0 such that $V''(r_0) > 0$, this implies $a = \text{const}$. □

We can now conclude that for any $T_{\mathrm{o}} > 0$, there is $\varepsilon_0 > 0$ such that for all $|\varepsilon| < \varepsilon_0$ a self-consistent profile corresponding to $T_{\mathrm{L}} = T_{\mathrm{o}} + \frac{\varepsilon}{2}$, $T_{\mathrm{R}} = T_{\mathrm{o}} - \frac{\varepsilon}{2}$ can be found. This profile is differentiable with respect to ε and the derivative satisfies for $x \notin \partial \Lambda_N$

$$0 = \frac{\partial}{\partial \varepsilon} F_x(\mathbf{T}(\varepsilon; T_{\mathrm{o}})) = \sum_{y \in \Lambda_N} \frac{\partial T_y}{\partial \varepsilon} \partial_{T_y} F_x(\mathbf{T}(\varepsilon; T_{\mathrm{o}})). \tag{6.21}$$

Therefore, we have $\sum_{y \in \Lambda_N} \mathcal{J}_{x,y} \frac{\partial T_y(0)}{\partial \varepsilon} = 0$. This shows that for $x \notin \partial \Lambda_N$,

$$\left. \frac{\partial T_x(\varepsilon; T_{\mathrm{o}})}{\partial \varepsilon} \right|_{\varepsilon=0} = \sum_{y \notin \partial \Lambda_N} (M^{-1})_{x,y} \frac{1}{2} \Bigg(\sum_{y' \in \partial_{\mathrm{R}} \Lambda_N} \mathcal{J}_{y,y'} - \sum_{y' \in \partial_{\mathrm{L}} \Lambda_N} \mathcal{J}_{y,y'} \Bigg), \tag{6.22}$$

where $M = (\mathcal{J}_{x,y})_{x,y \notin \partial \Lambda_N}$ is a strictly positive matrix, and thus invertible.

Recall the definition of entropy production given in (3.2). By (5.4) we have then always $\sigma(\mathbf{T}) \geq 0$, with equality when $\mathbf{T} = \mathbf{T}_{\mathrm{o}}$, a constant profile given by $T_{\mathrm{o}} > 0$. Since

$$\frac{\partial \sigma}{\partial T_x}(\mathbf{T}) = -\gamma_x \frac{\langle p_x^2 \rangle}{T_x^2} + \sum_y \gamma_y \frac{\partial_{T_x} \langle p_y^2 \rangle}{T_y}, \tag{6.23}$$

we have for the constant profile

$$\frac{\partial \sigma}{\partial T_x}(\mathbf{T}_{\mathrm{o}}) = -T_{\mathrm{o}}^{-1} \gamma_x + T_{\mathrm{o}}^{-1} \frac{\partial}{\partial T_x} \Bigg(\sum_y \gamma_y \langle p_y^2 \rangle \Bigg)_{\mathbf{T} = \mathbf{T}_{\mathrm{o}}}. \tag{6.24}$$

As mentioned earlier, for any profile $\sum_y \gamma_y \langle p_y^2\rangle = \sum_y \gamma_y T_y$, and thus we have proven that

$$\frac{\partial\sigma}{\partial T_x}(\mathbf{T}_\mathrm{o}) = 0. \tag{6.25}$$

A similar, but a slightly longer calculation, shows that

$$\frac{\partial^2\sigma}{\partial T_x \partial T_y}(\mathbf{T}_\mathrm{o}) = \frac{1}{T_\mathrm{o}^2}(\mathcal{J}_{x,y} + \mathcal{J}_{y,x}) = \frac{2}{T_\mathrm{o}^2}\mathcal{J}_{x,y}. \tag{6.26}$$

By dividing Λ_N into $R \neq \emptyset$ (the fixed thermostats) and R^c, we can conclude from the previous results that the symmetric matrix $M = (\mathcal{J}_{x,y})_{x,y\in R^c}$ is strictly positive. By (6.25) and (6.26), the Taylor expansion of σ around $\mathbf{T}_\mathrm{o}$ yields

$$\sigma(\mathbf{T}_\mathrm{o} + \varepsilon\mathbf{v}) = \frac{\varepsilon^2}{T_\mathrm{o}^2}\sum_{x,y\in\Lambda_N} \mathcal{J}_{x,y} v_x v_y + \mathcal{O}(\varepsilon^3). \tag{6.27}$$

This proves Theorem 5. For fixed ε and v_x, $x \in R$, the quadratic form corresponding to the leading term has a unique minimizer, given by $v_x^{(\min)} = v_x$, $x \in R$, and

$$v_x^{(\min)} = -\sum_{y\in R^c}\sum_{y'\in R}(M^{-1})_{xy}\mathcal{J}_{y,y'}v_{y'}, \quad \text{for } x \in R^c. \tag{6.28}$$

Let us next consider the case studied earlier, with the opposite boundaries fixed at two different temperatures T_L and T_R. Denote $\delta T = T_\mathrm{L} - T_\mathrm{R}$, which we assume to be positive, and $T_\mathrm{o} = (T_\mathrm{L} + T_\mathrm{R})/2$. Let us consider a sequence of T_L, T_R for which T_o remains fixed and $\delta T \to 0$. We assume that $\mathbf{T}$ is a sequence of profiles with boundary values on R equal to T_L and T_R, and which has a Taylor expansion

$$T_x = T_\mathrm{o} + g(x)\delta T + \mathcal{O}(\delta T^2) \tag{6.29}$$

where g is a function for which $g(x) = 1/2$ for $x \in \partial_\mathrm{L}\Lambda_N$ and $g(x) = -1/2$ for $x \in \partial_\mathrm{R}\Lambda_N$. By (6.27), the entropy production will be of the order $(\delta T)^2$, and the leading term is minimized by $g(x) = v_x^{(\min)}$ corresponding to $v_x = \pm\frac{1}{2}$, with $+$, if $x \in \partial_\mathrm{L}\Lambda_N$, and $-$, if $x \in \partial_\mathrm{R}\Lambda_N$.

We have proven in the beginning of this section, that the self-consistent profile can be chosen for all sufficiently small δT so that it is differentiable in the boundary temperatures. In particular, comparing (6.22) to (6.28) shows that

$$T_x^\mathrm{sc} = T_\mathrm{o} + \mathrm{g}^\mathrm{sc}(x)\delta T + \mathcal{O}(\delta T^2) \tag{6.30}$$

with $\mathbf{g}^\mathrm{sc} = \mathbf{v}^{(\min)}$. We have thus proven Theorem 6.

7 Conductivity of the Finite System

In the following we again set $\Lambda'_N = \Lambda_N \backslash \partial_\mathrm{R}\Lambda_N$, and consider, as in Sect. 5, a generic profile $\mathbf{T}$ which is invariant under periodic translations. Let $\langle\cdot\rangle$ be the expectation with respect to the corresponding stationary state. It is convenient now to use as a reference measure the inhomogeneous Gibbs measure $\nu_\mathbf{T} = G(\mathbf{T}; q, p)\mathrm{d}q\mathrm{d}p$, with

$$G(\mathbf{T}; q, p) = \frac{\exp(-\sum_x \mathcal{E}_x(q,p)/T_x)}{Z} \tag{7.1}$$

where $\mathcal{E}_x$ is defined in (2.1). Notice that S is automatically symmetric with respect to $\nu_{\mathbf{T}}$, while the adjoint of A is given by

$$-A + \sum_{x\in\Lambda'_N} \left(\frac{1}{T_{x+e_1}} - \frac{1}{T_x} \right) j_{x,x+e_1}. \tag{7.2}$$

Let us next inspect $\mathbf{T} = \mathbf{T}^{\mathrm{sc}}$ and denote by $\tilde{f}$ the density of the self-consistent stationary state with respect to $\nu_{\mathbf{T}^{\mathrm{sc}}}$. Let us fix $T_{\mathrm{o}} = \frac{T_{\mathrm{R}}+T_{\mathrm{L}}}{2}$ with $\varepsilon = \delta T = T_{\mathrm{L}} - T_{\mathrm{R}} > 0$, as before. Repeating the argument used in Sect. 2, we find that $\tilde{f}$ is smooth in ε, so a first order development in ε is justified. Using the expansion of the self-consistent profile, (6.29), shows that $u = \partial_\varepsilon \tilde{f}|_{\varepsilon=0}$ is solution of the equation

$$(-A + S(\mathbf{T}_{\mathrm{o}}))u = \sum_{x\in\Lambda'_N} \frac{\nabla_{e_1} \mathrm{g}^{\mathrm{sc}}(x)}{T_{\mathrm{o}}^2} j_{x,x+e_1}. \tag{7.3}$$

Explicit formulae for the derivatives of the self-consistent profile, $\mathrm{g}^{\mathrm{sc}}(x)$, are given in (6.22).

Recall the definition of the conductivity of the finite system, (3.14). Since we have already proven Theorems 1–6, the argument given before Theorem 7 in Sect. 3 provides a proof that $\kappa_N(T_{\mathrm{o}})$ is bounded in N. On the other hand, by (7.3),

$$\begin{aligned}\kappa_N(T_{\mathrm{o}}) &= \lim_{\delta T\to 0} \frac{2N+1}{\delta T} \frac{1}{|\Lambda'_N|} \sum_{x\in\Lambda'_N} \langle j_{x,x+e_1}\rangle \\ &= \lim_{\delta T\to 0} \frac{2N+1}{\delta T} \langle j_{0,e_1}\rangle = (2N+1)\langle u j_{0,e_1}\rangle_0. \end{aligned}\tag{7.4}$$

Define $\check{u}(q,p) = u(q,-p)$, and observe that, since $j_{x,x+e_1}$ is antisymmetric in p,

$$(A + S(\mathbf{T}_{\mathrm{o}}))\check{u} = -\sum_{x\in\Lambda'_N} \frac{\nabla_{e_1} \mathrm{g}^{\mathrm{sc}}(x)}{T_{\mathrm{o}}^2} j_{x,x+e_1}. \tag{7.5}$$

Thus

$$\begin{aligned}\kappa_N(T_{\mathrm{o}}) &= -(2N+1)\langle \check{u} j_{0,e_1}\rangle_0 = (2N+1)\int_0^\infty \partial_t \langle \check{u}(t) j_{0,e_1}(0)\rangle_0\, dt \\ &= \frac{1}{T_{\mathrm{o}}^2}\int_0^\infty \sum_{x\in\Lambda'_N} (-(2N+1)\nabla_{e_1}\mathrm{g}^{\mathrm{sc}}(x)) \langle j_{x,x+e_1}(t) j_{0,e_1}(0)\rangle_0\, dt \end{aligned}\tag{7.6}$$

where $\langle\cdot\rangle_0$ denotes taking the initial data distribution according to the equilibrium measure at the specified temperature T_{o}, and then considering the time-evolution corresponding to the stochastic process with all heat-bath temperatures set to T_{o}. We have used here the property that then $\langle \check{u}(t) j_{0,e_1}(0)\rangle_0 \to \langle\check{u}\rangle_0 \langle j_{0,e_1}\rangle_0 = 0$ for $t\to\infty$. This completes the proof of Theorem 7.

Repeating the same steps for $\mathbf{T} = \mathbf{T}^{\beta\mathrm{lin}}$, for which $\partial_\varepsilon T_x^{\beta\mathrm{lin}}\big|_{\varepsilon=0} = -\frac{x_1}{2N}$, proves also the validity of (3.19).

8 Conductivity of the Infinite System

We prove here Theorem 8 concerning the infinite system on $(\mathbb{R}^{2d})^{\mathbb{Z}^d}$ with all $\gamma_x = \gamma$ and all thermostats at temperature $T_{\rm o}$. This infinite dynamics has a unique invariant measure given by the Gibbs measure on $(\mathbb{R}^{2d})^{\mathbb{Z}^d}$ at temperature $T_{\rm o}$, defined by the usual DLR relations. We denote this measure by $\mu_{T_{\rm o}}$ and its expectation by $\langle\cdot\rangle_0$. Consequently we look at the dynamics starting from this equilibrium distribution.

We adapt here an argument used in [3]. Introduce on $L^2(\mu_{T_{\rm o}})$ a degenerate scalar product

$$\langle\langle \varphi, \psi\rangle\rangle = \sum_{x\in\mathbb{Z}^d} [\langle \varphi\tau_x\psi\rangle_0 - \langle\varphi\rangle_0\langle\psi\rangle_0], \tag{8.1}$$

where τ_x is the translation operator. The scalar product can also be obtained via the limit

$$\langle\langle \varphi, \psi\rangle\rangle = \lim_{n\to\infty} \mathrm{Cov}_{\mu_{T_{\rm o}}}(\Phi_n\varphi, \Phi_n\psi) = \lim_{n\to\infty} (\langle \Phi_n\varphi\Phi_n\psi\rangle_0 - \langle\Phi_n\varphi\rangle_0\langle\Phi_n\psi\rangle_0), \tag{8.2}$$

where Φ_n maps functions into the corresponding "fluctuation averages" in Λ_n, a square box of linear size n centered at 0. Explicitly,

$$(\Phi_n\psi)(q,p) = \frac{1}{\sqrt{|\Lambda_n|}} \sum_{x\in\Lambda_n} (\tau_x\psi)(q,p). \tag{8.3}$$

The scalar product is degenerate, since every function of the form $\phi = \psi - \tau_x\psi$ is in its kernel. We denote by $\mathcal{L}^2$ the corresponding Hilbert space of square integrable functions. More precisely, $\mathcal{L}^2$ is a space of classes of functions such that each of its elements can be identified with a function in $L^2(\mu_{T_{\rm o}})$ up to a translation.

Observe that A and S are still respectively anti-symmetric and symmetric with respect to the scalar product $\langle\langle\cdot,\cdot\rangle\rangle$. We also introduce the semi-norm

$$\|\varphi\|_1^2 = \langle\langle \varphi, (-S)\varphi\rangle\rangle \tag{8.4}$$

and let $\mathcal{H}_1$ denote the corresponding Hilbert space obtained by closing $\mathcal{L}^2$ with respect to $\|\cdot\|_1$. To see that $\|\varphi\|_1$ is a semi-norm, in particular, that it is positive, we can employ the easily derived identity

$$\|\varphi\|_1^2 = \lim_{n\to\infty} \langle \Phi_n\varphi(-S\Phi_n\varphi)\rangle_0. \tag{8.5}$$

Since S acts only on velocities, $\|\cdot\|_1$ has a kernel consisting of all functions which depend only on q, the position variables. Thus also $\mathcal{H}_1$ is a space of equivalence classes of functions.

Let $\lambda > 0$ be given and let u_λ be the solution of the resolvent equation

$$\lambda u_\lambda - Lu_\lambda = j_{0,e_1}. \tag{8.6}$$

The solution can be given explicitly in terms of the semigroup P^t generated by $L = A + S$,

$$u_\lambda(q,p) = \int_0^\infty e^{-\lambda t}(P^t j_{0,e_1})(q,p)\,dt. \tag{8.7}$$

Obviously,

$$C_0 := \langle\langle j_{0,e_1}, j_{0,e_1}\rangle\rangle = \sum_{x\in\mathbb{Z}^d} \langle j_{0,e_1} j_{x,x+e_1}\rangle_0 \le T_{\rm o}\langle (V'(q_{e_1} - q_0))^2\rangle_0 < \infty, \tag{8.8}$$

and thus $j_{0,e_1} \in \mathcal{L}^2$. Then $u_\lambda \in L^2(\mu_{T_0})$, and by stationarity $\langle u_\lambda \rangle_0 = 0$. We will show next that, in fact, $u_\lambda \in \mathcal{H}_1$. From (8.6) we obtain

$$\lambda \langle (\Phi_n u_\lambda)^2 \rangle_0 + \langle (\Phi_n u_\lambda)(-S)(\Phi_n u_\lambda) \rangle_0 = \langle (\Phi_n u_\lambda)(\Phi_n j_{0,e_1}) \rangle_0, \tag{8.9}$$

where we have used translation invariance of L and antisymmetry of A. Since $S j_{0,e_1} = -\gamma j_{0,e_1}$, an application of Schwarz inequality yields

$$\begin{aligned} \langle (\Phi_n u_\lambda)(\Phi_n j_{0,e_1}) \rangle_0 &= \gamma^{-1} \langle (\Phi_n u_\lambda)(-S)(\Phi_n j_{0,e_1}) \rangle_0 \\ &\le \gamma^{-1} \langle (\Phi_n u_\lambda)(-S)(\Phi_n u_\lambda) \rangle_0^{1/2} \langle (\Phi_n j_{0,e_1})(-S)(\Phi_n j_{0,e_1}) \rangle_0^{1/2} \\ &= \gamma^{-1/2} \langle (\Phi_n j_{0,e_1})^2 \rangle_0^{1/2} \langle (\Phi_n u_\lambda)(-S)(\Phi_n u_\lambda) \rangle_0^{1/2}. \end{aligned} \tag{8.10}$$

Consequently, we have

$$\langle (\Phi_n u_\lambda)(-S)(\Phi_n u_\lambda) \rangle_0 \le \gamma^{-1} \langle (\Phi_n j_{0,e_1})^2 \rangle_0 \stackrel{n\to\infty}{\longrightarrow} \gamma^{-1} C_0, \tag{8.11}$$

which implies that

$$\lambda \langle\langle u_\lambda, u_\lambda \rangle\rangle \le \gamma^{-1} C_0 \tag{8.12}$$

and

$$\|u_\lambda\|_1^2 \le \gamma^{-1} C_0. \tag{8.13}$$

Therefore, $u_\lambda \in \mathcal{H}_1$ and by (8.13), we can extract a subsequence, which we still denote with u_λ, weakly convergent in $\mathcal{H}_1$ to u_0.

Let $u_\lambda(p,q) = u_\lambda^s(p,q) + u_\lambda^a(p,q)$ where u_λ^s and u_λ^a are respectively symmetric and antisymmetric in the p's. Since j_{0,e_1} is antisymmetric in the p's, we have that $\langle\langle u_\lambda, j_{0,e_1} \rangle\rangle = \langle\langle u_\lambda^a, j_{0,e_1} \rangle\rangle$. Furthermore, S preserves the parity in p, while it is inverted by A. So we can decompose the resolvent equation as

$$\begin{aligned} \lambda u_\lambda^s - S u_\lambda^s - A u_\lambda^a &= 0, \\ \nu u_\mu^a - S u_\nu^a - A u_\nu^s &= j_{0,e_1}. \end{aligned} \tag{8.14}$$

Taking a scalar product of the first equation with u_ν^s, of the second with u_λ^a, and using the antisymmetry of A, we find

$$\begin{aligned} \langle\langle u_\lambda^a, j_{0,e_1} \rangle\rangle &= \nu \langle\langle u_\nu^a, u_\lambda^a \rangle\rangle + \langle\langle u_\lambda^a, (-S) u_\nu^a \rangle\rangle - \langle\langle u_\lambda^a, A u_\nu^s \rangle\rangle \\ &= \nu \langle\langle u_\nu^a, u_\lambda^a \rangle\rangle + \lambda \langle\langle u_\lambda^s, u_\nu^s \rangle\rangle + \langle\langle u_\lambda, (-S) u_\nu \rangle\rangle. \end{aligned} \tag{8.15}$$

Since

$$\int u_\lambda^a(p,q) \tilde{\mu}_{T_\mathrm{o}}(dp) = 0, \tag{8.16}$$

where $\tilde{\mu}_{T_\mathrm{o}}(dp)$ is the centered Gaussian product measure of variance T_o, and S has a spectral gap γ in $L^2(\tilde{\mu}_{T_\mathrm{o}}(dp))$, we have that

$$\langle\langle u_\lambda^a, u_\lambda^a \rangle\rangle \le \frac{1}{\gamma} \langle\langle u_\lambda, (-S) u_\lambda \rangle\rangle \le C_0 \gamma^{-2}. \tag{8.17}$$

In particular, $u_0^a \in \mathcal{L}^2$. Thus by taking first the limit as $\lambda \to 0$ we have $\lambda \langle\langle u_\lambda^s, u_\nu^s \rangle\rangle \to 0$, then as $\nu \to 0$ we have $\nu \langle\langle u_\nu^a, u_0^a \rangle\rangle \to 0$, and finally we obtain from (8.15)

$$\langle\langle u_0, j_{0,e_1} \rangle\rangle = \langle\langle u_0, (-S)u_0 \rangle\rangle = \|u_0\|_1^2. \tag{8.18}$$

On the other hand, we have

$$\begin{aligned}\langle\langle u_0, j_{0,e_1} \rangle\rangle &= \lim_{\lambda\to 0} \langle\langle u_\lambda, j_{0,e_1} \rangle\rangle = \lim_{\lambda\to 0} [\lambda \langle\langle u_\lambda, u_\lambda \rangle\rangle + \langle\langle u_\lambda, (-S)u_\lambda \rangle\rangle] \\ &\geq \lim_{\lambda\to 0} \lambda \langle\langle u_\lambda, u_\lambda \rangle\rangle + \|u_0\|_1^2. \end{aligned} \tag{8.19}$$

This implies

$$\lim_{\lambda\to 0} \lambda \langle\langle u_\lambda, u_\lambda \rangle\rangle = 0, \tag{8.20}$$

and

$$\|u_\lambda\|_1 \to \|u_0\|_1. \tag{8.21}$$

Therefore, $u_\lambda \to u_0$ strongly in $\mathcal{H}_1$.

Uniqueness of the limit follows by the following standard argument. Suppose that λ_n is the chosen subsequence such that u_{λ_n} converges to u_0, and suppose ν_m is another sequence such that u_{ν_m} converges to $\tilde{u}_0$. Then, similarly as we have done in (8.15)

$$\langle\langle u_{\lambda_n}^a, j_{0,e_1} \rangle\rangle = \nu_m \langle\langle u_{\nu_m}^a, u_{\lambda_n}^a \rangle\rangle + \lambda_n \langle\langle u_{\lambda_m}^s, u_{\nu_n}^s \rangle\rangle + \langle\langle u_{\lambda_n}, (-S)u_{\nu_m} \rangle\rangle \tag{8.22}$$

which implies

$$\langle\langle u_0^a, j_{0,e_1} \rangle\rangle = \langle\langle u_0, (-S)\tilde{u}_0 \rangle\rangle. \tag{8.23}$$

Using $u_{\nu_m}^a$ instead of $u_{\lambda_n}^a$, we find similarly

$$\langle\langle \tilde{u}_0^a, j_{0,e_1} \rangle\rangle = \langle\langle u_0, (-S)\tilde{u}_0 \rangle\rangle. \tag{8.24}$$

Combining these with (8.19) shows that $\|u_0 - \tilde{u}_0\|^2 = 0$, i.e., $u_0 = \tilde{u}_0$.

Thus the conductivity $\kappa(T_\mathrm{o})$ defined by (3.20) is independent of the subsequence chosen for λ. Moreover, we have

$$\kappa(T_\mathrm{o}) = T_\mathrm{o}^{-2} \langle\langle u_0, j_{0,e_1} \rangle\rangle = T_\mathrm{o}^{-2} \|u_0\|_1^2 \leq \frac{C_0}{T_\mathrm{o}^2 \gamma} \leq \frac{\langle V'(q_{e_1} - q_0)^2 \rangle_0}{T_\mathrm{o} \gamma}. \tag{8.25}$$

This completes the proof of Theorem 8.

9 Concluding Remarks

While all the results obtained in this paper are as expected, the difficulty of actually proving things about the NESS of systems with nonlinear dynamics is immense. This is well illustrated by the impossibility (for us) of obtaining a bound on the self-consistent temperature T of the second oscillator in a system consisting of three oscillators with $T_1 = T_\mathrm{L}$, $T_3 = T_\mathrm{R}$, and the Hamiltonian is as in (2.1) with $\gamma_x = \gamma > 0$. We certainly expect that T will satisfy $T_\mathrm{R} < T < T_\mathrm{L}$, but do not know how to prove this. All we know is that there exists a $T = \langle p_2^2 \rangle$, and that $\bar{j} = T_\mathrm{L} - \langle p_1^2 \rangle = \langle p_3^2 \rangle - T_\mathrm{R} > 0$. We also know for general N that when $T_L, T_R \to T_o$, then there is a self-consistent choice $T \to T_o$, and that this in this limit $(2N+1)\bar{j}/(T_L - T_R)$ is bounded and given by the Green-Kubo formula (3.18). Beyond this however we are stymied except when V and W are harmonic. In that case T is given by (3.13) without a correction term for any T_L, T_R, and due to explicit expressions $g^{sc}(x)$ can be analyzed in great detail, proving $T_R < T < T_L$.

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