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Successes and failures in the construction of NESS-states

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Abstract

We construct non-equilibrium states by coupling a large but finite system with quasifree evolution to two temperature baths of free fermions or bosons with different temperature. We are interested in the resulting behaviour of the temperature baths as well as in the consequences for the finite system, especially what happens in the limit when the finite system tends to infinity. As a special example we consider the Kronig–Penney model and the tight binding model. Here a heat current remains that changes the baths but does not allow a limiting behaviour when the finite system tends to infinity. For the random versions of these models, especially the Anderson model, the heat current disappears exponentially with the size of the system. We show that a limit state is attained that is independent of the time direction and does not show any kind of symmetry breaking.

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1. Introduction

We know how to construct equilibrium states in the thermodynamic limit as a limit of Gibbs states. However, we are also interested in whether there exist other time-invariant states, especially states that permit a heat flux. We can construct such states by considering quasifree states determined by a two-point function corresponding to a one-particle operator that commutes with the one-particle Hamiltonian. If this operator breaks reflection symmetry it leads to a heat current. However, these states are also invariant under space translation and we cannot obtain any temperature gradient that is related to the heat current.

The general idea to construct time-invariant states as it is offered in [1, 2] is to start with an arbitrary state and take its (or some) invariant mean with respect to time evolution. To mimic a temperature gradient we can take as initial state some arbitrary state on a large but finite system coupled to two infinite heat baths of different temperature. In these heat baths the time evolution is free. For an appropriate local Hamiltonian and an appropriate coupling

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we can assume that scattering theory between the real time evolution and the uncoupled time evolution applies. Then the invariant means correspond to the limits $t \to \pm\infty$ and depending on the time direction we obtain two different time-invariant states reflecting the existence of a heat current.

If the heat current corresponds to a temperature gradient we have to expect that it will decrease when the subsystem increases. If there is enough interaction in the subsystem one might expect that locally up to a negligible amount an equilibrium is obtained corresponding to a temperature that varies and leads to a temperature gradient of size $1/N$ if N is the length of the subsystem. Finally also the size of the heat current should be of size $1/N$.

Of course so far I do not know the tools to handle such an interacting system. Therefore I limit my research to systems I can control, where the increasing subsystem is also quasifree and the calculations take place on the one-particle level. This is still of some interest, because in general for these systems the limit is taken without any coupling to heatbaths, and one is just interested in the spectral properties in the thermodynamic limit. Now these spectral properties will give the main information on the limiting state; however, the coupling to the heatbaths is still powerful enough that we can apply scattering theory, where of course the time the system needs to reach its final state will in general increase with the size of the subsystem. The Hamiltonian corresponding to an infinite system with periodic interaction will determine which states are possible as time-invariant states, but which of these permitted states will be reached will be determined by the heat baths.

A natural choice for such subsystems are the regular ones, that is, the Kronig–Penney model with a differential equation and the tight binding model with a difference equation. In both cases scattering theory works. The Kronig–Penney model is more interesting insofar as some energy regions are forbidden and in these regions we have almost total reflection. In the permitted regions in both cases we have a heat current whose direction depends on the time direction. Inside the system, as that of the heat baths, we have space translation invariance on a microscopic scale, if we neglect the boundary region. The relevant scattering essentially only occurs at the boundary of the system to the heat baths, but we cannot get rid of the size of the system for increasing size but instead keep a heat current whose strength slightly fluctuates with the size of the system and does not tend to zero when the size of the interacting systems tend to infinity.

The next examples are again the Kronig–Penney model and the tight binding model, but now with random parameters and thus mimicking interaction. The tight binding model is known as the Anderson model. These models and their variations are well studied in the literature [3]. The main tool is Fuerstenberg's theorem [4], which guarantees that for almost all models in this context the thermodynamic limit allows only a point spectrum and therefore a heat current is not possible. But as long as the system is finite and coupled to the heat baths, we still have an absolutely continuous spectrum and can apply scattering theory. As for the Kronig–Penney model in the forbidden region, in the thermodynamic limit, the heat current will decrease exponentially with the size of the system, but now for all energies. But this does not imply that we have a vacuum inside the system. But neither will we obtain a state that we can interpret as a state with locally varying temperature and therefore reflecting the mixing power of interaction. We obtain a unique state, now independent of the time direction, that is quasifree with a two-point function which is a mean corresponding to the two temperatures and does not break the symmetry relation of the Hamiltonian. Nor can we speak of a temperature gradient as the state depends on space only insofar as the time evolution itself does not commute with space translation. Altogether we observe that it is possible to construct time-invariant states that reflect in some way the coupling to different temperature baths in quite different ways, but never in a way that we expect to happen in realistic models.

2. The models

We follow essentially the treatment in [3]. We only add that the system is infinite but, outside of a finite region, free. We arrange the free system in such a way that the total Hamiltonian has only an absolutely continuous spectrum. In this way the state on the free part of the system determines in the long run also the state inside of the finite part where the random potential mimics interaction between the particles. More precisely we consider the following models represented by their one-particle Hamiltonian.

Model 1. Kronig–Penney model in a finite region:

$$H = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \sum_{n=-N}^{n=N} \lambda\delta(x - nl), \qquad (-\infty < x < \infty) \quad \lambda > 0. \tag{1}$$

Model 2. Kronig–Penney model with varying strength and distance:

$$H = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \sum_{n=-N}^{n=N} \lambda_n\delta(x - l_n), \qquad (-\infty < x < \infty) \quad \lambda_n - \lambda_{n-1} > 0. \tag{2}$$

Model 3. Tight binding electron model: we describe the Hamiltonian as the quadratic form, so that it is evident that it is positive definite:

$$\langle\Psi|H|\Psi\rangle = \sum_{|n|>N} |\Psi_n - \Psi_{n-1}|^2 + \sum_{|n|\leqslant N} (\alpha|\Psi_n - \Psi_{n-1}|^2 + \beta_n|\Psi_n|^2), \tag{3}$$

where $\alpha < 1$ and $4\alpha + \beta < 4$, $0 \leqslant \beta_n = \beta\ \forall -N \leqslant n \leqslant N-1$, $\beta_N = 0$.

Model 4. Anderson model:

$$\langle\Psi|H|\Psi\rangle = \sum_{|n|>N} |\Psi_n - \Psi_{n-1}|^2 + \sum_{|n|\leqslant N} (\alpha|\Psi_n - \Psi_{n-1}|^2 + \beta_n|\Psi_n|^2), \tag{4}$$

where now $0 \leqslant \beta_n$ can vary but still has to satisfy $4\alpha + \beta_n < 4$.

All these Hamiltonians are self-adjoint with an absolutely continuous spectrum and can be characterized by their generalized eigenfunctions. We first concentrate on models 1 and 2. Following [3] we look for the generalized eigenfunctions. In the interval $l_n < x < l_{n+1}$ we write them as $\Psi(x) = A_n\cos(kx) + B_n\sin(kx)$ so that the values A_n, B_n are calculated by the transfer matrix T_n:

$$\begin{pmatrix} A_{n+1} \\ B_{n+1} \end{pmatrix} = T_n \begin{pmatrix} A_n \\ B_n \end{pmatrix}$$

$$T_n = \begin{bmatrix} \cos(k((l_{n+1} - l_n)) & \frac{1}{k}\sin(k(l_{n+1} - l_n)) \\ -k\sin(k(l_{n+1} - l_n)) + \lambda_n\cos(k(l_{n+1} - l_n)) & \cos(k(l_{n+1} - l_n)) + \frac{\lambda_n}{k}\sin(k(l_{n+1} - l_n)) \end{bmatrix}, \tag{5}$$

where we can take $l_{n+1} - l_n = 1\ \forall|n| > N$. The choice of how to describe the eigenfunctions is done in such a way that the transfer matrix T_n is real with determinant 1 so that we can apply Fuerstenberg's theorem [4]. Since the determinant is $\neq 0$ eigenfunctions cannot have finite support. The energy corresponding to the eigenfunctions is $E(k) = k^2$. The Hamiltonian is self-adjoint and by our condition on λ positive definite; therefore, k has to be real in both models 1 and 2.

Models 3 and 4 have essentially the same structure. Our choice of parameters follows from the fact that

$$0 \leqslant \langle \Psi | H_0 | \Psi \rangle = \sum_n |\Psi_n - \Psi_{n-1}|^2 \leqslant 4 \sum_n |\Psi_n|^2 \tag{6}$$

and therefore the energy spectrum is $[0, 4]$. The energy spectrum of H should coincide with the energy spectrum of H_0. This follows on one hand because for functions localized outside a finite region, the expectation values coincide and therefore the range of the spectrum can only be larger. That this does not happen is guaranteed by

$$\begin{aligned} 0 &\leqslant \alpha \langle \Psi | H_0 | \Psi \rangle \leqslant \langle \Psi | H | \Psi \rangle \\ &\leqslant \sum_{|n|>N} (|\Psi_n| + |\Psi_{n-1}|)^2 + \sum_{|n|\neq N} \alpha((|\Psi_n| + |\Psi_{n-1}|)^2 + \beta_n |\Psi_n|^2) \leqslant 4 \sum_n |\Psi_n|^2. \end{aligned} \tag{7}$$

The quadratic form of the Hamiltonian corresponds to the operator

$$(H\Psi)_n = -\alpha_{n+1}\Psi_{n+1} - \alpha_n \Psi_n + (\alpha_n + \alpha_{n-1} + \beta_n)\Psi_n. \tag{8}$$

Now the sequence $\{\Psi_n\}$ corresponding to a generalized eigenfunction of the Hamiltonian is determined by the transfer matrix

$$\begin{pmatrix} \Psi_{n+1} \\ \Psi_n \end{pmatrix} = \begin{bmatrix} \frac{\alpha_n + \alpha_{n-1} + \beta_n - E}{\alpha_{n+1}} & -\frac{\alpha_n}{\alpha_{n+1}} \\ 1 & 0 \end{bmatrix} \begin{pmatrix} \Psi_n \\ \Psi_{n-1} \end{pmatrix}. \tag{9}$$

As in models 1 and 2, the transfer matrix is real valued and has determinant $\neq 0$, so that eigenfunctions do not have compact support and therefore do not vanish in a region where the Hamiltonian acts as the free Hamiltonian. For the permitted energy values the absolute value of the eigenfunctions cannot decrease in the region without interaction. Therefore, proper eigenfunctions are excluded and the spectrum is determined by the behaviour outside a finite region and is absolutely continuous. For the model 4, we will apply Fuerstenberg's theorem for random sequences, which holds for transfer matrices with real coefficients and determinant 1. This makes it necessary that $\alpha_n = \alpha_{n+1}$ except at the transition points $|n| = N$. At these transition points we have to accept that $\alpha_n \neq \alpha_{n+1}$, otherwise we cannot satisfy $4\alpha_n + \beta_n < 4$ and cannot exclude bound states. Thus the transition matrix at these single points has not only determinant $\neq 1$ but also $\neq 0$, and can provide details of the scattering, but not create transfer if it is otherwise forbidden.

3. Scattering theory

The idea of how to obtain NESS-states is based on the application of scattering theory. As suggested in [1, 2] we consider a finite system with some local Hamiltonian coupled to two heat baths with different temperature. We take all systems to be one-dimensional. Therefore, we have the algebra built by bosonic or fermionic creation and annihilation operators over the Hilbertspace:

$$L^2(-\infty, -N) \oplus L^2[-N, N] \oplus L^2(N, \infty), \tag{10}$$

where the Hilbert spaces L^2 are either over the continuum (models 1 and 2) or over the lattice (models 3 and 4). The initial state is assumed to decompose into

$$\omega = \omega_{(-\infty,-N)}(\beta_-) \otimes \omega_{[-N,N]} \otimes \omega_{(-N,\infty)}(\beta_+). \tag{11}$$

There is no need to specify how the state looks like in the region $[-N, +N]$ except that we assume that it is quasifree. Therefore, the state is invariant under some Hamiltonian which corresponds to a Hamiltonian on the one-particle level of the form

$$\hat{H} = H^0_{(-\infty,-N)} \oplus H_{[-N,N]} \oplus H^0_{(N,\infty),} \tag{12}$$

where H^0 is the free Hamiltonian in the restricted regions corresponding to the four models with appropriately chosen boundary conditions. The spectrum of $\hat{H}$ contains an absolutely continuous part from the contribution of the heat baths and a pure point spectrum corresponding to the finite system. The time evolution on the algebra determined by this one-particle Hamiltonian is denoted with $\hat{\tau}_t$, whereas the real time evolution τ_t is determined by the one-particle Hamiltonians corresponding to the models 1–4. The state (11) will evolve in time and tend to the final NESS-state

$$\omega_\infty(A) = \lim_{t\to\infty} \omega(\hat{\tau}_{-t} \circ \tau_t A) \tag{13}$$

if we can show that scattering theory between the automorphisms applies. Since they are quasifree it suffices if it works between the two one-particle Hamiltonians.

The state is fixed by the two-point function

$$\omega(a^*(f)a(g)) = \langle g|\hat{\rho}|f\rangle, \qquad [\hat{H}, \hat{\rho}] = 0. \tag{14}$$

Therefore,

$$\omega_\infty(a^*(f)a(g)) = \lim_{t\to\infty} \langle g|\, \mathrm{e}^{\mathrm{i}Ht}\, \mathrm{e}^{-\mathrm{i}\hat{H}t}\, \hat{\rho}\, \mathrm{e}^{\mathrm{i}\hat{H}t}\, \mathrm{e}^{-\mathrm{i}Ht}|f\rangle. \tag{15}$$

Thus our only task is to evaluate the wave operator $\Omega = \lim_{t\to\infty} \mathrm{e}^{\mathrm{i}\hat{H}t}\, \mathrm{e}^{-\mathrm{i}Ht}$. H has an absolutely continuous spectrum and so has $\hat{H}$ apart from finitely many-bound states. Therefore the limit exists in the strong sense and has a range on the absolutely continuous part of $\hat{H}$. The adjoint therefore converges weakly which is sufficient for the existence of the limit in (15). In complete generality the wave operator can be expressed as an integral kernel in terms of the generalized eigenfunctions Ψ corresponding to H and Φ corresponding to $\hat{H}$:

$$\Omega(x, y) = \int_0 \mathrm{d}k \Phi_+(x, k)\bar{\Psi}_+(y, k) + \int_0 \mathrm{d}k \Phi_-(x, k)\bar{\Psi}_-(y, k). \tag{16}$$

The upper limit in the integral is $+\infty$ in model 1, and 2 and 2 in models 3 and 4 according to the energy range of the absolutely continuous spectrum. According to (12) $\Phi_+(x, k) = \chi_{(N,\infty)}(x) \sin(k(x - N))$, $\Phi_-(x, k) = \chi_{(-\infty,-N)}(x) \sin(k(x + N))$ are the generalized eigenfunctions corresponding to $\hat{H}$, the other eigenfunctions are proper eigenfunctions and do not contribute to the wave operator. $\Psi_\pm(y, k)$ are the generalized eigenfunctions corresponding to H where $\pm$ indicates whether the waves are going to the right or to the left. More precisely they have the form

$$\begin{aligned} &\Psi_+(x, k) = \mathrm{e}^{\mathrm{i}kx} + a(k)\, \mathrm{e}^{-\mathrm{i}kx}, \qquad -\infty < x < -N, \\ &\Psi_+(x, k) = b(k)\, \mathrm{e}^{\mathrm{i}kx}, \qquad N < x < \infty, \qquad k > 0 \end{aligned} \tag{17}$$

$$\begin{aligned} &\Psi_-(x, k) = c(k)\, \mathrm{e}^{-\mathrm{i}kx}, \qquad -\infty < x < -N, \\ &\Psi_-(x, k) = \mathrm{e}^{-\mathrm{i}kx} + d(k)\, \mathrm{e}^{\mathrm{i}kx}, \qquad N < x < \infty, \qquad k > 0, \end{aligned} \tag{18}$$

where we do not specify how they look like in the interval $-N < x < N$, though from there the values $a(k), b(k), c(k), d(k)$ have to be calculated.

They are complete in the sense that

$$\int_0 \mathrm{d}k[\bar{\Psi}_+(x, k)\Psi_+(y, k) + \bar{\Psi}_-(x, k)\Psi_-(y, k)] = \delta(x - y) \tag{19}$$

and they are orthogonal in the sense that

$$\int \mathrm{d}x \bar{\Psi}_+(k, x)\Psi_+(q, x) = \delta(k - q), \qquad \int \mathrm{d}x \bar{\Psi}_+(k, x)\Psi_-(q, x) = 0, \tag{20}$$

respectively, replacing appropriately the integral by a sum in models 3 and 4. That the wave operator has this form can be seen by the ansatz

$$\begin{aligned}\Omega(x,y) = \lim_{t\to\infty}\Bigg[&\int_0 \mathrm{d}k \int_0 \mathrm{d}q\, \mathrm{e}^{\mathrm{i}t(E(q)-E(k))}\bar{\Phi}_+(x,k)\int \mathrm{d}z\Phi_+(z,k)\bar{\Psi}_+(z,q)\Psi_+(y,q)\\ &+\int_0 \mathrm{d}k \int_0 \mathrm{d}q\, \mathrm{e}^{\mathrm{i}t(E(q)-E(k))}\bar{\Phi}_+(x,k)\int \mathrm{d}z\Phi_+(z,k)\bar{\Psi}_-(z,q)\Psi_- y,q)\\ &+\int_0 \mathrm{d}k \int_0 \mathrm{d}q\, \mathrm{e}^{\mathrm{i}t(E(q)-E(k))}\bar{\Phi}_-(x,k)\int \mathrm{d}z\Phi_-(z,k)\bar{\Psi}_+(z,q)\Psi_+(y,q)\\ &+\int_0 \mathrm{d}k \int_0 \mathrm{d}q\, \mathrm{e}^{\mathrm{i}t(E(q)-E(k))}\bar{\Phi}_-(x,k)\int \mathrm{d}z\Phi_-(z,k)\bar{\Psi}_-(z,q)\Psi_-(y,q)]\end{aligned}$$

and evaluating

$$\lim_{t\to\infty}\mathrm{e}^{\mathrm{i}t(E(q)-E(k))}\int \mathrm{d}z\Phi_\pm(z,k)\bar{\Psi}_\pm(z,q) = \delta(k-q)\delta(\pm),$$

where $E(k), E(q)$ are the energies of the generalized eigenfunctions characterized by k, q. For models 1 and 2, this reduces to concentrating on Gauss functions (compare [5]); for models 3 and 4 it follows from the convexity of $E(k)$ together with the distribution properties of $\lim_{y\to\pm\infty}\sum_{x=0}^{\infty}\mathrm{e}^{\mathrm{i}k(y+x)}$. Only the asymptotic behaviour of the generalized eigenfunctions contributes to the integral. Local parts do not contribute in the limit by Riemann–Lebesgue. The essential contribution has the form

$$\begin{aligned}&\lim_{t\to+\infty}\lim_{N\to\infty}\sum_{n=M}^{N}\mathrm{e}^{\mathrm{i}(k-q)n-\mathrm{i}t(\cos k-\cos q)}\\ &\quad=\lim_{t\to+\infty}\lim_{N\to\infty}\frac{\mathrm{e}^{\mathrm{i}(k-q)(N-t\frac{\sin(k/2-q/2)}{k-q}\sin(k/2+q/2))}-\mathrm{e}^{-\mathrm{i}t(k-q)\frac{\sin(k/2-q/2)}{k-q}\sin(k/2+q/2)}}{\mathrm{e}^{\mathrm{i}(k-q)}-1}\mathrm{e}^{\mathrm{i}(k-q)M}\\ &\quad=\delta(k-q)\lim_{t\to-\infty}\lim_{N\to\infty}\sum_{n=M}^{N}\mathrm{e}^{\mathrm{i}(k-q)n-it(\cos k-\cos q)}\\ &\quad=\lim_{t\to-\infty}\lim_{N\to\infty}\frac{\mathrm{e}^{\mathrm{i}(k-q)(N-t\frac{\sin(k/2-q/2)}{k-q}\sin(k/2+q/2))}-\mathrm{e}^{-\mathrm{i}t(k-q)\frac{\sin(k/2-q/2)}{k-q}\sin(k/2+q/2)}}{\mathrm{e}^{\mathrm{i}(k-q)}-1}\mathrm{e}^{\mathrm{i}(k-q)M}\\ &\quad=0,\end{aligned}$$

where we note that in the permitted region of k, q $\frac{\sin(k/2-q)/2}{k-q}\sin(k/2+q/2)$ is positive and bounded. The arguments for the Kronig–Penney model are essentially the same. Completeness and orthogonality is then a consequence of applying scattering theory with respect to the free evolution where both properties are well established. Note that completeness when examined for x, y both in the left and in the right region implements

$$|a(k)|^2+|c(k)|^2=1, \qquad |b(k)|^2+|d(k)|^2=1. \tag{21}$$

With our ansatz (11) the limit state will therefore read

$$\omega_\infty(a^*(f)a(g)) = \langle g|P_+\frac{1}{\mathrm{e}^{\beta_+H}\pm 1}+P_-\frac{1}{\mathrm{e}^{\beta_-H}\pm 1}|f\rangle \tag{22}$$

depending whether we consider fermions or bosons. Here $P_\pm$ are the projections on the generalized eigenfunctions $\Psi_\pm$. Therefore we can evaluate the heat current that is determined by the transition values $|b(k)|^2$ and $|c(k)|^2$. We are interested in how this heat current depends on N. In addition we are also interested in how the effect of $P_\pm$ is reflected locally and in which sense we can talk of a thermodynamic limit $N\to\infty$.

4. The thermodynamic limit

We can calculate the heat current in the left and right heat baths by

$$\begin{aligned} j_l &= \int_0 \mathrm{d}k k(\rho_{\beta_+}(k)(1-|a(k)|^2) - \rho_{\beta_-}(k)|c(k)|^2) \\ j_r &= \int_0 \mathrm{d}k k(\rho_{\beta_+}(k)|b(k)|^2 - \rho_{\beta_-}(k)(1-|d(k)|^2). \end{aligned} \tag{23}$$

Evidently from (21) it vanishes for equal temperature. From symmetry relations of the Hamiltonian, it follows that it is the same in the right and left region. However the state in the heat baths will depend on N in the sense that $a(k)$ and $d(k)$ in (17) can still depend on N and therefore also the generalized eigenfunctions will depend on N. How they depend on N in the various models will have to be clarified in detail.

In the interacting region we are especially interested in how the state looks like far away from the boundary. First we have to argue that the dynamics will converge to a limit. This happens if H_N converges to H_∞ in the strong resolvent sense. This can be seen by the following arguments.

Take a sequence of projections P_L such that $\langle\Psi|P_L H_N P_L|\Psi\rangle = \langle\Psi|P_L H_{\bar{N}} P_L|\Psi\rangle$ for $N < \bar{N}$. Therefore also for $z > 0$

$$\langle\Psi|P_L \frac{1}{P_L H_N P_L + z} P_L|\Psi\rangle = \langle\Psi|P_L \frac{1}{P_L H_{\bar{N}} P_L + z} P_L|\Psi\rangle. \tag{24}$$

Now we can apply

$$P\frac{1}{A}P = P\frac{1}{PAP}P + P\frac{1}{A}(1-P)\frac{1}{(1-P)\frac{1}{A}(1-P)}(1-P)\frac{1}{A}P.$$

Exponential decay of the kernels corresponding to unitaries and resolvents of the relevant operators are studied in detail in the literature (e.g. [6]). Therefore we know that for every ϵ we can find L_0 such that

$$\left\| P_L \frac{1}{H_N}(1-P_M) \right\| \langle \epsilon\ \forall (M-L)\rangle L_0, \qquad N > M. \tag{25}$$

This fact allows us to conclude that

$$\lim_{N\to\infty} \left\langle \Psi|P_L \frac{1}{H_N + z} P_L|\Psi \right\rangle = \left\langle \Psi|P_L \frac{1}{H_\infty + z} P_L|\Psi \right\rangle. \tag{26}$$

With increasing N, P_L can also be chosen to increase to 1. From (26) we have weak resolvent convergence. Estimating for $L - M > L_0$, $L < N$ and $\|\Psi\| < \epsilon + \|P_M\Psi\|$

$$\left\| (P_L + (1-P_L))\left(\frac{1}{H_\infty + z} - \frac{1}{H_N + z}\right) P_L\Psi \right\| \leqslant \left\| (1-P_L)\left(\frac{1}{H_\infty + z} - \frac{1}{H_N + z}\right) P_M\Psi \right\| + \epsilon$$

and using (24) and (25) again, we can strengthen the result to strong resolvent convergence. That allows us to take functions of H_N such that the limit of their local expectation values exist and can be written as

$$\lim_{N\to\infty} \langle f|\rho(H_N)|g\rangle = \langle f|\rho(H_\infty)|g\rangle, \tag{27}$$

where H_∞ corresponds to our models 1, 2, 3 and 4 with N replaced by ∞.

The systems corresponding to H_∞ in the various models are well analysed in the literature, also in the broader context, e.g. in [6] or more recently [7]. In particular, the clustering behaviour (25) is well under control. If H_∞ has a continuous spectrum as in models 1 and 3, (25) is a consequence of Riemann Lebesgue in essentially the same way as for free

systems. If the spectrum is pure point, then it is a consequence of the exponential decay of the eigenfunctions. Detailed analyses even for more general models can be found in [6]. We examine the consequences for the different models with the main interest in how far the models allow to take the limit $N \to \infty$ in

$$\lim_{N\to\infty}\lim_{t\to\infty}\langle g|\,\mathrm{e}^{\mathrm{i}H_N t}\,\mathrm{e}^{-\mathrm{i}\hat{H}_N t}\,\hat{\rho_N}\,\mathrm{e}^{\mathrm{i}\hat{H}_N t}\,\mathrm{e}^{-\mathrm{i}H_N t}|\,f\rangle.$$

Model 1 is the Kronig–Penney model. The transfer matrix at every point is the same. For a given energy parameter $E(k) = k^2$, its eigenvalues are either $\mathrm{e}^{\pm\mathrm{i}\kappa}$ satisfying

$$\cos(\kappa) = \cos(kl) + \frac{\lambda}{2k}\sin(kl) \tag{28}$$

or they are $\mathrm{e}^{\pm\kappa}$ satisfying

$$\cosh(\kappa) = \cos(kl) + \frac{\lambda}{2k}\sin(kl).$$

For the infinite systems Bloch's theorem tells us that only the first case is permitted and that we are limited to energy bands. For finite N we conclude that the generalized eigenvalues corresponding to the forbidden regions vanish exponentially fast at the boundaries $x = \pm N$. This means especially that $b(k)$, $c(k)$ are of order $\mathrm{e}^{-\kappa N}$ and the corresponding current vanishes exponentially fast. For the remaining part, however, we cannot get rid of the N-dependence. The easiest way to see this is to write the transfer matrix in bra-ket notation

$$T^{(n)} = \prod_{N}^{n+N} T_k = T^{(n+N)} = \mathrm{e}^{\mathrm{i}\kappa(n+N)}|\Psi_+\rangle\langle\Phi_+| + \mathrm{e}^{-\mathrm{i}\kappa(n+N)}|\Psi_-\rangle\langle\Phi_-|, \tag{29}$$

where $|\Psi_\pm\rangle$ are the eigenfunctions of T and $|\Phi_\pm\rangle$ are the eigenfunctions of T^* corresponding to the eigenvalues $\mathrm{e}^{\pm\mathrm{i}\kappa}$ and normalized such that $\langle\Phi_\pm|\Psi_\pm\rangle = 1$, $\langle\Phi_\mp|\Psi_\pm\rangle = 0$. $b(k)$ is then calculated from (17) via $T^{(N)}$ and therefore

$$\left\langle \begin{matrix}1\\ \mathrm{i}\end{matrix}\right| (\mathrm{e}^{\mathrm{i}\kappa 2N}|\Psi_+\rangle\langle\Phi_+| + |\,+\mathrm{e}^{-\mathrm{i}\kappa 2N}|\Psi_-\rangle\langle\Phi_-|) \left|\begin{matrix}1\\ \mathrm{i}\end{matrix}\right\rangle b(k) = 1. \tag{30}$$

This shows that $|b(k)|$ and therefore the contribution to the heat current (23) will depend on N without tending to any limit. Transfer in the forbidden region vanishes exponentially fast with N; here we can take the thermodynamic limit. In the region in which energy is transferred, the amount will however oscillate in N. This has a consequence both for the heat baths as for the interacting system. We can get rid of the dependence on N only by averaging over a region $N \pm L$ where $L \ll N$ but tends to infinity. More precisely we can consider the limit

$$\bar{\omega}(a^*(f)a(g)) = \lim_{N\to\infty}\frac{1}{2N^{1/2}}\sum_{c=-N^{1/2}}^{c=N^{1/2}}\omega_{N+c}(a^*(f)a(g)). \tag{31}$$

In this way a finite heat current will remain. According to our remark on the thermodynamic limit (25), (26), we examine both the state inside the bath and inside the interior far away from the boundary, both in the limit of increasing interior. It is invariant under the time evolution (in the sense of the thermodynamic limit either for the bath or interior) permitting a heat current and being non-reflection invariant. We average among states that are time invariant with respect to different time evolutions; in this sense we cannot talk about time invariance. If, however, we take into account that (26) holds far away from the boundary, the dependence on N disappears and the time evolutions coincide so that in this limit away from the boundary the state has to be considered time and space translation invariant but neither extremely space translation invariant nor extremely time translation invariant.

Model 3 is called 'tight binding electron model' in [3]. Again we have to calculate the eigenvalues of the transfer matrix (9):

$$\begin{aligned}\cos(\kappa) &= \cos\left(\frac{2\alpha_n + \beta_n - E}{2\alpha_n}\right)\\ \cosh(\kappa) &= \cosh\left(\frac{2\alpha_n + \beta_n - E}{2\alpha_n}\right)\end{aligned} \tag{32}$$

depending whether $\frac{2\alpha_n+\beta_n-E}{2\alpha_n}$ is smaller or larger than 1. The final reflection coefficient is slightly more complicated than (30) because there is the additional term when α_n, β_n change. However, as before for $\frac{2\alpha_n+\beta_n-E}{2\alpha_n} > 1$, the transfer coefficient decays exponentially fast with N, whereas for $\frac{2\alpha_n+\beta_n-E}{2\alpha_n} < 1$ the transfer coefficient is positive but fluctuates with N because again (30) gives the correct N-dependence of the matrix, and only the vectors have to be adjusted. Therefore, the conclusions for the heat current and the limiting state remain unchanged.

Our main interest lies in models 2 and 4. If the parameters are sufficiently random then we will argue that the transfer coefficient will vanish exponentially fast. Therefore, the state for the heat baths sufficiently away from the boundary will not change and we do not obtain a NESS-state there. At the boundary the coupling to the Kronig–Penney model and the Anderson model respectively will affect the boundary conditions, but due to the exponential decay these boundary conditions do not affect the state far away from the boundary.

Inside of the interacting region again there will be no heat current. Nevertheless according to (22) the projection operators for finite N $P_\pm$ remain with different weights. However they depend on N, and again we have to clarify what the consequences of this N-dependence in the thermodynamic limit are.

The main tool in the analysis is Fuerstenberg's theorem:

Theorem 1 (Fuerstenberg theorem)**.** *Let μ be a measure on $SL(2, R)$ which is the group of two-dimensional unimodular matrices transforming the real vector space R^2 into itself. Let G be the smallest subgroup of $SL(2, R)$ containing the support of μ. Assume that G is noncompact and no subgroup of G of finite index is reducible. Let $\{T_n; n = 1, 2, \ldots\}$ denote the sequence of mutually independent G-valued random variables with the common distribution μ. For every vector $|\Psi>$ with $||\Psi|| = 1$*

$$\lim_{n\to\infty} \frac{1}{n} \log \|T_n T_{n-1} .. T_1 \Psi\| = \gamma > 0 \tag{33}$$

with probability 1 where γ depends only on μ.

Note that the conditions on G are satisfied if it contains at least two elements of $SL(2, R)$ with no common eigenvector. Therefore varying λ_n, l_n in model 2 or α, β_n in model 4 we can easily meet the conditions. It follows that (29) the transfer matrix $T^{(N)} = \Pi T_N \ldots T_1$ between the incoming and outgoing wave becomes for almost all sequences $\{\lambda_n, l_n\}$, $\{\alpha, \beta_n\}$

$$T^{(N)} = \mathrm{e}^{\gamma N} |\Psi_{+,N}\rangle\langle\Phi_{+,N}| + \mathrm{e}^{-\gamma N} |\Psi_{-,N}\rangle\langle\Phi_{-,N}|, \tag{34}$$

where $|\Psi_{\pm,N}\rangle$, $|\Phi_{\pm,N}\rangle$ are also random vectors and γ is determined by the sequence. If the vector corresponding to the incoming wave is not orthogonal to $|\Phi_{+,N}\rangle$ then its weight $b(k)$ has to be exponentially small. That it is orthogonal happens with vanishing probability on N, according to (33). Altogether the heat current will decrease exponentially fast with N. At the boundary the phase relations between the incoming and the reflected wave may change; however, this does not affect the state of the heat bath far away from the boundary.

Considering the state inside the interacting region, we have to be more careful than for the regular Kronig–Penney model or the regular tight binding model. Remember that also inside

the interaction region (19) has to hold. Whereas in the previous case we could concentrate on the scattered part, i.e. the part of the continuous spectrum and the eigenfunctions corresponding to the forbidden region contributed only to an exponentially negligible amount, and now the continuous part does not exist. Therefore after having taken the limit $t \to \infty$, we remain with

$$\omega_{\infty,N}(a^*(f)a(g)) = \langle g|P_{+,N}\frac{1}{e^{\beta_+ H_N} \pm 1} + P_{-,N}\frac{1}{e^{\beta_- H_N} \pm 1}|f\rangle\,. \tag{35}$$

We can concentrate on local f, g so that in the thermodynamic limit H_N can be replaced by H_∞, but we still have to worry about the dependence on $P_{\pm,N}$. The generalized eigenfunctions of the Hamiltonian H_N are twofold degenerate: with $\Psi(x)$ resp. Ψ_n also $\bar{\Psi}(x)$ or $\bar{\Psi}_n$ being an eigenfunction. These eigenfunctions cannot be real, as can be seen in the free regime. Therefore, we have degeneracy; however, the decomposition $P_{\pm,N}$ highly depends on N. As stated we have strong resolvent convergence of H_N. To control (35) it is sufficient to argue that for localized $|f\rangle$ we can take the weak limit

$$\lim P_{\pm,N}|f\rangle = \frac{1}{2}|f\rangle. \tag{36}$$

Proof. We use the fact that H_N is twofold degenerate. We can write

$$\langle f|\,P_{\pm,N}g(H)\,|f\rangle = \int \mathrm{d}E|f(E,\omega_0)\Psi_{\pm,N}(E)|^2 g(E), \tag{37}$$

where $\Psi_{\pm,N}(E)$ is the generalized eigenfunction corresponding to the energy E and $f(E,\omega_0)$ corresponds to the spectral decomposition of f where we indicate by ω_0 its dependence on the fixed sequence. However, we know from resolvent convergence that its dependence on the part of the sequence sufficiently far apart can be ignored. Therefore, we can replace it by

$$f(E,\omega_0) = \int \mathrm{d}\mu_r(\omega)\, f(E,\omega), \tag{38}$$

where we integrate over all sequences restricted to those that coincide with the fixed sequence in a neighbourhood of the region in which f is located. Now we can use the fact that the sequences are random and the measure $\mathrm{d}\mu_r(\omega)$ is ergodic. Therefore we can interpret (37) as the expectation value of projections in a two-dimensional Hilbert space averaged by the ergodic measure to a c-number, so that we can argue that in (37) the dependence on $\pm$ disappears and therefore (36) holds.

From (35) and (36) it follows that

$$\begin{aligned}\omega_\infty(a^*(f)a(g)) &= \lim_{\Delta\to\infty}\langle g|P_{+,N}\frac{1}{e^{\beta_+ H_N} \pm 1} + P_{-,N}\frac{1}{e^{\beta_- H_N} \pm 1}|f\rangle \\ &= \frac{1}{2}\langle g|\frac{1}{e^{\beta_+ H_\infty} \pm 1} + \frac{1}{e^{\beta_- H_\infty} \pm 1}|f\rangle \quad \forall\, f, g, \Delta = \mathrm{Distance}[\mathrm{supp}(f,g), N],\end{aligned} \tag{39}$$

since $\Delta \to \infty$ implies $N \to \infty$. Therefore, after taking the limit $t \to \infty$ we can also take the limit $N \to \infty$ and obtain

$$\omega_\infty = \frac{1}{2}\langle g|\frac{1}{e^{\beta_+ H_\infty} \pm 1} + \frac{1}{e^{\beta_- H_\infty} \pm 1}|f\rangle. \tag{40}$$

Evidently the state that is finally reached when we couple the system to two heat baths with different temperature is not a temperature state, nor does it carry a heat current. But there is also no symmetry breaking that reflects the orientation and location in space. We have no possibility of assigning something like a temperature gradient to the system. The random interaction with the background cannot replace the random interaction between the particles themselves that should produce a temperature gradient.

5. Conclusion

We studied the effect of coupling a system to two heat baths of different temperature in the thermodynamic limit. The coupled systems were quasifree, either translation invariant or with random one-particle Hamiltonians. As a consequence in the thermodynamic limit, the spectra were either absolutely continuous or pure point. In the former case they permit a heat current that depends not only on the temperature of the heat baths but also on the size of the system, so that it does not allow a thermodynamic limit. In the latter case no heat current remains, though the final state of the system is still determined by the heat baths but without any kind of symmetry breaking.

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