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A Model of Heat Conduction

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We construct a model of a chain of atoms coupled at its ends to two reservoirs at different temperatures. In a weak coupling limit the atoms obey a stochastic evolution law and have an equilibrium state with a uniform temperature gradient along the chain.

KEY WORDS: Master equation; heat conduction; stochastic dynamics; nonequilibrium thermodynamics; Markov process.

1. INTRODUCTION

We consider a finite, one-dimensional chain of quantum mechanical atoms with nearest neighbor interactions coupled at the ends of two infinite quasi-free reservoirs at different temperatures, and study the heat flow along the chain. While such chains have been considered before,[2,11,13,15–18] our model has two variations which enable it to be asymptotically exactly soluble without being superconducting.

In order to obtain an exact evolution equation for the atoms, we pass to the weak coupling limit of the interactions between the ends of the chain and the two reservoirs. By itself this would cause heat entering the chain at one end to diffuse along it much more rapidly that it could leave at the other end, so that in the equilibrium state all atoms of the chain would have the same temperature. We therefore make the coupling between atoms of the same order of magnitude as the coupling between the ends of the chain and the two reservoirs, before passing to the weak coupling limit.

Our second variation is that we do not couple neighboring atoms directly but via intermediate states involving virtual particles. The coupling is arranged so that in the long term there can be no transfer of energy between the atoms and these particles, which nevertheless have the effect of destroying phase relationships between the atoms. While the means by which we achieve

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this effect is somewhat artificial, we conjecture that some mechanism of this type is necessary to obtain a model of heat conduction. Although we use intermediate reservoirs, our model differs from that of Refs. 16 and 18 in that we do not need to adjust the reservoir parameters in a self-consistent manner in order to prevent the transfer of heat between these reservoirs and the atoms. Moreover in our model this transfer vanishes for all states of the atoms, not just for the stationary state as in Refs. 16 and 18.

We now specify the model. If $1 \leqslant r \leqslant N$, the rth atom is associated with a Hamiltonian H_r on the finite-dimensional Hilbert space $\mathscr{H}_r$. We identify any operator A on $\mathscr{H}_n$ with the operator $A_1 \otimes A_2 \otimes \cdots \otimes A_N$ on

$$\mathscr{H}_A = \mathscr{H}_1 \otimes \cdots \otimes \mathscr{H}_N$$

where $A_r = 1$ for $r \neq n$ and $A_n = A$. The chain of atoms then has Hamiltonian

$$H_A = H_1 + \cdots + H_N$$

Let $\{\mathscr{F}_r\}_{r=0}^N$ be the Hilbert spaces in the GNS representation of $N+1$ infinite quasifree fermion reservoirs[1,9] with Hamiltonians K_r and cyclic vectors Ω_r such that $K_r\Omega_r = 0$ for $0 \leqslant r \leqslant N$. The collection of all reservoirs has Hilbert space

$$\mathscr{F} = \mathscr{F}_0 \otimes \cdots \otimes \mathscr{F}_N$$

Hamiltonian

$$H_R = K_0 + \cdots + K_N$$

and cyclic vector

$$\Omega = \Omega_0 \otimes \cdots \otimes \Omega_N$$

The Hamiltonian of the system plus reservoirs is taken to be

$$H = H_A + H_R + \lambda H_I$$

on the space $\mathscr{H}_A \otimes \mathscr{F}$, where

$$H_I = \sum_{r=0}^{N} A_r \otimes \phi_r$$

A_0 being a self-adjoint operator on $\mathscr{H}_0$, A_N a self-adjoint operator on $\mathscr{H}_N$, A_r a self-adjoint operator on $\mathscr{H}_r \otimes \mathscr{H}_{r+1}$ for $1 \leqslant r \leqslant N-1$, and ϕ_r a bounded linear smeared field operator on $\mathscr{F}_r$ for $0 \leqslant r \leqslant N$. Possible variations of the model are discussed at the end of Section 2, while a particular example is treated in Section 3.

Because the reservoirs are quasifree, their effects on the atoms are completely determined by the forms of the two-point functions

$$h_r(t) = \langle e^{iH_R t}\phi_r e^{-iH_R t}\phi_r\Omega, \Omega\rangle = \langle e^{iK_r t}\phi_r e^{-iK_r t}\phi_r\Omega_r, \Omega_r\rangle$$

which are continuous, positive-definite functions. In order to be able to apply the results of Ref. 3 we need the regularity assumption

$$\int_{-\infty}^{\infty} |h_r(t)|(1 + |t|)^{\epsilon}\, dt < \infty \tag{1}$$

for some $\epsilon > 0$. This implies that the Fourier transforms $\hat{h}_r(\omega)$ are non-negative continuous functions on $\mathbb{R}$.

Our crucial assumptions on the mode of action of the reservoirs can be phrased in terms of the two-point functions. We assume that

$$\hat{h}_0(-\omega) = e^{-\beta_L \omega}\hat{h}_0(\omega) \tag{2}$$

and

$$\hat{h}_N(-\omega) = e^{-\beta_R \omega}\hat{h}_N(\omega) \tag{3}$$

for all $\omega \in \mathbb{R}$, so that β_L and β_R are the inverse temperatures of the left and right reservoirs, respectively. We also assume that the normal modes of the intermediate reservoirs are limited by the condition

$$1 \leqslant r \leqslant N - 1 \qquad \text{and} \qquad |\omega| \geqslant E \Rightarrow \hat{h}_r(\omega) = 0 \tag{4}$$

where $E > 0$ is small enough that if ω and ω' are two different eigenvalues of H_A, then

$$|\omega - \omega'| \geqslant E$$

The existence of such an $E > 0$ is a consequence of the finite-dimensionality of $\mathscr{H}_A$.

2. THE WEAK COUPLING LIMIT

Denoting by $\mathscr{T}(\mathscr{H}_A)$ the space of trace class operators on $\mathscr{H}_A$, we have that the initial state ρ of the system is an element of

$$S = \{\rho \in \mathscr{T}(\mathscr{H}_A):\quad \rho \geqslant 0 \text{ and } \mathrm{tr}[\rho] = 1\}$$

The reservoir is taken to be initially in the stationary state $v = |\Omega\rangle\langle\Omega|$ and the system plus reservoir is supposed to be in the initial state $\rho \otimes v$. The state of the system at time $t > 0$ is then given in the interaction representation by

$$\rho_\lambda(t) = e^{iH_A t}\, \mathrm{tr}_{\mathscr{F}}[e^{-iHt}(\rho \otimes v)e^{iHt}]e^{-iH_A t}$$

where $\mathrm{tr}_{\mathscr{F}}$ is the partial trace with respect to the reservoir variables. We pass to the weak coupling limit $\lambda \to 0$ keeping the rescaled time $\tau = \lambda^2 t$ constant as in Refs. 3 and 14.

Theorem 1. For all $\rho \in S$ and $\tau \geqslant 0$

$$\lim_{\lambda \to 0} \rho_\lambda(\lambda^{-2}\tau) = [\exp(K^\natural \tau)]\rho \tag{5}$$

where

$$K^\natural(\rho) = \lim_{a \to \infty} \frac{1}{2a} \int_{-a}^{a} e^{iH_A s} K\{e^{-iH_A s} \rho e^{iH_A s}\} e^{-iH_A s}\, ds \tag{6}$$

$$K(\rho) = \sum_{r=0}^{N} K_r(\rho)$$

and $K_r : \mathscr{T}(\mathscr{H}_A) \to \mathscr{T}(\mathscr{H}_A)$ depend on A_r and h_r.

Proof. This is taken directly from Ref. 3, the fact that we have $N + 1$ reservoirs instead of just one necessitating only slight extra complications in the proof. The operator K_r is given by

$$K_r(\rho) = \int_0^\infty \{-A_r(t)A_r\rho h_r(t) + A_r(t)\rho A_r \overline{h_r(t)} + A_r\rho A_r(t)h_r(t) - \rho A_r A_r(t)\overline{h_r(t)}\}\, dt$$

where

$$A_r(t) = e^{iH_A t} A_r e^{-iH_A t}$$

Expanding $A_r(t)$ as a finite sum

$$A_r(t) = \sum_\omega A_{r,\omega} e^{-i\omega t} \tag{7}$$

where ω runs through all differences of eigenvalues of H_A, and using

$$\int_0^\infty h_r(t) e^{i\omega t}\, dt = \tfrac{1}{2}\hat{h}_r(\omega) + i s_r(\omega)$$

where both $\hat{h}_r$ and s_r are real, continuous functions on $\mathbb{R}$, we obtain, as in Ref. 3,

$$\begin{aligned} K_r^\natural(\rho) = \sum_\omega [&-A_{r,-\omega}A_{r,\omega}\rho\{\tfrac{1}{2}\hat{h}_r(\omega) + i s_r(\omega)\} \\ &+ A_{r,\omega}\rho A_{r,-\omega}\{\tfrac{1}{2}\hat{h}_r(\omega) - i s_r(\omega)\} \\ &+ A_{r,\omega}\rho A_{r,-\omega}\{\tfrac{1}{2}\hat{h}_r(\omega) + i s_r(\omega)\} \\ &- \rho A_{r,-\omega}A_{r,\omega}\{\tfrac{1}{2}\hat{h}_r(\omega) - i s_r(\omega)\}] \\ = \sum_\omega \hat{h}_r(\omega)&\{-\tfrac{1}{2}A_{r,-\omega}A_{r,\omega}\rho - \tfrac{1}{2}\rho A_{r,-\omega}A_{r,\omega} + A_{r,\omega}\rho A_{r,-\omega}\} \\ &- i\Big[\sum_\omega s_r(\omega)A_{r,-\omega}A_{r,\omega},\, \rho\Big] \end{aligned} \tag{8}$$

Each term in the first series describes a stochastic transition transferring energy between neighboring atoms, while each term in the second series

describes an energy level shift of the atoms, of second order in λ. Our hypotheses on the two-point functions allow us to be much more precise about the effect of each term $K_r^\natural$.

Theorem 2. If $1 \leqslant r \leqslant N-1$, then

$$K_r^\natural(\rho) = -i[D_r, \rho] + \hat{h}_r(0)\{-\tfrac{1}{2}A_{r,0}^2\rho - \tfrac{1}{2}\rho A_{r,0}^2 + A_{r,0}\rho A_{r,0}\} \tag{9}$$

where D_r and $A_{r,0}$ are both self-adjoint, commute with H_A, and lie in $\mathscr{L}(\mathscr{H}_r \otimes \mathscr{H}_{r+1})$.

Proof. Our assumptions on $\hat{h}_r$ in Eq. (4) imply that in the first sum of Eq. (8) all terms vanish except that for $\omega = 0$. Since

$$A_{r,\omega} = \lim_{a\to\infty} \frac{1}{2a}\int_{-a}^{a} e^{i\omega t}e^{iH_A t}A_r e^{-iH_A t}\,dt$$

$$= \lim_{a\to\infty} \frac{1}{2a}\int_{-a}^{a} e^{i\omega t}e^{i(H_r+H_{r+1})t}A_r e^{-i(H_r+H_{r+1})t}\,dt$$

it follows that both $A_{r,0}$ and

$$D_r = \sum_{\omega} s_r(\omega)A_{r,-\omega}A_{r,\omega} \tag{10}$$

lie in $\mathscr{L}(\mathscr{H}_r \otimes \mathscr{H}_{r+1})$. Equation (7) also implies that both $A_{r,0}$ and D_r commute with H_A.

Theorem 2 allows us to deduce that the intermediate reservoirs cannot transfer energy to or from the system of atoms.

Corollary 1. If $1 \leqslant r \leqslant N-1$, then $K_r^\natural$ conserves energy in the sense that

$$\mathrm{tr}[H_A\{\exp(K_r^\natural\tau)\}\rho] = \mathrm{tr}[H_A\rho] \tag{11}$$

for all $\rho \in S$ and $\tau \geqslant 0$.

Proof. It is immediate from the theorem that

$$K_r^\natural(H_A\rho) = H_A(K_r^\natural\rho) \tag{12}$$

for all $\rho \in \mathscr{T}(\mathscr{H}_A)$. This implies

$$\mathrm{tr}[\{\exp(K_r^\natural\tau)\}(H_A\rho)] = \mathrm{tr}[H_A\{\exp(K_r^\natural\tau)\}\rho]$$

Since also

$$\mathrm{tr}[K_r^\natural\sigma] = 0$$

for all $\sigma \in \mathscr{T}(\mathscr{H}_A)$

$$\mathrm{tr}[\{\exp(K_r^\natural\tau)\}\sigma] = \mathrm{tr}[\sigma]$$

for all $\tau \geqslant 0$. The corollary results by putting these remarks together.

Note. Equation (12) is much stronger than

$$K_r^{\natural}\{[H_A, \rho]\} = [H_A, K_r^{\natural}(\rho)] \tag{13}$$

which is an immediate consequence of the definition of $\natural$ in Eq. (6).

Corollary 2. If ρ_L is the Gibbs state

$$\rho_L = e^{-\beta_L H_1}/\mathrm{tr}[e^{-\beta_L H_1}]$$

of the first atom and σ is any state on $\mathscr{H}_2 \otimes \cdots \otimes \mathscr{H}_N$, then $\rho_L \otimes \sigma$ is a stationary state for the semigroup $\exp(K_0^{\natural}\tau)$. A similar result holds for $\exp(K_N^{\natural}\tau)$.

Proof. This is a direct quotation of Theorem 4.5 of Ref. 3.

We have shown that in the limit $\lambda \to 0$ the system of atoms evolves according to the irreversible dynamical equation

$$\frac{d\rho}{d\tau} = \sum_{r=0}^{N} K_r^{\natural}\rho \tag{14}$$

The terms $K_0^{\natural}$ and $K_N^{\natural}$ tend to drive the end atoms to their Gibbs states at the inverse temperatures β_L and β_R. The terms K_r with $1 \leqslant r \leqslant N-1$ effect a stochastic and conservative transfer of energy between the rth and $(r+1)$th atoms of the chain. The rate of flow of energy is proportional to λ^2 because of the time rescaling.

We end this section with comments on some possible variations of the model.

(i) We have seen that translation invariance of the chain is not necessary, and it is clear that the dimensionality and degree of interconnectedness of the array of atoms may be arbitrary.

(ii) The model may be solved with boson reservoirs as in Ref. 14 but one does not then have the possibility of β_L and β_R being negative.

(iii) If the reservoirs are not quasifree, one needs to impose rather strong conditions on the time decay of the n-point functions as $n \to \infty$. Their validity for general reservoirs is not known, although they are satisfied in some cases.[6]

(iv) We have presented our model in the weak coupling limit, but the same estimates deal with certain singular coupling limits, for which time rescaling is not necessary.[7,12]

(v) We have taken each of the atoms to be finite-dimensional, but one may deal with infinite-dimensional atoms whose Hamiltonians have pure point spectra by using the techniques of Refs. 4 and 5.

(vi) If the coupling between all pairs of atoms is effected by a single intermediate reservoir, then $K^{\natural}$ will contain more complicated terms involving

four atoms. A number of other variations on the interaction term H_I are possible.

(vii) In particular, by suitable choices, one may derive the stochastic dynamics of the Ising model in the weak coupling limit.[10]

3. EQUILIBRIUM STATE OF THE ATOMS

We describe a concrete example where the evolution equation (14) and the equilibrium state of the system of atoms may be explicitly determined. We let each $\mathscr{H}_r$ be two-dimensional and define the operators P_r, Q_r, R_r, and L_r on $\mathscr{H}_r$ by

$$P_r = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \qquad Q_r = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \qquad R_r = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \qquad L_r = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

We let the rth atom have Hamiltonian

$$H_r = \tfrac{1}{2}EP_r - \tfrac{1}{2}EQ_r$$

where $E > 0$. We let

$$A_0 = R_1 + L_1, \qquad A_N = R_N + L_N$$

while if $1 \leqslant r \leqslant N - 1$

$$A_r = (R_r + L_r) \otimes (R_{r+1} + L_{r+1})$$

The possible values of the operators $A_{r,\omega}$ are tabulated in Table I.

Since

$$\mathscr{V} = \{X \in \mathscr{L}(\mathscr{H}_A): \quad [X, H_r] = 0 \text{ all } r\}$$
$$= \{P_r, Q_r: \quad 1 \leqslant r \leqslant N\}''$$

is an Abelian von Neumann algebra of dimension 2^N, the set of states

$$S_0 = \{\rho \in \mathscr{V}: \quad \rho \geqslant 0 \text{ and } \mathrm{tr}[\rho] = 1\}$$

Table I

ω \ r	0	N	$1 \leqslant r \leqslant N - 1$
$-2E$	0	0	$R_r \otimes R_{r+1}$
$-E$	R_1	R_N	0
0	0	0	$R_r \otimes L_{r+1} + L_r \otimes R_{r+1}$
E	L_1	L_N	0
$2E$	0	0	$L_r \otimes L_{r+1}$

may be identified with the set of all probability measures on $\{0, 1\}^N$, the rth coordinate of a point in $\{0, 1\}^N$ being equal to one if the rth atom is excited.

Theorem 3. If $\rho \in S_0$, then

$$\begin{aligned} K^\natural(\rho) = {} & \hat{h}_0(E)\{-\tfrac{1}{2}P_1\rho - \tfrac{1}{2}\rho P_1 + L_1\rho R_1\} \\ & + \hat{h}_0(-E)\{-\tfrac{1}{2}Q_1\rho - \tfrac{1}{2}\rho Q_1 + R_1\rho L_1\} \\ & + \hat{h}_N(E)\{-\tfrac{1}{2}P_N\rho - \tfrac{1}{2}\rho P_N + L_N\rho R_N\} \\ & + \hat{h}_N(-E)\{-\tfrac{1}{2}Q_N\rho - \tfrac{1}{2}\rho Q_N + R_N\rho L_N\} \\ & + \sum_{r=1}^{N-1} \hat{h}_r(0)\{-\tfrac{1}{2}Q_{r+1}P_r\rho - \tfrac{1}{2}\rho P_r Q_{r+1} + R_{r+1}L_r\rho R_r L_{r+1} \\ & - \tfrac{1}{2}P_{r+1}Q_r\rho - \tfrac{1}{2}\rho P_{r+1}Q_r + R_r L_{r+1}\rho R_{r+1}L_r\} \end{aligned} \tag{15}$$

Moreover,

$$[\exp(K^\natural\tau)](S_0) \subseteq S_0 \tag{16}$$

for all $\tau \geqslant 0$, and $\exp(K^\natural\tau)$ describes a classical Markov semigroup on $\{0, 1\}^N$.

Proof. From Table I we see that every operator $A_{r,-\omega}A_{r,\omega}$ lies in $\mathscr{V}$, so that if $\rho \in S_0$, then the commutator in Eq. (8) vanishes. The first two terms in Eq. (15) then give $K_0^\natural(\rho)$, while the second two terms give $K_N^\natural(\rho)$. We show that if $\rho \in S_0$, each term of the series in Eq. (15) equals $K_r^\natural(\rho)$.

By Eq. (9), if $\rho \in S_0$, then

$$\begin{aligned} K_r^\natural(\rho) &= \hat{h}_r(0)\{-\tfrac{1}{2}A_{r,0}^2\rho - \tfrac{1}{2}\rho A_{r,0}^2 + A_{r,0}\rho A_{r,0}\} \\ &= \hat{h}_r(0)\{-\tfrac{1}{2}(R_r \otimes L_{r+1} + L_r \otimes R_{r+1})^2\rho \\ &\quad - \tfrac{1}{2}\rho(R_r \otimes L_{r+1} + L_r \otimes R_{r+1})^2 \\ &\quad + (R_r \otimes L_{r+1} + L_r \otimes R_{r+1})\rho(R_r \otimes L_{r+1} + L_r \otimes R_{r+1})\} \\ &= \hat{h}_r(0)\{-\tfrac{1}{2}(P_rQ_{r+1} + Q_rP_{r+1})\rho - \tfrac{1}{2}\rho(P_rQ_{r+1} + Q_rP_{r+1}) \\ &\quad + R_{r+1}L_r\rho R_rL_{r+1} + R_rL_{r+1}\rho R_{r+1}L_r\} \end{aligned}$$

since

$$R_r\rho R_r = L_r\rho L_r = 0$$

if $\rho \in S_0$.

Having established Eq. (15), we see that $K^\natural(\mathscr{V}) \subseteq \mathscr{V}$, so that

$$[\exp(K^\natural\tau)](\mathscr{V}) \subseteq \mathscr{V}$$

for all $\tau \geqslant 0$. Equation (16) follows since $\exp(K^\natural\tau)$ preserves positivity and trace.[3]

The classical Markov process, known as a Markov population process,[8] may be described as follows. The first atom becomes deexcited at the rate $\hat{h}_0(E)$ and excited at the rate $\hat{h}_0(-E) = e^{-\beta_L E}\hat{h}_0(E)$ because of its contact with the left reservoir. The Nth atom becomes deexcited at the rate $\hat{h}_N(E)$ and excited at the rate $\hat{h}_N(-E) = e^{-\beta_R E}\hat{h}_N(E)$ due to its contact with the right reservoir. If $1 \leqslant r \leqslant N-1$, excitations are exchanged between the rth and $(r+1)$th atoms in both directions at the same rate $\hat{h}_r(0)$. It is clear that if all the above coefficients are nonzero, the Markov process is irreducible, so that the process has a unique stationary state ρ_0.

We describe the temperature gradient along the chain in the stationary state by means of the map $\theta: S_0 \to \mathbb{C}^N$ defined by

$$(\theta\rho)_r = \mathrm{tr}[P_r\rho]$$

this representing the probability that the rth atom is excited.

Theorem 4. The stationary probabilities of excitation $\alpha_r = (\theta\rho_0)_r$ are obtained by solving the equations

$$\{\hat{h}_0(-E) + \hat{h}_0(E) + \hat{h}_1(0)\}\alpha_1 - \hat{h}_1(0)\alpha_2 = \hat{h}_0(-E)$$
$$-\hat{h}_{N-1}(0)\alpha_{N-1} + \{\hat{h}_N(-E) + \hat{h}_N(E) + \hat{h}_{N-1}(0)\}\alpha_N = \hat{h}_N(-E)$$

and if $2 \leqslant r \leqslant N-1$,

$$\hat{h}_{r-1}(0)\alpha_{r-1} - \{\hat{h}_{r-1}(0) + \hat{h}_r(0)\}\alpha_r + \hat{h}_r(0)\alpha_{r+1} = 0$$

Proof. If $\bar{K}: \mathbb{C}^N \to \mathbb{C}^N$ is the affine map

$$(\bar{K}\alpha)_1 = \hat{h}_0(-E)(1-\alpha_1) - \hat{h}_0(E)\alpha_1 - \hat{h}_1(0)\alpha_1 + \hat{h}_1(0)\alpha_2$$
$$(\bar{K}\alpha)_N = \hat{h}_N(-E)(1-\alpha_N) - \hat{h}_N(E)\alpha_N - \hat{h}_{N-1}(0)\alpha_N + \hat{h}_{N-1}(0)\alpha_{N-1}$$

while if $2 \leqslant r \leqslant N-1$,

$$(\bar{K}\alpha)_r = -\hat{h}_{r-1}(0)\alpha_r + \hat{h}_{r-1}(0)\alpha_{r-1} - \hat{h}_r(0)\alpha_r + \hat{h}_r(0)\alpha_{r+1}$$

then direct computation shows that

$$\bar{K}(\theta\rho) = \theta(K^\natural\rho)$$

for all $\rho \in S_0$. Since $K^\natural\rho_0 = 0$, it follows that $\bar{K}\alpha = 0$.

By their definition, the coefficients $\hat{h}_r(0)$, $\hat{h}_0(\pm E)$, and $\hat{h}_N(\pm E)$ are nonnegative. If they are strictly positive, the equations for α_r are uniquely soluble. If the chain has uniform conductivity $\gamma = \hat{h}_r(0)$, then the probability of excitation increases linearly from one end of the chain to the other. If γ is small compared with $\hat{h}_0(\pm E)$ and $\hat{h}_N(\pm E)$, then the temperatures of the end atoms are approximately equal to those of their adjacent reservoirs. It is also elementary to compute the heat flux between the two reservoirs in the stationary state.

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