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Quantum-mechanical harmonic chain attached to heat baths. II. Nonequilibrium properties

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We study nonequilibrium properties of a one-dimensional harmonic chain to whose ends independent heat baths are attached which are kept at different temperatures. Using the quantum Langevin equation approach, we determine the stationary nonequilibrium state for arbitrary temperatures and coupling strength to the heat baths. This allows us to discuss several typical nonequilibrium properties. We find that the heat flux through the chain is finite as the length of the chain goes to infinity, i.e., we recover the well-known fact that the lattice thermal conductivity of the perfect harmonic chain is infinite. In the quantal case, the heat flux j_{qm} is reduced compared with its classical value j_{cl} , $j_{qm} \propto (\bar{T}/\Theta_D)^3 j_{cl}$, where \bar{T} is the average temperature of the heat baths, and where Θ_D is the Debye temperature of the chain. Furthermore, we investigate the variance of the displacement operators and the temperature profile along the chain. In accordance with the infinite thermal conductivity we find a vanishing temperature gradient in the chain except in boundary layers at its ends.

I. INTRODUCTION

In the preceding paper,¹ henceforth referred to as I, we studied a large quantum-mechanical perfect harmonic chain to whose ends independent heat baths are attached. These heat baths induce fluctuations and dissipation in the chain. In the general case in which the heat baths are at different temperatures, in I, we set up the quantum Langevin equations² for the operators $x_n(t)$, $p_n(t)$, $n=1,2,\dots,N$, of the displacement and conjugate momentum operators, respectively, of all particles of the chain. Choosing fixed boundary conditions, we showed that an arbitrary initial state decays towards a uniquely determined stationary state. Because then the chain settles down in a Gaussian state, the thermal properties of the chain are determined by its second moments $\langle x_n x_m \rangle$, $\langle x_n p_m \rangle$, etc. In I, we specified then the heat baths being at equal temperatures so that the chain approaches thermal equilibrium. We found that in the classical case, the properties of the chain are independent of the coupling strength between the heat baths and chain whereas in the quantal case this is only true outside boundary layers of thickness $a\Theta_D/(2\pi T)$ at both ends of the chain, where a is the lattice constant, T is the temperature of the heat baths, and Θ_D is the Debye temperature of the chain. In the weak-coupling limit, we recovered the standard expressions obtained from the Gibbs state of the free chain. In this paper, we investigate the stationary nonequilibrium state that the chain approaches if the heat baths are at different temperatures $\beta_1 \neq \beta_N$.

Thermal properties of a classical perfect harmonic chain were investigated in detail by Rieder, Lebowitz,

and Lieb.³ They found that the heat flux is proportional to the temperature difference $T_1 - T_N$ and not to the temperature gradient $(T_1 - T_N)/N$, as required by Fourier's law of heat conduction. A simple argument due to Peierls, shows that the infinite thermal conductivity is common to all systems in which momentum destroying Umklapp processes are absent.⁴

In the classical and quantal case, nonequilibrium properties of one-dimensional harmonic chains were investigated in other models as well. In the approach put forward by Visscher and co-workers⁵ heat baths are attached not only at the ends of the chain but to all particles along the chain. The temperatures of these heat baths are determined by the requirement that in the stationary state, no heat flows between each particle and its heat bath. The action of these self-consistent heat baths maintain a constant finite temperature gradient in the middle of the chain which leads to a finite thermal conductivity.

A somewhat related quantum chain was studied by Davies.⁶ Here, heat baths are attached only to the particles at the ends. The coupling between the chain and heat baths is made of the same order of magnitude as the coupling between neighboring particles, and then the weak-coupling limit is considered. The chain is made nonsuperconducting by coupling neighboring particles not directly but via intermediate phase destroying virtual particles.

Bafaluy and Rubi⁷ investigated still another model studied first by Rubin and Greer,⁸ who, however, were primarily interested in chains with impurities; see Sec. VI for a brief discussion. In these models, at an initial time

$t=0$, one divides the infinite chain into two disconnected parts with one part kept at temperature T while the other part is kept at zero temperature. Then, one connects the two parts, and lets the chain evolve freely in time. As time goes to infinity, the chain approaches a stationary state in which the particles at the far left and right from the middle of the chain make up two heat baths at different temperatures. The remaining part of the middle is in a nonequilibrium state. In the classical and quantal case, Bafaluy and Rubi derived exact expressions for the heat flux.

In one dimension, a chain with two heat baths attached to its ends is closest to an idealized experiment which measures the thermal conductivity of bulk materials. Though the perfect harmonic chain is superconducting, studying the model of Rieder, Lebowitz, and Lieb in its quantal version, we gain interesting insights into nonequilibrium properties of large quantum systems.

This paper is organized as follows. In Sec. II, the stationary nonequilibrium covariance matrix is constructed and general properties of it are discussed. More specifically, in Sec. III, the heat flux is determined. The absence of long-range order is demonstrated in Sec. IV by means of the mean square of the difference of displacement operators $\langle (x_k - x_l)^2 \rangle$. In Sec. V, the temperature profile along the chain is discussed. Finally, Sec. VI provides a summary.

II. NONEQUILIBRIUM COVARIANCE MATRIX

Because the equations of motion of the particles of the harmonic chain are linear and the fluctuating forces Gaussian, cf. Eqs. (2.8)–(2.10) of paper I [abbreviated (I-2.8)–(I-2.10)], the stationary state of the chain is Gaussian too. The matrix of equal time correlation functions $\langle x_k(t)x_l(t) \rangle$, $\langle x_k(t)p_l(t) \rangle$, etc., the so-called covariance matrix, obeys a linear first-order differential equation whose form is the same in the classical and quantal case; cf. Eq. (I-3.5). It turns out that the covariance matrix has a time-independent imaginary part which is determined by the equal time commutators $[x_k(t), p_l(t)] = i\hbar\delta_{kl}$. We shall always split off this trivial contribution. The remaining real part of the covariance matrix $\underline{B}(t)$ is symmetrical and defined by

$$\underline{B}(t) = \begin{bmatrix} \langle x_k(t)x_l(t) \rangle & \langle \{x_k(t), p_l(t)\} \rangle \\ \langle \{p_k(t), x_l(t)\} \rangle & \langle p_k(t)p_l(t) \rangle \end{bmatrix}, \quad (2.1)$$

where $\langle \{x_k(t), p_l(t)\} \rangle$ denotes the symmetrized mean $\frac{1}{2}\langle x_k(t)p_l(t) + p_l(t)x_k(t) \rangle$, and where, for example, the term $\langle x_k(t)x_l(t) \rangle$ represents an $N \times N$ matrix with the corresponding elements. The relaxation of an initial state towards the stationary state is completely determined by the $2N \times 2N$ relaxation matrix \underline{A} , cf. Eq. (I-2.15),

$$\underline{A} = \begin{bmatrix} \underline{0} & -\underline{1} \\ \underline{g} & \underline{r} \end{bmatrix}, \quad (2.2)$$

where $\underline{0}$ and $\underline{1}$ are the zero and unit $N \times N$ matrix, respectively, and where \underline{g} and \underline{r} are given by, cf. Eqs. (I-2.16a) and (I-2.16b),

$$(\underline{g})_{kl} = -\delta_{k+1,l} + 2\delta_{kl} - \delta_{k-1,l}, \quad (2.3a)$$

$$(\underline{r})_{kl} = \delta_{kl}(\delta_{1k} + \delta_{Nk}). \quad (2.3b)$$

We recall from I that we measure time in units of the universe of the half Debye frequency and lengths in units of the lattice constant. Correspondingly, the heat baths are characterized by three dimensionless parameters γ , \hbar , and $\hbar\beta$; cf. Eqs. (I-2.12) and (I-2.13). Further, we set $k_B = 1$ so that $T = \beta^{-1}$ is the dimensionless temperature.

Because the relaxation matrix does not depend on the state of the heat baths, an initial state relaxes towards a nonequilibrium state according to the same law as towards an equilibrium situation. In any case, the stationary covariance matrix is the unique solution of the inhomogeneous matrix equation

$$\underline{A} \cdot \underline{B} + \underline{B} \cdot \underline{A}' = \underline{D}, \quad (2.4)$$

where the diffusion matrix carries the information about the state of the heat baths via the temperatures β_1 and β_N . It is symmetrical in accordance with the self-transposedness of \underline{B} .

In (I-3.21), we decomposed the diffusion matrix into two parts transforming evenly and oddly under the exchange of the heat baths $\beta_1 \leftrightarrow \beta_N$,

$$\underline{D} = \underline{D}_+ + \underline{D}_-, \quad (2.5)$$

where

$$\begin{aligned} \underline{D}_+ = & \frac{1}{2} \sum_{m=1}^N [D'^{pp}(m, \beta_1) + D'^{pp}(m, \beta_N)] \underline{S}_1(m) \\ & + \frac{1}{2} \sum_{m=1}^N [D^{xp}(m, \beta_1) + D^{xp}(m, \beta_N)] \underline{S}_2(m), \end{aligned} \quad (2.6a)$$

$$\begin{aligned} \underline{D}_- = & \frac{1}{2} \sum_{m=1}^N [D'^{pp}(m, \beta_1) - D'^{pp}(m, \beta_N)] \underline{T}_1(m) \\ & + \frac{1}{2} \sum_{m=1}^N [D^{xp}(m, \beta_1) - D^{xp}(m, \beta_N)] \underline{T}_2(m). \end{aligned} \quad (2.6b)$$

Here, the quantities $D'^{pp}(m, \beta)$, $D^{xp}(m, \beta)$, $m = 1, 2, \dots$, are given by, cf. Eqs. (I-B8) and (I-B9a)–(I-B9c),

$$\begin{aligned} D'^{pp}(m, \beta) = & \gamma \left[\frac{1}{\beta} \delta_{1m} + \frac{4}{\beta} \sum_{n=1}^{\infty} \tilde{\chi}_{1m}^0(i\nu_n) \right. \\ & - \frac{2}{\beta} \sum_{n=1}^{\infty} \tilde{\chi}_{1, m+1}^0(i\nu_n) \\ & \left. - \frac{2}{\beta} \sum_{n=1}^{\infty} \tilde{\chi}_{1, m-1}^0(i\nu_n) \right], \quad m = 1, 2, \dots, \end{aligned} \quad (2.7a)$$

$$D^{xp}(1, \beta) = \gamma \frac{\hbar}{\pi} \ln \left[\frac{\hbar\beta}{2\pi} \Omega_D \right], \quad (2.7b)$$

$$D^{xp}(m, \beta) = -\gamma \frac{2}{\beta} \sum_{n=1}^{\infty} \nu_n \frac{\tilde{\chi}_{1m}^0(i\nu_n)}{1 + \gamma \nu_n \tilde{\chi}_{11}^0(i\nu_n)}, \quad m = 2, 3, \dots, \quad (2.7c)$$

where $\nu_n = 2\pi n / (\hbar\beta)$, $\hat{\chi}_{nm}^0(\omega)$ is the dynamic susceptibility of the undamped harmonic chain, cf. Eq. (I-2.7), and Ω_D is an upper cutoff on the frequency distribution of the heat baths. Furthermore, the matrices $\underline{S}_i(m)$, $i=1,2$, are given by Eqs. (I-3.22) and (I-3.23), and $\underline{T}_i(m)$, $i=1,2$, by Eqs. (I-3.24) and (I-3.25).

Accordingly, there are two distinct contributions to the covariance matrix: the average thermal equilibrium state and the deviation thereof,

$$\underline{B} = \underline{B}_+ + \underline{B}_-, \quad (2.8)$$

where \underline{B}_+ and \underline{B}_- are the respective solutions of

$$\underline{A} \cdot \underline{B}_+ + \underline{B}_+ \cdot \underline{A}^t = \underline{D}_+, \quad (2.9a)$$

$$\underline{A} \cdot \underline{B}_- + \underline{B}_- \cdot \underline{A}^t = \underline{D}_-. \quad (2.9b)$$

It is our next aim to solve Eqs. (2.9a) and (2.9b) for \underline{B}_+ and \underline{B}_- . The reader who is not interested in technical details of the construction of the solution may skip the following paragraphs and may find the result in Eqs. (2.10), (I-4.3), (I-4.8), (I-4.13), (I-4.14), (2.13), (2.15), (2.17), (2.19b), (2.25), (2.30), (2.35), (2.36), (2.40), and (2.41). Unfortunately, for the general result it is not feasible to condense this chain of equations into one single expression. We shall discuss simple expressions for particular stationary quantities in the following sections.

The inhomogeneity in Eq. (2.9a) consists of half the sum of two equilibrium diffusion matrices at temperatures β_1^{-1} and β_N^{-1} , cf. Eq. (I-4.2). Consequently, \underline{B}_+ is given by the respective linear combination of equilibrium covariance matrices at β_1^{-1} and β_N^{-1} ,

$$\underline{B}_+ = \frac{1}{2} [\underline{B}_{\text{eq}}(\beta_1) + \underline{B}_{\text{eq}}(\beta_N)] . \quad (2.10)$$

In Eq. (I-4.3), $\underline{B}_{\text{eq}}$ was conveniently decomposed into a weak-coupling contribution $\underline{B}'_{\text{eq}}$ and a correction $\underline{B}''_{\text{eq}}$,

$$\underline{B}_{\text{eq}} = \underline{B}'_{\text{eq}} + \underline{B}''_{\text{eq}} , \quad (2.11)$$

where $\underline{B}'_{\text{eq}}$ and $\underline{B}''_{\text{eq}}$ are the respective solutions of

$$\underline{A} \cdot \underline{B}'_{\text{eq}} + \underline{B}'_{\text{eq}} \cdot \underline{A}^t = \sum_{m=1}^N D'^{\text{pp}}(m, \beta) \underline{S}_1(m) , \quad (2.12a)$$

$$\underline{A} \cdot \underline{B}''_{\text{eq}} + \underline{B}''_{\text{eq}} \cdot \underline{A}^t = \sum_{m=1}^N D^{\text{xp}}(m, \beta) \underline{S}_2(m) . \quad (2.12b)$$

An analogous decomposition applies to \underline{B}_- as well,

$$\begin{aligned} \underline{B}_- &= \underline{B}'_- + \underline{B}''_- \\ &= \begin{bmatrix} \underline{x}'_- & \underline{z}'_- \\ \underline{z}'^t_- & \underline{y}'_- \end{bmatrix} + \begin{bmatrix} \underline{x}''_- & \underline{z}''_- \\ \underline{z}''^t_- & \underline{y}''_- \end{bmatrix} \\ &= \begin{bmatrix} \langle \{x_k, x_l\}'_- \rangle & \langle \{x_k, p_l\}'_- \rangle \\ \langle \{p_k, x_l\}'_- \rangle & \langle \{p_k, p_l\}'_- \rangle \end{bmatrix} \\ &\quad + \begin{bmatrix} \langle \{x_k, x_l\}''_- \rangle & \langle \{x_k, p_l\}''_- \rangle \\ \langle \{p_k, x_l\}''_- \rangle & \langle \{p_k, p_l\}''_- \rangle \end{bmatrix} , \end{aligned} \quad (2.13)$$

where \underline{B}'_- and \underline{B}''_- are the respective solutions of

$$\begin{aligned} \underline{A} \cdot \underline{B}'_- + \underline{B}'_- \cdot \underline{A}^t &= \frac{1}{2} \sum_{m=1}^N [D'^{\text{pp}}(m, \beta_1) - D'^{\text{pp}}(m, \beta_N)] \\ &\quad \times \underline{T}_1(m) , \end{aligned} \quad (2.14a)$$

$$\begin{aligned} \underline{A} \cdot \underline{B}''_- + \underline{B}''_- \cdot \underline{A}^t &= \frac{1}{2} \sum_{m=1}^N [D^{\text{xp}}(m, \beta_1) - D^{\text{xp}}(m, \beta_N)] \\ &\quad \times \underline{T}_2(m) . \end{aligned} \quad (2.14b)$$

First, we determine \underline{B}'_- . For this purpose we observe that \underline{B}'_- may be represented as

$$\underline{B}'_- = \frac{1}{2} \sum_{m=1}^D [D'^{\text{pp}}(m, \beta_1) - D'^{\text{pp}}(m, \beta_N)] \underline{U}(m) , \quad (2.15)$$

where $\underline{U}(m)$ is the unique solution of

$$\underline{A} \cdot \underline{U}(m) + \underline{U}(m) \cdot \underline{A}^t = \underline{T}_1(m) . \quad (2.16)$$

According to Eq. (2.13), we write $\underline{U}(m)$ in block form,

$$\underline{U}(m) = \begin{bmatrix} \underline{u}_1(m) & \underline{u}_2(m) \\ \underline{u}_2^t(m) & \underline{u}_3(m) \end{bmatrix} . \quad (2.17)$$

Because $\underline{T}_1(m)$ is symmetrical, $\underline{u}_1(m)$ and $\underline{u}_3(m)$ are symmetrical too,

$$\underline{u}_1^t(m) = \underline{u}_1(m), \quad \underline{u}_3^t(m) = \underline{u}_3(m) , \quad (2.18)$$

whereas the “off-diagonal” terms in Eq. (2.17) are symmetrical by construction. Inserting Eq. (2.17) into Eq. (2.16) and using Eqs. (I-3.24), we obtain the following set of coupled matrix equations:

$$\underline{u}_2(m) + \underline{u}_2^t(m) = \underline{0} , \quad (2.19a)$$

$$-\underline{u}_3(m) + \underline{u}_1(m) \cdot \underline{g} + \gamma \underline{u}_2(m) \cdot \underline{r} = \underline{0} , \quad (2.19b)$$

$$-\underline{u}_3(m) + \underline{g} \cdot \underline{u}_1(m) + \gamma \underline{r} \cdot \underline{u}_2^t(m) = \underline{0} , \quad (2.19c)$$

$$\underline{g} \cdot \underline{u}_2(m) + \underline{u}_2^t(m) \cdot \underline{g} + \gamma [\underline{r} \cdot \underline{u}_3(m) + \underline{u}_3(m) \cdot \underline{r}] = \underline{t}_1(m) . \quad (2.19d)$$

Obviously Eq. (2.19b) is the transpose of Eq. (2.19c). From Eq. (2.19a) we infer the antisymmetry of $\underline{u}_2(m)$,

$$\underline{u}_2^t(m) = -\underline{u}_2(m) . \quad (2.20)$$

This is substituted into Eqs. (2.19c) and (2.19d). Next, we subtract Eq. (2.19b) from Eq. (2.19c),

$$\underline{g} \cdot \underline{u}_1(m) - \underline{u}_1(m) \cdot \underline{g} = \gamma [\underline{r} \cdot \underline{u}_2(m) + \underline{u}_2(m) \cdot \underline{r}] . \quad (2.21)$$

Equation (2.19d) now reads

$$\underline{g} \cdot \underline{u}_2(m) - \underline{u}_2(m) \cdot \underline{g} = \underline{t}_1(m) - \gamma [\underline{r} \cdot \underline{u}_3(m) + \underline{u}_3(m) \cdot \underline{r}] . \quad (2.22)$$

The right-hand side of Eq. (2.22) is a bordered matrix, that is, it has nonvanishing elements in the first and last rows and columns only,

$$\begin{aligned}
& [\underline{t}_1(m) - \gamma \underline{r} \cdot \underline{u}_3(m) - \gamma \underline{u}_3(m) \cdot \underline{r}]_{kl} \\
&= \delta_{mk} \delta_{1l} + \delta_{1k} \delta_{ml} - \delta_{N+1-m,k} \delta_{Nl} - \delta_{Nk} \delta_{N+1-m,l} \\
&+ \gamma \{ \delta_{1k} [\underline{u}_3(m)]_{1l} + \delta_{1l} [\underline{u}_3(m)]_{1k} \\
&+ \delta_{Nk} [\underline{u}_3(m)]_{Nl} + \delta_{Nl} [\underline{u}_3(m)]_{Nk} \} . \quad (2.23)
\end{aligned}$$

Under the condition that $\underline{u}_3(m)$ is antisymmetrical with respect to the reflection about the middle of the chain, i.e.,

$$[\underline{u}_3(m)]_{1k} = -[\underline{u}_3(m)]_{N+1-k,N} . \quad (2.24)$$

the solution of Eq. (2.22) is an antisymmetric Toeplitz matrix, see Appendix A,

$$[\underline{u}_2(m)]_{ij} = \begin{cases} -\phi_{i-j}, & i > j \\ 0, & i = j \\ \phi_{i-j}, & i < j \end{cases} \quad (2.25)$$

where the quantities ϕ_i depend on the label m , $\phi_i = \phi_i(m)$. As shown in Appendix A, the quantities $\phi_i(m)$, $i = 1, 2, \dots, N-1$, are given by

$$\phi_1(m) = \frac{1}{2} [\underline{t}_1(m) - \gamma \underline{r} \cdot \underline{u}_3(m) - \gamma \underline{u}_3(m) \cdot \underline{r}]_{11} , \quad (2.26a)$$

$$\begin{aligned}
\phi_i(m) &= [\underline{t}_1(m) - \gamma \underline{r} \cdot \underline{u}_3(m) - \gamma \underline{u}_3(m) \cdot \underline{r}]_{1i} , \\
& i = 2, 3, \dots, N-1 . \quad (2.26b)
\end{aligned}$$

Using Eq. (2.23), we easily obtain

$$\phi_i(m) = \delta_{im} - \gamma [\underline{u}_3(m)]_{1i}, \quad i = 1, 2, \dots, N-1 . \quad (2.27)$$

With Eq. (2.25), for the inhomogeneity in Eq. (2.21) we find the expression

$$\begin{aligned}
& \gamma [\underline{r} \cdot \underline{u}_2(m) + \underline{u}_2(m) \cdot \underline{r}]_{kl} \\
&= \gamma [\delta_{1k} \phi_{l-1}(m) - \delta_{1l} \phi_{k-1}(m) \\
&+ \delta_{Nk} \phi_{N+1-l}(m) - \delta_{Nl} \phi_{N+1-k}(m)] , \quad (2.28)
\end{aligned}$$

where we defined

$$\phi_0(m) = \phi_N(m) = 0 . \quad (2.29)$$

Hence the right-hand side of Eq. (2.21) is antisymmetrical with respect to the reflection along the diagonal and symmetrical with respect to the reflection along the crossdiagonal. In Appendix B, we show that one solution of Eq. (2.21) is an antisymmetric Hankel matrix, i.e.,

$$[\underline{u}_1(m)]_{ij} = \begin{cases} \psi_{i+j-1}, & i+j \leq N \\ 0, & i+j = N+1 \\ -\psi_{2N+1-i-j}, & i+j \geq N+2 \end{cases} \quad (2.30)$$

The quantities $\psi_i \equiv \psi_i(m)$, $i = 1, 2, \dots, N-1$, are determined by the inhomogeneity in Eq. (2.21),

$$\psi_i(m) = \gamma [\underline{r} \cdot \underline{u}_2(m) + \underline{u}_2(m) \cdot \underline{r}]_{1,i+1}, \quad i = 1, 2, \dots, N-2, \quad (2.31a)$$

$$\psi_{N-1}(m) = \frac{1}{2} \gamma [\underline{r} \cdot \underline{u}_2(m) + \underline{u}_2(m) \cdot \underline{r}]_{1N} . \quad (2.31b)$$

Using Eq. (2.28), we easily find

$$\psi_i(m) = \gamma \phi_i(m) . \quad (2.32)$$

The solution of Eq. (2.21) is, however, not unique. We could add to the solution (2.30) any symmetric matrix that commutes with \underline{g} . Because all eigenvalues of \underline{g} are nondegenerate, such a matrix must be a function of \underline{g} , $\underline{u}_1 = f(\underline{g})$. However, \underline{u}_1 must vanish as a consequence of the condition (2.24).

Up to now we expressed $\underline{u}_1(m)$ and $\underline{u}_2(m)$ in terms of the as yet unknown quantities $\phi_i(m)$, which depend on the elements of the first row of the matrix $\underline{u}_3(m)$. First we determine $\phi_i(m)$ by inserting Eqs. (2.25) and (2.30) into the first row of Eq. (2.19b). This yields

$$-\phi_{i-1}(m) + \left[2 + \frac{1}{\gamma^2} \right] \phi_i(m) - \phi_{i+1}(m) = \frac{1}{\gamma^2} \delta_{im} , \quad (2.33)$$

and Eq. (2.29) yields the boundary conditions,

$$\phi_0(m) = \phi_N(m) = 0 . \quad (2.34)$$

That is, $\phi_i(m)$ are the solutions of linear second-order difference equations. Using standard methods, we find in the limit $N \rightarrow \infty$,

$$\phi_i(m) = \frac{1}{2\gamma^2 \sinh(\delta)} (e^{-|i-m|\delta} - e^{-(i+m)\delta}) , \quad (2.35)$$

where the quantity δ is defined by

$$\frac{1}{\gamma} = 2 \sinh \left[\frac{\delta}{2} \right] . \quad (2.36)$$

Now with Eqs. (2.25) and (2.30) the matrices $\underline{u}_2(m)$ and $\underline{u}_1(m)$ follow immediately, and with Eq. (2.19b) the matrix $\underline{u}_3(m)$ follows. We note that this solution fulfills the symmetry relation Eq. (2.24), which we had to anticipate in order to obtain the solution of Eq. (2.22). Finally, with Eqs. (2.15), (2.17), (2.19b), (2.25), (2.30), (2.32), (2.35), and (2.36) the matrix \underline{B}_+ is completely determined.

\underline{B}'' can be obtained along the same lines as \underline{B}' . Analogously to Eq. (2.15), \underline{B}'' may be represented as

$$\underline{B}'' = \frac{1}{2} \sum_{m=1}^N [D^{xp}(m, \beta_1) - D^{xp}(m, \beta_N)] \underline{V}(m) , \quad (2.37)$$

where $\underline{V}(m)$, $m = 1, 2, \dots$, are the solutions of $\underline{A} \cdot \underline{V}(m) + \underline{V}(m) \cdot \underline{A}^t = \underline{T}_2(m)$ with $\underline{T}_2(m)$, $m = 1, 2, \dots$, as given by Eqs. (I-3.25a)–(I-3.25c). We find⁹

$$\underline{V}(m) = \begin{bmatrix} \underline{v}_1(m) & \underline{0} \\ \underline{0} & \underline{v}_3(m) \end{bmatrix} . \quad (2.38)$$

Here, $\underline{v}_1(m)$ and $\underline{v}_3(m)$ are antisymmetric Hankel matrices

$$\underline{v}_1(m) = \hat{h}(m-1) , \quad (2.39a)$$

$$\underline{v}_3(m) = -\hat{h}(m-2) + 2\hat{h}(m-1) - \hat{h}(m) , \quad (2.39b)$$

where

$$[\hat{h}(m)]_{kl} = \delta_{k+l, m+1} - \delta_{2(N+1)-k-l, m+1} , \quad (2.40)$$

and where we defined $\underline{h}(m) = \underline{0}$ for $m \leq 0$. That is, the matrices $\hat{\underline{h}}(m)$ have nonvanishing matrix elements on the $(N-m)$ th cocrossdiagonals only. Inserting Eqs. (2.39) into Eq. (2.37), we obtain

$$\underline{x}'' = \frac{1}{2} \sum_{m=1}^N [D^{xp}(m+1, \beta_1) - D^{xp}(m+1, \beta_N)] \hat{\underline{h}}(m), \quad (2.41a)$$

$$\begin{aligned} \underline{y}'' = \frac{1}{2} \sum_{m=1}^N \{ & -[D^{xp}(m+2, \beta_1) - D^{xp}(m+2, \beta_N)] \\ & + 2[D^{xp}(m+1, \beta_1) - D^{xp}(m+1, \beta_N)] \\ & - [D^{xp}(m, \beta_1) - D^{xp}(m, \beta_N)] \} \hat{\underline{h}}(m), \end{aligned} \quad (2.41b)$$

$$\underline{z}'' = \underline{0}. \quad (2.41c)$$

The decomposition of the equilibrium covariance matrix into a part depending on $D'^{pp}(m, \beta)$, $m = 1, 2, \dots$, and another one depending on $D^{xp}(m, \beta)$, $m = 1, 2, \dots$, corresponds to a decomposition into a bulk contribution and boundary layers at both ends of the chain. These boundary layers follow from the matrices \underline{x}''_{eq} and \underline{y}''_{eq} being of Hankel type and the decrease in magnitude of the quantities $D^{xp}(m, \beta)$ with increasing label m ; cf. Eqs. (I-C10)–(I-C13). While the quantities $D'^{pp}(m, \beta)$ decrease similarly as $D^{xp}(m, \beta)$, their contributions to \underline{x}''_{eq} and \underline{y}''_{eq}

are appreciable in the whole chain because these matrices have parts which are of Toeplitz type; cf. Eqs. (I-4.9) and (I-4.10a).

It is interesting that in the nonequilibrium state, an analogous decomposition emerges. The differences $[D^{xp}(m, \beta_1) - D^{xp}(m, \beta_N)]$, $m = 1, 2, \dots$, determine boundary layers in the covariance of displacement and momentum operators $\langle x_k x_l \rangle_-$ and $\langle p_k p_l \rangle_-$, while they do not contribute to the mixed moments $\langle \{x_k, p_l\} \rangle_-$. These latter moments are completely determined by the differences $[D'^{pp}(m, \beta_1) - D'^{pp}(m, \beta_N)]$, $m = 1, 2, \dots$, which govern also the moments $\langle x_k x_l \rangle_-$ and $\langle p_k p_l \rangle_-$ far from the ends of the chain. Hence the covariance matrix \underline{B} may conveniently be decomposed into a bulk and a boundary layer contribution

$$\underline{B} = \underline{B}' + \underline{B}'', \quad (2.42)$$

where \underline{B}' and \underline{B}'' are defined by, cf. Eqs. (I-4.1), (I-4.3), (2.8), (2.13), and (2.41c),

$$\underline{B}' = \underline{B}'_+ + \underline{B}'_- = \begin{bmatrix} \underline{x}'_+ + \underline{x}'_- & \underline{z}' \\ \underline{z}'^t & \underline{y}'_+ + \underline{y}'_- \end{bmatrix}, \quad (2.43a)$$

$$\underline{B}'' = \underline{B}''_+ + \underline{B}''_- = \begin{bmatrix} \underline{x}''_+ + \underline{x}''_- & \underline{0} \\ \underline{0} & \underline{y}''_+ + \underline{y}''_- \end{bmatrix}. \quad (2.43b)$$

The boundary layers have a particular simple form. Using Eqs. (I-4.13), (I-4.14), (2.40), and (2.41) we find

$$\begin{aligned} \underline{x}'' &= \underline{x}''_+ + \underline{x}''_- \\ &= \sum_{m=1}^N D^{xp}(m+1, \beta_1) \underline{i}(m) + \sum_{m=1}^N D^{xp}(m+1, \beta_N) \hat{\underline{i}}(m), \end{aligned} \quad (2.44a)$$

$$\begin{aligned} \underline{y}'' &= \underline{y}''_+ + \underline{y}''_- \\ &= \sum_{m=1}^N [-D^{xp}(m+2, \beta_1) + 2D^{xp}(m+1, \beta_1) - D^{xp}(m, \beta_1)] \underline{i}(m) \\ &\quad + \sum_{m=1}^N [-D^{xp}(m+2, \beta_N) + 2D^{xp}(m+1, \beta_N) - D^{xp}(m, \beta_N)] \hat{\underline{i}}(m), \end{aligned} \quad (2.44b)$$

where the matrices $\underline{i}(m)$ and $\hat{\underline{i}}(m)$, $m = 1, 2, \dots$, have nonvanishing elements only in their upper and lower $(N-m)$ th cocrossdiagonals, respectively,

$$[\underline{i}(m)]_{kl} \equiv \frac{1}{2} [\underline{h}(m) + \hat{\underline{h}}(m)]_{kl} = \delta_{k+1, m+1}, \quad (2.45a)$$

$$[\hat{\underline{i}}(m)]_{kl} \equiv \frac{1}{2} [\underline{h}(m) - \hat{\underline{h}}(m)]_{kl} = \delta_{2(N+1)-k-l, m+1}. \quad (2.45b)$$

It follows that in the nonequilibrium state, the boundary layer on each side is the same as in the equilibrium situation in which both heat baths were at the corresponding temperature. More specifically, all divergencies in nonequilibrium states are already present in equilibrium states, i.e., the diverging moments are

$$\langle p_i^2 \rangle \simeq \gamma \frac{\hbar}{\pi} \ln \left[\frac{\hbar \beta_i}{2\pi} \Omega_D \right], \quad i = 1, N, \quad (2.46)$$

while all other moments remain finite in the limit $\Omega_D \rightarrow \infty$.

III. HEAT FLUX

The heat flux across a plane separating the $(i-1)$ st particle from the i th particle is proportional to the work done on the i th particle by its left neighbor,

$$(j_{ph})_{i-1,i} = \frac{\omega_D^2}{4} \langle \{ (x_{i-1} - x_i), p_i \} \rangle = \frac{\omega_D^2}{4} \langle x_{i-1} p_i \rangle \quad (3.1)$$

(the subscript ph denotes that the parameter to which it is affixed has the correct physical dimensions). We define a dimensionless heat flux by $j = 4j_{ph}/\omega_D^2$. From Eqs. (2.15), (2.17), (2.25), (2.37), and (2.38) we find that the heat flux is constant along the chain $j_{i-1,i} = j$. The constancy of the heat flux was to be expected because the

sources and sinks of heat are placed at the ends of the chain. Using the quantum Langevin equations (I-2.8), we relate the heat flux to the work done by the fluctuating forces on both particles at the ends,

$$j = \lim_{t \rightarrow \infty} \langle \{E_1(t), p_1(t)\} \rangle - \gamma \langle p_1^2 \rangle \\ = - \left[\lim_{t \rightarrow \infty} \langle \{E_N(t), p_N(t)\} \rangle - \gamma \langle p_N^2 \rangle \right]. \quad (3.2)$$

In accordance with the discussion given in Sec. II, the heat flux is completely determined by the quantities $D'^{pp}(m, \beta)$, $m = 1, 2, \dots$,

$$j = \frac{1}{2} \sum_{m=1}^N [D'^{pp}(m, \beta_1) - D'^{pp}(m, \beta_N)] \phi_1(m). \quad (3.3)$$

Here, $\phi_1(m)$ are elements of Toeplitz matrices which read in the limit $N \rightarrow \infty$, cf. Eq. (2.35),

$$\phi_1(m) = \frac{1}{\gamma^2} e^{-m\delta}, \quad (3.4)$$

where δ is related to the damping constant by Eq. (2.36). Similarly, in Appendix A of I, we computed the quantities $D'^{pp}(m, \beta)$, $m = 1, 2, \dots$, in the thermodynamic limit. Hence, in Eq. (3.3), we can set the upper limit of summation equal to infinity,

$$j = \frac{1}{2\gamma^2} \sum_{m=1}^{\infty} [D'^{pp}(m, \beta_1) - D'^{pp}(m, \beta_N)] e^{-m\delta}. \quad (3.5)$$

Thus the heat flux through the chain is finite as the length of the chain goes to infinity, and we recover the well-known fact that the thermal conductivity of the perfect harmonic chain is infinite.

The heat flux may be decomposed into two contributions stemming from the contributions of the different heat baths,

$$j = \tilde{j}(\beta_1) - \tilde{j}(\beta_N), \quad (3.6)$$

where

$$\tilde{j}(\beta) = \frac{1}{2\gamma^2} \sum_{m=1}^{\infty} D'^{pp}(m, \beta) e^{-m\delta}. \quad (3.7)$$

Using Eqs. (2.7a), (I-A13) and (I-A14), it is readily shown that

$$\tilde{j}(\beta) = \frac{e^{-\delta}}{\gamma} \frac{1}{\beta} \left[\frac{1}{2} + 2 \sum_{n=1}^{\infty} e^{-\alpha_n} - \sum_{n=1}^{\infty} e^{-2\alpha_n} \right] \\ - \frac{e^{-2\delta}}{\gamma} \frac{1}{\beta} \sum_{n=1}^{\infty} 4 \sinh^2 \left(\frac{\alpha_n}{2} \right) \frac{e^{-2\alpha_n}}{1 - e^{-(\alpha_n + \delta)}}, \quad (3.8)$$

where the quantities α_n are related to the Matsubara frequencies,

$$\nu_n = \frac{2\pi}{\hbar\beta} n = 2 \sinh \left(\frac{\alpha_n}{2} \right). \quad (3.9)$$

In general, one cannot analytically evaluate these sums. A numerical computation shows that for arbitrary damping constants, $\tilde{j}(\beta)$ is a monotonically decreasing function of β , cf. Fig. 1,

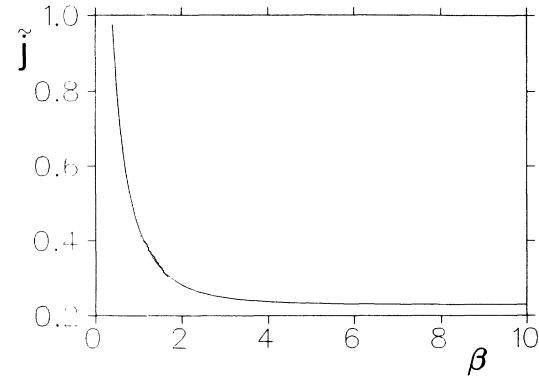


FIG. 1. Partial contributions of one heat baths at inverse temperature β to the heat flux as a function of β for $\gamma=1$ and $\hbar=1$.

$$\tilde{j}(\beta) > \tilde{j}(\bar{\beta}), \quad \beta < \bar{\beta}. \quad (3.10)$$

This inequality ensures that heat flows from the hotter to the colder end of the chain, as it should be.

For very high temperatures $\hbar\beta \rightarrow 0$, $\tilde{j}(\beta)$ approaches its classical value ($\beta^{-1} = T$),

$$\lim_{\hbar\beta \rightarrow 0} \tilde{j}(\beta) = \rho(\gamma) T, \quad (3.11)$$

where

$$\rho(\gamma) = \frac{e^{-\delta}}{\gamma}, \quad (3.12)$$

so that then the dependence on the temperature and damping constant factorizes. Although this is no longer true in the quantal case, the numerical evaluation of the sums clearly indicates that the dominant dependence on the damping constant is still determined by the same prefactor $\rho(\gamma)$; cf. Fig. 2. At constant temperature, $\rho^{-1}\tilde{j}$ decreases smoothly as the damping constant increases. Figure 2 shows further that this decrease is not uniform over the whole temperature range but becomes smaller as the

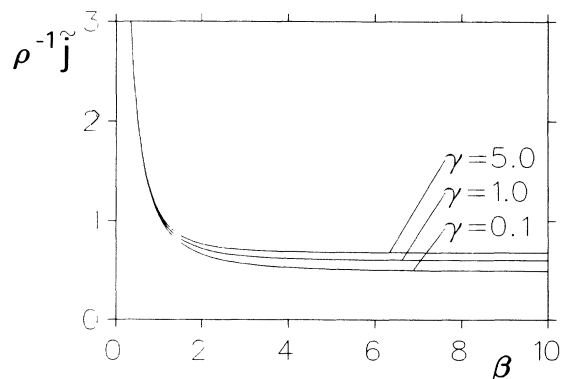


FIG. 2. Partial contribution of one heat bath to the heat flux divided by its classical damping dependence as a function of β for three different values of the damping constant and $\hbar=1$.

temperature is increased and vanishes in the classical limit. In the zero-temperature limit $\hbar\beta \rightarrow \infty$, $\tilde{j}(\beta)$ approaches a finite value $\tilde{j}(\infty)$. This property is due to quantal fluctuations which are present even in the absence of thermal excitations. In this respect, quantal fluctuations mimic a finite temperature T_{\hbar} , which we define by

$$\tilde{j}(\infty) = \rho(\gamma) T_{\hbar}. \quad (3.13)$$

T_{\hbar} depends weakly on the damping constant. From Eq. (3.8), with reasoning similar to that in Appendix C of I, we find

$$T_{\hbar} = \frac{32}{15\pi} \hbar, \quad \gamma \rightarrow 0, \quad (3.14a)$$

$$T_{\hbar} = \frac{4}{3\pi} \hbar, \quad \gamma \rightarrow \infty. \quad (3.14b)$$

From Eqs. (3.12) and (2.36), we easily find the asymptotic behavior of the prefactor $\rho(\gamma)$,

$$\rho(\gamma) \sim \gamma, \quad \gamma \rightarrow 0, \quad (3.15a)$$

$$\rho(\gamma) \sim \frac{1}{\gamma}, \quad \gamma \rightarrow \infty. \quad (3.15b)$$

At $\gamma = \sqrt{3}/2$, $\rho(\gamma)$ has a maximum; cf. Fig. 3. That is, in both the weak-, and strong-coupling limits the energy transfer between heat baths and harmonic chains goes to zero. The strong-coupling limit reminds us of properties of a highly absorbing dielectric medium which, according to the Kramers-Kronig dispersion relations, is highly reflecting as well.

Because the dependence of the heat flux on the damping constant is already almost entirely described by the prefactor $\rho(\gamma)$, we restrict the discussion of the temperature dependence of the heat flux to small damping constants $\gamma \ll 1$.

(i) *Both heat baths at high temperature.* For temperatures much above the Debye temperature $T_i \gg \Theta_D$, $i = 1, N$, we find

$$j_{cl} = \gamma(T_1 - T_N), \quad (3.16)$$

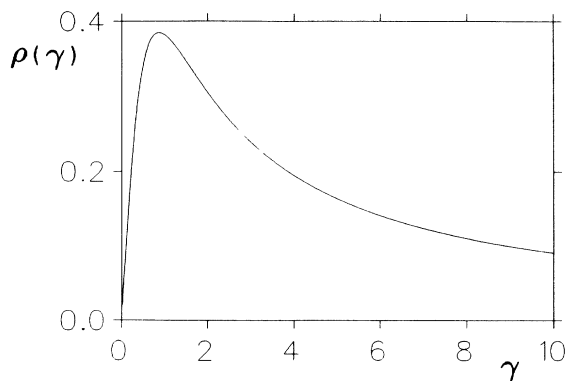


FIG. 3. Dependence of the partial contribution of one heat bath at $T=1$ to the classical heat flux as a function of the damping constant.

which agrees with the finding of Rieder, Lebowitz, and Lieb.³ Hence the heat flux through the classical perfect harmonic chain is proportional to the difference of the temperatures of the heat baths $T_1 - T_N$ and not to the gradient $(T_1 - T_N)/N$.

(ii) *One heat bath at high and the other at low temperature.* For, say, $T_1 \gg \Theta_D$ and $T_N \ll \Theta_D$, an asymptotic analysis reads

$$j = \gamma[T_1 - T_{\hbar}(\gamma \rightarrow 0)], \quad (3.17)$$

with $T_{\hbar}(\gamma \rightarrow 0)$ as given in Eq. (3.14a). That is, quantum-mechanical fluctuations induced by the heat bath at the lower temperature reduce the heat flux by a constant amount.

(iii) *Both heat baths at low temperatures.* We assume $T_i < \Theta_D/(10\pi)$. For a small temperature difference, we find in leading order

$$j_{qm} = \frac{1}{2} \left[\frac{4\pi\bar{T}}{\Theta_D} \right]^3 j_{cl}, \quad (3.18)$$

where $\bar{T} = (T_1 + T_N)/2$ is the average temperature and j_{cl} is the classical heat flux; cf. Eq. (3.16). Thus in the quantal case, the heat flux is strongly reduced compared with its classical value.

IV. COVARIANCE OF DISPLACEMENT OPERATORS

First we shall briefly recall the main results for the square of the difference of displacement operators $\sigma(k, l) = \langle (x_k - x_l)^2 \rangle$ in thermal equilibrium (cf. Sec. IV of I). In the classical case, $\sigma_{eq}(k, l)$ is independent of the damping constant and grows linear with the separation $|k - l|$, cf. Eq. (I-4.22),

$$\sigma_{eq}(k, l) \simeq |k - l|T, \quad \hbar \rightarrow 0. \quad (4.1)$$

In the quantum regime, the quantity $\sigma_{eq}(k, l)$ depends on the damping constant inside boundary layers of thickness $\hbar\beta/\pi$ at both ends of the chain. Outside these boundary layers, i.e., for $\hbar\beta/\pi < k, l < N - \hbar\beta/\pi$, we find two different regimes defined by the separation $|k - l|$, cf. Eqs. (I-4.23),

$$\sigma_{eq}(k, l) \simeq \begin{cases} \frac{\hbar}{\pi} [\ln(|k - l|) + 2], & |k - l| \leq \frac{\hbar\beta}{\pi}, \\ |k - l|T + \frac{\hbar}{\pi} \left[\ln \left[\frac{\hbar\beta}{\pi} \right] + 1 \right], & |k - l| \geq \frac{\hbar\beta}{\pi}. \end{cases} \quad (4.2a)$$

$$\sigma_{eq}(k, l) \simeq \begin{cases} \frac{\hbar}{\pi} [\ln(|k - l|) + 2], & |k - l| \leq \frac{\hbar\beta}{\pi}, \\ |k - l|T + \frac{\hbar}{\pi} \left[\ln \left[\frac{\hbar\beta}{\pi} \right] + 1 \right], & |k - l| \geq \frac{\hbar\beta}{\pi}. \end{cases} \quad (4.2b)$$

According to Eq. (2.10), the part $\sigma_+(k, l)$ of $\sigma(k, l)$ that transforms evenly under the exchange of the heat baths is determined by its equilibrium expressions,

$$\sigma_+(k, l) = \frac{1}{2} [\sigma_{eq}(k, l)|_{\beta_1} + \sigma_{eq}(k, l)|_{\beta_N}]. \quad (4.3)$$

Hence the oddly transforming part $\sigma_-(k, l)$ remains to be determined.

Because $\underline{x}_- = \underline{x}'_- + \underline{x}''_-$ is antisymmetrical with respect to the reflection about the middle of the chain, cf. Eqs. (2.13), (2.15), (2.17), (2.30), (2.40), and (2.41a), k and l may be restricted to $k, l < N/2$. Together with Eqs. (2.32) we obtain

$$\langle x_k x_l \rangle_- = \frac{\gamma}{2} \sum_{m=1}^{\infty} [D'^{pp}(m, \beta_1) - D'^{pp}(m, \beta_N)] \phi_{k+l-1}(m) + [D^{xp}(k+l, \beta_1) - D^{xp}(k+l, \beta_N)], \quad (4.4)$$

where the quantities $D'^{pp}(m, \beta)$ and $D^{xp}(m, \beta)$ are given by Eqs. (2.7a)–(2.7c) and $\phi_k(m)$ by Eqs. (2.35) and (2.36).

(i) *Classical limit.* If both heat baths are at very high temperatures $\hbar\beta_i \ll 1$, $i=1, N$, the only nonvanishing diffusion matrix element is $D'^{pp}(1, \beta) = \gamma T$; cf. Eqs. (I-3.16a) and (I-3.16b). In this case, from Eq. (4.4) we find

$$\sigma_-(k, l) = 2(T_1 - T_N) \sinh^2 \left[(k-l) \frac{\delta}{2} \right] e^{-(k+l-1)\delta}. \quad (4.5)$$

For small damping constants, $1/\gamma \simeq \exp(\delta/2) \gg 1$, we find in leading order

$$\sigma_-(k, l) = \frac{1}{2}(T_1 - T_N) \gamma^{4l-2}, \quad k > l. \quad (4.6)$$

That is, $\sigma_-(k, l)$ decreases exponentially with a rate determined by the smaller one of the two particles labeled k and l .

For large damping constants $1/\gamma \simeq \delta \ll 1$, we distinguish two cases. First, for $k+l < \gamma$, we set the exponential function in Eq. (4.5) equal to unity,

$$\sigma_-(k, l) = \frac{1}{2}(T_1 - T_N) \frac{(k-l)^2}{\gamma^2}, \quad k-l < \gamma. \quad (4.7)$$

For $k+l > \gamma$ we find

$$\sigma_-(k, l) = \frac{1}{2}(T_1 - T_N) \frac{(k-l)^2}{\gamma^2} e^{-(k+l-1)/\gamma}, \quad k-l < \gamma. \quad (4.8)$$

Hence, in the classical case, the quantity $\sigma_-(k, l)$ vanishes both in the weak- and strong-coupling limit.

(ii) *Quantal limit.* In this case, we assume that both heat baths are at very low temperatures $\hbar\beta_1, \hbar\beta_N \gg 1$. Consequently, the temperature difference is very small too. We investigate $\sigma_-(k, l)$ only outside the boundary layers, i.e., for $k, l > \hbar\beta_i/\pi$, so that the quantities $D^{xp}(m, \beta)$, $m=1, 2, \dots$ do not contribute to Eq. (4.4). We can analytically evaluate the series in Eq. (4.4) for small and large damping constants.

For small damping constants, from Eqs. (2.35) and (2.36) we have

$$\lim_{\gamma \rightarrow 0} \phi_k(m) = \delta_{km}. \quad (4.9)$$

Inserting Eq. (4.9) into Eq. (4.4) and using the low-temperature approximation of Appendix C of I, we find

$$\sigma_-(k, l) \simeq \begin{cases} -32\gamma^2 \frac{\hbar}{\pi} (k-l)^2 \left[\left[\frac{\pi}{\hbar\beta_1} \right]^5 \exp \left[-\frac{2\pi(k+l)}{\hbar\beta_1} \right] - \left[\frac{\pi}{\hbar\beta_N} \right]^5 \exp \left[-\frac{2\pi(k+l)}{\hbar\beta_N} \right] \right], & |k-l| < \frac{\hbar\beta_i}{\pi} \\ -8\gamma^2 \frac{\hbar}{\pi} \left[\left[\frac{\pi}{\hbar\beta_i} \right]^3 \exp \left[-\frac{4\pi}{\hbar\beta_1} l \right] - \left[\frac{\pi}{\hbar\beta_N} \right]^3 \exp \left[-\frac{4\pi}{\hbar\beta_N} l \right] \right], & k-l > \frac{\hbar\beta_i}{\pi} \end{cases} \quad (4.10a)$$

$$\sigma_-(k, l) \simeq \begin{cases} -32\gamma^2 \frac{\hbar}{\pi} (k-l)^2 \left[\left[\frac{\pi}{\hbar\beta_1} \right]^5 \exp \left[-\frac{2\pi(k+l)}{\hbar\beta_1} \right] - \left[\frac{\pi}{\hbar\beta_N} \right]^5 \exp \left[-\frac{2\pi(k+l)}{\hbar\beta_N} \right] \right], & |k-l| < \frac{\hbar\beta_i}{\pi} \\ -8\gamma^2 \frac{\hbar}{\pi} \left[\left[\frac{\pi}{\hbar\beta_i} \right]^3 \exp \left[-\frac{4\pi}{\hbar\beta_1} l \right] - \left[\frac{\pi}{\hbar\beta_N} \right]^3 \exp \left[-\frac{4\pi}{\hbar\beta_N} l \right] \right], & k-l > \frac{\hbar\beta_i}{\pi} \end{cases} \quad (4.10b)$$

For large damping constants, from Eqs. (2.35) and (2.36) it is readily shown that

$$\phi_k(m) \simeq \frac{1}{\gamma^2} \times \begin{cases} m, & m \leq k \\ k, & m \geq k \end{cases}. \quad (4.11)$$

The quantity $\sigma_-(k, l)$ then has the same dependence on k and l as in Eqs. (4.10),

$$\sigma_-(k, l) \simeq \begin{cases} 8 \frac{\hbar}{\pi} (k-l)^2 \left[\left[\frac{\pi}{\hbar\beta_1} \right]^3 \exp \left[-\frac{2\pi(k+l)}{\hbar\beta_1} \right] - \left[\frac{\pi}{\hbar\beta_N} \right]^3 \exp \left[-\frac{2\pi(k+l)}{\hbar\beta_N} \right] \right], & |k-l| < \frac{\hbar\beta_i}{\pi} \\ 2 \frac{\hbar}{\pi} \left[\left[\frac{\pi}{\hbar\beta_i} \right] \exp \left[-\frac{4\pi}{\hbar\beta_1} l \right] - \left[\frac{\pi}{\hbar\beta_N} \right] \exp \left[-\frac{4\pi}{\hbar\beta_N} l \right] \right], & k-l > \frac{\hbar\beta_i}{\pi} \end{cases}, \quad (4.12a)$$

$$\sigma_-(k, l) \simeq \begin{cases} 8 \frac{\hbar}{\pi} (k-l)^2 \left[\left[\frac{\pi}{\hbar\beta_1} \right]^3 \exp \left[-\frac{2\pi(k+l)}{\hbar\beta_1} \right] - \left[\frac{\pi}{\hbar\beta_N} \right]^3 \exp \left[-\frac{2\pi(k+l)}{\hbar\beta_N} \right] \right], & |k-l| < \frac{\hbar\beta_i}{\pi} \\ 2 \frac{\hbar}{\pi} \left[\left[\frac{\pi}{\hbar\beta_i} \right] \exp \left[-\frac{4\pi}{\hbar\beta_1} l \right] - \left[\frac{\pi}{\hbar\beta_N} \right] \exp \left[-\frac{4\pi}{\hbar\beta_N} l \right] \right], & k-l > \frac{\hbar\beta_i}{\pi} \end{cases}. \quad (4.12b)$$

In any case we find only small corrections to the average thermal equilibrium contribution.

Finally, we come back to the discussion of the covariance matrix \underline{B} in the weak- and strong-coupling limit. In Sec. III, we showed that for all temperatures, the heat flux through the chain vanishes in the weak- as well as in the strong-coupling limit. From Eqs. (4.6), (4.7), and (4.8) we see that in both limits the classical chain is in the average thermal equilibrium state, for $\hbar \rightarrow 0$,

$$\lim_{\gamma \rightarrow 0} \underline{B} = \lim_{\gamma \rightarrow 0} \frac{1}{2} [\underline{B}_{\text{eq}}|_{\beta_1} + \underline{B}_{\text{eq}}|_{\beta_N}], \quad (4.13)$$

$$\lim_{\gamma \rightarrow \infty} \underline{B} = \lim_{\gamma \rightarrow \infty} \frac{1}{2} [\underline{B}_{\text{eq}}|_{\beta_1} + \underline{B}_{\text{eq}}|_{\beta_N}].$$

Strictly speaking, in the quantal case this is true only in the weak-coupling limit, cf. Eqs. (4.10), while in the strong-coupling limit \underline{B}_- approaches a finite value, cf. Eqs. (4.12), whose magnitude is infinitely small.

V. TEMPERATURE PROFILE

Even if both heat baths are at equal temperature $\beta_1 = \beta_N$, the kinetic energy of a particle varies with its position in the chain according to Eqs. (I-4.7b), (I-4.13b), and (I-4.14),

$$\begin{aligned} \langle p_k^2 \rangle \equiv \zeta_k(\beta) = & \frac{1}{\beta} + \frac{4}{\beta} \sum_{n=1}^{\infty} \tilde{\chi}_{kk}^0(i\nu_n) - \frac{2}{\beta} \sum_{n=1}^{\infty} \tilde{\chi}_{k,k+1}^0(i\nu_n) \\ & - \frac{2}{\beta} \sum_{n=1}^{\infty} \tilde{\chi}_{k,k-1}^0(i\nu_n) \\ & + [-D^{xp}(2k+1, \beta) + 2D^{xp}(2k, \beta) \\ & - D^{xp}(2k-1, \beta)] . \end{aligned} \quad (5.1)$$

We recall that these expressions are obtained for $k < N/2$ in the limit $N \rightarrow \infty$. Only in the classical limit this expression becomes k independent,

$$\begin{aligned} \langle p_k^2 \rangle = & \frac{1}{2} [\zeta_k(\beta_1) + \zeta_k(\beta_N)] + \frac{1}{2\gamma} [D'^{pp}(2k-1, \beta_1) - D'^{pp}(2k-1, \beta_N)] - \frac{1}{2\gamma} \sum_{m=1}^{\infty} [D'^{pp}(m, \beta_1) - D'^{pp}(m, \beta_N)] \phi_{2k-1}(m) \\ & + \frac{1}{2} \{ -[D^{xp}(2k+1, \beta_1) - D^{xp}(2k+1, \beta_N)] + 2[D^{xp}(2k, \beta) - D^{xp}(2k, \beta_N)] \\ & - [D^{xp}(2k-1, \beta_1) - D^{xp}(2k-1, \beta_N)] \} , \end{aligned} \quad (5.5)$$

where the $\phi_k(m)$'s are given by Eqs. (2.36) and (2.37).

An analytic result for the temperature profile can be obtained only in the high-temperature (classical) limit. In this case, the only nonvanishing element of the diffusion matrix is $D'^{pp}(1, \beta) = \gamma T$, cf. Eqs. (I-3.16), and thus from Eq. (2.5) we recover the result obtained by Rieder, Lebowitz, and Lieb,³

$$\langle p_1^2 \rangle \equiv T(1, \gamma) = T_1 - \frac{1}{2}(T_1 - T_N) \frac{1}{\gamma^2} e^{-\delta} , \quad (5.6a)$$

$$\begin{aligned} \langle p_k^2 \rangle \equiv T(k, \gamma) = & \frac{1}{2}(T_1 + T_N) - \frac{1}{2}(T_1 - T_N) \frac{1}{\gamma^2} e^{-(2k-1)\delta} , \\ & k = 2, 3, \dots, \frac{N}{2} . \end{aligned} \quad (5.6b)$$

This is a quite unexpected result because the kinetic temperature drops *below* the average temperature near the hotter end and raises *above* near the colder one. The kinetic temperature is constant in the middle of the chain and varies only over a length $l(\gamma)$ near the ends,

$$l(\gamma) = \frac{1}{2\delta} , \quad (5.7)$$

which approaches its limits as

$$l(\gamma) \sim \begin{cases} \frac{1}{4 \ln(1/\gamma)} , & \gamma \rightarrow 0 \\ \frac{1}{2}\gamma , & \gamma \rightarrow \infty . \end{cases} \quad (5.8)$$

In Figs. 4(a) and 4(b), the temperature profile is shown for a small ($\gamma = 0.1$) and a large ($\gamma = 10.0$) damping constant, respectively.

In the remaining temperature regimes, we choose typical pairs of temperature, namely $T_1 = 10.0$ and $T_N = 0.1$,

$$\lim_{\hbar \rightarrow 0} \langle p_k^2 \rangle = T . \quad (5.2)$$

It is easily checked numerically that for every fixed damping constant, $\langle p_k^2 \rangle$ decreases monotonically with temperature,

$$\langle p_k^2 \rangle|_{\beta} > \langle p_k^2 \rangle|_{\bar{\beta}} \quad \beta < \bar{\beta} . \quad (5.3)$$

In nonequilibrium states, this one-to-one correspondence can be used to define a local temperature at each site k ,

$$\beta_k = \zeta_k^{-1}(\langle p_k^2 \rangle) , \quad (5.4)$$

where $\langle p_k^2 \rangle$ is the second moment of momentum at the site k in the considered nonequilibrium state. We emphasize that in Eq. (5.4), the dependence on the particle label k comes about from both ζ_k and $\langle p_k^2 \rangle$. In the nonequilibrium state, from Eqs. (2.8), (2.10), (2.13), (2.15), (2.17), (2.19b), (2.25), (2.30), (2.32), and (2.41b) we find

and $T_1 = 0.1$ and $T_N = 0.02$, and determine numerically the temperature profile from Eqs. (5.4) and (5.5) for $\hbar = 1$. The results are represented in Figs. 4(c)–4(f).

For small damping constants, we see in Figs. 4(c) and 4(e) that quantal fluctuations enhance the temperature as we move from the middle of the chain towards its ends. The enhancement is smaller near the end which is coupled to the heat bath held at the higher temperature.

For large damping constants, the temperature profile has more structure. If the temperature of one heat bath is high while that of the other one is low, the temperature increases as we move from the middle of the chain towards the colder end while it starts to decrease towards the hotter one but increases for the second nearest particle from the end; cf. Fig. 4(d). If the temperatures of both heat baths are low, the temperature starts to increase towards both ends of the chain and drops near the colder end; cf. Fig. 4(f). As in the classical case, a deeper understanding of these strange findings is lacking. The definition of kinetic temperature has been ruled out as a possible reason by numerical computation in Refs. 10–12.

VI. SUMMARY AND CONCLUSIONS

In this paper, we investigated in detail stationary properties of a one-dimensional quantum-mechanical harmonic chain in a nonequilibrium state. We started from an algebraic equation for the matrix of the second moments which was derived in the preceding paper where primarily thermal equilibrium was considered.

In thermal equilibrium, in accordance with the predictions of equilibrium statistical mechanics, we find that

thermal properties of the particles outside boundary layers at both ends of the chain are completely determined by the Gibbs state of the free chain. Inside these boundary layers properties of the particles depend both on the temperature and coupling strength between the chain and heat baths.

For a stationary nonequilibrium state, the covariance matrix can be decomposed into contributions from the average thermal equilibrium and deviation thereof. Both contributions have parts which vanish well inside the chain. In thermal nonequilibrium, the boundary layer at each end is the same as in thermal equilibrium if both

heat baths were at the temperature of the heat bath at that side. The boundary layer contributions vanish in the classical limit. The deviations from the average thermal equilibrium state determine the moments $\langle x_{i-j} p_i \rangle$, $j=1,2,\dots$, which are constant along the chain. Most interesting is $\langle x_{i-1} p_i \rangle$, which is proportional to the heat flux through the chain. We find that the heat flux approaches a finite value as the length of the chain goes to infinity. That is, we recover the well-known fact that the thermal conductivity of a harmonic crystal is infinite. If both heat baths are at very low temperatures, the heat flux is strongly reduced compared with its classical value.

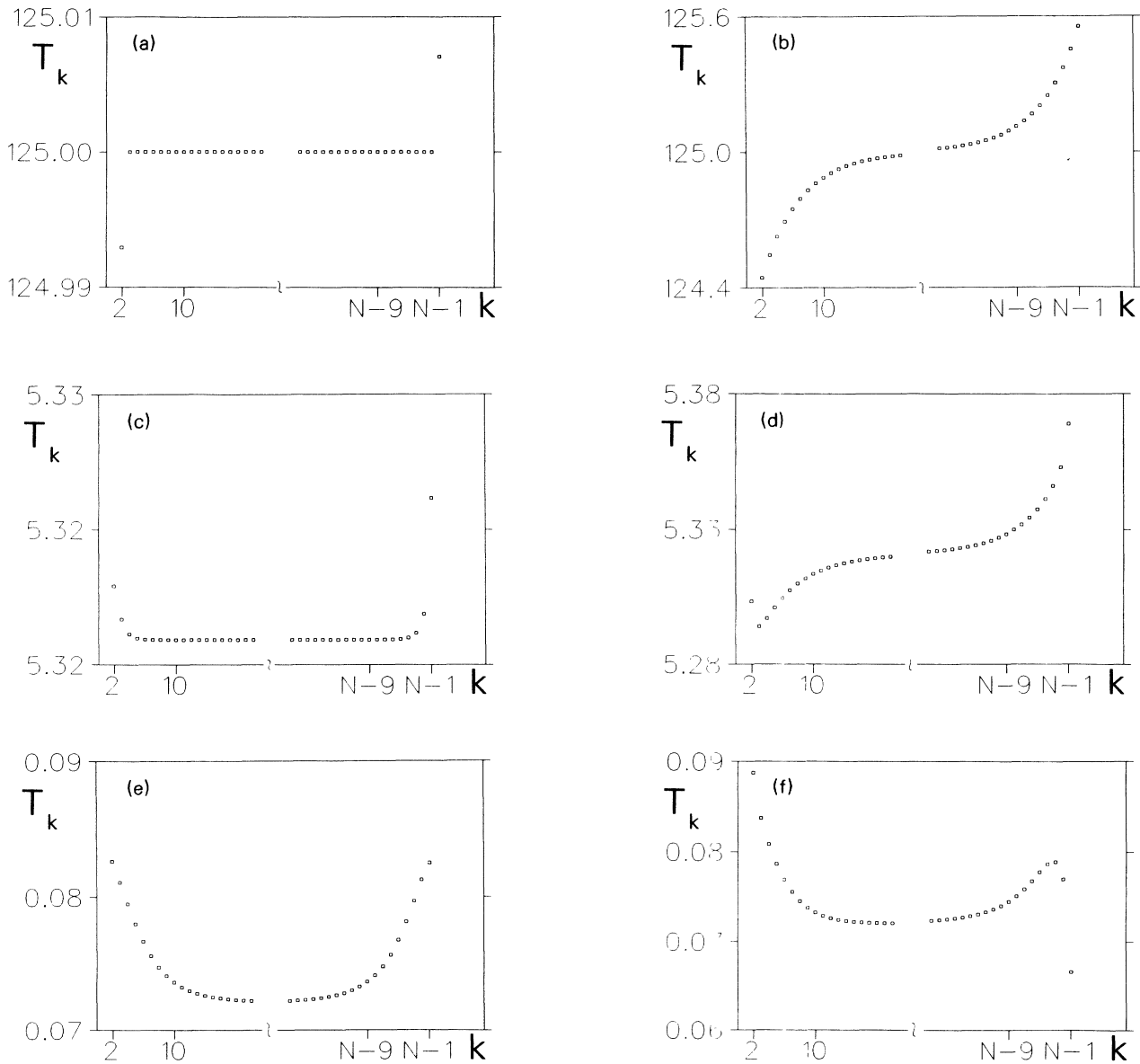


FIG. 4. Temperature profile along the chain for $\hbar=1$ for different values of the dimensionless temperatures and damping constant: (a) $T_1=200$, $T_N=50$, $\gamma=0.1$; (b) $T_1=200$, $T_N=50$, $\gamma=10.0$; (c) $T_1=10.0$, $T_N=0.1$, $\gamma=0.1$; (d) $T_1=10.0$, $T_N=0.1$, $\gamma=10.0$; (e) $T_1=0.1$, $T_N=0.02$, $\gamma=0.1$; (f) $T_1=0.1$, $T_N=0.02$, $\gamma=10.0$.

For large separation $|k-l|$, the mean square of the difference of displacement operators $\langle (x_k - x_l)^2 \rangle$ is determined by the contribution from the average thermal equilibrium state, $\langle (x_k - x_l)^2 \rangle \simeq \bar{T}|k-l|$, where $\bar{T} = \frac{1}{2}(T_1 + T_N)$ is the mean temperature of the heat baths. This absence of long-range order is common to all one-dimensional systems with short-range forces. Finally, for all temperatures, the mean kinetic energy defines a local temperature at all sites. If the temperatures of the two heat baths are different, we find in accordance with the infinite thermal conductivity that the temperature is constant inside the chain. That is, similar to the Kapitza resistance between dissimilar substances at low temperatures, the temperature varies only near the ends of the chain.

The deficiencies of the harmonic approximation are well known and for classical systems have been removed by different means. Most analytical work was done on isotopically disordered harmonic chains, i.e., chains with randomly varying mass of the particles. For fixed concentration of impurities, the thermal conductivity λ is investigated as a function of the length N of the chain. For a chain with fixed ends one finds $\lambda \propto N^{1/2}$ and for a chain with free ends $\lambda \propto N^{-1/2}$.^{13,14} The latter tells us that a disordered harmonic chain is a poorer heat conductor than ordinary bulk material. These results are in good agreement with numerical calculations.¹⁵ In chains with nonlinear interactions evidence for Fourier's law of heat conduction was found numerically in Refs. 10–12 and 16.

Neither in disordered nor in nonlinear quantum systems has the heat flux been investigated up to now. We expect that quantum-mechanical interference enhances the effect of disorder which might lead to a normal heat conductivity. It is therefore important to study in detail quantal versions of isotopically disordered harmonic chains. Generalizations to non-Ohmic heat baths with frequency-dependent damping and the treatment of finite-size effects are straightforward.

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APPENDIX A: TOEPLITZ MATRIX

We seek to find the solution of the matrix equation

$$\underline{g} \cdot \underline{x} - \underline{x} \cdot \underline{g} = \underline{b}, \quad (\text{A1})$$

where \underline{g} is the tridiagonal matrix

$$(g)_{ij} = -\delta_{i+1,j} + 2\delta_{ij} - \delta_{i-1,j}, \quad (\text{A2})$$

and where \underline{b} is a bordered matrix, i.e., it has nonvanishing elements only in the first and last rows and columns, which is symmetrical with respect to the reflection along the diagonal and antisymmetrical with respect to the reflection along the crossdiagonal,

$$(\underline{b})_{1n} = (\underline{b})_{n1}, \quad (\text{A3a})$$

$$(\underline{b})_{1n} = -(\underline{b})_{N+1-n,N}. \quad (\text{A3b})$$

Hence only $N-1$ quantities determine \underline{b} . Because we are looking for antisymmetric solutions,

$$\underline{x}' = -\underline{x}, \quad (\text{A4})$$

the solution \underline{x} of Eq. (A1) is uniquely defined.

In component form, the matrix equation (A1) reads $[(\underline{x})_{ij} = x_{ij}, (\underline{b})_{ij} = b_{ij}]$, we set

$$-x_{i-1,j} - x_{i+1,j} + x_{i,j+1} + x_{i,j-1} = b_{ij}. \quad (\text{A5})$$

Using the antisymmetry of \underline{x} , we find for $i=j$,

$$-2(x_{i-1,i} + x_{i+1,i}) = b_{ii}. \quad (\text{A6})$$

Hence, for $i=2, 3, \dots, N-1$,

$$x_{i+1,i} = -x_{i-1,i} = x_{i,i-1}, \quad (\text{A7})$$

i.e., the elements on the first codiagonal are identical. From Eq. (A5) we find for $i=1, N$,

$$x_{12} = \frac{1}{2}b_{11}, \quad (\text{A8a})$$

$$x_{N-1,N} = -\frac{1}{2}b_{NN}, \quad (\text{A8b})$$

which is in accordance with Eq. (A3b) because $(\underline{x})_{N-1,N} = -(\underline{x})_{12}$.

We proceed further by induction. We show that elements on the n th codiagonal are identical assuming that the same holds for the n' th codiagonal $n' < n$. Since it has been shown for the first one, the proof is then complete. That is, we assume

$$x_{i,i+n'} = x_{i-1,i-1+n'}, \quad n' < n. \quad (\text{A9})$$

We set $j=i+n-1$ in Eq. (A5) and obtain

$$\begin{aligned} &(-x_{i-1,i+n-1} + x_{i,i+n}) \\ &+ (-x_{i+1,i+1+(n-2)} + x_{i,i+1+(n-2)}) = b_{i,i+n-1}. \end{aligned} \quad (\text{A10})$$

For $i=2, 3, \dots, N-n-1$,

$$\begin{aligned} &(-x_{i-1,i+n-1} + x_{i,i+n}) \\ &+ (-x_{i+1,i+1+(n-2)} + x_{i,i+1+(n-2)}) = 0. \end{aligned} \quad (\text{A11})$$

Using Eq. (A9), we infer

$$x_{i-1,i-1+n} = x_{i,i+n}, \quad (\text{A12})$$

i.e., the elements on the n th codiagonal are identical. For $i=1, N+1-n$, we find

$$x_{1,1+n} = b_{1n}, \quad (\text{A13a})$$

$$x_{N-n,N} = b_{N+1-n,N}, \quad (\text{A13b})$$

which is again compatible with Eq. (A3b) because $x_{N-n,N} = -x_{N+1-n,N}$.

As a summary, we proved that the antisymmetric solution of (A1) is a Toeplitz matrix,

$$\underline{x} = \begin{bmatrix} 0 & \phi_1 & \phi_2 & \cdots & \cdots & \cdots & \cdots & \phi_{N-2} & \phi_{N-1} \\ -\phi_1 & 0 & \phi_1 & \phi_2 & \cdots & & & & \phi_{N-2} \\ -\phi_2 & -\phi_1 & 0 & \phi_1 & \phi_2 & & & & \\ \vdots & & & & & & & & \\ \vdots & & & & & & & & \\ & & & & & & -\phi_2 & -\phi_2 & 0 & \phi_1 & \phi_2 \\ -\phi_{N-2} & & & & & & -\phi_2 & -\phi_1 & 0 & \phi_1 \\ -\phi_{N-1} & -\phi_{N-2} & & & & & -\phi_2 & -\phi_1 & 0 \end{bmatrix}, \quad (\text{A14})$$

where its elements are given by the elements of the bordered matrix

$$\phi_1 = \frac{1}{2}b_{11}, \quad (\text{A15a})$$

$$\phi_i = b_{1i}, \quad 2 \leq i \leq N-1. \quad (\text{A15b})$$

APPENDIX B: HANKEL MATRIX

Again, we consider the matrix equation

$$\underline{g} \cdot \underline{x} - \underline{x} \cdot \underline{g} = \underline{b}, \quad (\text{B1})$$

where \underline{g} is the tridiagonal matrix as given in Eq. (A2) and where \underline{b} is now a bordered matrix which is antisymmetrical with respect to the reflection along the diagonal and symmetrical with respect to the reflection along the

crossdiagonal,

$$(\underline{b})_{1n} = -(\underline{b})_{n1}, \quad (\text{B2a})$$

$$(\underline{b})_{1n} = (\underline{b})_{N+1-n, N}. \quad (\text{B2b})$$

Hence $N-1$ quantities determine \underline{b} . Under the additional assumption that \underline{x} is symmetrical,

$$\underline{x}^t = \underline{x}, \quad (\text{B3})$$

it follows that \underline{x} is determined only up to an arbitrary function of \underline{g} ,

$$\underline{x}' = \underline{x} + f(\underline{g}). \quad (\text{B4})$$

Here, we verify that a particular solution \underline{x} is of Hankel type,

$$\underline{x} = \begin{bmatrix} \psi_1 & \psi_2 & \psi_3 & \cdots & \cdots & \psi_{N-1} & 0 \\ \psi_1 & \psi_3 & & & \psi_{N-1} & 0 & -\psi_{N-1} \\ \psi_3 & & & & & & \\ \vdots & & & & & & \\ \vdots & & & & & & \\ -\psi_{N-1} & 0 & -\psi_{N-1} & & & -\psi_3 & -\psi_2 \\ 0 & -\psi_{N-1} & & -\psi_3 & -\psi_2 & -\psi_1 \end{bmatrix}, \quad (\text{B5})$$

i.e., it has identical elements on the cocrossdiagonals.

The calculation is straightforward. In component form, the matrix equation (B1) reads $[(\underline{x})_{ij} = x_{ij}, (\underline{b})_{ij} = b_{ij}]$

$$-x_{i-1,j} - x_{i+1,j} + x_{i,j-1} + x_{i,j+1} = b_{ij}. \quad (\text{B6})$$

For $j = N+2-i-n$, we find

$$\begin{aligned} & (-x_{i-1, N+2-(i-1)-(n+1)} + x_{i, N+2-i-(n+1)}) \\ & + (-x_{i+1, N+2-(i+1)-(n-1)} + x_{i, N+2-i-(n-1)}) \\ & = b_{i, N+2-i-n}. \end{aligned} \quad (\text{B7})$$

We set $i = 2, 3, \dots, N-n$, and obtain

$$\begin{aligned} & (-x_{i-1, N+2-(i-1)-(n+1)} + x_{i, N+2-i-(n+1)}) \\ & + (-x_{i+1, N+2-(i+1)-(n-1)} + x_{i, N+2-i-(n-1)}) = 0. \end{aligned} \quad (\text{B8})$$

Both sets of parentheses vanish since they are differences of elements of the matrix x of the same cocrossdiagonal. Next, we set $i = 1$,

$$\begin{aligned} & x_{1, N+1-(n-1)} + (-x_{2, N-(n-1)} + x_{1, N+1-(n-1)}) \\ & = b_{1, N+1-n}. \end{aligned} \quad (\text{B9})$$

For $n = 2, 3, \dots, N-1$, we have

$$x_{1, N-n} = b_{1, N+1-n}. \quad (\text{B10})$$

Inserting the explicit form of the Hankel matrix \underline{x} , $\psi_n = (\underline{x})_{1, N+1-n}$, cf. Eq. (B5), we find

$$\psi_n = b_{1, n+1}, \quad n = 2, 3, \dots, N-1. \quad (\text{B11})$$

For $n = 1$ we have

$$x_{1, N-1} - x_{2N} = b_{1N}. \quad (\text{B12})$$

Using $x_{1n} = x_{N+1-n, N}$ we find

$$x_{1,N-1} = \frac{1}{2}b_{1N} . \quad (\text{B13})$$

It follows that

$$x_{N-1} = \frac{1}{2}b_{1N} . \quad (\text{B14})$$

Similarly, for $j = N - i + n$,

$$\begin{aligned} &(-x_{i-1,N-(i-1)+(n+1)} + x_{i,N-i+(n+1)}) \\ &+ (-x_{i+1,N-(i+1)+(n+1)} + x_{i,N-i+(n+1)}) = b_{i,N-i+n} . \end{aligned} \quad (\text{B15})$$

We set $i = n, n+1, \dots, N-1$,

$$\begin{aligned} &(-x_{i-1,N-(i-1)+(n+1)} + x_{i,N-i+(n+1)}) \\ &+ (-x_{i+1,N-(i+1)+(n+1)} + x_{i,N-i+(n+1)}) = 0 . \end{aligned} \quad (\text{B16})$$

As above, both sets of parentheses vanish. Next, we set $i = N$,

$$(-x_{N-1,n} + x_{N,n-1}) + x_{N,n+1} = b_{Nn} . \quad (\text{B17})$$

For $n = 2, 3, \dots, N-1$, we have

$$x_{N,n+1} = b_{Nn} . \quad (\text{B18})$$

Using Eq. (B5), we find

$$\psi_n = -b_{N,N-n}, \quad n = 2, 3, \dots, N-1 . \quad (\text{B19})$$

For $n = 1$,

$$x_{N,2} = \frac{1}{2}b_{N1} , \quad (\text{B20})$$

and it follows that

$$x_{N-1} = -\frac{1}{2}b_{N1} . \quad (\text{B21})$$

Note that Eqs. (B19) and (B21) are compatible with Eqs. (B11) and (B14), respectively, because \underline{b} is antisymmetrical with respect to the reflection along the crossdiagonal.

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