Heat and Mass Transfer 34 (1999) 453–459 © Springer-Verlag 1999

Hamiltonian description of the heat conduction

E. Magyari, B. Keller

Abstract It is shown that the linear boundary value problems of the heat conduction in a homogeneous slab can be mapped on the initial value problem for a Hamiltonian motion whose phase-space trajectories are subject to an additional restriction, the "arrival condition". The physical consequences of this formal analogy for the macroscopic heat conduction are discussed in detail.

List of symbols

a	thermal diffusivity
a_n	semiaxes of ellipses
b_n	semiaxes of ellipses
$\mathrm{Bi}_{1,2}$	Biot numbers
c	specific heat
d	slab-thickness
$g(x)$	initial temperature profile
H	Hamiltonian
$\mathbf{H}$	Hamiltonian matrix
I	transfer invariant
n	natural number
N_n	normalization
p	canonical momentum
$\mathbf{P}$	propagator
q	heat flux
t	time
x	position coordinate

Greek symbols

$\alpha_{1,2}$	heat transfer coefficients
δ	infinitesimal difference
δ_{mn}	Kronecker symbol
λ	thermal conductivity
ϕ	state-vector
ϑ	temperature field
θ	generalized coordinate
Ω	frequency; eigenvalue
τ	relaxation time

Subscripts

P	Poisson-bracket

Superscripts

n	eigenvalues, eigenstates
$\cdot$	t-derivative (dot)
$'$	x-derivative (dash)

Received on 27 April 1998

E. Magyari
B. Keller
Chair for the Physics of Buildings
Institute of Building Technology
Swiss Federal Institute of Technology (ETH) Zürich
Ch-8093 Zürich, Switzerland

Correspondence to: E. Magyari

1 Introduction

The Hamiltonian description developed originally for mechanical systems (Sir W. R. Hamilton, 1835) has become in the meantime one of the most powerful tools of theoretical physics, playing a central role in statistical and quantum mechanics, classical and quantum field theories, as well as in the contemporary theories of deterministic chaos in conservative dynamical systems (see e.g. [1]). In his celebrated work [2] Herbert Goldstein describes this outstanding role of Hamiltonian formulation with the words: "The equal status accorded to coordinates and momenta as independent variables encourages a greater freedom in selecting the physical quantities to be designated as "coordinates" and "momenta". As a result we are led to newer, more abstract ways of presenting the physical content of mechanics. While often of considerable help in practical applications to mechanical problems, these more abstract formulations are primarily of interest to us today because of their essential role in constructing the more modern theories of matter".

Our aim in the present paper is to point out, in agreement with Goldstein's remark, that the Hamiltonian formalism also allows (in addition to some computational advantages) a deeper insight in the abstract as well as in the physical content of the macroscopic heat conduction. For the sake of simplicity we restrict our arguments in this paper to the case of the one dimensional heat conduction in media with constant thermophysical properties.

2 Mapping the heat conduction on a Hamiltonian motion

The starting point of our considerations is the energy conservation equation and Fourier's law:

$$\left.\begin{aligned} &\rho c\frac{\partial\vartheta}{\partial t}(x,t)+\frac{\partial q}{\partial x}(x,t)=0 \\ &q(x,t)=-\lambda\frac{\partial\vartheta}{\partial x}(x,t)\ . \end{aligned}\right\} \quad 0<x<d, t\geq 0 \qquad (1\mathrm{a,b})$$

We assume a homogenous slab of thickness d, subject to the most general linear and homogeneous boundary conditions:

$$\alpha_1\vartheta(0,t)-\lambda\frac{\partial\vartheta}{\partial x}(0,t)=0$$
$$\alpha_2\vartheta(d,t)+\lambda\frac{\partial\vartheta}{\partial x}(d,t)=0\ . \quad (2a,b)$$

("Newton heat loss", [7]) and to the general initial condition:

$$\vartheta(x,0)=g(x)\qquad 0\le x\le d\ . \quad (3)$$

The temperature of the environment is considered constant and is chosen as origin of the temperature scale. The usual methods in heat conduction (see e.g. [3–7]) reduce the system (1) by elimination of q to Fourier's well known (second order) partial differential equation for ϑ. By contrast, the essential point of the Hamiltonian approach developed below is to renounce to this operation and to preserve ϑ and q instead as independent dynamic variables satisfying the first order system (1) with its straightforward physical message.

In this way, the separation ansatz $\vartheta(x,t)=\theta(x)f(t)$ and $q(x,t)=-p(x)f(t)$, where the minus sign was introduced for later convenience, leads to:

$$\vartheta(x,t)=\theta(x)\mathrm{e}^{-\frac{t}{\tau}}\quad\text{and}\quad q(x,t)=-p(x)\mathrm{e}^{-\frac{t}{\tau}}\ . \quad (4a,b)$$

Here τ is the separation constant defined as $\dot{f}/f=-1/\tau$ and the space-dependent parts $\theta(x)$ and $p(x)$ of ϑ and $-q$, respectively satisfy the first order system:

$$\theta'=\frac{1}{\lambda}p,\quad p'=-\lambda\Omega^2\theta\quad\text{with }\Omega^2=\rho c/\lambda\tau\ . \quad (5a,b,c)$$

This system may now be converted easily into the Hamiltonian form:

$$\theta'=\frac{\partial H}{\partial p},\quad p'=-\frac{\partial H}{\partial\theta} \quad (6a,b)$$

with the Hamilton function

$$H=\frac{1}{2\lambda}p^2+\frac{1}{2}\lambda\Omega^2\theta^2\ . \quad (7)$$

It is now immediately seen that, if one considers x as the "time variable" of motion of a hypothetical point-particle of *mass* λ, coordinate θ, momentum p and total energy H, then the heat conduction described by Eqs. (5) may be put in a one-to-one correspondence with an abstract mechanical motion, which is nothing than the harmonic oscillation of a spring-mass system of spring constant $k=\lambda\Omega^2$. The oscillations are carried out with the (circular) frequency Ω in a finite "time interval" extending from the "initial instant" $x=0$ to a prescribed "arrival time" $x=d$, respectively. Already the possibility of this formal mapping of the heat conduction problem onto a Hamiltonian motion has interesting physical consequences as:

1). The Hamiltonian (7) is the generator of any infinitesimal configuration-change:

$$\{\delta\vartheta;\delta q\}=\{\vartheta(x+\delta x,t)-\vartheta(x,t);q(x+\delta x,t)-q(x,t)\} \quad (8)$$

of the temperature and flux fields $\{\vartheta(x,t);q(x,t)\}$ at any fixed time t. Accordingly, the relationship connecting the values $\{\theta(x_1),p(x_1)\}$ to $\{\theta(x_2),p(x_2)\}$ is a canonical transformation for any $x_1,x_2\in[0,d]$, which in turn leads for $x_1=0$ and $x_2=x$ to the general solution of the heat conduction problem (see Eqs. (22) below).

2). As x varies from 0 to d, the field configurations change not somehow, but in such a way that the Hamiltonian (7) remains unchanged:

$$H=\frac{1}{2\lambda}[p(x)]^2+\frac{1}{2}\lambda\Omega^2[\theta(x)]^2=\text{constant}\equiv I\ . \quad (9)$$

The constant value I of H is determined by the values of θ and p on the boundaries:

$$I=\frac{1}{2\lambda}[p(0)]^2+\frac{1}{2}\lambda\Omega^2[\theta(0)]^2$$
$$=\frac{1}{2\lambda}[p(d)]^2+\frac{1}{2}\lambda\Omega^2[\theta(d)]^2. \quad (10)$$

On this ground, $I=H$ will be referred to as configuration- or transfer invariant of the system. The existence of this conservation-law is a direct consequence of the translation-symmetry (i.e of invariance under $x\to x+\text{const.}$) of Eqs. (6).

3). The temperature θ (as a generalized coordinate) and the heat flux p (as the conjugate momentum) play totally equivalent and interchangeable physical roles. This becomes more transparent by transcribing (the slightly asymmetrical) Eq. (6) with the aid of the Poisson brackets [2] into the fully symmetric form:

$$\theta'=[\theta,H]_P,\quad p'=[p,H]_P\ . \quad (11a,b)$$

Once recognized, this equivalence can also be proven directly. It originates namely from the simple fact that (for constant thermophysical properties) both the fields $\vartheta(x,t)$ and $q(x,t)$ satisfy, as an immediate consequence of (1), the same Fourier-type equations:

$$\frac{\partial\vartheta}{\partial t}=a\frac{\partial^2\vartheta}{\partial x^2}\quad\text{and}\quad\frac{\partial q}{\partial t}=a\frac{\partial^2 q}{\partial x^2} \quad (12a,b)$$

respectively, where $a=\lambda/\rho c$ denotes the thermal diffusivity of the slab. This is in full agreement with the existence of a canonical transformation able to convert in any Hamiltonian system the "old" momenta in the "new" coordinates and the "old" coordinates in the "new" momenta, respectively, [2]. The difference between temperature and heat flux is thus (for constant thermophysical properties) practically one of nomenclature only, in agreement with (11). The symmetric character of the two fields $\vartheta(x,t)$ and $q(x,t)$ as independent dynamical variables on equal footing with respect to their evolution-equations (12) is also preserved by the boundary conditions (2). Indeed, by taking into account (1) and (4), the conditions (2), as linear relationships between the boundary values of ϑ and $\partial\vartheta/\partial x$ may immediately be transcribed in similar linear relationships between the corresponding boundary values of q and $\partial q/\partial x$:

$$\lambda\Omega^2 q(0,t) + \alpha_1 \frac{\partial q}{\partial x}(0,t) = 0$$
$$\lambda\Omega^2 q(d,t) - \alpha_2 \frac{\partial q}{\partial x}(d,t) = 0 \qquad (13\text{a, b})$$

or, equivalently

$$\lambda\Omega^2 p(0) + \alpha_1 p'(0) = 0$$
$$\lambda\Omega^2 p(d) - \alpha_2 p'(d) = 0 \ . \qquad (13'\text{a, b})$$

Therefore, the heat conduction problem considered can be described in a "ϑ-picture" as well as in a "q-picture" in a completely equivalent manner. This equivalence results often in some practical advantages. Thus, by comparing (2) to (13) one immediately sees that a Neumann-problem for the first equation (12), reduces to a (usually more familiar) Dirichlet-problem for the second one (i.e., according to the nomenclature of [6]: Eq. (12a) with homogeneous boundary conditions of the second kind, is equivalent to Eq. (12b) with homogeneous boundary conditions of the first kind). Some differences of "technical" nature between the two pictures mentioned, resulting from the presence of Ω in Eqs. (13′), will be discussed in the next section.

Let us now discuss the mechanical meaning of the boundary conditions (2) shortly. For the canonical conjugate variables θ and p they become:

$$p(0) = \alpha_1\theta(0) \quad \text{and} \quad p(d) = -\alpha_2\theta(d) \ . \qquad (14\text{a, b})$$

These equations show that the boundary conditions of the heat conduction problem are converted in the framework of the Hamiltonian approach in simple proportionality requirements for the coordinates and momenta in the initial ($x = 0$) and the final ($x = d$) instant of the mechanical motion, the coefficients of proportionality being precisely the heat transfer coefficients α_1 and α_2 at the front- and the backside of the slab, respectively. With given initial data $\theta(0)$ and $p(0)$, condition (14a) determines the solution of the mechanical problem unequivocally for any value of the continuous parameter Ω. Condition (14b) requires then additionally that the trajectory of motion started in the point $\{\theta(0), p(0)\}$ of the phase-space, arrives in the final instant of motion ($x = d$) in a certain point $\{\theta(d), p(d)\}$ fixed a priori. As we shall show in the next section, the effect of this additional "arrival requirement" is a severe restriction on the allowed frequencies Ω of the abstract harmonic oscillator. As expected, the sequence of these frequencies of the Hamiltonian problem turns out to be equivalent to the eigenvalues encountered in the traditional approaches [3–7] of the heat conduction problems. The "initial position" $\theta(0)$ of the oscillator is then determined by the "true" initial condition (3) of the heat conduction problem, which in turn requires (except for certain very special cases) to represent $\vartheta(x,t)$ as a linear superposition of all the allowed states of the oscillator, with amplitudes attenuated in time according to Eqs. (4).

We close this section by writing down, as a direct outflow of the transfer-invariant (9) and the boundary conditions (14), two useful relationships connecting the possible values of θ and p at the two boundaries of the slab:

$$\theta(d) = \pm\sqrt{\frac{\alpha_1^2 + \lambda^2\Omega^2}{\alpha_2^2 + \lambda^2\Omega^2}} \cdot \theta(0),$$
$$p(d) = \mp\frac{\alpha_2}{\alpha_1}\sqrt{\frac{\alpha_1^2 + \lambda^2\Omega^2}{\alpha_2^2 + \lambda^2\Omega^2}} \cdot p(0) \ . \qquad (15\text{a, b})$$

The transfer-invariant (9) yields therefore direct physical information about the configuration change of the thermophysical field $\{\vartheta(x,t), q(x,t)\}$, without detailed knowledge of the explicit solution of the problem.

3
Solution by the "propagator-method"

This section is devoted to the "propagator approach", a formal method for solving the Hamiltonian Eqs. (5) with interesting physical spin-offs, especially concerning the heat conduction problem in composite media. To this end we first transcribe the system (5) into the compact 2×2-matrix form:

$$\phi'(x) = \mathbf{H} \cdot \phi(x) \qquad (16)$$

where the column matrix $\phi(x)$ as state vector of the field configuration and the quadratic matrix $\mathbf{H}$ as Hamiltonian matrix of the system are defined as:

$$\phi(x) = \begin{pmatrix} \theta(x) \\ p(x) \end{pmatrix} \quad \text{and} \quad \mathbf{H} = \begin{pmatrix} 0 & \frac{1}{\lambda} \\ -\lambda\Omega^2 & 0 \end{pmatrix} \qquad (17\text{a, b})$$

respectively. The matrix-differential equation (16) can now be considered formally as a "usual" ordinary differential equation of the first order, whose (formal) solution is immediate:

$$\phi(x) = e^{\mathbf{H}x} \cdot \phi(0) \equiv \mathbf{P}(x;0) \cdot \phi(0) \qquad (18)$$

where for the exponential-matrix $e^{\mathbf{H}x}$ the shortcut notation $\mathbf{P}(x;0)$ was introduced.

Now, by expanding the exponential-matrix $e^{\mathbf{H}x}$ in a Taylor series of its exponent-matrix $\mathbf{H}x$ and by taking into account the property

$$\mathbf{H}^n = \begin{cases} (-1)^{\frac{n}{2}}\Omega^n \cdot \mathbf{1} & \text{for } n = 2,\ 4,\ 6, \ldots \\ (-1)^{\frac{n-1}{2}}\Omega^{n-1} \cdot \mathbf{H} & \text{for } n = 1,\ 3,\ 5, \ldots \end{cases} \qquad (19)$$

of the Hamiltonian matrix (17), we obtain after some algebra:

$$\mathbf{P}(x;0) = \mathbf{1} \cdot \cos\Omega x + \mathbf{H} \cdot \frac{\sin\Omega x}{\Omega} \qquad (20)$$

which, written out explicitly reads as:

$$\mathbf{P}(x;0) = \begin{pmatrix} \cos\Omega x & \dfrac{\sin\Omega x}{\lambda\Omega} \\ -\lambda\Omega\sin\Omega x & \cos\Omega x \end{pmatrix} \qquad (21)$$

(the symbol $\mathbf{1}$ denotes above the 2×2 unity-matrix).

The physical meaning of the matrix $\mathbf{P}$ results by inspection of Eq. (18) at the first glance: It "transfers" or "propagates" the mechanical state of the hypothetical oscillator from the starting moment of motion $x = 0$ into a later state at an instant $x \leq d$. On this ground, $\mathbf{P}(x;0)$ will be referred to as transfer matrix or propagator of the system. This "transfer" corresponds in the heat conduction problem to a mapping of the thermophysical field

$\{\vartheta(x,t); q(x,t)\}$ for a fixed instant of the real time t from its configuration $\{\theta(0), p(0)\}$ at the boundary $x = 0$ into the configuration $\{\theta(x), p(x)\}$ at a distance $x \le d$ within the slab. The transfer matrix $\mathbf{P}(x;0)$ is thus equivalent to the finite canonical transformation mentioned in the precedent section, which yields the explicit solution of the problem. Indeed, the latter results from (18) immediately, by taking into account (21) and (14a), as:

$$\begin{aligned} \theta(x) &= \left(\cos\Omega x + \frac{\alpha_1}{\lambda\Omega}\sin\Omega x\right)\theta(0) \\ p(x) &= -\lambda\Omega\left(\sin\Omega x - \frac{\alpha_1}{\lambda\Omega}\cos\Omega x\right)\theta(0) \ . \end{aligned} \tag{22a,b}$$

Let us now examine the crucial effect of the boundary condition (14b) on this unique solution of the "initial value" problem specified by Eq. (14a) where Ω, which depends according to (5) on the separation constant τ, is still considered as a continuous free-parameter of the problem. To this end we substitute in (22) $x = d$, divide the resulting equations side by side to each other and recall Eq. (14b). Thus, we obtain as an additional effect of the second boundary condition (14) to the first one the following restriction, or selection rule for the allowed frequencies of our oscillator:

$$\tan\Omega d = \frac{(\alpha_1+\alpha_2)\Omega\lambda}{(\Omega\lambda)^2 - \alpha_1\alpha_2} \equiv \frac{(\mathrm{Bi}_1+\mathrm{Bi}_2)\Omega d}{(\Omega d)^2 - \mathrm{Bi}_1\mathrm{Bi}_2} \tag{23}$$

Here, $\mathrm{Bi}_{1,2}$ denote the Biot numbers defined as $\mathrm{Bi}_{1,2} = \alpha_{1,2}d/\lambda$, [6].

In (23) we now recover the well known transcendental equation which determines the infinite sequence of the eigenvalues $\Omega = \Omega_n$, $n = 1, 2, 3, \ldots$, encountered in the traditional approaches of the heat conduction problems, [3–7]. Therefore, these eigenvalues (which all are non-degenerate, i.e. distinct) represent precisely the allowed frequencies i.e. the eigenfrequencies of the abstract harmonic oscillator of the Hamiltonian description. According to equation (5c), the eigenfrequencies also determine the exponential relaxation times $\tau_n = 1/a\Omega_n^2$ of the field configurations $\{\theta_n(x), p_n(x)\}$. The symmetric roles played by the temperature and flux components θ_n and p_n become manifest again. Indeed, the x-derivative of Eq. (16) and the properties (19) of the Hamiltonian matrix yield:

$$\phi_n''(x) = \mathbf{H}\cdot\phi_n'(x) = \mathbf{H}^2\phi_n(x) = -1\cdot\Omega_n^2\phi_n(x) \ . \tag{24}$$

This is however the concise form of equations $\theta_n'' = -\Omega_n^2\theta_n$ and $p_n'' = -\Omega_n^2 p_n$ which are nothing than Eqs. (12), after the variables x and t have been separated.

Let us now discuss shortly the mechanical meaning of the "true" initial condition (3). One immediately sees that if there accidentally happens that the initial temperature profile $g(x)$ coincides with one of the eigenstates of the oscillator, i.e.

$$g(x) = \left(\cos\Omega_n x + \frac{\alpha_1}{\lambda\Omega_n}\sin\Omega_n x\right)\theta_n(0) \tag{25}$$

then, and only then, the unique solution of the heat conduction problem is simply:

$$\begin{aligned} \vartheta(x,t) &= \theta_n(x)\mathrm{e}^{\frac{t}{\tau_n}} = g(x)\mathrm{e}^{-a\Omega_n^2 t} \\ q(x,t) &= -p_n(x)\mathrm{e}^{\frac{t}{\tau_n}} = -\lambda\cdot g'(x)\mathrm{e}^{-a\Omega_n^2 t} \ . \end{aligned} \tag{26a, b}$$

If, however the initial temperature profile $g(x)$ is not an eigenstate of the oscillator, condition (3) can only be satisfied by a linear superposition of the form:

$$\begin{aligned} \vartheta(x,t) &= \sum_{n=1}^{\infty}\theta_n(x)\mathrm{e}^{-\frac{t}{\tau_n}} \\ &= \sum_{n=1}^{\infty}\theta_n(0)\cdot\left(\cos\Omega_n x + \frac{\mathrm{Bi}_1}{\Omega_n d}\sin\Omega_n x\right)\mathrm{e}^{-a\Omega_n^2 t} \end{aligned} \tag{27}$$

The coefficients $\theta_n(0)$ can now be determined by subjecting (27) to the initial condition (3) and by taking into account the orthogonality of the functions $\theta_n(x)$. In this way we recover in the propagator approach the well known results [3–7]:

$$\begin{aligned} \theta_n(x) &= \left(\cos\Omega_n x + \frac{\mathrm{Bi}_1}{\Omega_n d}\sin\Omega_n x\right)\cdot\theta_n(0) \\ p_n(x) &= -\lambda\Omega_n\left(\sin\Omega x - \frac{\mathrm{Bi}_1}{\Omega_n d}\cos\Omega_n x\right)\cdot\theta_n(0) \end{aligned} \tag{28a, b}$$

$$\int_0^d \theta_n(x)\theta_m(x)\mathrm{d}x = N_n\delta_{nm} \tag{29}$$

$$\theta_n(0) = \frac{1}{N_n}\int_0^d g(x)\left(\cos\Omega_n x + \frac{\mathrm{Bi}_1}{\Omega_n d}\sin\Omega_n x\right)\mathrm{d}x \tag{30}$$

$$\begin{aligned} N_n = &\left(1 + \frac{\mathrm{Bi}_1^2}{\Omega_n^2 d^2}\right) \\ &\times\left(1 + \frac{\mathrm{Bi}_1}{Bi_1^2 + \Omega_n^2 d^2} + \frac{\mathrm{Bi}_2}{Bi_2^2 + \Omega_n^2 d^2}\right)\frac{d}{2} \ . \end{aligned} \tag{31}$$

Obviously, all the remaining Eq. (5)–(21) of the present paper are valid in this general case for every eigenstate of the oscillator separately. In other words, every eigenstate of the oscillator is characterized by its own Hamiltonian (7), configuration-invariant (10), Hamiltonian matrix (17b), propagator (21) and satisfies the conditions (14) individually. Therefore, we may interpret the general solution (27) as a linear superposition of the independent eigenstates of an abstract harmonic oscillator with eigenfrequencies Ω_n, spring constants $k_n = \lambda\Omega_n^2$ and initial positions $\theta_n(0)$ given by Eq. (30). We underline that the initial positions $\theta_n(0)$ of the mechanical oscillator are prescribed here not somehow but are determined in a self-consistent way as the projections (Fourier coefficients) of the initial temperature distribution $\vartheta(x,0) = g(x)$ on the eigenstates $\theta_n(x)$ of the oscillator itself. Finally, it is worthwhile to spend some attention to the problem of orthogonality of the components $\theta_n(x)$ and $p_n(x)$ of the configuration-eigenstates $\phi_n(x)$. By contrast to the temperature components whose well known orthogonality is given by (29), the flux components p_n as given by (28b) are neither orthogonal to each other, nor to the temperature components θ_n. The reason for this lack of orthogonality resides in the Ω_n-dependence of the boundary conditions (13′), as mentioned in Section 2. There seems also that the "ϑ- and q-pictures", in spite of the symmetry of their evolution equations (12) and boundary conditions (2) and (13) are not equally adequate to the description of the heat conduction problems. This is however not the case. We are faced here not with a basic but with a "technical" problem only. As it is well known from linear algebra, by choosing certain linear combinations of the linearly independent "vectors" $p_n(x)$ given in (28b), one always can construct a new orthogonal q-base, by following the classical orthogonalization procedure of Schmidt, [8].

4 Geometrical interpretation and discussion

As argued in Section 2, the Hamiltonian (9) of the mechanical motion associated with the heat conduction remains unchanged as the position coordinate runs across the slab. This means geometrically that in the two-dimensional phase-space $\{\theta, p\}$ the representative point $M_n = \{\theta_n(x), p_n(x)\}$ of the nth eigenstate of the mechanical oscillator moves on an ellipse $\theta_n^2/a_n^2 + p_n^2/b_n^2 = 1$ with semiaxes $|a_n| = (2I_n/\lambda\Omega_n^2)^{1/2}$ and $|b_n| = (2\lambda I_n)^{1/2}$. According to (28a, b), the semiaxes are obtained as the absolute values of

$$a_n = \sqrt{1 + \left(\frac{\mathrm{Bi}_1}{\Omega_n d}\right)^2} \cdot \theta_n(0)$$

and

$$b_n = \alpha_1 \cdot \sqrt{1 + \left(\frac{\Omega_n d}{\mathrm{Bi}_1}\right)^2} \cdot \theta_n(0) \tag{32}$$

respectively. Here, the eigenfrequencies Ω_n are the (positive) roots $\Omega_1 < \Omega_2 < \Omega_3 < \cdots$ of the transcendental Eq. (23) and the initial position of the oscillator $\theta_n(0)$ in the nth eigenstate is given by Eq. (30) and (31). The semiaxes of the elliptic trajectories are connected to the eigenfrequencies by the simple relationship

$$\Omega_n = \frac{1}{\lambda}\frac{|b_n|}{|a_n|} \tag{33}$$

The number of cycles C_n described by M_n on the ellipse as x runs from 0 to d, is given by the ratio of the slab thickness d and the period $T_n = 2\pi/\Omega_n$ of motion, i.e.

$$C_n = \frac{\Omega_n d}{2\pi} = \frac{d}{2\pi\lambda}\frac{|b_n|}{|a_n|} \tag{34}$$

Thus, the Fourier series of the temperature and flux fields may be put in the form

$$\vartheta(x,t) = \sum_{n=1}^{\infty} \theta_n(x) \cdot \mathrm{e}^{-a\Omega_n^2 t} = \sum_{n=1}^{\infty} a_n \cdot \mathrm{e}^{-a\Omega_n^2 t} \cdot \cos\left(\Omega_n x - \arctan\frac{\mathrm{Bi}_1}{\Omega_n d}\right) \tag{35}$$

$$q(x,t) = -\sum_{n=1}^{\infty} p_n(x) \cdot \mathrm{e}^{-a\Omega_n^2 t} = \sum_{n=1}^{\infty} b_n \cdot \mathrm{e}^{-a\Omega_n^2 t} \cdot \sin\left(\Omega_n x - \arctan\frac{\mathrm{Bi}_1}{\Omega_n d}\right) \tag{36}$$

These equations show that (a) the amplitude spectrum $\{|a_n|\}$ and $\{|b_n|\}$ of the temperature $\vartheta(x,t)$ and the flux field $q(x,t)$ coincides with the sequence of the semiaxes $|a_n|$ and $|b_n|$ of the elliptic phase-space trajectories of the oscillator in its eigenstates, respectively, (b) the contributions of the individual eigenstates of the oscillator to the thermophysical field $\{\vartheta, q\}$ do relaxe in the real time t exponentially, and (c) the relaxation rates depend to the eigenfrequencies of the mechanical oscillator according to $\tau_n = 1/a\Omega_n^2$.

As an illustration, in Fig. 1 the semiaxes $|a_n|$ and $|b_n|$ corresponding to the first four eigenstates of the oscillator are shown as obtained for a constant initial temperature distribution of $g(x) = \mathrm{const.} = 1$ K (above the temperature of the ambient) and the parameter values $d = 0.1$ m, $\lambda = 0.1\ \mathrm{W \cdot m^{-1} \cdot K^{-1}}$, $\alpha_1 = 1\ \mathrm{W \cdot m^{-2} \cdot K^{-1}}$ and $\alpha_2 = 0.01\ \mathrm{W \cdot m^{-2} \cdot K^{-1}}$. The corresponding eigenfrequencies obtained by numerical solving of Eq. (23) are $\Omega_1 = 8.68\ \mathrm{m^{-1}}$, $\Omega_2 = 34.28\ \mathrm{m^{-1}}$, $\Omega_3 = 64.39\ \mathrm{m^{-1}}$ and $\Omega_4 = 95.30\ \mathrm{m^{-1}}$, respectively.

The geometrical meaning of the boundary conditions (14) may now be described as follows. Taking into account that the starting condition (14a) does not specify both the initial data $\theta(0)$ and $p(0)$ but their ratio α_1 only, it is only

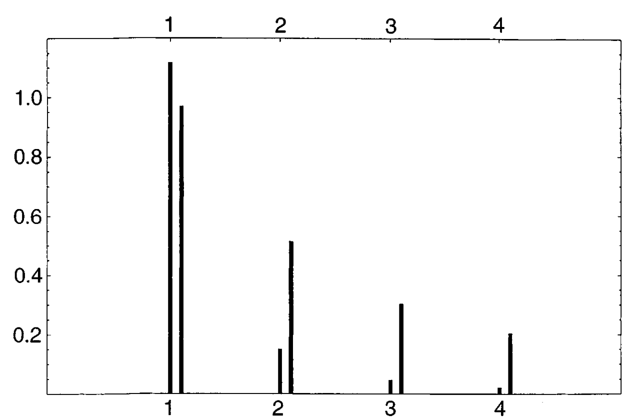

Fig. 1. The semiaxes $a_1 = 1.116, a_2 = 0.15, a_3 = 0.047$, and $a_4 = 0.021$ (left bars) and $b_1 = 0.968, b_2 = 0.513, b_3 = 0.303$, and $b_4 = 0.204$ (right bars) of the elliptic phase-space trajectories of the oscillator in its first four eigenstates, representing the first four lines of the amplitude spectrum of the temperature $\vartheta(x,t)$ and flux field $q(x,t)$, respectively (parameter values as given in the text)

able to specify the laws of motion (22) up to the arbitrary initial position $\theta(0)$ of the oscillator. It also leaves the continuous frequency spectrum Ω of the oscillator (depending on the separation constant τ) entirely free. The amplitude-freedom of the oscillator is then removed by the "true" initial condition (3) which supplies for $\theta_n(0)$ the explicit formula (30) in a self consistent way, as explained in Section 3. The frequency-freedom on the other hand, is lifted by the "arrival condition" (14b) which acts similarly to a quantization rule, namely it selects out from the continuous frequency spectrum of the initial-value problem an infinite but denumerable set of discrete values, the eigenfrequencies Ω_n of the oscillator, given by the positive roots of Eq. (23). Therefore, the two-point boundary conditions (14) play for the abstract mechanical motion the role of the "two-instant" conditions which hold for every eigenstate of the oscillator separately, i.e.:

$$p_n(0) = \alpha_1\theta_n(0) \text{ and } p_n(d) = -\alpha_2\theta_n(d). \qquad (37a, b)$$

This means geometrically that in the phase-plane $\{\theta, p\}$ all the starting points $\{\theta_n(0), p_n(0)\}$ and all the arrival points $\{\theta_n(d), p_n(d)\}$ of the elliptic trajectories corresponding to the eigenstates of the oscillator (i.e. to the Fourier components of the thermophysical field at the boundaries of the slab) lie on the same straight lines $p = \alpha_1\theta$ and $p = -\alpha_2\theta$, respectively. The slopes of these straight lines (both of them passing through the origin) are precisely the heat transfer coefficients α_1 and $-\alpha_2$, respectively. This circumstance may be immediately seen in Fig. 2 which shows the ellipses corresponding to the amplitude spectra of Fig. 1, i.e. to the first four Fourier components $\{\theta_n(d), p_n(d)\}$ of the thermophysical field.

We close this Section by writing down some special solutions of the eigenvalue Eq. (23). It is a widely spread opinion that (for finite values of both α_1 and α_2) this

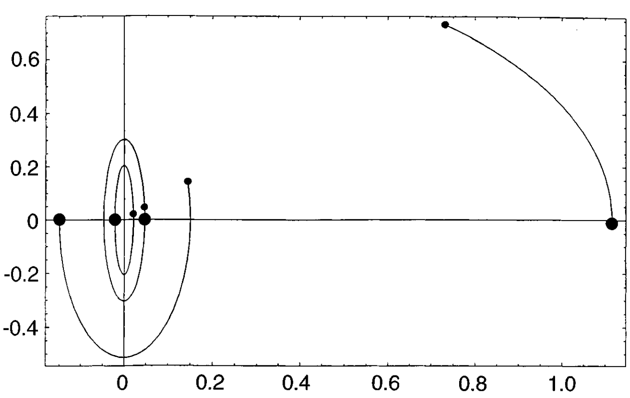

Fig. 2. As x varies from 0 to d the representative points $M_n = \{\theta_n(x), p_n(x)\}$ of the first four eigenstates of the thermophysical field (for parameter values as in Fig. 1) describe (by moving clockwise) elliptic trajectories which all issue from the same starting line (small dots) of slope $\arctan(\alpha_1) = 45°$ and stop after a number of cycles C_n at the same finishing line (big dots) of slope $\arctan(-\alpha_2) = -0.57°$. The biggest ellipse corresponds to the ground state of frequency $\mathbf{\Omega}_1$. The other ones become with increasing eigenfrequency $\mathbf{\Omega}_n$ of the mechanical oscillator smaller and smaller. The number of cycles described by the points M_n on the corresponding ellipses are $C_1 = 0.14, C_2 = 0.54, C_3 = 1.02$ and $C_4 = 1.52$, respectively

transcendental equation is only tractable by numerical methods. This statement actually holds, except for a great number of (physically interesting) special values of d for which one of the eigenvalues Ω_n always can be calculated in an exact algebraic form. Perhaps, the most exotic one of these special cases is obtained if the slab thickness coincides with one of the values d_n of the infinite sequence

$$d_n = \frac{(2n-1)\pi}{2}\frac{\lambda}{\sqrt{\alpha_1\alpha_2}}, \quad n = 1, 2, 3, \ldots \qquad (38)$$

It is easy to prove that is this case

$$\Omega^* = \frac{\sqrt{\alpha_1\alpha_2}}{\lambda} \qquad (39)$$

represents precisely the nth positive root of Eq. (23). Thus, to $n = 1$ there corresponds the slab thickness $d_1 = (\pi/2)\lambda(\alpha_1 \cdot \alpha_2)^{-1/2}$ and (39) yields the most persistent eigenvalue of the spectrum, the ground-state frequency Ω_1. For $n = 2, 3, \ldots$ the frequency Ω^* shifts to the second, third etc. place of the sequence $\Omega_1 < \Omega_2 < \Omega_3 < \cdots$. If one considers e.g. a slab of concrete with $\lambda = 1.8\ \mathrm{W \cdot m^{-1} \cdot K^{-1}}$, $a = 6.8 \cdot 10^{-7}\ \mathrm{m^2\,s^{-1}}$ and the standard indoor and outdoor heat transfer coefficients $\alpha_1 = 10\ \mathrm{W \cdot m^{-1} \cdot K^{-1}}$ and $\alpha_2 = 20\mathrm{W \cdot m^{-1} \cdot K^{-1}}$, one obtains for $n = 1$ a usual thickness of $d_1 \cong 0.2$ m, the frequency of $\Omega_1 = 7.86\ \mathrm{m^{-1}}$ and a relaxation time of the ground state of $\tau_1 = 6.62$ h, respectively. The next eigenfrequencies of the spectrum (calculated numerically) are $\Omega_2 = 19.66\ \mathrm{m^{-1}}$, $\Omega_3 = 33.83\ \mathrm{m^{-1}}$, and $\Omega_4 = 48.83\ \mathrm{m^{-1}}$, respectively. It is also worthwhile to notice that for the slab thickness' (38), the number of cycles (34) described by the representative point of the mechanical oscillator along the ellipse is

$$C_n = \frac{\Omega^* d_n}{2\pi} = \frac{2n-1}{4} \qquad (40)$$

This means physically that the nth positive root of Eq. (23) is then and only then given by the exact formula (39), when the slab thickness $d = d_n$ amounts exactly $2n - 1$ quarter-periods of the corresponding mechanical oscillation. From mathematical point of view, the exotic character of the solution (38) and (39) consists in the fact that it coincides with each a singular point of the left and the right hand side of (23), respectively. Due to this fact, this solution can not be found by numerical procedures applied to the form (23) of the eigenvalue equation directly. If however the numerical approach is applied instead to the reciprocal equation of (23), i.e. to $\cot \Omega_n d = 1/\text{r.h.s}$, the singularities mentioned go over into zeros of the new equation and the existence of the special solution (38) and (39) becomes immediately manifest. It can then be identified also by numerical calculations easily.

5
Summary and conclusions

The main results of this paper may be summarized as follows.

1. The heat conduction problem in a homogeneous slab $0 \le x \le d$ with the most general linear and homogeneous boundary conditions can be put (for a fixed time t) in a one-to-one correspondence with the Hamiltonian motion

of an abstract harmonic oscillator in the "time-interval" $x \in [0, d]$. The two-point boundary value problem of heat conduction specified according to (2) by the temperature and the heat flux at the front $(x = 0)$- and the backside $(x = d)$ of the slab, corresponds in this way to a mechanical "two-instant-problem", specified by the "starting"- and the "arrival"-conditions (14a,b) with respect to the coordinate and the momentum of the oscillator at the initial $(x = 0)$ and final $(x = d)$ "instant" of motion, respectively.

2. The laws of motion for the position coordinate and the momentum of the oscillator in its eigenstates correspond to the individual terms of the Fourier series (35) and (36) of the temperature $\vartheta(x, t)$ and of the flux field $q(x, t)$, respectively. The contributions of the individual eigenstates to these fields are not equally important. They are weighted by the eigenfrequencies of the oscillator through the "relaxation factor" $\exp(-a\Omega_n^2 t)$, so that after a long time (i.e. for $t \gg \tau_n = 1/a\Omega_n^2$) only the ground state of the oscillator (i.e. the state corresponding to the lowest eigenvalue Ω_1) survives. This means geometrically that with time the ellipses of Fig. 2 e.g. start to disappear successively. Those corresponding to big frequencies "die out" first, being followed by the low-frequency ones, until the steady state corresponding to the ambient temperature is reached. For some special (and for the practice significant) values of the slab thickness, the ground-state frequency can be calculated in the exact algebraic form (39).

3. The Hamiltonian approach reveals the existence of a configuration- or transfer-invariant of the thermophysical field $\{\vartheta, q\}$. This is a quadratic form of the space-dependent parts of the temperature and flux fields whose value remains invariant as x changes from 0 to d within the slab. The transfer-invariant yields in this way explicit relationships connecting the field configurations for two different values of x (in particular at the two boundaries), without any detailed knowledge about the solution of the heat conduction problem.

4. As an immanent feature of any Hamiltonian system results that the space-dependent part of the temperature and the flux field as generalized coordinate and conjugate momentum, respectively play in the heat conduction totally equivalent and interchangeable roles. There always exists a canonical transformation which maps these dynamical variables on each other. The difference between temperature and heat flux is thus (in a homegeneous slab with constant thermophysical properties) practically one of nomenclature only.

5. The transfer-matrix or propagator makes it possible to map the thermophysical field $\{\vartheta, q\}$ for any fixed time t from its configuration at the boundary $x = 0$ on its configuration at any $x \leq d$ by a simple matrix-multiplication, which leads at the same time to the explicit solution of the heat conduction problem. This configuration-transfer from $x = 0$ to $x \leq d$ takes place in such a way that the Hamiltonian (9) remains unchanged.

6. The propagator method can be extended to the case of a composite slab directly. The transfer matrix of the latter is obtained simply by multiplying the transfer matrices of type (21) corresponding to the individual layers of the composite, respectively.

References

1. **Benest D; Froeschle C eds.** (1994) Chaos and Diffusion in Hamiltonian Systems, Editions Frontiers, Gif-sur Yvette Cedex
2. **Goldstein H** (1980) Classical Mechanics, Chapter 9, Addison-Wesley Publ.Co., Reading, Massachusetts
3. **Grigull U; Gröber Erk** (1988) Die Grundgesetze der Wärmeleitung, Springer Verlag, Berlin
4. **Eckert ERG; Drake Jr RM** (1971) Analysis of Heat and Mass Transfer, McGraw-Hill, New York
5. **Carslaw HS; Jaeger JC** (1995) Conduction of Heat in Solids (2nd Edn), Clarendon Press, Oxford
6. **Özisik MN** (1993) Heat conduction (2nd Edn), Wiley-Interscience Publ., New York
7. **Hill JM; Dewynne JN** (1987) HeatConduction, Blackwell Sci. Publ., Oxford
8. **Morse PM; Feshbach H** (1953) Methods of Theoretical Physics, Chapter 8, McGraw-Hill, Inc., New York