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Temperature and entropy production operator in Fourier heat conduction

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The Hamilton-Lagrange formalism of the field theory of irreversible nonequilibrium thermodynamics has been developed in the last few years. Consequently, we have a good opportunity to introduce the canonical quantization for the parabolic differential equations, such as Fourier heat conduction. This procedure might tell us how quantum features arise in the system under consideration and how we may get to the quantum field theory of irreversible processes. We introduce the temperature and the entropy production operator in the case of the heat equation, and we show that the eigenvalues of the entropy production operator are discrete and real quantities.

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I. INTRODUCTION

The Hamilton-Lagrange formalism is widely used in the different disciplines of physics [1–3]. This mathematical method enables us to gain a deeper insight into the physical processes. However, the Hamilton formalism of fields was developed only for those theories where the operators in the field equations were self-adjoint. There were several attempts to construct a Hamiltonian variational principle for thermodynamics in which the equations of motion contain non-self-adjoint operators, too, such as the first time derivative operator. Nowadays, we know of a few successful results [4–14] that are different in some ways but all of them based on Hamilton's principle. From these methods, we get back the equations of motion; however, the goal of our investigation is to obtain more than just the field equations, e.g., the attainment of quantization. We have worked out a possible description of nonequilibrium thermodynamics in an essentially complete form of the Hamilton-Lagrange formalism for those cases where we restricted ourselves to convection- and source-free systems, and we have obtained constant coefficients in the differential equations [4–7]. In this paper, we would like to show how we are able to obtain the first steps towards the canonical quantization for one of the simplest cases of the irreversible processes, the Fourier heat conduction. In the microscopic theory of irreversible processes, Prigogine [15] handled the entropy as an operator in order to introduce the concept of irreversibility into the extension of the formalism of classical and quantum mechanics. Presently, there are some works on the problem of discrete quantities in thermodynamics [16,17]. In this paper, we attain the temperature and entropy production operator in the field theory of heat conduction using the usual quantization procedure [18–22].

II. THE LAGRANGIAN AND THE HAMILTONIAN OF HEAT CONDUCTION

We start from the Lagrange density function

$$L = \frac{1}{2}\dot{\varphi}^2 + \frac{1}{2}\frac{\lambda^2}{c_v^2}(\Delta\varphi)^2, \tag{1}$$

where λ is the heat conduction coefficient and c_v is the specific heat capacity. The dot denotes the partial time derivative and Δ is the Laplace operator. φ is a field quantity that is defined in this way:

$$T = -\dot{\varphi} - \frac{\lambda}{c_v}\Delta\varphi, \tag{2}$$

where T is the temperature. From Hamilton's principle we get the Euler-Lagrange equation for φ

$$-\ddot{\varphi} + \frac{\lambda^2}{c_v^2}\Delta\Delta\varphi = 0. \tag{3}$$

If we take into account Eq. (2), we get back the Fourier heat equation

$$\dot{T} - \frac{\lambda}{c_v}\Delta T = 0. \tag{4}$$

In the following, we would like to calculate the Lagrangian of the system. For this we calculate φ in Fourier series,

$$\varphi = \sum_k \sqrt{\frac{2}{V}}(C_k \cos kx + S_k \sin kx), \tag{5}$$

where the coefficients C_k and S_k are the function of time, V is the volume, and k is the wave number. The time derivative and Laplacian of φ can be calculated,

$$\dot{\varphi} = \sum_k \sqrt{\frac{2}{V}}(\dot{C}_k \cos kx + \dot{S}_k \sin kx), \tag{6}$$

$$\Delta\varphi = \sum_k -k^2\sqrt{\frac{2}{V}}(C_k \cos kx + S_k \sin kx). \tag{7}$$

The Lagrangian of the system is obtained by the integration of a Lagrange density function over the volume

$$L = \int L\,dV = \frac{1}{2}\sum_k \left[(\dot{C}_k^2 + \dot{S}_k^2) + \frac{\lambda^2}{c_v^2}k^4(C_k^2 + S_k^2)\right]. \tag{8}$$

1063-651X/95/52(1)/623(4)/$06.00

From the Lagrange formalism we obtain the canonically conjugated quantities

$$P_k^{(C)} = \dot{C}_k, \tag{9}$$

$$P_k^{(S)} = \dot{S}_k, \tag{10}$$

from which it is easy to express the Hamiltonian of the field. The Hamiltonian is

$$\begin{aligned} H &= \dot{C}\frac{\partial L}{\partial \dot{C}} + \dot{S}\frac{\partial L}{\partial \dot{S}} - L \\ &= \sum_k \left(\frac{1}{2}P_k^{(C)2} - \frac{1}{2}\frac{\lambda^2}{c_v^2}k^4 C_k^2 + \frac{1}{2}P_k^{(S)2} - \frac{1}{2}\frac{\lambda^2}{c_v^2}k^4 S_k^2\right) \\ &= \sum_k \left(\frac{1}{2}P_k^{(C)2} - \frac{1}{2}\frac{\lambda^2}{c_v^2}k^4 C_k^2\right) \\ &\quad + \sum_k \left(\frac{1}{2}P_k^{(S)2} - \frac{1}{2}\frac{\lambda^2}{c_v^2}k^4 S_k^2\right), \end{aligned} \tag{11}$$

which can be devided into two sums. Now we can say that we have obtained the Hamiltonian of the system which is the function of time only.

III. THE QUANTIZATION

If we introduce the following expressions:

$$C_k^- = \frac{P_k^{(C)}}{\sqrt{2}} - \frac{\lambda k^2}{\sqrt{2}c_v}C_k, \tag{12}$$

$$C_k^+ = \frac{P_k^{(C)}}{\sqrt{2}} + \frac{\lambda k^2}{\sqrt{2}c_v}C_k, \tag{13}$$

$$S_k^- = \frac{P_k^{(S)}}{\sqrt{2}} - \frac{\lambda k^2}{\sqrt{2}c_v}S_k, \tag{14}$$

$$S_k^- = \frac{P_k^{(S)}}{\sqrt{2}} + \frac{\lambda k^2}{\sqrt{2}c_v}S_k, \tag{15}$$

the Hamilton operator can be obtained in the simplest form

$$\mathcal{H} = \sum_k (C_k^+ C_k^- + S_k^+ S_k^-). \tag{16}$$

After these, let $P_k^{(C)}$, C_k, $P_k^{(S)}$, and S_k be operators that obey the following commutation rules:

$$[P_k^{(C)}, C_l] = h\delta_{kl}, \tag{17}$$

$$[P_k^{(S)}, S_l] = h\delta_{kl}, \tag{18}$$

from which we get the commutation rules of C_k^+, C_k^- and S_k^+, S_k^-. Moreover, C_k^+, C_k^- commutates with S_k^+, S_k^- because these are independent coordinates,

$$C_k^- C_l^+ - C_l^+ C_k^- = \frac{\lambda}{c_v}k^2 h\delta_{kl}, \tag{19}$$

$$S_k^- S_l^+ - S_l^+ S_k^- = \frac{\lambda}{c_v}k^2 h\delta_{kl}. \tag{20}$$

We have to examine the property of these operators. If Ψ is the eigenfunction of $\mathcal{H}$,

$$\mathcal{H}\Psi = \alpha\Psi, \tag{21}$$

with the eigenvalue α, it can be admitted that $C_k^+\Psi$ is an eigenfunction of $\mathcal{H}$,

$$\mathcal{H}C_k^+\Psi = \left(\alpha + \frac{\lambda}{c_v}k^2 h\right)C_k^+\Psi, \tag{22}$$

with the eigenvalue $\alpha + \frac{\lambda}{c_v}k^2 h$ and $C_k^-\Psi$ is an eigenfunction of $\mathcal{H}$, too,

$$\mathcal{H}C_k^-\Psi = \left(\alpha - \frac{\lambda}{c_v}k^2 h\right)C_k^-\Psi, \tag{23}$$

with the eigenvalue $\alpha - \frac{\lambda}{c_v}k^2 h$. These show that C_k^+ is a creation operator that increases the state with $\frac{\lambda}{c_v}k^2 h$ quantum, C_k^- is a destruction operator that decreases the state with $\frac{\lambda}{c_v}k^2 h$ quantum.

IV. THE TEMPERATURE AND ENTROPY PRODUCTION OPERATOR

We obtain the conserved current J of the field from the canonical tensor (thermodynamic tensor) [4–7]

$$J = \int (\dot{\varphi}\nabla\Delta\varphi - \nabla\dot{\varphi}\Delta\varphi)\, dV, \tag{24}$$

and after substituting Eqs. (6) and (7) we can express it with the coefficients C_k and S_k

$$\begin{aligned} J &= \int \frac{2}{V}\left\{\left[\sum_k (\dot{C}_k \cos kx + \dot{S}_k \sin kx)\right]\left[\sum_l l^3 (C_l \sin lx - S_l \cos lx)\right]\right. \\ &\quad \left. + \left[\sum_k k(\dot{C}_k \sin kx - \dot{S}_k \cos kx)\right]\left[\sum_l (-l^2)(C_l \cos lx + S_l \sin lx)\right]\right\} dV \\ &= \sum_k 2k^3 (\dot{S}_k C_k - \dot{C}_k S_k). \end{aligned} \tag{25}$$

If we take into account Eqs. (12)–(15), we get the conserved current operator of the field

$$\mathcal{J} = \sum_k \frac{2c_v}{\lambda} k (S_k^- C_k^+ - C_k^- S_k^+). \tag{26}$$

We would like to introduce the temperature T as an operator. When we use the connection between T and field φ, and Eqs. (6) and (7), then the temperature can be written

$$T = -\sum_k \sqrt{\frac{2}{V}} (\dot{C}_k \cos kx + \dot{S}_k \sin kx) + \sum_k \sqrt{\frac{2}{V}} \frac{\lambda k^2}{c_v} (C_k \cos kx + S_k \sin kx). \tag{27}$$

We read from Eqs. (12) and (15) that

$$C_k = \frac{c_v}{\sqrt{2}\lambda k^2} (C_k^+ - C_k^-), \tag{28}$$

$$S_k = \frac{c_v}{\sqrt{2}\lambda k^2} (S_k^+ - S_k^-), \tag{29}$$

and we substitute these into the formula of temperature (27). Now we obtain the temperature operator that contains the time derivatives of the operators

$$\mathcal{T} = -\sum_k \sqrt{\frac{1}{V}} \frac{c_v}{\lambda k^2} \left[(\dot{C}_k^+ - \dot{C}_k^-) \cos kx + (\dot{S}_k^+ - \dot{S}_k^-) \sin kx \right] + \sum_k \sqrt{\frac{1}{V}} \left[(C_k^+ - C_k^-) \cos kx + (S_k^+ - S_k^-) \sin kx \right]. \tag{30}$$

We know that the time derivative of an operator can be expressed as a Poisson bracket of the operator and the Hamilton operator

$$\dot{C}_k^+ = \frac{1}{h} [C_k^+, \mathcal{H}] = -\frac{\lambda}{c_v} k^2 C_k^+, \tag{31}$$

$$\dot{C}_k^- = \frac{1}{h} [C_k^-, \mathcal{H}] = \frac{\lambda}{c_v} k^2 C_k^-, \tag{32}$$

$$\dot{S}_k^+ = \frac{1}{h} [S_k^+, \mathcal{H}] = -\frac{\lambda}{c_v} k^2 S_k^+, \tag{33}$$

$$\dot{S}_k^- = \frac{1}{h} [S_k^-, \mathcal{H}] = \frac{\lambda}{c_v} k^2 S_k^-. \tag{34}$$

Using these equations the temperature operator is

$$\mathcal{T} = \sum_k 2 \sqrt{\frac{1}{V}} (C_k^+ \cos kx + S_k^+ \sin kx). \tag{35}$$

Let us define a new operator $\mathcal{X}$ for the theory

$$\mathcal{X} = \sum_k 2 \sqrt{\frac{1}{V}} \frac{c_v}{\lambda} k (S_k^- \cos kx - C_k^- \sin kx). \tag{36}$$

If we calculate the following integral:

$$\int \mathcal{T} \mathcal{X} \, dV = \sum_k \frac{2c_v}{\lambda} k (S_k^- C_k^+ - C_k^- S_k^+), \tag{37}$$

we recognize the current operator $\mathcal{J}$ on the right-hand side. Now, in this manner we are able to introduce the inverse of the temperature operator

$$\mathcal{T}^{-1} = \frac{\mathcal{X}}{|\,\mathcal{J}\,|} = \sum_k 2 \sqrt{\frac{1}{V}} \frac{c_v k}{\lambda \,|\,\mathcal{J}\,|} (S_k^- \cos kx - C_k^- \sin kx). \tag{38}$$

This operator is neccessary and important when expressing the classical entropy production density [23] in the operator formalism. In this way, this operator can be formulated

$$\sigma = \lambda \nabla \mathcal{T}^{-1} \nabla \mathcal{T}^{-1}, \tag{39}$$

i.e.,

$$\sigma = \lambda \left[\sum_k 2 \sqrt{\frac{1}{V}} \frac{c_v k^2}{\lambda \,|\,\mathcal{J}\,|} (-S_k^- \sin kx - C_k^- \cos kx) \right] \times \left[\sum_l 2 \sqrt{\frac{1}{V}} \frac{c_v l^2}{\lambda \,|\,\mathcal{J}\,|} (-S_l^- \sin lx - C_l^- \cos lx) \right]. \tag{40}$$

If we integrate over the volume we get the entropy production operator of the infinite field

$$\Sigma = \sum_k \frac{2c_v^2 k^4}{\lambda \,|\,\mathcal{J}\,|^2} (C_k^- C_k^- + S_k^- S_k^-). \tag{41}$$

This operator contains only annihilation operators. Let Ψ be an eigenfunction of $\mathcal{H}$ with the eigenvalue α

$$\mathcal{H}\Psi = \alpha \Psi. \tag{42}$$

It is easy to prove that $\Sigma\Psi$ is an eigenfunction of $\mathcal{H}$

$$\mathcal{H}\Sigma\Psi = \left(\alpha - \frac{2\lambda}{c_v} k^2 h \right) \Sigma\Psi \tag{43}$$

with the eigenvalue $\alpha - \frac{2\lambda}{c_v} k^2 h$. This means that the entropy production operator decreases the state in steps

$$\frac{2\lambda}{c_v} k^2 h. \tag{44}$$

While the system tends to the equilibrium state, the entropy production decreases with these quanta.

V. CONSEQUENCES

The present paper shows that the concept of quantization can be introduced into an irreversible process with the help of a scalar field using Hamilton-Lagrange formalism. However, this is not simply the quantization problem of a free scalar field because Fourier's heat equation contains a non-self-adjoint operator and pertains to a nonconservative field. We go through the mathematical method step by step and we obtain the Hamiltonian, temperature, and entropy production operator. The internal energy operator is equivalent to the temperature operator $\mathcal{E} = c_v \mathcal{T}$, and this indicates that we have obtained discrete energy levels. The interesting thing is that we can increase or decrease the energy density in steps with the Newtonian and/or non-Newtonian work. We think this may be the key to studying the interaction and overlapping of different (without respect to the reversible or irreversible) disciplines of physics. We probably have a good opportunity to link, e.g., the thermal and electromagnetic fields. In this way we can speak about nonequilibrium heat radiation.

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