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Quantized heat transport in small systems: A phenomenological approach

F. Vázquez,[1,*] F. Márkus,[1,†] and K. Gambár[2,‡]
[1]*Department of Physics, Budapest University of Technology and Economics, Budafoki út 8, H-1521 Budapest, Hungary*
[2]*Department of Atomic Physics, Roland Eötvös University, Pázmány Péter sétány 1/A, H-1117 Budapest, Hungary*

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Recent progress in nanoscale materials science has pushed the basic research on physical effects while going to such length scales. Particularly, the study of size effects on heat conductivity has attracted much theoretical and experimental interest. In this work we explore the possibilities to study such kinds of phenomena through the quantization of the dynamic equations of a class of nonlinear heat transport macroscopic models. We develop a quantization procedure to search the energy level structure of one-dimensional nanosystems. The procedure may have applications in other fields of the physics of mesoscopic systems.

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I. INTRODUCTION

The heat transport problem in small systems with the characteristic mean free path of the energy carriers being comparable with the system's dimensions has attracted the interest of both theoretical and experimental researchers [1–8]. The quantization nature of heat transport phenomena at such length scales was shown by the measurement by Schwab *et al.* [9] of the maximum energy value transported per phonon mode in phonon waveguides in the ballistic, one-dimensional limit. For each transmission mode the quantum of thermal conductance g_0 depends directly of the temperature as [10–12]

$$g_0 = \frac{\pi^2 k_B^2 T}{3h}. \tag{1}$$

The quantum character of the heat conductance is obtained with different methods to calculate the phonon transmission coefficients [13,14].

The influence of the size sample on the heat conductivity has been particularly analyzed from different macroscopic approaches. Within the extended irreversible thermodynamics framework, Alvarez and Jou [15,16] found a theoretical size-dependent thermal conductivity and fitted it to well established experimental and numerical measurements of the heat conductivity in nanodevices. The model was obtained (by including nonlocal and memory effects) through the continued-fraction expression of a wave number and frequency-dependent effective thermal conductivity. Some approaches have proposed two kinds of contributions to heat transport, namely, a ballistic part and a diffusive one [15,17] allowing to deal with the nanoscale and the macroscopic length.

In this paper we introduce the quantization of macroscopic models of heat transport in small systems. It is not known to what extent quantized macroscopic theories of heat conduction can give information on the transport properties of small systems and questions concerning the interpretation of the quantized values of energy arising from such theoretical formalisms remain to be answered. It is claimed that they can similarly be applied not only to solid as to noncrystalline disordered materials such as gases and liquids but also to the several length scales between nanoscale and macroscopic scale. Two of us have been working in this direction since some years ago. The simple case of one-dimensional linear heat conduction (Fourier transport) was discussed in [18–20]. Through this series of works it has been outlined the canonical quantization of dissipative processes. Here, we address a class of nonlinear heat transport models to make a connection with some of the recent results on the quantum features of the dissipative energy conduction in small systems [9,21]. We are interested in the general problem of the structure of the energy levels as predicted by nonlinear macroscopic heat conduction theories. The nonlinear properties of small systems pose new mathematical challenges to the quantization process. Our aim is to sketch a way to deal with them. We start in Sec. II by assuming a heat conductivity depending on the size of the sample. Then we introduce a Lagrangian formalism that contains the nonlinearities of the dissipative transport of energy introduced by the space-dependent heat conductivity. In Sec. III we establish the basic steps to canonically quantize the classical temperature field derived from the nonlinear transport equations of Sec. II. A key step is the definition of the commutation rules of the basic conjugated variables that determine all the subsequent quantization procedure. We take the quantum of the action, denoted by h^*, which has been determined in a previous paper [20]. In Sec. IV we study a one-dimensional two-level system to illustrate the use of the formalism. We use Alvarez and Jou's results [15] to calculate the heat conductivity distribution in a discrete set of heat conductors. We end the paper with some comments and a conclusion.

II. LAGRANGIAN FORMALISM OF NONLINEAR HEAT TRANSPORT

On the way toward the canonical quantization procedure first we need to find the Hamiltonian formulation of the non-

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[*] Corresponding author. On sabbatical leave from Departamento de Física, Facultad de Ciencias, Universidad de Morelos, México; vazquez@buzon.uaem.mx

[†] markusferi@tvn.hu; markus@phy.bme.hu

[‡] gakati@gmail.com; gambar@ludens.elte.hu

linear heat equation. We show how the field equation (equation of motion), the Lagrangian, the canonically conjugated variables, and the Hamiltonian can be obtained [19].

We start from the source- and convective-free heat transport which is described by the balance equation of the internal energy u, $\partial u/\partial t + \mathrm{div}\,\mathbf{J}_q = 0$, taking into account the internal energy current density $\mathbf{J}_q$. The temperature T can be introduced to the description taking into account the caloric equation (density $\varrho = 1$) $du = c_v dT$, and the constitutive Fourier law $\mathbf{J}_q = -\lambda\,\mathrm{grad}\,T$.

Here, c_v is the specific heat and λ is the heat conductivity. By combining the mentioned equations we find the basic transport equation

$$c_v(\mathbf{r},T)\frac{\partial T}{\partial t} - \mathrm{grad}\,\lambda(\mathbf{r},t,T)\mathrm{grad}\,T - \lambda(\mathbf{r},t,T)\Delta T = 0, \quad (2)$$

where it has been assumed the most general dependence of the coefficients c_v and λ on the space-time and the temperature field. We remind the reader briefly that in the special case $c_v = \mathrm{const}$ and $\lambda = \mathrm{const}$, the well-known transport equation $c_v \partial T/\partial t = \lambda \Delta T$ is obtained.

In the further examination we restrict ourselves to the one-dimensional case, and we consider the coefficients $c_v = \mathrm{const}$ and $\lambda = \lambda(x)$. The $\lambda(x)$ is taken as a given function of the space variable x; this restriction is important in the application of variational calculus. We define the potential field φ by the following relation with the temperature [19,22]

$$T = -c_v\frac{\partial \varphi}{\partial t} - \mathrm{grad}\,\lambda\;\mathrm{grad}\,\varphi - \lambda\Delta\varphi.$$

Now we take the functional

$$L = \frac{1}{2}\left(c_v\frac{\partial\varphi}{\partial t}\right)^2 + \frac{1}{2}(\mathrm{grad}\,\lambda\;\mathrm{grad}\,\varphi + \lambda\Delta\varphi)^2$$

as the Lagrangian density.

By abbreviating the differentiating operations as follows $\frac{\partial}{\partial t}\to\dot{}\,$, $\frac{\partial}{\partial x}\to{}'$, the functional L can be written as

$$L = \frac{1}{2}c_v^2\dot{\varphi}^2 + \frac{1}{2}(\lambda'\varphi' + \lambda\varphi'')^2. \quad (3)$$

The Fourier's equation as Euler-Lagrange equation expressed by the potential φ becomes $0 = -c_v^2\ddot{\varphi} + \lambda'(\lambda'\varphi' + \lambda\varphi'')' + \lambda(\lambda'\varphi' + \lambda\varphi'')''$, i.e.,

$$0 = -c_v^2\ddot{\varphi} + [\lambda(\lambda\varphi')'']'. \quad (4)$$

Substituting the temperature $T = -c_v\dot{\varphi} - \lambda'\varphi' - \lambda\varphi'' = -c_v\dot{\varphi} - (\lambda\varphi')'$ we get the heat equation [Eq. (2) in the case in which $c_v = \mathrm{const}$ and $\lambda = \lambda(x)$]. Finally, the heat transport equation takes the form

$$c_v\dot{T} - (\lambda T')' = 0.$$

Now we define the conjugated momentum related to the potential field φ as

$$P = \frac{\partial L}{\partial\dot{\varphi}} = c_v^2\dot{\varphi}. \quad (5)$$

The Hamiltonian density is easily obtained as usual

$$H = P\dot{\varphi} - L = \frac{1}{2c_v^2}P^2 - \frac{1}{2}[(\lambda\varphi')']^2 \quad (6)$$

or

$$H = \frac{1}{2}\left[\frac{1}{c_v}P + (\lambda\varphi')'\right]\left[\frac{1}{c_v}P - (\lambda\varphi')'\right]. \quad (7)$$

Generally, to achieve the operator formulation it is needed to calculate the Hamiltonian in that form which can be expressed as a product like in Eq. (7) (for linear heat conduction [18]).

III. CANONICAL QUANTIZATION PROCEDURE

In this section we generalize the quantization procedure of parabolic differential Eq. (18) for the nonlinear heat equation based on the Lagrangian formalism of Sec. II. In the previous work [18] we have shown for the linear case that by expressing the potential field φ in Fourier series and integrating the Hamiltonian density over the whole space, the Hamiltonian of the whole space can be expressed by the Fourier coefficients. Since the Hamiltonian density can be written as a product like in Eq. (7), the global Hamiltonian can consequently be given as a quadratic form by the Fourier coefficients, thus allowing us to introduce the operator formalism, i.e., the creation, the annihilation and the number operators can be constructed. Finally, the quantum number operators and the quanta appear in the description. In the present work the reader can follow the whole extended formulation for the nonlinear case in which the linear case is also involved, naturally.

Presently, the difficulty is in the space dependence of the heat conductivity. We show a simplified calculus (simplified in the sense of the approximation of heat conductivity), but later we point out that the whole procedure can be widened and applied for more general cases.

First, we consider the following expansions for the quantities φ and λ,

$$\varphi(x) = \sum_{l=0}^{\infty}\sqrt{\frac{2}{V}}(C_l\cos lx + S_l\sin lx),$$

$$\lambda(x) = \sum_{n=0}^{\infty}(A_n\cos nx). \quad (8)$$

In fact, we are assuming that the potential and the heat conductivity can be approximated by Fourier's series. (The last one is also a part of a Fourier series, but now we show the procedure with this reduced form for the sake of simplifying the mathematical expressions. This simplification does not destroy the essence of the quantization procedure.)

Accepting this condition, accordingly with Eq. (5), the conjugated momentum becomes

$$P = c_v^2\dot{\varphi}(x) = c_v^2\sum_{l=0}^{\infty}\sqrt{\frac{2}{V}}(\dot{C}_l\cos lx + \dot{S}_l\sin lx).$$

The first term of the Lagrangian given by Eq. (3) integrated in the total volume is

$$\int_{\text{all space}} \frac{1}{2} c_v^2 \dot{\varphi}^2 dV = \frac{1}{2} c_v^2 \sum_{l=0}^{\infty} (\dot{C}_l^2 + \dot{S}_l^2).$$

We can define the following canonically conjugated momenta to C_l and S_l:

$$P_l^{(C)} = c_v^2 \dot{C}_l,$$

$$P_l^{(S)} = c_v^2 \dot{S}_l. \tag{9}$$

The first term of the Hamiltonian by Eq. (6) integrated in the total volume:

$$\int_{\text{all space}} \frac{1}{2c_v^2} P^2 dV = \frac{1}{2c_v^2} \sum_{l=0}^{\infty} (P_l^{(C)^2} + P_l^{(S)^2}). \tag{10}$$

To obtain the second term of the Hamiltonian Eq. (6) we need to calculate:

$$\begin{aligned}\frac{1}{2}[(\lambda\varphi')']^2 = {} & \frac{1}{2}\sum_{n,m,l,p=0}^{\infty} A_n A_m l^2 p^2 \cos(nx)\cos(mx)[C_l C_p \cos(lx)\cos(px) + C_l S_p \cos(lx)\sin(px) + C_p S_l \sin(lx)\cos(px) \\ & + S_l S_p \sin(lx)\sin(px)] + \frac{1}{2}\sum_{n,m,l,p=0}^{\infty} A_n A_m lp \sin(nx)\sin(mx)[C_l C_p \sin(lx)\sin px - C_l S_p \sin(lx)\sin(px) \\ & - C_p S_l \cos(lx)\sin(px) + S_l S_p \cos(lx)\cos(px)] - \sum_{n,m,l,p=0}^{\infty} A_n A_m l p^2 m \cos(nx)\sin(mx)[- C_l C_p \sin(lx)\cos px \\ & - C_l S_p \sin(lx)\sin(px) + C_p S_l \cos(lx)\cos(px) + S_l S_p \cos(lx)\sin(px)].\end{aligned} \tag{11}$$

As it stands, this complicated expression involves crossed terms such as $C_l C_p$, $C_l S_p$, etc. Nevertheless, in the present $\lambda(x)$ dependence given by Eq. (8), the integration over the whole space eliminates all the terms of the form $C_l S_p$, and a basis change can always transform the bilinear form Eq. (11) into a quadratic bilinear form. This procedure will be illustrated in Sec. IV with a specific example. We have assumed the above simple expansion [Eq. (8)] for the heat conductivity in order to eliminate crossed terms in the integration, but mention must be made that we can handle such kinds of terms by carrying out a more complicated diagonalization procedure. The expression of the Hamiltonian density after the diagonalization and basis change has then the form

$$\begin{aligned}H = \frac{1}{2}\sum_{k=1}^{\infty} \Bigg(& \frac{1}{c_v^2} P_k'^{(C)^T} \mathbf{M}^{P'^{(C)}} P_k'^{(C)} + \frac{1}{c_v^2} P_k'^{(S)^T} \mathbf{M}^{P'^{(S)}} P_k'^{(S)} \\ & - C_k'^{T} \mathbf{M}^{C'} C_k' - S_k'^{T} \mathbf{M}^{S'} S_k' \Bigg),\end{aligned} \tag{12}$$

having been the vectors and matrices transformed under the operations $\mathbf{D}C$, $\mathbf{D}S$ and $\mathbf{D}^T\mathbf{M}\mathbf{D}$, respectively, $\mathbf{D}$ is the diagonalizing matrix and the superscript T denotes the transposed vector or matrix. We note that the lower limit in the summation of Eq. (12) has been changed to 1 because for $l=p=0$ the term $\frac{1}{2}[(\lambda\varphi')']^2$ vanishes [see Eq. (11)]. Moreover, the $0-0$ element of matrices $\mathbf{M}^{C'}$ and $\mathbf{M}^{S'}$ also vanish and, as will be seen below, the operators $\mathbf{C}_0^-$, $\mathbf{C}_0^+$ and $\mathbf{S}_0^-$, $\mathbf{S}_0^+$ commute, respectively.

We now introduce a set of operators $\mathbf{C}_k$, $\mathbf{P}_k^{(C)}$ and $\mathbf{S}_k$, $\mathbf{P}_k^{(S)}$ associated to the dynamic conjugated variables C_k', $P_k'^{(C)}$ and S_k', $P_k'^{(S)}$ which obey the following commutation rules: $[\mathbf{P}_k^{(C)}, \mathbf{C}_l] = h^* \delta_{kl}$ and $[\mathbf{P}_k^{(S)}, \mathbf{S}_l] = h^* \delta_{kl}$, with h^* the quantum of the action which takes the value $2h_p/k_B$ (h_p is the Planck constant; k_B is the Boltzmann constant) [20]. Each pair of noncommuting conjugated variables obeys an uncertainty relation

$$\Delta C_k' \Delta P_k'^{(C)} \geq \int_{\text{all space}} \langle [\mathbf{P}_k^{(C)}, \mathbf{C}_k] \rangle_{\psi} dV,$$

$$\Delta S_k' \Delta P_k'^{(S)} \geq \int_{\text{all space}} \langle [\mathbf{P}_k^{(S)}, \mathbf{S}_k] \rangle_{\psi} dV,$$

where

$$\int_{\text{all space}} \langle [\mathbf{P}_k^{(C)}, \mathbf{C}_k] \rangle_{\psi} dV = \int_{\text{all space}} \langle [\mathbf{P}_k^{(S)}, \mathbf{S}_k] \rangle_{\psi} dV = h^*.$$

At this step we define the operators

$$\mathbf{C}_k^{\pm} = \frac{1}{c_v} \sqrt{\frac{1}{2} \mathbf{M}_{kk}^{P^{(C)}}} \mathbf{P}_k^{(C)} \pm \sqrt{\frac{1}{2} \mathbf{M}_{kk}^{C}} \mathbf{C}_k$$

and

$$\mathbf{S}_k^{\pm} = \frac{1}{c_v} \sqrt{\frac{1}{2} \mathbf{M}_{kk}^{P^{(S)}}} \mathbf{P}_k^{(S)} \pm \sqrt{\frac{1}{2} \mathbf{M}_{kk}^{S}} \mathbf{S}_k.$$

Comparing the matrices in these equations with the matrices in Eq. (12) we can see: $\mathbf{M}_{kk}^{P^{(C)}} \to \mathbf{M}^{P'^{(C)}}$; $\mathbf{M}_{kk}^{C} \to \mathbf{M}^{C'}$; $\mathbf{M}_{kk}^{P^{(S)}} \to \mathbf{M}^{P'^{(S)}}$; $\mathbf{M}_{kk}^{S} \to \mathbf{M}^{S'}$. After this, it can then be verified that the Hamiltonian density operator reads

$$\mathbf{H} = \frac{1}{2}\sum_{k=1}^{\infty}(\mathbf{C}_k^+\mathbf{C}_k^- + \mathbf{C}_k^-\mathbf{C}_k^+ + \mathbf{S}_k^+\mathbf{S}_k^- + \mathbf{S}_k^-\mathbf{S}_k^+).$$

The commutation rules for the operators $\mathbf{C}_k^{\pm}$ and $\mathbf{S}_k^{\pm}$ must be

$$[\mathbf{C}_k^-,\mathbf{C}_l^+] = \frac{1}{2c_v}\sqrt{\mathbf{M}_{kk}^{P(C)}\mathbf{M}_{ll}^C}h^*\delta_{kl} \tag{13}$$

and

$$[\mathbf{S}_k^-,\mathbf{S}_l^+] = \frac{1}{2c_v}\sqrt{\mathbf{M}_{kk}^{P(S)}\mathbf{M}_{ll}^S}h^*\delta_{kl}. \tag{14}$$

In order to build in the quantum occupation number operator it is necessary first to specify four additional operators

$$\mathbf{N}_k^{(C)\pm} = \frac{2c_v}{h^*\sqrt{\mathbf{M}_{kk}^{P(C)}\mathbf{M}_{kk}^C}}\mathbf{C}_k^{\pm}\mathbf{C}_k^{\mp}$$

and

$$\mathbf{N}_k^{(S)\pm} = \frac{2c_v}{h^*\sqrt{\mathbf{M}_{kk}^{P(S)}\mathbf{M}_{kk}^S}}\mathbf{S}_k^{\pm}\mathbf{S}_k^{\mp}.$$

Then the quantum occupation number operator $\mathbf{N}_k$ becomes

$$\mathbf{N}_k = \frac{1}{2}(\mathbf{b}_k^+\mathbf{b}_k^- + \mathbf{b}_k^-\mathbf{b}_k^+),$$

where the operators $\mathbf{b}_k^{\pm}$ are the creation and annihilation operators as it will be shown below. They are given by the relations

$$\mathbf{b}_k^+\mathbf{b}_k^- = \frac{1}{2}(\mathbf{N}_k^{(C)+} + \mathbf{N}_k^{(S)+}), \quad \text{and} \quad \mathbf{b}_k^-\mathbf{b}_k^+ = \frac{1}{2}(\mathbf{N}_k^{(C)-} + \mathbf{N}_k^{(S)-}).$$

Note that

$$[\mathbf{b}_k^-,\mathbf{b}_l^+] = \delta_{kl}, \tag{15}$$

accordingly with the commutation rules Eqs. (13) and (14).

We define the energy operator of the thermal field as $\mathbf{E} = \Sigma_k \mathbf{E}_k$, with

$$\mathbf{E}_k = \frac{1}{c_v}(\sqrt{\mathbf{M}_{kk}^{P(C)}\mathbf{M}_{kk}^C} + \sqrt{\mathbf{M}_{kk}^{P(S)}\mathbf{M}_{kk}^S})h^*\mathbf{N}_k. \tag{16}$$

Observe that the Hamiltonian operator can now be written in terms of the creation and annihilation operators as follows:

$$\mathbf{H} = \sum_k \frac{h^*}{c_v}(\sqrt{\mathbf{M}_{kk}^{P(C)}\mathbf{M}_{kk}^C} + \sqrt{\mathbf{M}_{kk}^{P(S)}\mathbf{M}_{kk}^S})(\mathbf{b}_k^+\mathbf{b}_k^- + \mathbf{b}_k^-\mathbf{b}_k^+). \tag{17}$$

When applied to the eigenstate $|n_k\rangle$ the occupation number operator gives

$$\mathbf{N}_k|n_k\rangle = \frac{1}{2}(\mathbf{b}_k^+\mathbf{b}_k^- + \mathbf{b}_k^-\mathbf{b}_k^+)|n_k\rangle = n_k|n_k\rangle,$$

moreover,

$$\mathbf{N}_k\mathbf{b}_k^{\pm}|n_k\rangle = (n_k \pm 1)|n_k\rangle.$$

In this way, we have that $\mathbf{b}_k^+$ and $\mathbf{b}_k^-$ are the creation and the annihilation operators, respectively.

The ground state $|\mathrm{Gr}\rangle$ is defined as the state which is annihilated by all the operators $\mathbf{b}_k^-$, i.e., $\mathbf{b}_k^-|\mathrm{Gr}\rangle = 0$. The effect of the Hamiltonian operator, Eq. (17), on the ground state can be obtained if the Hamiltonian is written, as usual, in ordered form

$$\mathbf{H} = :\mathbf{H}: + E_{\mathrm{Gr}},$$

where

$$:\mathbf{H}: = \sum_k \frac{2h^*}{c_v}(\sqrt{\mathbf{M}_{kk}^{P(C)}\mathbf{M}_{kk}^C} + \sqrt{\mathbf{M}_{kk}^{P(S)}\mathbf{M}_{kk}^S})\mathbf{b}_k^+\mathbf{b}_k^-,$$

and

$$E_{\mathrm{Gr}} = \sum_k \frac{h^*}{c_v}(\sqrt{\mathbf{M}_{kk}^{P(C)}\mathbf{M}_{kk}^C} + \sqrt{\mathbf{M}_{kk}^{P(S)}\mathbf{M}_{kk}^S}). \tag{18}$$

Then $\mathbf{H}|\mathrm{Gr}\rangle = E_{\mathrm{Gr}}|\mathrm{Gr}\rangle$, E_{Gr} being the energy of the ground state. If we apply the energy operator $\mathbf{E}$ to the ground state we should obtain the value E_{Gr}. Observe that this is the case if the ground state is $|\mathrm{Gr}\rangle = |1_1 1_2 1_3 \ldots\rangle$ since, accordingly with Eq. (16),

$$\begin{aligned}\mathbf{E}|\mathrm{Gr}\rangle &= \sum_k \frac{h^*}{c_v}(\sqrt{\mathbf{M}_{kk}^{P(C)}\mathbf{M}_{kk}^C} + \sqrt{\mathbf{M}_{kk}^{P(S)}\mathbf{M}_{kk}^S})|1_1\ 1_2\ 1_3 \ldots\rangle \\ &= E_{\mathrm{Gr}}|\mathrm{Gr}\rangle.\end{aligned}$$

The ground state is so characterized by the presence of one quantum of energy in each energy level $k = 1, 2, 3, \ldots$

Finally, we can calculate the energy which excites the ground state by considering the two quanta state $|2_k\rangle = |1_1 1_2 \ldots 2_k \ldots\rangle = \mathbf{b}_k^+|\mathrm{Gr}\rangle$. We let the Hamiltonian operator $\mathbf{H}$ to act over $|2_k\rangle$ as follows:

$$\begin{aligned}\mathbf{H}|2_k\rangle &= \mathbf{E}_{2,k}\mathbf{b}_k^+|\mathrm{Gr}\rangle \\ &= \left[\sum_{k'} \frac{2h^*}{c_v}(\sqrt{\mathbf{M}_{k'k'}^{P(C)}\mathbf{M}_{k'k'}^C} + \sqrt{\mathbf{M}_{k'k'}^{P(S)}\mathbf{M}_{k'k'}^S})\mathbf{b}_{k'}^+\mathbf{b}_{k'}^-\right. \\ &\quad \left. + E_{\mathrm{Gr}}\right]\mathbf{b}_k^+|\mathrm{Gr}\rangle = \left[\frac{2h^*}{c_v}(\sqrt{\mathbf{M}_{kk}^{P(C)}\mathbf{M}_{kk}^C} + \sqrt{\mathbf{M}_{kk}^{P(S)}\mathbf{M}_{kk}^S})\right. \\ &\quad \left. + E_{\mathrm{Gr}}\right]|2_k\rangle,\end{aligned}$$

where we used Eq. (15), the relation $\mathbf{b}_{k'}^-\mathbf{b}_k^+ = [\mathbf{b}_{k'}^-, \mathbf{b}_k^+] + \mathbf{b}_k^+\mathbf{b}_{k'}^-$, and the fact that $\mathbf{b}_{k'}^-|1_k\rangle = 0$. Then $\mathbf{E}_{2,k}$, the energy of the two quanta energy level k, is given by

$$\mathbf{E}_{2,k} = \frac{2h^*}{c_v}(\sqrt{\mathbf{M}_{kk}^{P(C)}\mathbf{M}_{kk}^C} + \sqrt{\mathbf{M}_{kk}^{P(S)}\mathbf{M}_{kk}^S}) + E_{\mathrm{Gr}}.$$

The necessary energy for the system jumps to the k energy level, the excitation energy ϵ_k, is therefore

$$\epsilon_k = \frac{2h^*}{c_v}(\sqrt{\mathbf{M}_{kk}^{P(C)}\mathbf{M}_{kk}^C} + \sqrt{\mathbf{M}_{kk}^{P(S)}\mathbf{M}_{kk}^S}). \tag{19}$$

The excitation energy ϵ_k given by this equation is the minimum energy to be introduced to the system to change

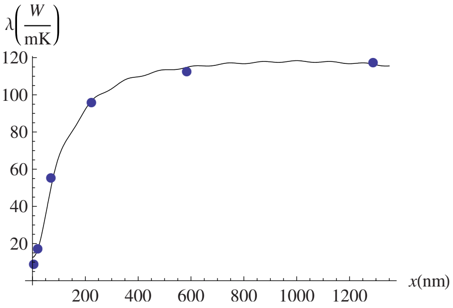

FIG. 1. (Color online) Thermal conductivity (λ) in W/mK versus the position x within the system constituted by conductor subsystems in thermal contact. Solid line is the 16 coefficients model for λ. The points are the heat conductivity of the conductor subsystems plotted at the middle point of each one. The sequence of subsystem sizes was generated through the relation $L_i=L_1+i^{2.8}\Delta L$, with $L_1=0.1\times10^{-7}$ m and $\Delta L=0.1\times10^{-7}$ m. Other parameters are $\lambda_0=115$ W/mK and $l=40$ nm which correspond to silicon.

the energy to a higher value and to reach the successive excited states above the ground state. The distribution function of the quantum occupation numbers in each energy level depends on the specific external constrictions imposed to the system and particularly on its size.

IV. NONLINEAR HEAT CONDUCTION IN TWO-LEVEL SYSTEMS

In this section we give an example of the previous formalism to calculate the lowest two excitation energies in a mesoscopic system in the nanolength scale. As usual in any macroscopic theory, some external information must be supplied to get a complete physical description. We remind the reader that such extra input is the Fourier expansion of λ in Eq. (8). Let us then consider a one-dimensional heat conductor constituted by N conductor "subsystems" in thermal contact with lengths L_i ($L_i<L_{i+1}$) for $i=1,\ldots,N$ in x direction and unitary area in the y-z plane. Each subsystem is considered homogeneous with x-size dependent heat conductivity $\lambda_i=\lambda(L_i)$ given by [15]

$$\lambda(L)=\frac{\lambda_0L^2}{2\pi^2l^2}\left[\sqrt{1+4\pi^2K_n^2}-1\right],\qquad(20)$$

where λ_0 is the bulk heat conductivity, l the mean free path of the heat carriers, L the size of each subsystem and the Knudsen number is defined as $\mathrm{K_n}=l/L$. We obtain the heat conductivity as a continuous function of position x by taking into account the first 16 terms in the Fourier expansion, Eq. (8). Let x_i be the middle point of subsystem L_i given by $x_i=L_1+L_2+\ldots+L_i/2$, where $i=2,\ldots,N$ and $x_1=L_1/2$. We then assign $\lambda(x_i)=\lambda_i$, and we fit coefficients A_n in the Fourier expansion to the values of the conductivity of the subsystems as a function of the position. The fitted curve obtained from Eq. (8) is shown in Fig. 1. Dots are the heat conductivity of the subsystems plotted at the middle point of each one. The following are the numerical values of the Fourier coefficients: $A_0=101.7$ W/mK, $A_1=-26.1$ W/mK, $A_2=-16.8$ W/mK, $A_3=-11.7$ W/mK, $A_4=-8.2$ W/mK, $A_5=-6.0$ W/mK, $A_6=-4.5$ W/mK, $A_7=-3.5$ W/mK, $A_8=-2.7$ W/mK, $A_9=-2.2$ W/mK, $A_{10}=-1.8$ W/mK, $A_{11}=-1.5$ W/mK, $A_{12}=-1.3$ W/mK, $A_{13}=-1.1$ W/mK, $A_{14}=-0.9$ W/mK, and $A_{15}=-0.8$ W/mK. We have taken $c_v=10^2$ J/kg K which corresponds to silicon at 50 K [23].

We now assume that only two energy levels $k=1,2$ are being occupied in each subsystem of the system. Of course, this restrictive assumption would require to be examined in terms of the distribution of the occupation numbers in the different energy levels k, but this distribution is unknown at the present stage. It will be a subject of further research. This preliminary assumption is made for the sake of simplicity and only to display an illustrative case. Nevertheless, as it will be seen, the results may have a physical sense when compared with experimental results on the quantum of heat conductance. Summing then the subindexes n and m from 0 to 15, subindexes l and p from 1 to 2 and integrating over the whole space we get from Eq. (11) an expression containing terms that are proportional to C_1C_2 and S_1S_2, but not so for terms that are proportional to C_1S_2, C_2S_2, etc. This expression can be written in matrix notation as that displayed in Eq. (12). As mentioned in Sec. III, the whole bilinear form can be transformed in a quadratic bilinear form by diagonalizing the matrices $\mathbf{M}_C$ and $\mathbf{M}_S$ and with the help of Eq. (10). The quadratic bilinear form of the Hamiltonian takes then the form

$$\begin{aligned}H=\frac{1}{2c_v^2}\Bigg[&(P_1'^{(C)}\quad P_2'^{(C)})\mathbf{M}_{P(C)}^D\begin{pmatrix}P_1'^{(C)}\\P_2'^{(C)}\end{pmatrix}\\&+(P_1'^{(S)}\quad P_2'^{(S)})\mathbf{M}_{P(S)}^D\begin{pmatrix}P_1'^{(S)}\\P_2'^{(S)}\end{pmatrix}\Bigg]+(C_1'\quad C_2')\mathbf{M}_C^D\begin{pmatrix}C_1'\\C_2'\end{pmatrix}\\&+(S_1'\quad S_2')\mathbf{M}_S^D\begin{pmatrix}S_1'\\S_2'\end{pmatrix}.\end{aligned}\qquad(21)$$

Here, the matrices $\mathbf{M}_C^D$ and $\mathbf{M}_S^D$ the transformed vectors

$$(P_1'^{(C)}\quad P_2'^{(C)}),\quad(P_1'^{(S)}\quad P_2'^{(S)}),$$

$$(C_1'\quad C_2')\ \text{and}\ (S_1'\quad S_2'),$$

depend on the coefficients A_0, $A_1,\ldots,A_{15}$ and the transformed vectors additionally depend on the nonprimed vectors. It must be said that in the limit $A_1,A_2,\ldots\to0$, we recover all the results for the case in which $\lambda=$const given in [18].

The matrices in Eq. (21) are then

$$\mathbf{M}_{P(C)}^D=\begin{pmatrix}1&0\\0&1\end{pmatrix},\quad\mathbf{M}_{P(S)}^D=\begin{pmatrix}1&0\\0&1\end{pmatrix},$$

$$\mathbf{M}_C^D=\begin{pmatrix}0.015&0\\0&0.20\end{pmatrix},\quad\mathbf{M}_S^D=\begin{pmatrix}0.013&0\\0&0.019\end{pmatrix},$$

and the transformed vectors are shown in the Appendix. We use Eq. (19) to calculate the two first excitation energies of the system. The result is $\epsilon_1=6.969\times10^{-14}$ J and $\epsilon_2=1.8293\times10^{-13}$ J. We can compare them with the energy density of the bulk, which can be considered on the order of $E_b=10^4$ J/m^3. This approximated value for the energy density has been calculated by using the known relation $E = \varrho c_v T$ and considering that the mass density for silicon is 2329 $\mathrm{kg/m^3}$ and that the sample has a temperature of $\sim 10^{-2}$ K. Observe that for a nanofilm sample size of about 100 nm length and 10^{-6} $\mathrm{m^2}$ cross section with a 10^{-13} $\mathrm{m^3}$ volume, the difference in the order of magnitude with respect to the calculated excitation energies is 10^5. This ratio is displayed only to give a comparative insight of the magnitude of excitation energies with respect of the energy of the bulk. From the expression for the universal quantum of conductance given by Schwab *et al.*, Eq. (1), we can obtain the energy transferred per unit temperature difference and unit time, $\epsilon = 7.582 \times 10^{-14}$ J. In order to get this we have taken the value 8×10^{-2} K for the temperature T to satisfy the saturation condition ($T \ll T_\infty = 8 \times 10^{-1}$ K) for which the measured thermal conductance equals 16 times the quantum of conductance g_0 in the experiments described in Ref. [9]. For temperatures $T \ll T_\infty$ the measured thermal conductance is not dependent on any other physical or geometric parameters. Note the similarity of the energy ϵ with the minimum excitation energy ϵ_1 of the first energy level given by our quantized formalism. It must be mentioned that this agreement does depend on the temperature of the system since the quantum of the conductance g_0 depends on it. In the present formalism we have considered the specific heat c_v as a constant. A possibility to elucidate how critical with respect to temperature is the agreement of our results with the experimental data is to assume that c_v depends on temperature. This point is left to future research.

V. SUMMARY AND CONCLUSION

We have developed a procedure to quantize the energy of a nonlinear thermal system by using an analogous but modified technique to the canonical quantization method of classical mechanics. The nonlinearity of the system was introduced through the heat conductivity. The set of quantum operators obey commutation rules which were written in terms of the quantum of the action $h^* = 2h/k_B$ [20]. We defined the lowest energy state, the ground state $|\mathrm{Gr}\rangle$, as that for which $\mathbf{b}_k^- |\mathrm{Gr}\rangle = 0$, being $\mathbf{b}_k^-$ the quantum annihilation operator. The ground energy was found to be given by

$$E_{\mathrm{Gr}} = \sum_k \frac{h^*}{c_v} \left(\sqrt{\mathbf{M}_{kk}^{P^{(C)}} \mathbf{M}_{kk}^{C}} + \sqrt{\mathbf{M}_{kk}^{P^{(S)}} \mathbf{M}_{kk}^{S}} \right),$$

where the matrix elements $\mathbf{M}_{kk}$ depend on the coefficients of the Fourier expansion of the nonlinear heat conductivity of the system. We have given an example of the application of the formalism to a nanosized system. We were able to calculate the energies to get the excited states of the system. Our main result concerns the structure of quantized energy levels. The system has a ground energy E_{Gr} which, for the two-level case studied in Sec. IV, has the value 2.5262×10^{-13} J, and successive excited levels given by $E_{\mathrm{Gr}} + \epsilon_1$, $E_{\mathrm{Gr}} + \epsilon_2, \ldots$, etc. These energy levels are got by the system through thermal interactions with the surroundings.

We have found a value for the minimum excitation energy $\epsilon_1 (= 6.969 \times 10^{-14}$ J) reasonably similar in magnitude to that of the energy of the measured thermal conductance (7.582×10^{-14} J) from Ref. [9]. This makes the quantization method developed in this work to appear as a promising technique to deal with the confinement effects on heat transport in nanoscaled systems.

We finish this section by sketching some future work. It would be interesting to determine the distribution function of the quantum occupation numbers $\mathbf{N}_k$ which depends on its size and particularly on the specific external constraints imposed to the system, which determine its temperature. It is possible to introduce in the nonlinear equations of the system the wave component if one recurs to relaxationlike models of heat transport. Finally, as it may be apparent, some other transport phenomena such as electric transport could be quantized in a way similar to that which we have designed in this paper.

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APPENDIX

After the diagonalization process of Eq. (6) the transformed vectors are given by

$$P_1'^{(C)} = P_1^{(C)} - 0.0083 P_2^{(C)},$$

$$P_2'^{(C)} = 0.0083 P_1^{(C)} + P_2^{(C)},$$

$$P_1'^{(S)} = P_1^{(S)} - 0.1088 P_2^{(S)},$$

$$P_2'^{(S)} = 0.1088 P_1^{(S)} + P_2^{(S)},$$

$$C_1' = C_1 - 0.0083 C_2,$$

$$C_2' = 0.0083 C_1 + C_2,$$

$$S_1' = S_1 - 0.1088 S_2,$$

$$S_2' = 0.1088 S_1 + S_2.$$

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