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On conduction heat transfer in metals

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ABSTRACT

The classical heat equation is characterized both by the instantaneous propagation of a physical interaction and by the lack of a particle that carries the heat. Metals have a particular feature: their atoms form a lattice with electrons traveling through the solid. This paper provides a conduction heat model for metals. The model replaces atoms by potential barrier and assigns the heat transport to electrons and, in some cases, photons. To emulate the transitory solution of Schrödinger's equation, the potential barrier is fragmented in others so that, the electron is losing energy packets while interacting with the sub-barriers. With this approach, the energy distribution is obtained for electrons and, in addition, it is derived a velocity expression for the heat spread through a metal. Last but not least, the classical solution of the heat equation is obtained but now the electron energy limits the heat diffusion avoiding the infinite range of the classical solution.

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1. Introduction

Since the 19th century, many efforts have been made to explain a wave behavior for heat in different ways and, consequently, to associate some speed which the heat propagation (for an comprehensive chronological revision [1,2]). One general classification of those heat theories could be made from the differential equation order: parabolic heat equations, hyperbolic heat equations and other theories (namely two temperature model and a relativistic heat equation).

First steps relating thermal flux **q** and temperature gradient ∇T were taken by means of Fourier's law. To consider the time variation of energy the classical parabolic heat equation arises, describing an energetic balance between internal energy, heat source and thermal diffusion.

$$\rho c_P \frac{\partial T}{\partial t} - \kappa \nabla^2 T = S \tag{1}$$

where ρ , c_p and κ are the density, the specific heat and the thermal conductivity of material, *t* is the time and *S* describes the source energy per unit of time and volume. The special behavior of this equation represents a paradox in the present: a physical phenomenon spreading with infinity velocity. To avoid this anomaly, some authors have proposed to use a modified Fourier's law [1,2]

$$\mathbf{q} + \tau \frac{\partial \mathbf{q}}{\partial t} = -\kappa \nabla T \tag{2}$$

here τ is the relaxation time; the inverse of τ is the frequency to activate the wave behavior of heat. The propagation speed *C* would relate τ and thermal diffusivity $\alpha = \kappa/(\rho c)$ through the equation

$$C = \sqrt{\frac{\alpha}{\tau}}$$
(3)

If Eq. (2) is inserted in the classical parabolic equation, it becomes an hyperbolic heat equation. However, at very short times ($t \simeq \tau$), the balance of energy is destroyed, thus violating the fundamental law of energy conservation [3,4]. Moreover, this theory does not identify the particles carrying the heat, another important skill in contemporary physics.

The third element in the classification is not a unique theory; on the contrary, it groups models with some special characteristics. In this paper, those having an interest are two temperatures and relativistic theories. The behavior of laser heating of metals is explained in Refs. [5–7]. From a point of view of interaction radiation-atom, the source *S* deposits electromagnetic energy on electrons, Eq. (4), that spend a finite time τ – as was the case before, a relaxation time – to change their states, Ref. (5). After this, an energy exchange between electrons and the lattice is generated, Ref. (6). This process lasts until the thermal equilibrium between electrons and lattice is reached: this interval receives the name of thermalization time. Last but not least, energy is propagated through the material. These three steps define the two temperature model. The equations are

$$c_e \frac{\partial T_e}{\partial t} = -\nabla \mathbf{q} - G(T_e - T_l) + S \tag{4}$$

$$\tau \frac{\partial \mathbf{q}}{\partial t} + \kappa \nabla T_e + \mathbf{q} = 0 \tag{5}$$



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Fig. 1. A causal representation of the photon–matter interaction. Once a photon γ_0 is absorbed by an potential barrier at t=0, another photon γ_r will be simultaneously reflected. A third photon γ and an electron e^- will be generated after a time τ .

$$c_l \frac{\partial T_l}{\partial t} = G(T_e - T_l) \tag{6}$$

where *G* is the electron–phonon coupling factor and the subscripts *e* and *l* are assigned to electron and lattice characteristics, i.e. c_l represents the heat capacity of the lattice. Together, Eqs. (4) and (5) form a hyperbolic model for electrons with a heat propagation velocity similar to Eq. (3). However, Eq. (6) predicts an infinity speed for phonons. Therefore, this theory combines both hyperbolic and parabolic equations, but only predicts a finite heat propagation speed for times close to relaxation time of electrons; after this interval, the heat propagation becomes infinite once again.

The authors Ali and Zhang [4,8] advance a relativistic heat theory. Their key idea is a weaker interpretation of principle of relativity: any field or matter has its own limiting speed, for example the light velocity for electromagnetic fields. Then, for heat conduction, the maximum speed at which the information can be transmitted would be the phonon velocity *C* through the material. In this four-dimensional space, the gradient operator would take the shape

$$\Box = \frac{-i}{C} \frac{\partial}{\partial t} \mathbf{o} + \nabla \tag{7}$$

where $i = \sqrt{-1}$ is the imaginary constant and **o** is a time unit vector in Minkowski algebra. From the relativistic flux vector

$$\mathbf{q} = -\kappa \Box T = \frac{i\kappa}{C} \frac{\partial T}{\partial t} \mathbf{o} - \kappa \nabla T \tag{8}$$

the four-dimensional energy balance becomes a hyperbolic heat equation.

$$c\frac{\partial T}{\partial t} + \Box \cdot \mathbf{q} = S \tag{9}$$

According to the authors, the advantages of this formulation over the hyperbolic equations mentioned above are first, the fact of that the energy is conserved and, second unlike the models above where C was only related to electrons, this theory takes into account the dependence of heat speed on thermal properties varying with temperature, on the presence of fields, on geometrical behavior, etc. However, there are two disadvantages in this theory: it does not give any expression for C and, furthermore, it does not set which particle transports the heat.

Metals have a particular feature: their atoms form a regular lattice. This elementary idealization allows to develop a model which consists of electrons moving freely until they interact with the lattice. The aim of this paper is to provide a conduction heat model from this idealization. This theory should explain what particles are responsible for heat transfer, how fast the heat spreads and the physical process to produce heat.

2. Quantum model of heat

Quantum electrodynamics is based on the interaction of charged particles and fields by means of the exchange of photons. We will now begin a journey through metals where we are going to find only photons and electrons. Suppose photons reaching the atoms of some kind of matter. Let us only consider those photons with energy between infrared and ultraviolet range, i.e. thermal photons. Since it is possible that the substance be passed through by some photons, let us only deal with those matter that interacts with thermal photons, i.e. non-transparent materials.

A theory about thermal conduction should consider both conventional and new heat sources-ovens, stoves, natural light, lasers, etc.; therefore, the energy range should include from infrared to partially ultraviolet photons: $[1.242 \times 10^{-3}, \simeq 25]$ eV, approximately. With this range in mind, the oscillation of an iron atom (rest mass 52 GeV, approx.) as a consequence of the collision with a thermal photon would be extremely improbable. The smaller first ionization potential in the periodic table belongs to francium, 3.83 eV, and the larger is for helium, 24.587 eV. These energies limit the chance of interactions so the Compton effect is prevented and the photoelectric effect should be considered only in certain circumstances. Nevertheless, the photoelectric effect could not justify the interaction of an infrared photon with all materials. A satisfactory explication lies in the fact that the electrical fields of the photon and electron interact with each other [9]. Thus, a photon passing close enough to an atom could be represented as a wave interacting with a potential barrier. Fig. 1 shows this event: at t=0 the photon γ_0 reaches the potential barrier V_0 and simultaneously another photon γ_r is reflected, after a time τ a third photon γ and an electron e^- arises from the barrier (on those situations where this is possible). At this point, some clarifications are needed to properly understand, Fig. 1:

- The energy primacy of γ_r , γ or e^- allows to sort the materials in reflective, transparent and absorbent substances. For example, the matter is reflective when the energy of γ_r is greater than the sum of the other two. In the case of Fig. 1, it represents one of the three possible situations.
- The number of arising photons and/or electrons depends on the physical involved laws; therefore, γ and e⁻ represent the photons and electrons that appear after a time τ. However, the time τ is not necessarily the same time for all the photons and electrons, i.e. γ_i or e_i⁻ emerges after a lapse τ_i.
- The real geometry of the barrier would be smoother than Fig. 1 and its height would also vary over time, for instance when an electron is emitted. Therefore, the model described in Fig. 1 gives a very rough idea of the reality, but it will help to explain some questions.

Continuing with this idea, a solid metal could be modeled by means of a periodic potential. Each atom or molecule will be replaced by a potential barrier, a in width, which is placed at distance b from another neighboring barriers, Fig. 2. The ensemble will form a one-dimensional grid with a lattice parameter a+b.

Let us see what happens when a photon γ_0 hits this grid, now metal. First, the electrical field of the photon interacts with the barrier and, immediately, a reflected photon appears. The remaining energy will be absorbed during the time τ – delay time for

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