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The design of a thermal rectifier

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Abstract. – The idea that one can build a solid-state device that lets heat flow more easily in one way than in the other, forming a heat valve, is counter-intuitive. However, the design of a thermal rectifier can be easily understood from the basic laws of heat conduction. Here we show how it can be done. This analysis exhibits several ideas that could in principle be implemented to design a thermal rectifier, by selecting materials with the proper properties. In order to show the feasibility of the concept, we complete this study by introducing a simple model system that meets the requirements of the design.

While electronics has been able to control the flow of charges in solids for decades, the control of heat flow still seems out of reach, and this is why, when a paper showed for the first time how to build a "thermal rectifier" [1], the thermal analogue of the electrical diode, it attracted a great deal of attention [2]. The idea that one can build a solid-state device that lets heat flow more easily in one way than in the other, forming a heat valve, is counter-intuitive and may even appear in contradiction with thermodynamics. Actually, this is not the case, and the design of a thermal rectifier can be easily understood from the basic laws of heat conduction. Here we show how it can be done. This analysis exhibits several ideas that could in principle be implemented to design a thermal rectifier, by selecting materials with the proper properties. In order to show the feasibility of the concept, we complete this study by introducing a simple model system that meets the requirements of the design. Such devices could be useful in nanotechnology, and particularly to control he heat flow in electronic chips.

Let us consider the heat flow along the x-direction, in a material in thermal contact with two different heat baths at temperatures T_1 for $x = 0$ and T_2 for $x = L$ (fig. 1a). We consider the general case of an inhomogeneous material with a local thermal conductivity $\lambda(x, T)$ which depends not only on space but also on temperature. To discuss the main ideas only the x-dependence is introduced, but the same analysis can be extended to a more general case, at the expense of heavier calculations.

The heat flow J_f is given by

$$J_f = -\lambda[x, T(x)] \frac{\mathrm{d}T(x)}{\mathrm{d}x} , \tag{1}$$

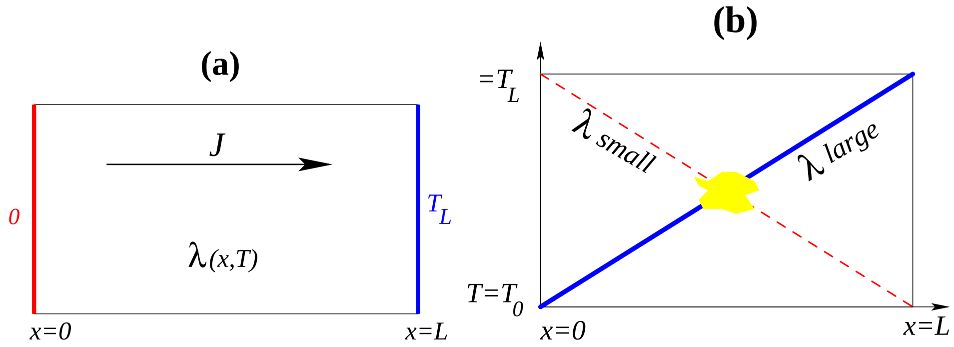

Fig. 1 – (a) Schematic picture of the device. (b) Schematic view of the requests on $\lambda(x,T)$ to get a rectifier.

so that the temperature distribution is

$$T(x) = T_1 + \int_0^x \frac{J_f}{\lambda[\xi, T(\xi)]} \, \mathrm{d}\xi \; . \tag{2}$$

Solving this equation with the boundary condition $T(x = L) = T_2$ determines the value of J_f. A numerical solution of eq. (2) can be obtained by an iterative scheme, starting from an initial temperature distribution $T_i(x)$ which is inserted in the r.h.s. of the equation to get an updated distribution from the l.h.s., and repeating the process until the desired convergence is achieved. A simple linear temperature distribution is a good starting point for $T_i(x)$ and, for non-singular thermal conductivities $\lambda(x,T)$, the convergence is fast.

If the boundary conditions are reversed, imposing temperature T_2 for $x = 0$ and temperature T_1 for $x = L$, the same process leads to another temperature distribution, and a different flux J_r. The rectifying coefficient can be defined as

$$R = \left| \frac{J_r}{J_f} \right| \; . \tag{3}$$

In general, for arbitrary $\lambda(x,T)$, there is no condition that imposes that R should be unity.

From this analysis, it is easy to understand qualitatively how a thermal rectifier can be built by selecting the appropriate function $\lambda(x,T)$, as shown in fig. 1b. In the (x,T)-plane, the temperature distributions for the forward and reverse boundary conditions follow roughly the two diagonals (fig. 1b). Of course, as shown by the exact results presented below, this is only an approximation, but it is nevertheless sufficient to provide a guide for the choice of $\lambda(x,T)$. If the thermal conductivity is large when the point (x,T) lies on one diagonal and small along the other, the forward and reverse heat flows will be significantly different, *i.e.* the device will rectify the heat flow. Strictly speaking, the two conditions are not compatible in the centre, but by choosing an intermediate value of λ when $x = L/2$ and $T = (T_1 + T_2)/2$, the rectifying effect is preserved.

Figure 2a shows an example for a particular choice of the local thermal conductivity coefficient $\lambda(x,T)$ which meets this requirement. Solving eq. (2) with the forward and reverse boundary conditions for this choice of λ gives temperature distributions $T_f(x)$ and $T_r(x)$, which are not invariant by the reversal of the x-axis although the boundary conditions have such a symmetry. As a result, the system shows a strong rectifying effect: the reverse heat flux is one order of magnitude larger than the forward flux, for our choice of boundary conditions.

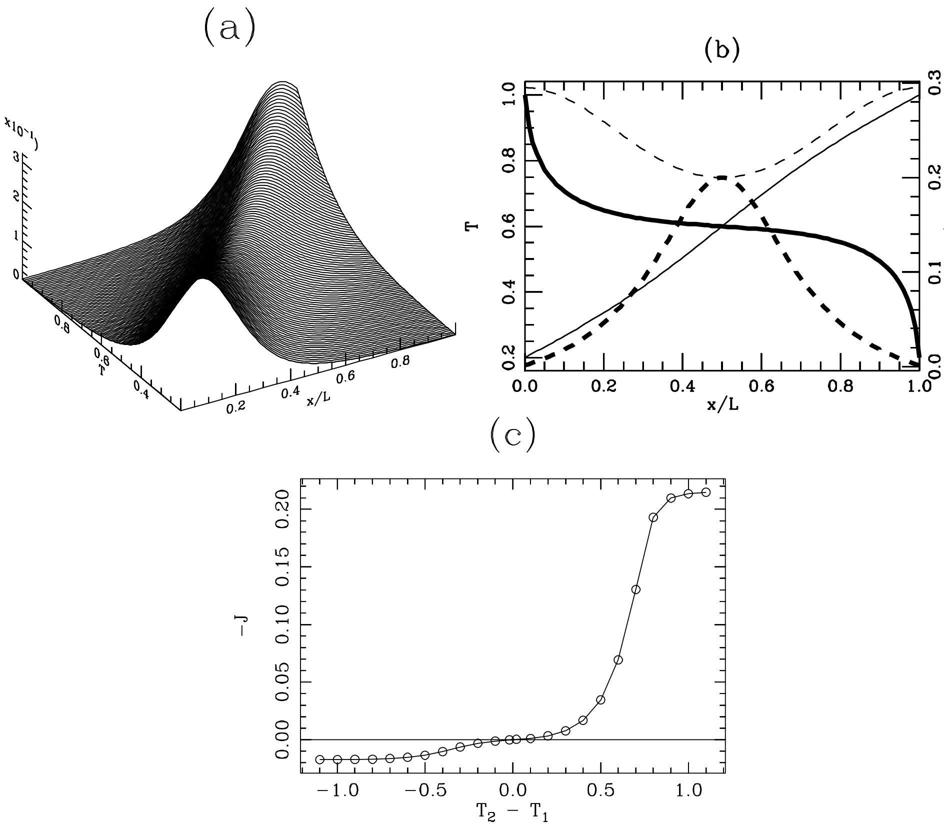

Fig. 2 – Example of temperature distributions for a particular choice of the thermal conductivity coefficient $\lambda(x,T) = \dfrac{1 - 0.8/\cosh^2(L/2-x)}{\cosh\left[a(L/2-x) + b\big(T - (T_1+T_2)/2\big)\right]}$ $(a = 7,\ b = 1)$. The boundary temperatures are $T_1 = 1.0$ and $T_2 = 0.2$, in arbitrary scale. (a) Variation of $\lambda(x,T)$. (b) The temperature distributions (solution of eq. (2)) (full lines) and the variation *vs.* space of the local conductivity $\lambda[x,T(x)]$ (dashed lines) are shown for the forward boundary condition ($T(x=0) = T_1$, $T(x=L) = T_2$) (thick lines) and reverse boundary condition (thin lines). For this choice of $\lambda(x,T)$, the rectifying coefficient is $J = |J_r/J_f| = 11.5$. (c) Variation of the heat flow J across the system, as a function of the temperature difference $T_2 - T_1$ for a fixed value of $T_1 = 0.2$.

Figure 2c shows the variation of the reverse and forward flux as a function of the temperature difference $T_2 - T_1$ for a given value of T_1. It has a shape that reminds the characteristic of an electrical diode, except for high $|T_2 - T_1|$ where a saturation appears because $\lambda(x,T)$ decreases in this range of temperatures.

The case presented on fig. 2 looks of course artificial because we have chosen a peculiar distribution $\lambda(x,T)$ to meet the requirements that were suggested by our analysis of eq. (2). Before considering a model system that could be the basis of a solid-state rectifier, let us examine some simpler designs, that would be more practical to build.

One possibility is to juxtapose two homogeneous materials with thermal conductivities $\lambda_1(T)$ and $\lambda_2(T)$ that have opposite behaviours, $\lambda_1(T)$ decreasing sharply around some temperature T_c and $\lambda_2(T)$ rising sharply around the same temperature, as shown in fig. 3. As

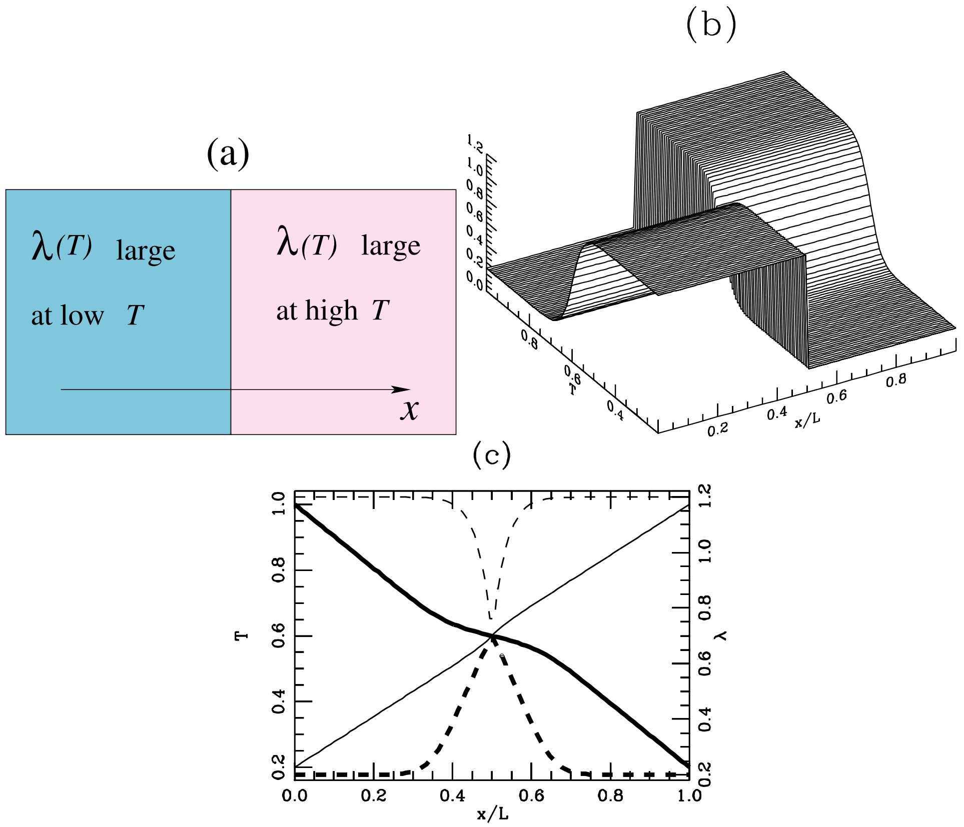

Fig. 3 – Thermal rectifier made by the juxtaposition of two different homogeneous materials which have a thermal conductivity that depends highly on temperature. The boundary temperatures are $T_1 = 1.0$ and $T_2 = 0.2$ in arbitrary scale. (a) Schematic view of the device. (b) Variation of $\lambda(x,T)$. (c) The temperature distributions (solution of eq. (2)) (full lines) and the variation *vs.* space of the local conductivity $\lambda[x,T(x)]$ (dashed lines) are shown for the forward boundary condition ($T(x=0)=T_1$, $T(x=L)=T_2$) (thick lines) and reverse boundary condition (thin lines). For this choice of $\lambda(x,T)$, the rectifying coefficient is $J = |J_r/J_f| = 4.75$.

shown in this figure this ensures that the average heat conductivity is higher along one diagonal of the (x,T)-plane than along the other and this can lead to a significant value of the rectifying coefficient, which of course depends on the exact value of $\lambda(x,T)$ and the temperatures at which the device is operated.

An even simpler design can be considered by combining a material having a temperature-dependent thermal conductivity $\lambda_1(T)$ with a material that has a temperature-independent conductivity λ_2, as shown in fig. 4. Anticipating on the results of the model that we discuss below, we have chosen $\lambda_2 \gg \lambda_1$, which would be the case, for instance, if the rectifier were built by combining some composite material with moderate heat conductivity $\lambda_1(T)$ with a good thermal conductor. Although the rectifying coefficient is smaller in this case which is not optimised, this simple design nevertheless shows a significant rectifying effect for the heat flow.

Thus it appears that designing the simplest thermal rectifier only requires a material with a thermal conductivity that varies significantly as a function of temperature. In a previous study [1], we showed that the nonlinearity of the vibrational modes in a soft material can be

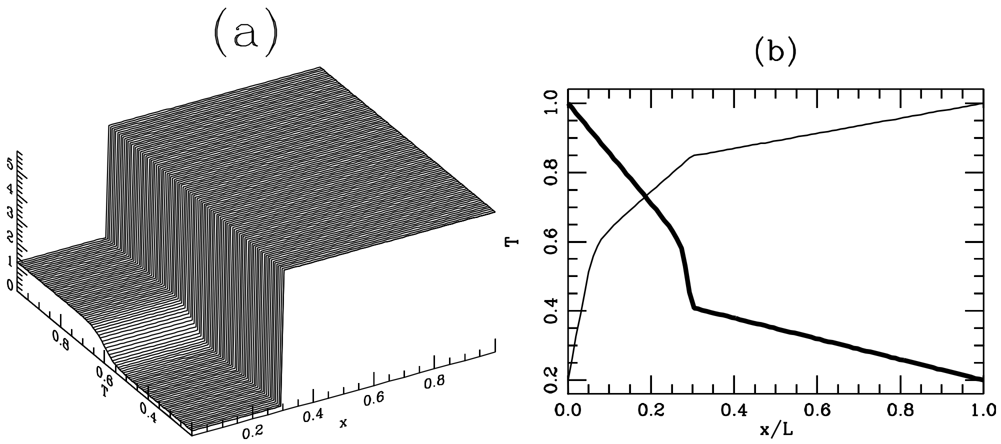

Fig. 4 – Thermal rectifier made by the juxtaposition of two different homogeneous materials, one of which has a thermal conductivity that drops below some temperature. The boundary temperatures are $T_1 = 1.0$ and $T_2 = 0.2$ in arbitrary scale. (a) Variation of $\lambda(x,T)$. (b) The temperature distributions (solution of eq. (2)) for the forward boundary condition ($T(x=0) = T_1$, $T(x=L) = T_2$) (thick line) and reverse boundary conditions (thin line). For this choice of $\lambda(x,T)$, the rectifying coefficient is $J = |J_f/J_r| = 1.37$.

used for this purpose. Let us illustrate this with a simple one-dimensional model system. We consider a one-dimensional lattice of nonlinear oscillators described by the Hamiltonian

$$H = \sum_{n=1}^{N} \frac{p_n^2}{2m} + \frac{1}{2}C(y_n - y_{n-1})^2 + V_n(y_n) \ , \tag{4}$$

where y_n designates the position of particle n, p_n its momentum, m its mass, and $V_n(y_n) = D_n[\exp(-a_n y_n) - 1]^2$ is a nonlinear on-site potential. The heat flow is carried by the phonon modes of the lattice. In a nonlinear lattice the effective frequency of these modes depends on their amplitude, *i.e.* on the local temperature. An approximate calculation of the frequency shift of the modes can be made in the self-consistent phonon approximation [3]. If one considers a lattice made of homogeneous domains in which the parameters of the potential, D_n, a_n, are constant, the thermal conductivity is essentially controlled by the matching of the phonon bands at the boundaries of the domains. As the bands depend on temperature due to nonlinearity, the thermal conductivity λ depends on temperature.

Figure 5 shows the self-consistent phonon bands in a nonlinear lattice made of two different regions. In the homogeneous right-hand side region, the frequencies of the vibrational modes are only weakly temperature dependent and do not vary in space. Phonons propagate easily in this region which has a high heat conductivity λ_2 which is almost temperature independent. In the left-hand side region, the phonon bands of the two types of stripes do not match at low temperature. The discontinuities scatter phonons and the heat conductivity λ_1 is low at low temperature ($T = 0.1$). But, as T is raised, the self-consistent phonon frequencies in the stripes with the highest nonlinearity ($a' = 2.0$) drop and overlap with the frequencies in the other stripes. The thermal conductivity λ_1 raises sharply at high temperature ($T = 0.4$). This analysis based on self-consistent phonon calculations is confirmed by numerical simulations in which the ends of a lattice similar to the left-hand side region are thermalized by Langevin thermostats at two slightly different temperatures T and $T + \Delta T$ with $\Delta T = 0.01$. The

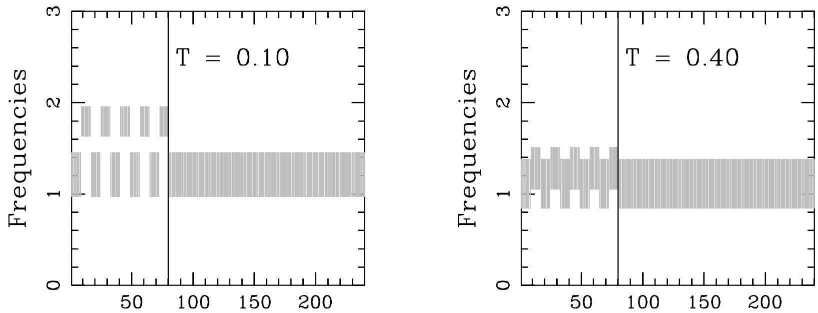

Fig. 5 – Phonon bands obtained in the self-consistent phonon approximation for a nonlinear lattice described by Hamiltonian (4) with 240 sites, at two temperatures (in energy units). The lattice is divided into two regions. In the right-hand side region ($n > 80$) the lattice is homogeneous with $D_n = D = 0.50$ and $a_n = a = 1.0$. In the left-hand side region ($1 \leq n \leq 80$) the lattice is made of stripes of 8 sites each, in which two parameter sets for the nonlinear potential alternate, $D_n = D = 0.5$, $a_n = a = 1.0$ on the one hand, and $D_n = D' = 0.375$, $a_n = a' = 2.0$ on the other hand.

value of $\lambda_1(T)$ is then estimated by measuring the heat flux $J(T)$ across the lattice [1] and using $\lambda_1(T) = J(T)\ \Delta x/\Delta T$, where Δx is the length of the lattice segment used for the measurement (132 sites). Figure 6a shows the result of this numerical measurement of $\lambda_1(T)$ and fig. 6b shows the forward and reverse temperature distributions in the nonlinear lattice in contact with two thermal baths at temperatures $T_1 = 0.1$ and $T_2 = 0.35$. These curves are very similar to the theoretical curves of fig. 4b, which indicates that the nonlinear lattice is able to lead to the kind of thermal conductivity distribution $\lambda(x, T)$ shown in fig. 4a. It behaves as a thermal rectifier.

In conclusion, we have shown that a simple calculation of the heat flowing through a material which has a thermal conductivity that depends on space *and* temperature indicates that thermal rectifiers, in which the heat flows more easily in one direction than in the other, can be designed. A nonlinear lattice model, investigated by numerical simulation, confirms the validity of the analysis and shows that materials meeting the necessary requirements to build

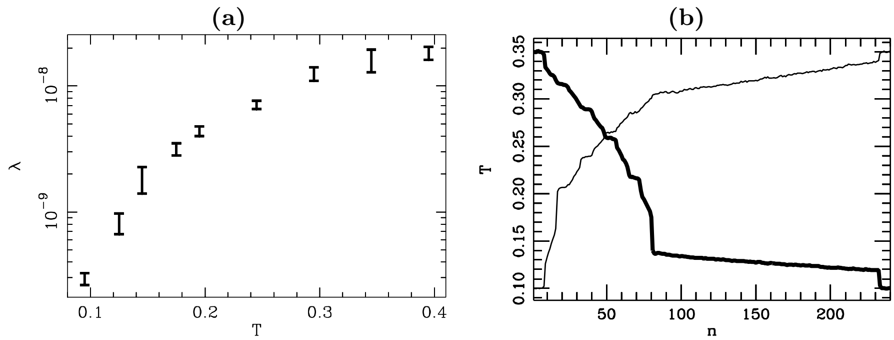

Fig. 6 – a) Variation *vs.* temperature of the thermal conductivity of the composite nonlinear lattice making the left-hand side region of the model introduced in fig. 5. b) Temperature distributions observed in the simulation of the nonlinear lattice described in the caption of fig. 5 in contact with two thermal baths at temperatures $T_1 = 0.1$ and $T_2 = 0.35$. The rectifying coefficient deduced from the simulation is $R = |J_f/J_r| = 1.39$.

thermal rectifiers could exist. This nonlinear lattice can be viewed as a simplified description of a layer of soft molecules deposited on a substrate which has a very small thermal conductivity such as a glass. But, since our analysis shows that any material which has a temperature-dependent thermal conductivity can be used, one can think of other possibilities such as composite materials or solids in the vicinity of a phase transition.

Moreover, in a practical design one could take advantage of another degree of freedom that we have not exploited in our simple analysis: geometry. For instance, changing the width of the conducting layer is an easy way to control the spatial dependence of $\lambda(x, T)$. We have verified that this allows the design of a thermal rectifier made of a single homogeneous material, having a temperature-dependent thermal conductivity $\lambda(T)$ by selecting the proper shape of the conducting layer.

The simplicity of the concept suggests that, after the selection of the optimal material, it could be used in various applications in nanotechnology, such as, for instance, the control of the heat flow in electronic chips.

REFERENCES

[1] TERRANEO M., PEYRARD M. and CASATI G., *Phys. Rev. Lett.*, **88** (2002) 094302.
[2] See, for instance, *Nature Science Update*: `http://www.nature.com/nsu/020304/020304-2.html` or *New Sci.*, 9 March issue (2002) 6.
[3] DAUXOIS T., PEYRARD M. and BISHOP A. R., *Phys. Rev. E*, **47** (1993) 684.