The form of energy termed heat that typically derives from lattice vibrations, i.e. the phonons, is usually considered as waste energy and, moreover, deleterious to information processing. However, with this colloquium, we attempt to rebut this common view: By use of tailored models we demonstrate that phonons can be manipulated like electrons and photons can, thus enabling controlled heat transport. Moreover, we explain that phonons can be put to beneficial use to carry and process information. In a first part we present ways to control heat transport and how to process information for physical systems which are driven by a temperature bias. Particularly, we put forward the toolkit of familiar electronic analogs for exercising phononics; i.e. phononic devices which act as thermal diodes, thermal transistors, thermal logic gates and thermal memories, etc. These concepts are then put to work to transport, control and rectify heat in physical realistic nanosystems by devising practical designs of hybrid nanostructures that permit the operation of functional phononic devices and, as well, report first experimental realizations. Next, we discuss yet richer possibilities to manipulate heat flow by use of time varying thermal bath temperatures or various other external fields. These give rise to a plenty of intriguing phononic nonequilibrium phenomena as for example the directed shuttling of heat, a geometrical phase induced heat pumping, or the phonon Hall effect, that all may find its way into operation with electronic analogs.

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I. INTRODUCTION

When it comes to the task of transferring energy, nature has at its disposal tools such as electromagnetic radiation, conduction by electricity and also heat. The latter two tools play a dominant role from a technological viewpoint. The conduction of heat and electric conduction are, however, two fundamental energy transport mechanisms of comparable importance, although never been treated equally in science. Modern infor-
mation processing rests on micro electronics, which after the invention of the electronic solid-state transistor \cite{Bardeen1948}, and other related devices, sparked off an unparalleled technological development, the state of the art being electric integrated circuitry. Without any doubt, this technology markedly changed many aspects of our daily life. Unfortunately, a similar technology which builds on electronic analogs via the constructive use of heat flow has not yet been realized by mankind, although several attempts have been repeatedly undertaken. In everyday life, however, signals encoded by heat prevail over those by electricity. Therefore, the potential of using heat control may result in an even more abundant and unforeseen wealth of applications. A legitimate question then is: Does phononics, i.e., the counterpart technology of electronics present only a dream?

Admittedly, it indeed is substantially more difficult to control a priori the flow of heat in a solid than it is to control the flow of electrons. The source of this imbalance is that, unlike electrons, the carriers of heat – the phonons – are quasi-particles in the form of energy bundles that possess neither a bare mass nor a bare charge. Although isolated phonons by itself do not influence each other, interactions involving phonons become of importance in the presence of condensed phases. Some examples that come to mind are phonon polaritons, i.e. the interaction of optical phonons with infrared photons, the generic phonon-electron interactions occurring in metals and semi-metal structures, phonon-spin interactions, or the phonon-phonon interaction in presence of nonlinearity. Therefore, heat flow features aspects which in many ways are distinct from charge and matter flow. Nonetheless, there occur in condensed phases many interesting cross-interplays as it is encoded with the reciprocal relations of the Onsager form for mass, heat and charge flow, of which thermoelectricity \cite{Callen1960, Dubi2011} or thermophoresis, i.e. the Soret vs. its reciprocal Dufour effect \cite{Callen1960}, are typical exemplars. Therefore, capitalizing on the rich physical diversities involving phonon transport as obtained with recent successes in nano-technology may open the door to turn phononics from a dream into a reality.

With this Colloquium we shall focus on two fundamental issues of phononics; - i.e. the manipulation of heat energy flow on the nanoscale and the objective of processing information by utilizing phonons. More precisely, we shall investigate the possibilities to devise elementary building blocks for doing phononics; namely we study the conceptual realization and its possible operation of a thermal diode which rectifies heat current, a thermal transistor that is capable to switch and amplify heat flow and last but not least a thermal memory device.

The objective of controlling heat flow on the nanoscale necessarily rests on the microscopic laws that govern heat conduction, stability aspects or thermometric issues. For these latter themes the literature provides the readers with several comprehensive reviews and features already. For heat flow and/or related thermoelectric phenomena on the micro-/nano- and molecular scales we refer the readers to the excellent treatises by \cite{Lepri2003, Casati2005, Galperin2007, Dhar2008, Li2005b, Zhang2010, Pop2010}, and recently also by \cite{Dubi2011}. We further demarcate our presentation from the subjects of refrigeration on mesoscopic scales and thermometry \cite{Giazotto2006} and, as well, as our title suggests, also do not address per se in greater detail the issue of conventional way of manipulating heat flow upon changing thermal conductivity by means of various phonon scattering mechanisms in nano- and heterostructures \cite{Chen2005, Zimen2001}. For compelling recent developments and advances in this latter area we refer the interested readers to the recent surveys by \cite{Balandin2005} and \cite{Balandin2007}, together with the original literature cited therein.

In this spirit, a primary building block for doing phononics is a setup that rectifies heat flow; i.e. a thermal rectifier/diode. Such a device acts as a thermal conductor if a positive thermal bias is applied while in the opposite case of a negative thermal bias it undergoes poor thermal conduction, thus effectively acting as a thermal insulator, or possibly also vice versa. The concept of such a thermal diode is sketched in Fig. 1.

![Thermal diode](image)

**FIG. 1** (color). Sketch of the modus operandi of a thermal diode. When the left end of the diode is at a higher temperature as compared to its right counterpart heat is allowed to flow almost freely. In contrast, when the right end is made hotter in reference to the left end the transduction of heat becomes strongly diminished.

The concept of a thermal diode involves, just as in its electronic counterpart, the presence of a symmetry breaking mechanism. This symmetry breaking is most conveniently realized by merging two materials exhibiting different heat transport characteristics. Historically, \cite{Starr1935} working at Rensselaer Polytechnic Institute in New York built a junction composed of a metallic copper part which he joined with its cuprous oxide phase; thus proving the working principle of rectifying heat in such a structure. Starr’s thermal rectifier is physically based on an asymmetric electron-phonon interaction oc-
curring in the interface of the two dissimilar materials. There exist a plenty of such macroscopic rectifiers which function via the difference of the material response due to temperature bias and/or other externally applied control fields such as strain, etc., (Roberts and Walker, 2011).

The focus in this colloquium will be on a thermal rectification scenario that is induced by phonon transport occurring on the nanoscale. The concept of such a thermal rectifier for heat was put forward by Terraneo et al. (2002). The authors therein proposed to use a three-segment structure composed of different nonlinear lattice segments. The underlying physical mechanism relies on the resonance phenomenon for the temperature dependent power spectrum vs. frequency as a result of the nonlinear lattice dynamics. Subsequently, it has been shown that a modified two-segment setup (Li et al., 2005a, 2004) yields considerably improved rectification characteristics as compared to the original three-segment setup (Terraneo et al., 2002). These pioneering works in turn ignited a flurry of activities, manifesting different advantageous features and characteristics. The theoretical and numerical efforts culminated in a first experimental validation of such a thermal rectifier in 2006: The device itself is based on an asymmetric nanotube structure (Chang et al., 2006). The concept of this latter thermal diode together with its explicit experimental setup is depicted with Fig. 2.

The thermal diode presents an important first step towards phononics. For performing logic operations and useful circuitry, however, additional control mechanisms for heat are required. This comprises the task of devising (i) the thermal analog of an electronic transistor, (ii) thermal logic gates and, as well, (iii) a thermal memory. The physical concept of these salient phononic building blocks will be elucidated in Sect. II. The main physical feature that enters the function of such phonon devices is the occurrence of negative differential thermal resistance (NDTR); the latter being a direct consequence of the inherently acting nonlinear dynamics with its intriguing nonlinear response to an externally applied thermal bias.

With Sect. III we investigate how to put these thermal phononic concepts to “action” by using realistic nanoscale structures. The actual operations of such devices rest on extended molecular dynamics simulations which serve as a guide for implementing its experimental realization. The control of heat flow in the above mentioned phononic building blocks is managed mainly by applying a static thermal bias. More intriguing control of transport emerges when the manipulations are made explicitly time-dependent or by use of different external forces such as the application of magnetic fields. As detailed with Sec. IV such manipulation scenarios then generate new roadways towards fine-tuned control and counterintuitive response behaviors. Originally, such dynamic control has been implemented for anomalous particle transport by taking the system dynamics out-of-equilibrium: Doing so results in intriguing phenomena such as Brownian motor (ratchet-like) transport, absolute negative mobility and alike (Astumian and Hänggi, 2002; Hänggi and Marchesoni, 2009; Hänggi et al., 2005). A similar reasoning can be put to work for shuttling heat in appropriately designed lattice structures, as detailed in Sect. IV. In Sect. V, we summarize our main findings, discuss yet some additional elements for phononic concepts and reflect on future potential and visions to advance the field of phononics from its present infancy towards a mature level.

II. PHONONICS DEVICES: THEORETICAL CONCEPTS

A. Thermal diode: Rectification of heat flow

The task of directing heat for information processing as in electronics requires a toolkit with suitable building blocks, namely those nonlinear components that mimic the role of diodes, transistors, and alike, known from electronic circuitry. A first challenge then is to design the blueprints for such components that function for heat control analogous to the building blocks for electronics.
This objective is best approached by making use of the nonlinear dynamics present in anharmonic lattice structures in combination with the implementation of a system inherent symmetry breaking. We start with the discussion of the theoretical design for thermal diodes that rectify heat flow.

1. Two-segment thermal diode

In order to achieve thermal rectification, we exploit the nonlinear response mechanism as it derives from inherent temperature-dependent power spectra. An everyday analog of such a nonlinear frequency response is a playground swing when driven into its large amplitude regime via parametric resonance. The response is optimized whenever the natural frequencies match those of the perturbations. Likewise, energy can be transported across two different segments when the corresponding vibrational frequency response characteristics overlap.

More precisely, whenever the power spectrum in one part of the device matches with its neighboring part, we find that heat energy is exchanged efficiently. In the absence of such overlapping spectral properties, the exchange of energy becomes strongly diminished. Particularly, the response behavior of realistic materials is typically anharmonic by nature. As a consequence, the corresponding power spectra become strongly dependent on temperature, see in Appendix A, Subsect. 3. If an asymmetric system is composed of different parts with differing physical parameters the resulting temperature-dependence of the power spectra will differ likewise.

Based on these insights, a possible working principle of a thermal diode goes as follows: If a temperature bias makes the spectral features of different parts overlap with each other, we obtain a favorable energy exchange. In contrast, if for the opposite temperature bias the spectral properties of the different parts fail to overlap appreciably a strong suppression of heat transfer occurs. In summary, this match/mismatch of spectral properties provides the salient mechanism for thermal rectification, see in Fig. 3(b) and (c).

Because the power spectra of an arbitrary nonlinear material typically become temperature-dependent, the use of any asymmetric nonlinear system is expected to display an inequivalent heat transport upon reversal of the temperature bias. It is, however, not a simple task to design a device that results in physical designated and technologically feasible thermal diode properties. After having investigated a series of possible setups we designed a thermal diode model that performs efficiently over a wide range of system parameters \( \text{Li et al.} (2004) \). The blueprint of this device consists of two nonlinear segments which are weakly coupled by a linear spring with strength \( k_{\text{int}} \). Each segment is composed of a chain of particles in which each individual particle is coupled with its nearest neighbors by linear springs. This whole nonlinear two-segment chain is each subjected to a cosinusoidal varying on-site potential (illustrated by the large wavy curve) is connected to the right (blue) segment possessing a relatively weak on-site potential. (b) In the case that the temperature \( T_L \) in the left segment is colder than the corresponding right temperature \( T_R \), i.e. \( T_L < T_R \), the power spectrum of the particle motions of the left segment is weighted at high frequencies. This is so because of the difficulty experienced by the dwelling particles to overcome the large barriers of the on-site potential. In contrast, the power spectrum of the right segment is weighted at low frequencies. As a result, the overlap of the spectra is weak, implying that the heat current \( J \) becomes strongly diminished. (c) Here the situation is opposite to panel (b). With \( T_L > T_R \) the particles can now move almost freely between neighboring barriers. Consequently the power spectrum extends to much lower frequencies, yielding an appreciable overlap with the right placed segment. This in turn causes a sizable heat current. Panel (d). Heat current \( J \) vs. the relative temperature bias \( \Delta \), as defined in the inset, for three different values of the reference temperature \( T_0 \). Adapted from \( \text{Wang and Li} (2008a) \) and \( \text{Li et al.} (2004) \).
on-site potential; the latter is provided by the coupling to a substrate. These individual chains are therefore described by a Frenkel-Kontorova (FK) lattice dynamics, cf. Appendix. The scheme of this thermal diode is depicted in Fig. 3(a).

The key feature of this FK-diode setup is the chosen difference in the strength of the corresponding on-site potential. At low temperature, the particles are confined in the valleys of the on-site potential. Thus the power spectrum is weighted in the high frequency regime. At high temperatures the particles assume sufficiently large kinetic energies so that thermal activation (Hanggi et al. 1990) across the inhibiting barriers becomes feasible. The corresponding power spectrum is then moved towards lower frequencies. By setting the strength of the on-site potential in the two segments at distinct different levels, see Fig. 3(a), we achieve the desired strong thermal rectification. Note that the barrier height of the on-site potential for the right segment is chosen sufficiently small so that the corresponding particles are allowed to move almost freely, both in the low and in the high temperature regime. In the case that the left end is set at the low temperature, its power spectrum is weighted within the high frequency regime. This in turn causes an appreciable mismatch with the right segment, see Fig. 3(b). In the opposite case, when the left end is set at the high temperature, its weighted power spectrum moves towards lower frequencies, thus matching considerably with the right segment, see Fig. 3(c).

In Fig. 3(d) the resulting stationary heat current $J$ (see in Appendix A) vs. the relative temperature bias $\Delta$ is depicted for three values of the reference temperatures $T_0$ (Li et al. 2004). The relation between the dimensionless temperature and the actual physical temperature can be found in the Appendix as well. It is shown that when $\Delta > 0$ (i.e. $T_L > T_R$), the heat current gradually increases with increasing $\Delta$, i.e. the setup behaves as a ‘good’ thermal conductor; in contrast, when $\Delta < 0$ ($T_L < T_R$), the heat current remains small. The two-segment structure thus behaves as a ‘poor’ thermal conductor, i.e. it mimics a thermal insulator.

For a given setup, the heat current through the system is mainly controlled by its interface coupling strength $k_{\text{int}}$. Figure 4 depicts the temperature profiles for different $k_{\text{int}}$ and for two oppositely chosen bias strengths. There occurs a large temperature jump at the interface. The size of the jump is larger for negative bias $\Delta$ (filled symbols in Fig. 4) than for positive bias $\Delta$. In the case with negative bias the temperature gradient inside each lattice segment almost vanishes; implying that the resulting heat current is very small. This behavior is opposite to the case with positive bias (open symbols in Fig. 4).

2. Asymmetric Kapitza resistance

The interface thermal resistance (ITR), also known as the Kapitza resistance, measures the interfacial resistance to heat flow (Pollack 1969; Swartz and Pohl 1980). It is defined as, $R_0 = \Delta T / J$, where $J$ is the heat flow (per area) and $\Delta T$ denotes the temperature jump between two sides of the interface. The origin of the Kapitza resistance can be traced back to the heterogeneous electronic and/or vibrational properties of the different materials making up the interface at which the energy carriers become scattered. The amount of relative transmission depends on the available energy states on either of the two sides of the interface. Originally, this phenomenon was discovered by Kapitza in 1941 in experiments detecting super-fluidity of He II (Kapitza, 1941).

The high thermal rectification in the above discussed model setups is mainly due to this interface effect. In order to further improve the performance (Li et al. 2005a) studied the ITR in a lattice consisting of two weakly coupled, dissimilar anharmonic segments, exemplified by a (FK)-chain segment and a neighboring Fermi-Pasta-Ulam (FPU) chain segment.

Not surprisingly, the ITR in such a setup depends on the direction of the applied temperature bias. A quantity that measures the degree of overlap of power spectra between left(L) and right(R) segments reads

$$S = \frac{\int_{0}^{\infty} P_L(\omega)P_R(\omega)d\omega}{\int_{0}^{\infty} P_L(\omega)d\omega \int_{0}^{\infty} P_R(\omega)d\omega}.$$  \hspace{1cm} (1)

Extensive numerical simulations then reveal that $R_+ / R_- \sim (S_+ / S_-)^{\delta_R}$ with $\delta_R = 1.68 \pm 0.08$, and $|J_+ / J_-| \sim (S_+ / S_-)^{\delta_J}$, with $\delta_J = 1.62 \pm 0.10$. The notation $+/−$ indicates the case with a positive thermal bias,
Δ > 0, and a negative thermal bias, Δ < 0, respectively. These findings thus support the strong dependence of thermal resistance on this very overlap of power spectra.

The physical mechanism of the asymmetric ITR between dissimilar anharmonic lattices can therefore be related to the match/mismatch of the corresponding power spectra. As temperature increases, the power spectrum of the FK lattice shifts downwards, towards lower frequencies. In contrast, the power spectrum of the FPU-segment, however, shifts upwards, towards higher frequencies. Due to these opposing shifts, it becomes evident that upon a reversing the thermal bias the amount of match/mismatch in such a FK-FPU setup can even exceed that of the above considered FK-FK setup. Conceptually this results in an even stronger thermal rectification.

B. Negative differential thermal resistance: The thermal transistor

The design and the experimental realization of the thermal diode presents a striking first step towards the goal of doing phononics. A next challenge to be overcome is then a design for a thermal transistor, which allows for an a priori control of heat flow much alike the familiar control of charge flow in a Field Effect Transistor. Like its electronic counterpart, a thermal transistor consists of three terminals: The drain (D), the source (S), and the gate (G). When a constant temperature bias is applied between the drain and the source, the thermal current flowing between source and drain can be fine-tuned by the temperature that is applied to the gate. Most importantly, because the transistor is able to amplify a signal, the changes in the heat current through the gate can induce an even larger current change from the drain to the source.

Towards the eventual realization of such a thermal transistor device we consider the concept depicted with Fig. 5(a). It uses a one-dimensional anharmonic lattice structure where the temperature at its ends are fixed at $T_D$ and $T_S$ ($T_D > T_S$), respectively. An additional, third heat bath at temperature $T_O$ controls the temperature at node O, so as to control the two heat currents $J_D$ and $J_S = J_D + J_O$. Let us next define the current amplification factor $\alpha$. This quantity describes the amplification ability of the thermal transistor, as the change of the heat current $J_D$ (or $J_S$, respectively), divided by the change in gate current $J_O$, which acts as the control signal. This amplification quantity explicitly reads

$$\alpha = \left| \frac{\partial J_D}{\partial J_O} \right|.$$  

Eq. (2) can be recast in terms of the differential thermal resistance of the segment $S$, i.e.,

$$r_S \equiv \left( \frac{\partial J_S}{\partial T_O} \right)_{T_S=\text{const}}^{-1}$$  

and that of the neighboring segment $D$, i.e.,

$$r_D \equiv -\left( \frac{\partial J_D}{\partial T_O} \right)_{T_D=\text{const}}^{-1}$$

to yield

$$\alpha = \left| \frac{r_S}{r_S + r_D} \right|.$$  

FIG. 5 (color online). Concept of a thermal transistor. Panel (a). A one-dimensional lattice is coupled at its two ends to heat baths at temperature $T_D$ and $T_S$ with $T_D > T_S$. A third heat bath with temperature $T_S < T_O < T_D$ can be used to control the temperature at the node O, so as to control the heat currents $J_D$ and $J_S$. Panel (b). In an extended regime, as the temperature $T_O$ increases, the thermal bias $(T_D - T_O)$ at the interface decreases while the power spectrum in the left segment of the control node (wine-color) increasingly matches with the power spectrum of the neighboring segment that is connected to the drain D (red). This behavior is depicted with the insets where the corresponding power spectra of the left-sided and right-sided interface particles are depicted for three representative values of $T_O$, as shown by the three arrows. The resulting drain current $J_D$ increases with increasing overlap until it reaches a maximum, and starts to decrease again.

For a transistor to work it is thus necessary that the current amplification factor obeys $\alpha > 1$. This implies a negative differential thermal resistance (NDTR); i.e., it requires a transport regime wherein the heat current decreases with increasing thermal bias. Such behavior occurs with the thermal diode characteristics depicted with Fig. 5(d); note the behavior for the case with filled (blue) triangles with $\Delta$ increasing from $\sim [-0.5, -0.2]$. It should be pointed out that such an (NDTR)-behavior is in no conflict with any physical laws.

While negative differential electric resistance has long been realized and extensively studied (Esaki, 1958), the

1 Note that this NDTR should not be confused with absolute neg-
The concept of NDTR has been proposed more recently only \cite{Li et al. 2004, 2006a}. With temperature $T_O$ increasing, the sensitively temperature-dependent power spectra of the two segments match increasingly better which not only offsets the effect of a decreasing thermal bias ($T_D - T_O$) but even induces an increasing heat current. This behavior is illustrated in Fig. 5(b).

A system displaying NDTR constitutes the main ingredient for operation of a thermal transistor. The scheme of a thermal transistor is shown in Fig. 6(a). In order to make this setup physically more realistic, a third segment (G) is connected to the node O. This is done so, because in an actual device it is difficult to directly control the temperature of node O, being located inside the device. Using different sets of parameters, this thermal transistor can work either as a thermal switch, Fig. 6(b), or also as a thermal modulator, Fig. 6(c).

The key prerequisite for a thermal transistor, i.e. the NDTR phenomenon has been investigated in various other systems recently, e.g. for high dimensional lattice models \cite{Lo et al. 2008}. A gas-liquid transition has also been utilized in the design of a thermal transistor \cite{Komatsu and Ito 2011}. The condition for the existence of a NDTR regime is more stringent than that of obtaining merely thermal rectification. The crossover from existence to nonexistence of NDTR have been investigated for a set of different lattice structures, both by analytical and numerical means \cite{He et al. 2009, Shao et al. 2009}. Because the NDTR in these lattice models basically derives from an interface effect, it is plausible that with a too large interface coupling strength $k_{int}$ or a too long lattice length, it is rather the thermal resistance of the involved segments than the interface resistance that rules the NDTR. As a consequence, the NDTR effect typically becomes considerably suppressed. We therefore expect that NDTR can experimentally be realized with nano-scale materials, for example using nano-tubes, nano-wires, etc., see \cite{Chang et al. 2007, 2008, 2006}. This issue is addressed in greater detail with Sect. III below.

C. Thermal logic gates

The phenomenon of NDTR provides not only the function for thermal switching and thermal modulating, but also the essential input in devising thermal logic gates. Setups for all major thermal logic gates able to perform thermal logic operations are given in this section, Fig. 7.

![FIG. 6 (color online). Thermal transistor. (a) Sketch of a thermal transistor device. Just as in the case of an electronic transistor, it consists of two segments (the Source and the Drain) and, as well, a third segment (the Gate) where the control signal is injected. The temperatures $T_D$ and $T_S$ are fixed at high, $T_A$, and low, $T_C$, values. The negative differential thermal resistance (NDTR) occurs at the interface between O and $O'$. This part then makes it possible that over a wide regime of parameters, when the gate temperature $T_G$ rises, not only $J_S$ but also $J_D$ may increase. Using different system parameters allow then different function, this being either a thermal switch (panel (b)) or also a thermal modulator (panel (c)). Panel (b). Function of a thermal switch: At three working points where $T_G = 0.04, 0.09$ and 0.14, the heat current $J_D$ equals $J_S$, yielding $J_G = J_S - J_D$ vanishing identically. These three working points correspond to (stable) “off”, (unstable) “semi-on” and (stable) “on” states, at which $J_D$ differs substantially. We can switch, i.e., forbid or allow heat flowing by setting $T_G$ at these different values. Panel (c). Function of a thermal modulator. Over a wide temperature interval of gate temperature $T_G$, depicted via the hatched working region, the heat current $J_D$ remains very small, i.e. it remains inside the hatched regime, while the two heat currents $J_S$ and $J_D$ can be continuously controlled from low to high values. Adapted from \cite{Li et al. 2006a}.](image-url)
form logic operations have been put forward recently (Wang and Li [2007]).

In digital electric circuits, two boolean states “1” and “0” are encoded by two different values of voltage, while in a digital thermal circuit these boolean states can be defined by two different values of temperature $T_{on}$ and $T_{off}$. In the following we discuss the way to realize such individual logic gates.

A most fundamental logic gate is the signal repeater which ‘digitizes’ the input. Namely, when the input temperature is lower/higher than a critical value $T_c$, with $T_{off} < T_c < T_{on}$, the output is set at $T_{off}/T_{on}$, respectively. This does not present a simple task; it must take into account that small errors may accumulate, thus leading eventually to incorrect outputs.

The thermal repeater can be obtained by use of thermal switches. Let us inspect again the thermal switch shown in Fig. 5(a), in which the $T_G$-dependence of the heat currents $J_D$, $J_S$ and $J_G$ is illustrated with Fig. 5(b). When the gate temperature $T_G$ is set very close but not precisely at $T_{off}/T_{on}$, then the heat current in the gate segment makes the temperature in the junction node $O$ approach more closely $T_{off}/T_{on}$. Therefore, upon connecting such switches in series, which involves plugging the output (from node $O$) of one switch into the gate of the next one, the final output will asymptotically approach that of an ideal repeater, i.e. $T_{off}/T_{on}$, whichever is closer to the input temperature $T_G$.

A NOT gate reverses the input; it yields the response “1” whenever it receives “0”, and vice versa. This requires that the output temperature falls when the input temperature rises, and vice versa. This feature can be realized by injecting the signal from the node $G$ and collecting the output from the node $O'$, cf. Fig. 6(a). The NDTR between the nodes $O$ and $O'$ again plays the key role. A higher temperature $T_G$ induces a larger thermal current $J_D$, $J_S$ and $J_G$ is illustrated with Fig. 6(b). When the gate temperature $T_G$ is set very close but not precisely at $T_{off}/T_{on}$, then the heat current in the gate segment makes the temperature in the junction node $O$ approach more closely $T_{off}/T_{on}$. Therefore, upon connecting such switches in series, which involves plugging the output (from node $O$) of one switch into the gate of the next one, the final output will asymptotically approach that of an ideal repeater, i.e. $T_{off}/T_{on}$, whichever is closer to the input temperature $T_G$.

Similarly, an AND gate is a three-terminal (two inputs and one output) device. The output is “0” if either of the inputs are “0”. Because we now have the thermal signal repeater at our disposal, an AND gate is readily realized by plugging two inputs into the same repeater. It is clear that when both inputs are “1”, then the output is also “1”; and when both inputs are “0”, then the output is also “0”. By adjusting some parameters of the repeater, we are able to make the final output to be “0” when the two inputs are opposite, therefore realizing a thermal AND gate. An OR gate, which exports “1” whenever the two inputs are opposite, can also be realized in the similar way.

D. Thermal memory

Towards the goal of an all phononic computing, yet another indispensable element, besides thermal logic gates, are thermal memory elements that enable the storage of information via its encoding by heat or temperature.

A possible such setup acting as a thermal memory has been proposed by Wang and Li (2008a). Its blueprint has much in common with the working scheme for the thermal transistor, cf. Fig. 3(a). Adjusting parameters appropriately, negative differential thermal resistance can be induced between the chain segments connecting to node $O$ and node $O'$, respectively. With fixed $T_S$ and $T_D$, obeying $T_S < T_D$, and a heat bath at temperature $T_G$ that is coupled to the node $G$, three possible

FIG. 7 (color online). Negative response and thermal NOT gate. (a) Temperature of the node $O'$ as a function of $T_G$ for the setup shown in Fig. 5(a). In a wide range of $T_G$, $T_{out}$ decreases as $T_G$ increases. (b) Function of the thermal NOT gate. The thin (blue) line indicates the function of an ideal NOT gate. Inset: Structure of a two-resistor voltage divider, the counterpart of a temperature divider, which supplies a voltage lower than that of the battery. The output of the voltage divider is: $V_{out} = V R_2/(R_1 + R_2)$. Adapted from [Wang and Li (2007)].
working points for \( T_G \), i.e., \( T_{\text{off}} \), \( T_{\text{semi-on}} \) and \( T_{\text{on}} \) can be realized. At these three working points the gate current vanishes, \( J_C = 0 \), thus balancing perfectly \( J_S \) and \( J_D \). Upon analyzing the slope of \( J_C \) at these very points two of these, i.e., \( (T_{\text{off}}, T_{\text{on}}) \) denote stable working points and the intermediate one, \( T_{\text{semi-on}} \), is unstable. Notably, these working states remain stationary when the heat bath that is coupled to terminal \( G \) is removed. Now, however, the corresponding temperatures at these working points exhibit fluctuations. As is well known from stochastic bistability (Hänggi et al., 1991), small fluctuations around these working points drive the system consistently back to the stable working points and away from the unstable working point. Accordingly, the system possesses two long lived meta-stable states, \( T_O = T_{\text{on}} \) and \( T_O = T_{\text{off}} \), while \( T_O = T_{\text{semi-on}} \) is unstable.

The stability of these so adjusted thermal states at \( T_{\text{on}} \), \( T_{\text{off}} \) implies that these states remain basically unchanged over an extended time span in spite of thermal fluctuations. This holds true even if a small external perturbation, for example imposed by a small thermometer, reading the temperature at the node \( O \), is applied.

The working principle of a Write-and-Read cycle of this so designed thermal memory is depicted with Fig. 3. Starting out at time \( t = 0 \) from a random initial preparation of all particles making up the memory device the local temperature at site \( O \) relaxes to its stationary value \( T_O \sim 0.18 \) (initializing stage). For the case in panel (b) in Fig. 3 the Writer, being prepared at its boolean temperature \( T_{\text{off}} \) is next connected to the site \( O \) (writing stage). As can be deduced from panel Fig. 3(b), the temperature \( T_O \) quickly relaxes during this writing cycle to this boolean value, and maintains this value over an extended time span, even after the Writer is removed (maintaining stage). More importantly, \( T_O \) self-recoveries to this setting temperature \( T_{\text{off}} \) after being exposed to the small perturbation as induced by the Reader (a small thermometer) during the following data-reading stage. The data stored in the thermal memory are therefore precisely read out without destroying the memory state.

In panel Fig. 3(c), the Write-and-Read process corresponding to the opposite boolean writing temperature value, i.e. \( T_O = T_{\text{on}} \), is depicted. Accordingly, this so engineered Write-and-Read cycle with its two possible writing temperatures \( T_{\text{off}} \) and \( T_{\text{on}} \) does accomplish the task of a thermal memory device.

III. PUTTING PHONONS TO WORK

In the foregoing Sec. II, we have investigated various setups involving stylized nonlinear lattice structures in order to manipulate heat flow. We next discuss how to put these concepts into practical use with physically realistic systems. In doing so we consider numerical studies of suitably designed nanostructures which exhibit the designated thermal rectification properties. This discussion is then followed with first experimental realizations of a thermal diode and the thermal memory.

Among the plenty of physical materials that come to mind, low dimensional nanostructures like nanotubes, nanowires and graphene likely offer optimal choices to realize the desired thermal rectification features obtained with nonlinear lattice studies. It is known from theoretical studies (Dhar, 2008; Lepri et al., 2003; Saito and Dhar, 2010) and experimental validation (Chang et al., 2008; Ghosh et al., 2010), that the characteristics of heat flow (such as the validity of the Fourier Law (Dhar, 2008; Lepri et al., 2003; Saito and Dhar, 2010)) sensitively depends on spatial dimensionality and the absence or presence of (momentum) conservation laws.
This is even more the case for nano materials, wherein due to the limited size, the discrete phonon spectrum (Yang et al., 2010) results in a distinct dependence of the thermal quantities on the specific geometrical configuration, mass distribution and ambient temperature. Overall, this makes nanosized materials promising candidates for phononics. Because the experimental determination of thermal transport properties is not straightforward the combined use of theory and numerical simulation is indispensable in devising phononics devices. Moreover, novel atomistic computational algorithms have been developed which facilitate the study of experimentally relevant system sizes (Li et al., 2010).

A. Thermal diodes from asymmetric nanostructures

Carbon nanotubes (CNTs) have recently attracted attention for applications in nanoscale electronics, mechanical and thermal devices. CNTs possess a high thermal conductivity at room temperature (Kim et al., 2001) and phonon mean free paths that extend over the length scale of structural ripples; thus providing ideal phonon waveguide properties (Chang et al., 2007).

Let us consider thermal rectification in single-walled carbon nanotube (SWCNT) based junctions (Wu and Li, 2007). A typical (n, 0)/(2n, 0) intramolecular junction structure is shown in Fig. 9(a) in which the structure contains two parts, namely, a segment with a (n, 0) SWCNT and a segment made of a (2n, 0) SWCNT. These two segments are connected by m pairs of pentagon-heptagon defects. By use of non-equilibrium molecular dynamics (NEMD) simulations, one finds that the heat flux from the (2n, 0) to (n, 0) tube exceeds that from the (n, 0) tube to the (2n, 0) segment. The corresponding thermal rectification increases upon raising the temperature bias.

Another beneficial feature is that the rectification is only weakly dependent on the detailed structure of the interface, assuming that the connecting region is sufficiently short. This is so because heat is predominantly carried by long wavelength phonons, which are scattered mainly by large defects. Just as with nonlinear lattice models, the match/mismatch of the energy spectra around the interface is the underlying mechanism for rectification. Furthermore, in the elongated structure (Wu and Li, 2008) the heat flux becomes smaller than that of the non-deformed structure; its temperature dependence, however, becomes more pronounced, due to the intrinsic tensile stress.

The carbon nanocone depicted in Fig. 9(b) is yet another carbon based material exhibiting a high asymmetric geometry. Its thermal properties were investigated by Yang et al. (2008). A temperature difference, Δ, between the two ends of nanocone is introduced, being positive when the bottom of nanocone is at a higher temperature, and is negative in the opposite case. It was found that the nanocone behaves as a “good” thermal conductor under positive thermal bias and as a “poor” thermal conductor when exposed to a negative thermal bias. This suggests that the heat flux runs preferentially along the direction of decreasing diameter.

In order to compare the impact of mass-asymmetry versus geometry-asymmetry for thermal rectification a nanocone structure with a graded mass distribution was discussed (Yang et al., 2008). The mass of the atoms of the nanocone are devised to change linearly; that is, the top atoms possess a minimum mass MC12 and the bottom atoms are at the maximum mass of 4MC12, with MC12 being the mass of 12C atom. NEMD results then yield a rectification ratio, $|J_+ - J_-|/|J_-|$, that is 10% for a nanocone with uniform masses and is 12% for the mass-graded nanocone (at identical thermal bias Δ). This 2% increase for the mass-graded distribution evidences that the role of geometric asymmetry is more effective in boosting thermal rectification.

These geometric asymmetric SWCNT junctions all exhibit thermal rectification. Compared to the SWCNT setup, it is easier, however, to control the shape of graphene by the nano cutting technology such as helium ion microscope. Graphene nanoribbons (GNRs), cf. Fig. 9(c), present promising elements for nanoelectronics and nanophononics. For instance, Yang et al. (2009) have demonstrated tunable thermal conduction in GNRs. They studied the direction dependent heat flux in asymmetric structural GNRs, and explored the impacts of both, GNR shape and size, for the rectification ratio. Two types of GNRs were considered: trapezia-shaped GNR and two-rectangular GNRs of different width, Fig. 9(c).

These two types of GNRs behave as a “good” thermal
conductors under positive thermal bias (i.e. bottom end at higher temperature) and as a “poor” thermal conductor under negative thermal bias (i.e. top end at higher temperature). This finding is similar to the rectification phenomena observed in carbon nanocone structures (Yang et al., 2008), which again results from the amount of match/mismatch between the respective phonon spectra.

It is interesting to note that the rectification ratios of GNRs are substantially larger than those in nanocone and SWCNT junctions. With $\Delta = 0.5$, the rectification ratio of the nanocone is 96% (Yang et al., 2008) and that of SWCNT intramolecular junction is only around 15% (Wu and Li, 2007), while the rectification ratio in GNRs is about 270% and 350% for two-rectangular GNRs and the trapezia-shaped GNR, respectively. The rectification ratio of trapezia-shaped GNR is thus larger than that of two-rectangular GNR under the same thermal bias difference. This feature is consistent with the phenomenon that the carbon nanocone (i.e. the geometric graded structure) possesses a larger rectification ratio than the two-segment carbon nanotube $(n, 0)/(2n, 0)$ intra-molecular junction. The phonon spectra change continuously in the graded structures which implies a more efficient control of heat flux. Similar rectification features were observed in graphene nanoribbons by Hu et al. (2009).

Yet another advantage of a GNR based thermal rectifier is its weak dependence on length. Because energy is transported ballistically in graphene, the heat flux is essentially independent on size. Both $J_+$ and $J_-$ are saturated when the GNR length is longer than $\sim 5.1$ nm, yielding that the rectification ratio remains constant around 92%. Moreover, compared to a setup composed of a single-layer graphene, an even larger rectification ratio can be achieved in few-layer asymmetric structures, this being a consequence of layer-layer interactions (Zhang and Zhang, 2011).

Thermal rectification can also be realized with a topological graphene setup such as the Möbius graphene strip (Jiang et al., 2010). Fig. 3(d). The advantage of this topology induced thermal rectification is that it is practically insensitive to temperature and size of the system. In this structure, the asymmetry originates from the intrinsic topological configuration.

Because phonons are strongly scattered due to the mismatch in vibrational properties of the materials forming the interface, which in addition depends on the sign of applied thermal bias, this produces an asymmetric Kapitza contact resistance. Capitalizing on this idea a silicon-amorphous polyethylene thermal rectifier was designed (Hu et al., 2008). The result is that the heat current from the polymer to the silicon is larger than vice versa. To examine the origin of the thermal rectification, the density of states of phonons on each side of the interface was investigated. The phonon density of states significantly softens in the polymer as it becomes warmer. This increases the density of states in the polymer at low frequencies. Those low frequency acoustic modes in silicon thus increase their transmission probability, yielding an enhanced thermal transport.

The setups discussed thus far are all operating in steady state. A transient thermal transport exhibiting a time-dependent thermal rectification has been investigated for a Y-SWCNT junction by Gonzalez Nova et al. (2009). From their molecular dynamics simulation it is reported that a heat pulse propagates unimpeded from the stem to the branches, undergoing little reflection. For the reverse temperature bias, however, there is a substantial reflection back into the branches. The transmission coefficient from the stem to the branches is more than four times that of the reverse direction.

Let us reflect again on the choice of materials suitable in obtaining those theoretically predicted thermal rectification features. A thermal rectifier constitutes a two-terminal thermal device whose working principle rests upon the different overlap of the temperature dependent phonon spectra. For this to occur strong anharmonicity plays an important factor. Given the above discussion of geometric asymmetric structures a strong intrinsic anharmonicity corresponds to diffusive phonon transport. However, diffusive phonon transport presents not a necessary condition for thermal rectification. In the asymmetric GNRs, phonon transport is almost ballistic. The conclusion is that thermal rectification exists for both, ballistic and diffusive phonon transport, assuming that a match/mismatch of the phonon spectrum of the two ends is present. This difference in phonon spectra can originate from different sources, as for example from an asymmetric mass distribution, different geometry, size or spatial dimension.

Despite an abundance of parameter dependent rectification studies (Hu et al., 2006; Wu and Segall, 2009; Wu et al., 2009; Yang et al., 2007), these were rarely tested against experiments. All those NEMD-studies rely on mathematically idealized material Hamiltonians, which in practice may still be far from physical reality. Only in situ experiments thus present the ultimate test bed for a validation of the wealth of available theoretical results and, even more importantly, dictate the necessary next steps towards an implementation of phononics.

B. In situ thermal diodes from mass-graded nanotubes: Experiment

On the experimental side, a pioneer thermal diode work has been performed by Chang et al. (2006). In their experiment, cf. Fig. 10, carbon nanotubes (CNTs) and boron nitride nanotubes (BNNTs) were gradually deposited on the surface with the heavy molecules located along the length of the nanotube in order to establish an asymmetric mass distribution. As an important test, it has been experimentally checked that in unmodified NTs with uniform mass distribution the thermal conductance is indeed independent of the direction of the applied ther-
C. Solid-state-based thermal memory: Experiment

Apart from the experimental demonstration of a nanoscale thermal rectifier, a thermal memory device has recently also brought into operation experimentally by Xie et al. (2011). In their work, see in Fig. 11(a), a single-crystalline VO2 nanobeam is used to store and retain thermal information with two temperature states as input $T_{in}$ and output $T_{out}$, which serve as the logical boolean units “1” (= HIGH) and “0” (= LOW), for writing and reading. This has been achieved by exploiting a metal-insulator transition. A nonlinear hysteretic response in temperature was obtained in this way. A voltage bias across the nanobeam has been applied to tune the characteristics of the thermal memory. One finds that the hysteresis loop becomes substantially enlarged, see in Fig. 11(b), and is shifted towards lower temperatures with increasing voltage bias. Moreover, the difference in the output temperature $T_{out}$ between its “HIGH” and
"LOW" temperature states increases substantially with increasing voltage bias. To demonstrate the repeatability of the thermal memory, they have performed repeated Write(High)-Read-Write(Low)-Read cycles using heating and cooling pulses to the input terminal, see panel (c) in Fig. [11] for more details. Repeated cycling over 150 times proves the reliable and repeatable performance of this thermal memory.

**IV. SHUTTLING HEAT AND BEYOND**

The function of the various thermal electronic analog devices discussed in Sect. II used a heat control mechanism which is based on a static thermal bias. In order to obtain an even more flexible control of heat energy, being comparable with the richness available known for electronics, one may design intriguing phononic devices which utilize temporal, ac gating modulations as well. Such forcing makes possible the realization of a plentitude of novel phenomena such as the heat ratchet effect, absolute negative heat conductance or the realization of Brownian (heat) motors, to name but a few (Astumian and Hänggi, 2002; Hänggi and Marchesoni, 2009; Ren and Li, 2010). Among the necessary pre-requisites to run such heat machinery are thermal noise, nonlinearity, unbiased nonequilibrium driving of deterministic or stochastic nature and a symmetry breaking mechanism. This then carries the setup away from thermal equilibrium, thereby circumventing the second law of thermodynamics, which otherwise would impose a vanishing directed transport (Hänggi and Marchesoni, 2009).

Dwelling on similar ideas used in Brownian motors for directing particle flow, an efficient pumping or shuttling of energy across spatially extended nano-structures can be realized via modulating either one or more thermal bath temperatures, or applying external time-dependent fields, such as mechanical/electric/magnetic forces. This gives rise to intriguing phononic phenomena such as a priori directed shuttling of heat against an external thermal bias or the pumping of heat that is assisted by a geometrical-topological component.

**A. Classical heat shuttling**

In the following we shall elucidate the objective for shuttling heat against an externally applied thermal bias. A salient requirement for the modus operandi of heat motors is the presence of a spatial or dynamic symmetry breaking.

A possible scenario consists in coupling an asymmetric nonlinear structure to two baths; i.e., a left(L) and right(R) heat bath which can be modeled by classical Langevin dynamics. Applying a periodically time-averaged temperature in one or both heat baths, \( T_{L(R)}(t) = T_{L(R)}(t + 2\pi/\omega) \), possessing the same average temperature \( T_{L(R)}(t) = T_0 \), then brings the system out-of-equilibrium. Noteworthy is that this so driven system is unbiased; i.e., it exhibits a vanishing average thermal bias \( \Delta T(t) = T_L(t) - T_R(t) = 0 \).

The asymptotic heat flux \( J(t) \) assumes the periodicity of the external driving period \( 2\pi/\omega \) and the time-averaged heat flux \( J \) follows as the cycle-average over a full temporal period: \( J = \frac{1}{2\pi} \int_0^{2\pi/\omega} J(t)dt \). Consequently, a nonzero average heat flux \( J \neq 0 \) emerges which then provides the seed to even shuttle heat against a net thermal bias \( \Delta T(t) \neq 0 \).

A first possibility to introduce the necessary symmetry breaking is to use an asymmetric material such as two coupled FK-FK lattices where two segments possess different thermal properties (Li et al., 2008; Ren and Li, 2010), see in Fig. [12]. The directed heat transport can be extracted out of unbiased temperature fluctuations by harvesting the static thermal rectification effect (Li et al., 2004).

Yet another possibility is to break the symmetry dynamically by exploiting the nonlinear response induced by the harmonic mixing mechanism, stemming from a time-varying two-mode modulation of the bath temperature(s), i.e., \( T_{L(R)}(t) = T_0[1 \pm A_1 \cos(\omega t) \pm A_2 \cos(2\omega t + \varphi)] \). The second harmonic driving term \( A_2 \cos(2\omega t + \varphi) \) causes the intended nonlinear frequency mixing (Li et al., 2009).

In the adiabatic limit; i.e., if \( \omega \to 0 \), a nonzero heat flux \( J \neq 0 \) can be obtained due to the nonlinearity of the heat conductance response. The preferred direction of such heat flow is determined by the intrinsic thermal diode properties. In contrast, in the fast driving limit \( \omega \to \infty \), the left- and right-end of the system will es-

**FIG. 12** (color online). Action of a heat Brownian motor in two coupled asymmetric FK-FK lattices. The heat baths are subjected to periodic modulations in the form \( T_L(t) = T_0[1 + \Delta + A \textrm{sgn}(\sin(\omega t))] \) and \( T_R(t) = T_0(1 - \Delta) \). The dimensionless reference temperature is set as \( T_0 = 0.09 \) (see the Appendix A.2 for the expressions of corresponding dimensionless units). Note that in distinct contrast to Fig. [3] (d) the ratchet effect now yields with a modulation strength \( A \neq 0 \) a nonvanishing heat flow at zero bias \( \Delta = 0 \). Applying a substantial rocking strength, \( A = 0.5 \), the current bias characteristics can be manipulated as to inhibit a negative differential thermal resistance (NDTR) regime at negative bias values \( \Delta \). Adapted from Li et al. (2008).
sentially experience a time-averaged constant temperature. This then mimics thermal equilibrium, yielding \( J \to 0 \). Remarkably, by modulating the driving frequency \( \omega \) through the characteristic thermal response frequency of the system, the intriguing phenomenon of a heat current reversal can be observed \cite{Li et al., 2008, 2009}. For this two segment system, an optimal heat current can be obtained around this characteristic frequency even when the two isothermal baths are oscillating in synchrony with \( T_L(t) = T_R(t) \), and the current reversal can be realized by tuning the system size \cite{Ren and Li., 2011}. In the harmonic mixing mechanism the directed heat current is found to be proportional to the third-order moment \( (\Delta T(t)/2T_0)^3 \), i.e., \( J \propto A_L^2 A_R \cos \varphi \) \cite{Li et al., 2009}. This enables a more efficient way of manipulating heat: the direction of heat current can be reversed by merely adjusting the relative phase shift \( \varphi \) of the second harmonic driving.

Apart from using the FK-lattice as a source of nonlinearity, other schemes of heat motors can be based on a Fermi-Pasta-Ulam (FPU) lattice structure, a Lennard-Jones interaction potential \cite{Li et al., 2009}, or also a Morse lattice structure \cite{Gao and Zheng, 2011}.

Besides a manipulation of bath temperatures, the shutting of heat can be realized by use of a combination of time-dependent mechanical control in otherwise symmetrical structures. Depending on specific nonlinear system setups, an emerging directed heat current can be controlled by adjusting the relative phase among the acting drive forces \cite{Marathe et al., 2007} or the driving frequency \cite{Ai et al., 2010}. Multiple resonance structures for the heat current vs. the driving frequency of external forces can occur as well \cite{Zhang et al., 2011}. It can be further demonstrated that for strict harmonic systems, periodic-force driving fails to shuttle heat. Moreover, it has been shown that even for anharmonic lattice segments composed of an additional energy depot, it is not possible to pump heat from a cold reservoir to a hot reservoir by merely applying external forces \cite{Marathe et al., 2007, Zhang et al., 2011}.

It is elucidative to compare these setups with the Feynman ratchet-and-pawl device of a heat pump \cite{Van den Broek and Kawal, 2000, van den Broek and Van den Broek, 2008, Hanggi and Marchesoni, 2009, Komatsu and Nakagawa, 2009}. The latter is a consequence of Onsager’s reciprocal relation in the linear response regime: if a thermal bias generates a mechanical output, then an applied force will direct a heat flow as a conjugate behavior. Therefore, conjugated processes can be utilized for heat control as well. Other well-known thermally conjugated processes are the Seebeck, Thomson and Peltier effects in thermoelectrical devices, where the thermal bias induces electrical currents, or vice versa. Recently, such a nanoscale magnetic heat engine and pump has been investigated for a magneto-mechanical system, which either operate as an engine via the application of a thermal bias to convert heat into useful work, or act as a cooler via applying magnetic fields or mechanical force fields to pump heat \cite{Bauer et al., 2010}.

![Figure 13](image_url)

**B. Quantum heat shuttling**

The efficient shuttling of heat via a time-dependent modulation of bath temperatures can be extended into the quantum regime when tunneling and other quantum fluctuation effects come into play. In clear contrast to the realm of electron shuttling \cite{Galperin et al., 2007, Hanggi and Marchesoni, 2009, Hanggi et al., 2002, Joachim and Ratner, 2003, Remacle et al., 2005}, however, this aspect of shuttling quantum heat is presently still at an initial stage, although expected to undergo increasing future activity.

1. **Molecular wire setup**

In the following we consider one specific such case in some detail. Let us consider a setup with a typical
molecular wire for which the heat transport is generally governed by both, electrons and phonons. A schematic setup based on a stylized molecular wire is sketched with Fig. 13(a) (Zhan et al., 2009). The single electronic level $E_1$ can be conveniently modulated by a gate voltage and $\omega_1$ denotes the vibrational frequency for a single phonon mode. The lead temperatures $T_{L(R)}(t)$ undergo an adiabatically slow periodic modulation for both electron and phonon reservoirs. The latter is experimentally accessible by use of a heating/cooling circulator (Lee et al., 2003). In an adiabatic driving regime, the asymptotic ballistic electron and phonon heat currents $J_{Q}^{\text{el}}(t)$ and $J_{Q}^{\text{ph}}(t)$ can be calculated via the celebrated Landauer-like expressions (Gomez et al., 2003): i.e.,

$$J_{Q}^{\text{el}}(t) = \int_{-\infty}^{\infty} \frac{d\varepsilon}{2\pi\hbar} (\varepsilon - \mu) T^{\text{el}}(\varepsilon) [f(\varepsilon, T_{L}(t)) - f(\varepsilon, T_{R}(t))],$$

$$J_{Q}^{\text{ph}}(t) = \int_{0}^{\infty} \frac{d\omega}{2\pi} \hbar \omega T^{\text{ph}}(\omega) [n(\omega, T_{L}(t)) - n(\omega, T_{R}(t))].$$

where $T^{\text{el}}(\varepsilon)$ and $T^{\text{ph}}(\omega)$, respectively, denote the temperature independent transmission probability for electrons with energy $\varepsilon$ and phonons with angular frequency $\omega$. Here, the functions $f(\varepsilon, T_{L}(t)) = [\exp(\varepsilon - \mu)/k_{B}T_{L}(t)] + 1)^{-1}$ and $n(\omega, T_{L}(t)) = [\exp(\hbar \omega/k_{B}T_{L}(t)) - 1)^{-1}$ where $l = L,R$, denote the Fermi-Dirac distribution and the Bose-Einstein distribution, respectively. These functions both inherit a time-dependence which derives from the applied adiabatic periodic temperature modulation.

Then, a finite total heat current $J_{Q}$ emerges, reading

$$J_{Q} = J_{Q}^{\text{el}}(t) + J_{Q}^{\text{ph}}(t).$$

This heat current $J_{Q}$ results as a consequence of the nonlinear dependence of quantum statistics on temperature, see in Fig. 13(b); note that in presence of modulation $J_{Q}$ is nonzero even for vanishing thermal bias $\Delta T_{\text{bias}}$. This ballistic heat transport is a pure quantum effect which will not occur in the classical diffusive limit, being approached at ultrahigh temperatures. The efficient manipulation of heat shuttling can be realized by applying the above-mentioned harmonic mixing mechanism. Since the heat transport is carried also by electrons, adjusting the gate voltage gives rise to a intriguing control of heat current with the result that the direction of heat current experiences multiple reversals.

The quantum heat shuttling of a dielectric molecular wire can also be achieved upon periodically modulating the molecular levels while this molecular wire is connected to two heat baths that are characterized by distinct spectral properties (Segal and Nitzan, 2006). Interestingly, the pumping of quantum heat can be operated arbitrarily close to the Carnot efficiency by a tailored stochastic modulation of the molecular levels (Segal, 2008, 2009). Time-dependent phonon transport in the non-adiabatic regime and strong driving perturbations has numerically been investigated by use of the nonequilibrium Green’s function (NEGF) approach (Gomez et al., 2011; Wang et al., 2008) for the case of coupled harmonic oscillator chains: There, the coupling to the reservoirs is held at different temperatures with the latter switched on suddenly (Cuansing and Wang, 2010).

2. Pumping heat via geometrical phase

As discussed above, a one-parameter modulation, e.g. via the left-sided contact temperature $T_{L}(t)$ is typically sufficient for quantum mechanical shuttling and rectification of heat, as sketched with Fig. 13(a).

It should be noted, however, that a cyclic modulation involving at least two control parameters generally induces additional current contributions beyond its mere dynamic component. This is so because with a variation evolving in a (parameter) space of dimension $d \geq 2$ one typically generates geometrical properties (i.e. a nonvanishing, gauge invariant curvature) in the higher-dimensional parameter space of the governing dynamical laws for the observable, in this case the heat flow. This geometrical properties in turn affect the resulting flow within an adiabatic or even non-adiabatic parameter variation. With a cyclic adiabatic variation of multiple parameters this contribution to the emerging flow is thus of topological origin. It has been popularized in the literature under the label of a geometrical, finite curvature or (Berry)-phase phenomenon (Sinitsyn, 2008). As a consequence, one needs to consider the total heat flow to be composed of two contributions, reading:

![FIG. 14](color online). Quantum heat pumping via a geometrical phase. (a) A schematic representation of a single molecular junction. (b) Quantum heat transfer across the molecular junction is generated via an adiabatic two-parameter variation of the left bath temperature $T_{L}(t)$ and the right bath temperature $T_{R}(t)$, which maps onto a closed (7) circle. The arrow indicates the direction of the modulation protocol. (c) Geometrical phase induced heat current, $J_{\text{geom}}$, versus the angular modulation frequency $\Omega$. The straight line corresponds to the analytic result while the open circles denote the simulation results. For further details we refer the reader to (Ren et al., 2010).
\[ J_{\text{tot}} = J_{\text{dyn}} + J_{\text{geom}} . \] (9)

Here, the geometrical contribution is proportional to the adiabatic small modulation frequency \( \Omega \); implying that this correction is typically quite small in comparison with its non-vanishing dynamical contribution. Therefore, to observe this component it is advantageous to use a two-parameter variation such that the dynamic component vanishes identically.

A sole geometrical contribution can be implemented, for example, by modulating the two bath temperatures in a way that the trajectory in the plane spanned by the two temperatures describes a circle, c.f. Fig. 14(b), – in which case there results a sole Berry-phase-induced heat current \( J_{\text{geom}} \), while its dynamical component, \( J_{\text{dyn}} \), is identically vanishing, \( J_{\text{dyn}} = 0 \) [Ren et al., 2010]. Also, different from the case of an irreversible, dynamical heat flux, this geometrical contribution can be reversed upon simply reversing the protocol evolution. The latter operation thus provides a novel and convenient method for controlling energy transport. In [Ren et al., 2010] the authors have demonstrated such nonvanishing quantum heat pumping as the result of a nonvanishing geometrical phase. This situation is depicted with Fig. 14(c).

A similar geometrical phase effect can also be present in classical setups; e.g., for coupled harmonic oscillators in contact with Langevin heat baths. In this case it has been demonstrated that with a modulation of the two bath temperatures in time the geometrical phase phenomenon emerges only for the higher order moments of the heat flow; that is to say only beyond the average heat flux. Only when nonlinearity or temperature-dependent parameters in an interacting system are present can the geometrical phase manifest itself in producing a nonvanishing heat current.

Moreover, the finite Berry-phase heat pump mechanism in both, quantum and classical systems has been demonstrated to cause a breakdown of the so termed “heat-flux fluctuation theorem”, the latter being valid for a time-independent heat flux transfer. This fluctuation theorem [Campisi et al., 2011; Saito and Dhar, 2007] can be restored only under special conditions in the presence of a vanishing Berry curvature [Ren et al., 2010].

C. Topological phonon Hall effect

It is known that a geometrical Berry phase yields profound effects on electronic transport properties in various Hall effect setups [Xiao et al., 2010]. Due to the very different nature of electrons and phonons, the phonon Hall effect (PHE) has been discovered only recently in a paramagnetic dielectric [Strohm et al., 2007], and subsequently confirmed by yet a different experimental setup [Inyushkin and Taldenkov, 2007]. In particular one observes a transverse heat current in the direction perpendicular to the applied magnetic field and to the longitudinal temperature gradient, see in Fig. 15. The discovery of this novel PHE renders the magnetic field to be another flexible degree of freedom for phonon manipulation towards the objective of energy and information control in phononics.

Since then, several theoretical explanations have been proposed [Kagan and Maksimov, 2008; Sheng et al., 2006; Wang and Zhang, 2010b; Zhang et al., 2010a] to understand the PHE by considering the spin-phonon coupling. The spin-phonon coupling has two possible origins: (i) It either derives from the magnetic vector potential in ionic crystal lattices, where the vibration of atoms with effective charges will experience the Lorentz force under magnetic fields [Holz, 1972], or (ii) it results from a Raman (spin-orbit) interaction [Ioselevich and Capellmann, 1993; Kornig, 1933; Orbach, 1961; Van Vleck, 1940]. It has been shown that by introducing spin-phonon couplings, a ballistic system without nonlinear interaction even exhibits the possibility of thermal rectification [Zhang et al., 2010b].

Similar to the various Hall effects occurring for electrons, a topological explanation of the PHE has been provided in [Zhang et al., 2010a, 2011a]. The heat flow in the PHE is ascribed to two separate contributions: the normal flow responsible for the longitudinal phonon transport, and the anomalous flow manifesting itself as the Hall effect of the transverse phonon transport. A general expression for the transverse phonon Hall conductivity is obtained in terms of the Berry curvature of phononic band structures. The associated topological Chern number (a quantized integer) for each phonon band is defined via integrating the Berry curvature over the first Brillouin zone. For the two dimensional honeycomb and kagome-lattice, the authors observed phase transitions in the PHE, which correspond to the sudden change of the underlying band topology. The physical mechanism is rooted in the touching and splitting of the phonon bands [Zhang et al., 2010a, 2011a].

Therefore, much alike for electrons in topological insulators [Hasan and Kane, 2010], the design of a family of novel phononic devices – topological thermal insulators – is promising, with the bulk being an ordinary thermal insulator while the edge/surface constitutes an extraordinary thermal conductor.
V. SUMMARY, SUNDRIES AND OUTLOOK

With this Colloquium we took the reader on a tour presenting the state of the art of the topic termed ‘Phononics’, an emerging research direction which is expected to chime in the future with conventional ‘Electronics’. Particularly, we surveyed and explained various physical mechanisms that are exploited in devising the elementary phononic toolkit: namely, a thermal diode/rectifier, thermal transistor, thermal logic gate and thermal memory. These building blocks for doing phononic electronics are rooted in the application of suitable static or dynamic control schemes for shuttling heat. We further reviewed recent attempts to realize such phononic devices which all are based on nanostructures and discussed first experimental realizations.

A. Challenges

In spite of the rapid developments of phononics in both science and technology, we should stress that this objective is still at its outset. To put these phononic devices to work, there remain lots of ambitious theoretical and severe experimental challenges to be overcome. For example, much work is still required for the physical realization of the phononic toolbox and for entering the next stage of assembling operating networks that are both scalable and stable under ambient conditions.

Theory.– Interface thermal resistance. As we have pointed out the underlying mechanism for thermal rectifier/diode is based on an asymmetric interface thermal resistance. However, thus far a truly comprehensive theory for this effect is lacking.

The current approaches for thermal transport across an interface, such as the acoustic mismatch (AMM) theory [Little, 1959] and the diffusive mismatch (DMM) theory [Swartz and Polik, 1989], are based on the assumption that phonon transport proceeds via a combination of either ballistic or diffusive transport on either side of the interface. Both schemes offer limited accuracy for nanoscale interfacial resistance predictions [Stevens et al., 2007], due to the neglect of the atomic details of actual interfaces. Specifically, the acoustic mismatch model assumes that phonons are transported across the interface without being scattered; i.e. they are ballistic while the diffuse mismatch model assumes the opposite, namely that the phonons are scattered diffusively. Thus, the effects of scattering on the interfacial thermal resistance act as upper and lower limits for real situation. In fact, both notions for real situation. In fact, both notions for real situation. In fact, both notions for real situation.

Yet another fact of thermal rectification and negative differential thermal resistance is the role of (strong) nonlinearity. How to set up a transport theory by incorporating nonlinearity in both, the quantum regime and the classical regime presents a challenge. The non-equilibrium Green’s (NEGF) function method [Wang et al., 2008] certainly serves as an elegant mathematical framework. However, when sophisticated phonon-phonon interactions (which derive from anharmonicity), and alike, become increasingly important (this being so in realistic nanostructures), the NEGF presents a cumbersome task. In the classical regime, an effective phonon theory has proven useful in characterizing heat conduction [Li and Li, 2007; Li et al., 2006b]. Several classical studies have been advanced [He et al., 2011, 2008, 2009], which may as well be extended into the quantum regime.

Experiment.– Experimental realization of practical phononic device depends on how to measure its thermal conductivity accurately. To this end, one needs to get rid of the contact thermal resistance. Thus far no well defined scheme capable to eradicate such contact thermal resistance has been put forward.

It also should be noted that presently the prime elementary phononic building block, i.e. the thermal rectifier, has been realized on the micrometer scale [Chang et al., 2006] and on the millimeter scale [Kobayashi et al., 2009; Sawaki et al., 2011] only. The challenge for experimentalists is to make the sample smaller, for example towards a dozens of nanometers or even a few nanometers only. This then would boost the rectification to much larger values and simultaneously would allow detecting the asymmetric interface thermal resistance. The primary challenge ahead, however, is to validate the negative differential thermal resistance, i.e. the key element necessary in realizing the thermal transistor.

For electronic-like function a networking towards a phononic-like logic operation is indispensable. In the event that this task could be achieved successfully could then facilitate the desirable operation of an all-phononic computer.

B. Future prospects

As emphasized above, the area of phononics lingers still in its infancy, yet it is at the verge of blossoming up.

From phononics to acoustics, and vice versa. – As we elucidated throughout this Colloquium the physical principle of phononic devices rests in the manipulation of phonon bands/spectra. This idea can be generalized to control any elastic/mechanical energy. For example,
inspired by the thermal diode, an acoustic diode has been proposed by Liang et al. (2009) and subsequently realized experimentally by use of a nonlinear acoustic medium and phononic crystal Liang et al. (2010), and a sonic crystal geometry Liu et al. (2011). Boechler et al. (2011) have demonstrated experimentally elastic energy switching and rectification. There is little doubt that in parallel to phononics, namely an acoustic transistor, logic gate and possibly even a computer device may be realized in the foreseeable future. The ideas and concepts in controlling acoustic waves can as well be exploited for phononics. For example, phononic crystals have been demonstrated to be useful in manipulating acoustic wave propagation Liu et al. (2000). This concept has been extended recently to control heat flow on the nanoscale Hopkins et al. (2011); Landry et al. (2008); McGaughey et al. (2006); Yu et al. (2010). It would not come as a too big surprise when someday concepts such as a “heat-cloak”, “super heat lens”, etc., come alive via the implementation of phononic concepts by use of acoustic meta-materials Fang et al. (2006); Guenneau et al. (2007); Yang et al. (2004); Zhang and Liu (2004). In fact, active research is presently pursued in controlling and manipulating mechanical/elastic energy which ranges from long wavelength elastic waves to very short wavelength thermal waves, a glimpse of this activity can be adapted from the Proceedings of the world first conference on ‘Phononics’ El-Kady and Hussein (2011).

PhoXonics: phonons plus photonics, and beyond. – Another promising prospect is based on the combination of phononics with photonics to control and manage photon and phonon energy concomitantly Maldovan and Thomas (2006). This synergy might potentially enable one to use the solar energy more wisely. For instance, a single-molecule phonon field-effect transistor has been designed wherein phonon conductance is controlled by a back-gate electric field Menezes et al. (2010). Moreover, as temperature is the commonly applied control parameter for chemical and biological reactions, phononic devices may also find application for the local control of temperatures, for example in regulating molecular self-assembling processes with the “Lab-on-a-Chip” technology.

Phononics and electronics. – Electrons carry as well heat. Therefore one can control the heat flow carried by electrons with the help of electric/magnetic fields. For example, by asymmetrically coupling a quantum dot to its two leads one can construct a heat rectifier Scheibner et al. (2008); – upon applying a gate voltage it is possible to operate a heat transistor Saira et al. (2007). These kind of devices combined with phononic circuits may then carry the potential to manipulate dissipation of heat and cooling in nanoscale and molecular devices. Overall, there is also the potential that hybrid structures composed of electronic and phononic elements may lead to beneficial applications.

From heat conduction to radiation. – In this colloquium, our proposed phononic devices are based on the control of heat conduction, being assisted by lattice vibrations. A similar idea can be generalized to control heat radiation. Indeed, Fan and collaborators at Stanford proposed a photon-mediated “thermal rectifier through vacuum” Otev et al. (2010) which makes constructive use of the temperature dependence of underlying electro-magnetic resonances. In the same spirit, Fan’s group Zhu et al. (2012) revealed negative differential thermal conductance through vacuum; this in turn allows for the blueprint of a transistor for heat radiation.

Finally, let us end with a celebrated quote by Winston Churchill: “This is not the end. It is not even the beginning of the end. But it is, perhaps, the end of the beginning.”

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Appendix: Nonlinear Lattice Models

1. Lattice models

In this Appendix we introduce three archetype one-dimensional (1D) lattice models commonly used in the
investigation of heat transport. These are (i) the linear Harmonic lattice, (ii) the nonlinear Fermi-Pasta-Ulam $\beta$ (FPU-$\beta$) lattice and (iii) the Frenkel-Kontorova (FK) lattice. The simplest harmonic lattice serves as the basic model from which the FPU-$\beta$ lattice and FK lattice are derived by complementing the dynamics with a nonlinear inter-atom interaction in the FPU-case and an on-site potential in the FK-case, respectively.

For a 1D harmonic lattice with $N$ atoms the normal modes of the lattice vibrations are known as phonons. The corresponding harmonic lattice Hamiltonian explicitly reads

$$H = \sum_{i=1}^{N} \left[ \frac{p_i^2}{2m} + \frac{k_0}{2}(x_i - x_{i-1} - a)^2 \right], \quad (A1)$$

wherein the dynamical variables $p_i$ and $x_i$ $i = 1, ..., N$, denote the momentum and position degrees of freedom for the $i$-th atom and $x_0 \equiv x_1 - a$. The parameters $m$, $k_0$, $a$ denote the mass of the atom, the spring constant and the lattice constant, respectively. The position variable $x_i$ can be replaced by the displacement from equilibrium position as $\delta x_i = x_i - ia$ which we denote by the same symbol $x_i \equiv \delta x_i$ henceforth. The Hamiltonian of Eq. (A1) with $\delta x_0 = \delta x_1$ thus simplifies, reading:

$$H = \sum_{i=1}^{N} \left[ \frac{p_i^2}{2m} + \frac{k_0}{2}(x_i - x_{i-1})^2 \right]. \quad (A2)$$

This form explicitly depicts the translational invariance of the free chain which implies momentum conservation.

Applying next periodic boundary conditions $x_0 \equiv x_N$, the harmonic lattice of Eq. (A2) can be decomposed into the sum of noninteracting normal modes (phonons) with the dispersion relation reading

$$\omega(q) = 2\sqrt{\frac{k_0}{m} |\sin(q/2)|}, \quad 0 \leq q \leq 2\pi \quad (A3)$$

where the continuous spectrum is due to the adoption of thermodynamical limit $N \to \infty$. The harmonic lattice possesses an acoustic phonon branch with $\omega(q) \to 0$ as $q \to 0$.

Although the 3D harmonic lattice model yields a satisfactory explanation for the temperature dependence of experimentally measured specific heat, it turns out that this very model of noninteracting phonon modes fails to describe a Fourier Law for heat transport. In pioneering work [Rieder et al., 1967] the authors proved that for this 1D harmonic lattice the heat transport is ballistic; this is due to the absence of phonon-phonon interactions. In order to take the phonon-phonon interactions into account, the harmonic chain model must be complemented with nonlinearity.

If a quartic inter-atom potential is added, one arrives at the FPU-$\beta$ lattice with the corresponding Hamiltonian reading:

$$H = \sum_{i=1}^{N} \left[ \frac{p_i^2}{2m} + \frac{k_0}{2}(x_i - x_{i-1})^2 + \frac{\beta_0}{4}(x_i - x_{i-1})^4 \right], \quad (A4)$$

where the parameter $\beta_0$ is the nonlinear coupling strength. Historically, the FPU-$\beta$ lattice has been put forward by Fermi, Pasta and Ulam [Fermi et al., 1955] to study the issue of ergodicity of a nonlinear system dynamics. For some excellent reviews of the original FPU problem we refer the readers to Refs. [Berman and Izrailev, 2005; Ford, 1992]). Surprisingly, the FPU-$\beta$ lattice still fails to obey Fourier’s law and the heat conductivity $\kappa$ diverges with the system size proportional to $\kappa \propto N^\alpha$ with $0 < \alpha < 1$ [Lepri et al., 1997]. This divergent behavior has recently been experimentally verified for a system setup using quasi-1D nanotubes [Chang et al., 2008]. The phonon modes of FPU-$\beta$ lattice are also acoustic-like after re-normalization of the nonlinear part, due to the conservation of total momentum.

If a periodic on-site substrate potential is added to the harmonic chain, one arrives at the FK lattice. Its Hamiltonian is given by

$$H = \sum_{i=1}^{N} \left[ \frac{p_i^2}{2m} + \frac{k_0}{2}(x_i - x_{i-1})^2 + \frac{V_0}{4\pi^2} \left( 1 - \cos \frac{2\pi x_i}{a} \right) \right], \quad (A5)$$

where parameter $V_0/4\pi^2$ denotes the nonlinear on-site coupling strength. Here we only consider the commensurate case where the on-site potential assumes the same spatial periodicity as the harmonic lattice. Notably this model with an on-site potential now breaks momentum conservation. Among the various phenomenological models that mimic solid state systems the FK model has been shown to provide a suitable theoretical description for possible nonlinear phenomena such as the occurrence of commensurate-incommensurate phase transitions [Floria and Mazo, 1996], kink-like structures and alike [Braun and Kivshar, 1998, 2004]. It has attracted interest since it was first proposed by Frenkel and Kontorova [Frenkel and Kontorova, 1938, 1939] in order to study various surface phenomena. Recently it has been established that the FK lattice indeed does exhibit normal heat conduction and thus obeys the Fourier law [Hu et al., 1998]. This normal behavior is attributed to the optical phonon mode where the phonon mode opens a gap as the momentum conservation is broken with the on-site potential.

2. Local temperature and heat flow

Dimensionless units constitute practical tools for the theoretical analysis and numerical simulations. Here we provide a brief introduction to the dimensionless units used in this report for the various lattice model setups.
Let us start with the simplest lattice model of 1D Harmonic lattice of Eq. (A2). For the harmonic lattice contacting a heat bath specified by a temperature $T$, there are four independent parameters $m, a, k_0$ and $k_B$ where $k_B$ denotes the Boltzmann constant. The dimensions of all the physical quantities that typically enter the issue of heat transport can be expressed by the proper combination of these four independent parameters because there are only four fundamental physical units involved: length, time, mass and temperature.

As a result, one can introduce the dimensionless variables by measuring lengths in units of $[a]$, momenta in units of $[a(mk_0)^{1/2}]$, temperature in units of $[k_0a^2/k_B]$, frequencies in units of $[(k_0/m)^{1/2}]$, energies in units of $[k_0a^2]$ and heat currents in units of $[a^2k_0^{3/2}]/(2\pi m^{1/2})]$. In particular, the Hamiltonian of Eq. (A2) can be transformed into a dimensionless form if we implement the following substitutions:

\[ H \rightarrow H[k_0a^2], p_i \rightarrow p_i[a(mk_0)^{1/2}], x_i \rightarrow x_i[a], \quad (A6) \]

where the so transformed dynamical variables yield the dimensionless variables to obtain

\[ H = \sum_{i=1}^{N} \left[ \frac{\dot{p}_i^2}{2} + \frac{1}{2} (x_i - x_{i-1})^2 \right], \quad (A7) \]

Typical physical values for atom chains are as follows: $a \approx 10^{-10}$ m, $\omega_0 \approx 10^{13}$ sec$^{-1}$, $m \approx 10^{-26} - 10^{-27}$ kg, $k_B = 1.38 \times 10^{-23}$ J K$^{-1}$, we have $[k_0a^2/k_B] \approx (10^2-10^3)$K. This in turn implies that room temperature corresponds to a dimensionless temperature $T$ of the order $0.1 - 1$ [Hu et al. 1998].

To obtain the dimensionless FPU-β lattice from Eq. (A4), one cannot scale the five parameters $k_B = a = m = k_0 = \beta_0 = 1$ because one of them is redundant. Applying the substitutions of Eq. (A6), we obtain the dimensionless form for the FPU-β Hamiltonian:

\[ H = \sum_{i=1}^{N} \left[ \frac{\dot{p}_i^2}{2} + \frac{1}{2} (x_i - x_{i-1})^2 + \frac{\beta}{4} (x_i - x_{i-1})^4 \right], \quad (A8) \]

with the dimensionless parameter $\beta \equiv \beta_0a^2/k_0$. It is evident that the dimensionless nonlinear coupling strength $\beta$ is generally not equal to unity. However, it can be shown that upon adjusting $\beta$ becomes equivalent to vary the system energy or its temperature.

The dimensionless FK Hamiltonian can also be obtained by use of Eq. (A6):

\[ H = \sum_{i=1}^{N} \left[ \frac{\dot{p}_i^2}{2} + \frac{1}{2} (x_i - x_{i-1})^2 + \frac{V}{4\pi^2} [1 - \cos(2\pi x_i)] \right], \quad (A9) \]

where the dimensionless on-site coupling strength $V \equiv V_0/k_0a^2$.

Thus far, we dealt with homogeneous lattice Hamiltonians. For thermal devices with more than one segment, each segment may possess its own set of parameters such as a different spring constant or nonlinear coupling strength. In those cases, the reference parameter, for instance $k_0$, used to define a transformation in Eq. (A6) may be chosen to correspond to a natural parameter of the corresponding segment. In particular, the dimensionless Hamiltonian for each individual segment of a coupled FK-FK lattice may be written as

\[ H = \sum_{i=1}^{N} \left[ \frac{\dot{p}_i^2}{2} + \frac{k}{2} (x_i - x_{i-1})^2 + \frac{V}{4\pi^2} [1 - \cos(2\pi x_i)] \right], \quad (A10) \]

where $k$ is measured with the reference to a parameter $k_0$ which is introduced a priori.

Next we discuss the results for expressing temperature and heat current in dimensionless units. In our classical simulations we typically used Langevin thermostats with coupling the “contact” or end particles to the heat baths at their corresponding temperature. More precisely, one adds to the corresponding Newtonian equation of motion a Langevin fluctuating term which satisfies the fluctuation-dissipation relation, e.g. see in Hänggi et al. (1994). Towards this goal we made use of the equipartition theorem of classical statistical mechanics to define, for example, the local temperature $T_i$ via its average atomic kinetic energy; i.e.,

\[ k_B T_i \equiv \left\langle \frac{p_i^2}{m} \right\rangle \rightarrow T_i \equiv \left\langle \frac{p_i^2}{k_0a^2} \right\rangle, \quad (A11) \]

where the arrow indicates the dimensionless substitution $T_i \rightarrow T_i[k_0a^2/k_B]$ and $p_i \rightarrow p_i[a(mk_0)^{1/2}]$, and $\langle \cdots \rangle$ denotes the (long) time-average or, equivalently, its ensemble-average in numerical simulations, thus implicitly assuming ergodicity (in mean value).

Unlike temperature, the expression for the heat current is model dependent. To arrive at a compact expression we first rewrite the 1D lattice Hamiltonian in the more general form:

\[ H = \sum_{i} \left[ \frac{\dot{p}_i^2}{2} + V(x_{i-1}, x_i) + U(x_i) \right], \quad (A12) \]

where $V(x_{i-1}, x_i)$ denotes the inter-atom potential and $U(x_i)$ is the on-site potential. As a result of the continuity equation for local energy, the local, momentary heat current can be expressed as [Lepri et al. 2003]:

\[ J_i = -\dot{x}_i \frac{\partial V(x_{i-1}, x_i)}{\partial x_i}. \quad (A13) \]

Consequently, the expression of heat current depends only on the form of the inter-atom potential $V(x_{i-1}, x_i)$. One should notice that although the on-site potential $U(x_i)$ does not enter into the expression of heat current explicitly, it does, however, influence the heat current implicitly through the dynamical equations of motions.

The heat currents itself are again obtained via the time average over an extended time span. For steady state setups with fixed bath temperatures the resulting
heat currents are time-independent and, as well, independent of the particular site index \(i\) within the particular chain segment. Likewise, with periodically varying bath temperatures \(T(t)\), the resulting ensemble average is also time-periodic; an additional time-average over the temporal period of \(T(t)\) yields the cycle-averaged, time-independent heat flux. Alternatively, an explicit long time average again produces this very time-independent value for the heat current.

3. Power spectra of FPU-\(\beta\) and FK lattices

The power spectrum (or power spectral density) describes the distribution of a system’s kinetic energy falling within given frequency intervals. For a homogeneous lattice composed of identical particles the velocity \(v_i(t) = \dot{q}_i(t)\) of a particle located at site \(i\) becomes independent of position \(i\); the power spectrum then can be conveniently calculated by the Fourier transform of the corresponding velocity degree of freedom to yield:

\[
P(\omega) = \lim_{t_0 \to \infty} \frac{1}{t_0} \int_0^{t_0} v(t)e^{-i\omega t}dt.
\]

(A14)

In doing so, the power spectrum of the FPU-\(\beta\) model of Eq. (A3) depends on the temperature. In the low temperature regime the FPU-\(\beta\) dynamics is close to a harmonic lattice, yielding \(0 < \omega < 2\). In contrast, in the high temperature regime it is the anharmonic part that starts to dominate. In this latter regime an approximate theoretical estimate then yields \(0 < \omega < C_0(T\beta)^{1/4},\) with \(C_0 = 2\sqrt{2\pi} \Gamma(3/4)^{3/4}/\Gamma(1/4) \approx 2.22\), where \(\Gamma\) denotes the Gamma function \([Li~et~al.,~2005a]\). Therefore, upon increasing the temperature then causes a rightward shift of the power spectrum towards higher frequencies. The Parseval’s theorem then dictates that the area below the curve is proportional to the average kinetic energy of the particle; i.e., \(\int_0^\infty P(\omega)d\omega \sim \langle E_{kin}\rangle\).

For the FK model in Eq. (A10) the form of the power spectrum depends sensitively on temperature. In the low temperature limit, the atoms are confined in the valley of the on-site potential. Upon linearizing Eq. (A10) the phonon band can be extracted to read:

\[
\sqrt{V} < \omega < \sqrt{V + 4k}.
\]

(A15)

In contrast, in the high temperature limit the on-site potential can be neglected; thus the system dynamics becomes effectively reduced to a harmonic chain dynamics, whose phonon band extends to:

\[
0 < \omega < 2\sqrt{k}.
\]

(A16)

The crossover temperature \(T_c\) can be approximated as: \(T_c \approx V/(2\pi)^2\). Its value depends on the height of on-site potential. This in turn implies different values for the two segments of the thermal diode setup, see Fig. 16. This difference is at the heart of the thermal rectifying mechanism.

FIG. 16 (color online). Temperature dependent power spectra. The variation of the power spectrum at different temperatures vs. the angular frequency \(\omega\) (both in dimensionless units) in an FK-lattice with 10000 sites for two different sets of parameters in (a) and (b). The features of these nonlinear FK-power spectra provide the seed for the \textit{modus operandi} in a thermal diode setup as discussed in Sec II.A.1. The panel (a) is for a FK-coupling strength of \(V=5\) and a strength for the spring constant of \(k=1\); panel (b) is for a coupling strength \(V=1\) and a spring constant value set at \(k=0.2\).

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