Thermal Logic Gates: Computation with Phonons

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Logic gates are basic digital elements for computers. We build up thermal logic gates that can perform similar operations as their electronic counterparts. The thermal logic gates are based on nonlinear lattices, which exhibit very intriguing phenomena due to their temperature dependent power spectra. We demonstrate that phonons, the heat carriers, can also be used to carry information and processed accordingly. The possibility of nanoscale experiments is discussed.

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As two fundamental energy transport phenomena with similar importance in nature [1], electric conduction and thermal conduction have never been treated equally. The invention of the electronic transistor [2] and other relevant devices that control electric flow has led to an impressive technological development that has changed many aspects of our daily life. However, similar devices in controlling heat flow are still not available even though many experimental attempts have been made to design such devices [3–7]. Recent years have witnessed some important progress; for example, a thermal rectifier has been proposed by using the property of temperature-dependent power spectra in nonlinear lattices [8–15], and molecular level thermal machines that pump heat from a cold to a hot reservoir have been suggested [16,17]. Merely a few years after the theoretical models of a thermal rectifier, a nanoscale solid-state thermal rectifier has been demonstrated experimentally by asymmetrically deposited nanotubes [18]. Moreover, based on the new phenomenon of negative differential thermal resistance [9], we have also built up a thermal transistor model [19] which controls heat flow like a field-effect-transistor does for the electric current.

On the other hand, phonons and other vibrational excitons in low-dimensional adsorbed dielectric and semiconductor nanostructures might also play an important role in information transmission [20].

In this Letter we present thermal logic gates that can do basic logic calculations. This may provide the possibility that in the near future, phonons, which are traditionally regarded as the heat carriers, can also carry information and can be processed accordingly, like electrons and photons. In other words, the “phononic computer,” an alternative to the existing electronic computer, may also be possible.

In an electric (chemical) [21] logic gate, the power supplies that fix the voltages (chemical concentrations) of some points are necessary. Similarly, in a thermal logic gate, power supplies that keep the temperatures of some points are necessary, too. The temperatures of the power supplies are labeled as T_+ and T_-, $T_+ > T_-$. In any linear electric circuit in which all the resistances are constants, when the voltage of one node is changed by a battery connected to it, the voltage of any other node may also change, but must be in the same way, and the latter change must NOT be greater than the former one, namely, *super response* and *negative response* are not allowed. This is also true for thermal circuits. Therefore, nonlinear devices are necessary for any thermal logic gate.

The nonlinear device that we use in this Letter is the thermal transistor, which is depicted in Fig. 1(a). Two weakly coupled nonlinear segments, D and S, are connected to power supplies with temperature $T_+(=0.2)$ and $T_-(=0.03)$, respectively. The control segment G is coupled to the “input signal” with temperature T_G. Each segment is modeled by a one-dimensional Frenkel-Kontorova (FK) lattice [22] whose Hamiltonian reads

$$H_{\rm FK} = \sum_i \left[\frac{1}{2}\dot{x}_i^2 + \frac{1}{2}k(x_i - x_{i-1})^2 + U_i(x_i)\right], \qquad (1)$$

where k is the spring constant and $U_i(x) = 1 - \frac{V}{(2\pi)^2} \times \cos 2\pi x$ corresponds to the on-site potential. The FK model describes a chain of harmonic oscillators subject to an external sinusoidal potential. This is similar to the case by putting a polymer chain or a nanowire on top of an adsorbed sheet [20]. Since the momentum conservation is broken in such a lattice, heat conduction obeys Fourier's law [23]. For simplicity, we have set the masses of all particles to unit. The spring constant k and the on-site potential strength V in different terminals are different. Terminal D is coupled to terminal S by a spring of constant $k_{\rm int}$, and terminal S is coupled to control terminal G by a spring of constant $k_{{\rm int}_G}$. $k_{\rm int}$ is the most important parameter of the thermal transistor. It controls the magnitude and position of the “negative differential thermal resistance” effect discussed below. More details can be found in Fig. 3(a) in Ref. [19].

In our computer simulation, power supplies and input signals are simulated by Langevin heat baths, and we have checked that our results do not depend on the particular heat bath realization (e.g., Nose-Hoover heat baths). We integrate the differential equations of motion by using the 5th-order Runge-Kutta algorithm. The simulations are per-

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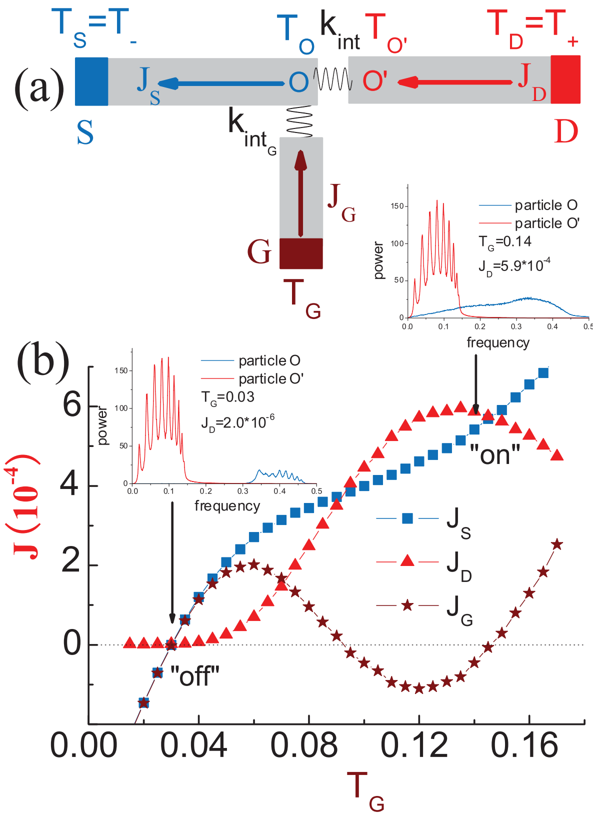

FIG. 1 (color). (a) Configuration of the thermal transistor. (b) Heat currents through three terminals D, S, and G versus temperature T_G. The NDTR is clearly seen in a wide region, namely, J_D increases when temperature T_G is increased. At $T_G = T_{\mathrm{on}}$ and T_{off}, J_G is exactly zero. Insets: power spectra of particles O and O' near off and on states. Power spectrum of O depends sensitively on temperature. It matches that of O' much better at the on state than at the off state, thus making much higher J_D at the on state although the temperature difference between terminal D and particle O is much larger at the off state.

formed long enough to allow the system to reach a nonequilibrium stationary state and the local heat flux, $J_i \equiv k\langle \dot{x}_i(x_i - x_{i-1})\rangle$, is constant in each segment. Temperature of a particle is defined as the average of twice the kinetic energy, $T_i = \langle \dot{x}_i^2 \rangle$.

If the lattice in segment D is linear, then as the temperature difference in this segment is decreased by increasing T_O, one expects a decrease in J_D. However, because the FK lattice is nonlinear, one actually obtains an increased J_D, as demonstrated in Fig. 1(b). In this figure, when T_G (T_O is always very close to T_G) changes from $T_{\mathrm{off}}(= 0.03)$ to $T_{\mathrm{on}}(= 0.14)$, the temperature difference $T_D - T_O$ is decreased, but the current J_D increases from 2×10^{-6} to 5.9×10^{-4}. This is the so-called negative differential thermal resistance (NDTR), an essential physical principle for the thermal transistor [19]. The NDTR can be understood from studying the vibrational spectra of interface particles O and O'. One should recall that in our model, the heat is conducted by lattice vibration. Therefore, when one combines two segments of different lattices, the overlap of the vibration spectra of the interface particles mainly determines the heat current. If the two spectra overlap, the heat can easily go through; otherwise, it is much more difficult. The FK lattice has a temperature-dependent vibrational spectrum. At the high and low temperature limits, the power spectra concentrate on low ($\omega \in [0, 2\sqrt{k}]$) and high ($\omega \in [\sqrt{V}, \sqrt{V + 4k}]$) frequencies, respectively. More details can be found in Refs. [9,14]. As shown in the inset of Fig. 1(b), at $T_G = T_{\mathrm{off}}$, the spectra of O and O' do not overlap; thus, the heat current at this point is very small, whereas at $T_G = T_{\mathrm{on}}$, the overlap is much better; thus, although the temperature difference at the interface is much smaller, the heat current is, however, much larger.

NDTR provides the keys for thermal logic gates, e.g., super response and negative response, which are necessary for the thermal signal repeater and the NOT gate. In the central region of Fig. 2(a), when temperature T_G is changed, temperature T_O changes even greater than T_G, which makes T_O always be closer to T_{on} or T_{off}, whichever is closer, than T_G is. This can be understood by considering the direction of heat flow in segment G when T_G is slightly different from $T_{\mathrm{on}}/T_{\mathrm{off}}$. Also see Fig. 2(b). $T_{O'}$ changes in the opposite way of T_G. This can be understood by considering change of heat flow J_D versus T_O. As T_G increases (in this case the thermal resistance between G and O is very

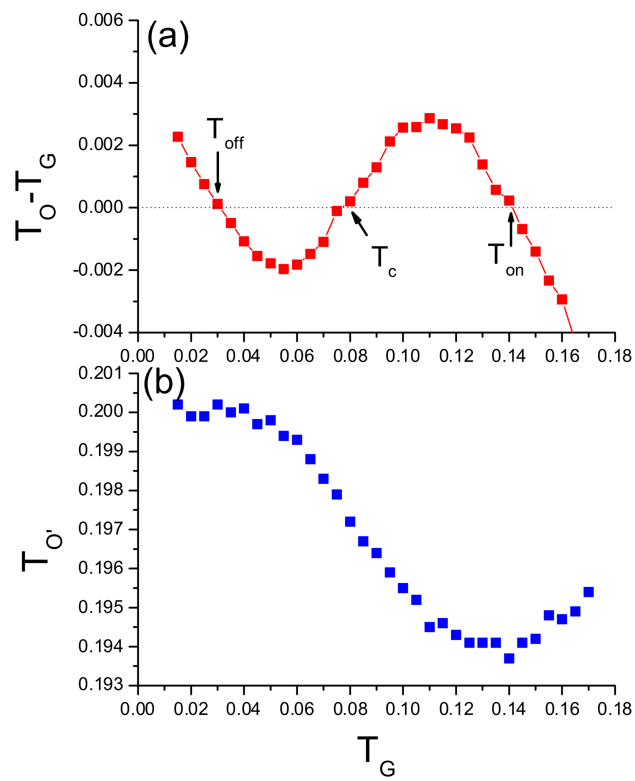

FIG. 2 (color online). (a) $T_O - T_G$ versus T_G. Notice the super response that in the central region, $T_O - T_G$ increases when T_G increases; namely, T_O increases even greater than T_G. (b) $T_{O'}$ versus T_G. Notice the negative response that $T_{O'}$ decreases as T_G increases.

small; thus, T_O is always close to T_G) thanks to the NDTR effect, heat flow J_D increases, which makes temperature difference $T_D - T_{O'}$ increase; namely, $T_{O'}$ decreases. As was mentioned above, these super response and negative response are not possible in any linear circuit. In the following, we show how to build thermal gates by combining thermal transistors. Hereafter in this Letter, symbols O, O', D, S, and G particularly indicate the corresponding nodes of the transistor shown in Fig. 1(a).

In a digital electric circuit, two standard values of voltage are used to indicate states "1" and "0." Similarly we use two standard values of temperature T_{on} and T_{off}, and hereafter we fix $T_{\text{on}} = 0.16$ and $T_{\text{off}} = 0.03$.

The most fundamental logic gate is the signal repeater, which is a two-terminal device (one input and one output) whose function is to standardize an input signal. Its response function, T_{output} as a function of T_{input}, is

$$T_{\text{output}} = T_{\text{off}}, \quad \text{if } T_{\text{input}} < T_c, \qquad T_{\text{output}} = T_{\text{on}}, \quad \text{if } T_{\text{input}} > T_c. \tag{2}$$

Namely, when the input signal is lower or higher than a critical value T_c ($T_{\text{off}} < T_c < T_{\text{on}}$), the output is exactly $T_{\text{off}}/T_{\text{on}}$. This is not a trivial device, without which small errors may accumulate, thus eventually leading to a wrong calculation.

This ideal repeater can be realized by several two-terminal devices whose response functions have two *stable* fixed points at T_{on} and T_{off}. Therefore, if we connect them in a series, namely, plug the output of one device to the input of the next one, the final output is closer and closer to an ideal repeater. It is easily seen that in such a device, super response, i.e., the change of T_{output} is greater than that of T_{input}, is necessary; otherwise, the two fixed points at T_{on} and T_{off} cannot both be stable. Such a device cannot be realized by any linear thermal circuit; however, it can be simply realized by a thermal transistor by using terminal G as input and node O as output [Fig. 2(a)]. $T_G = T_{\text{on}}$ and T_{off} are the two stable fixed points, and there still exists an unstable fixed point at $T_G = T_c$, which separates the attraction basins of the two stable fixed points.

As an example, we show a repeater consists of six thermal transistors in Fig. 3(a). Its function is shown in Fig. 3(b). It is very close to an ideal repeater.

A NOT gate reverses the input; namely, if $T_{\text{input}} = T_{\text{on}}/T_{\text{off}}$, then $T_{\text{output}} = T_{\text{off}}/T_{\text{on}}$. This requires that when T_{input} increases T_{output} decreases, and vice versa, which corresponds to the negative response, which is, as mentioned above, again realized by a thermal transistor by inputting a signal to G and then collecting output from O'; see Fig. 2(b). Notice that $T_{O'}$ is always higher than T_c (in fact, even higher than T_{on}) and thus will always be treated as "on" by the next device. In order to solve this

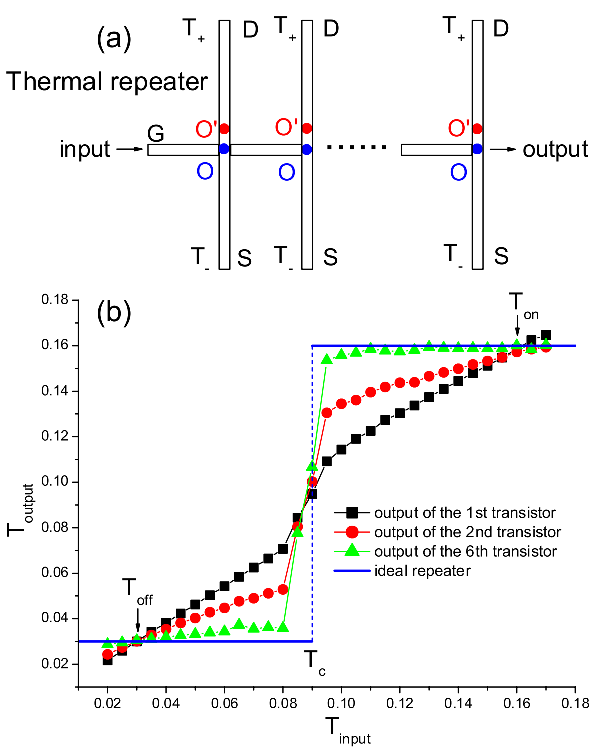

FIG. 3 (color online). (a) Structure of a thermal repeater. (b) Function of a thermal repeater that contains six thermal transistors. The outputs are better and better as the number of transistors is increased. The final output from the 6th transistor is very close to that of an ideal repeater.

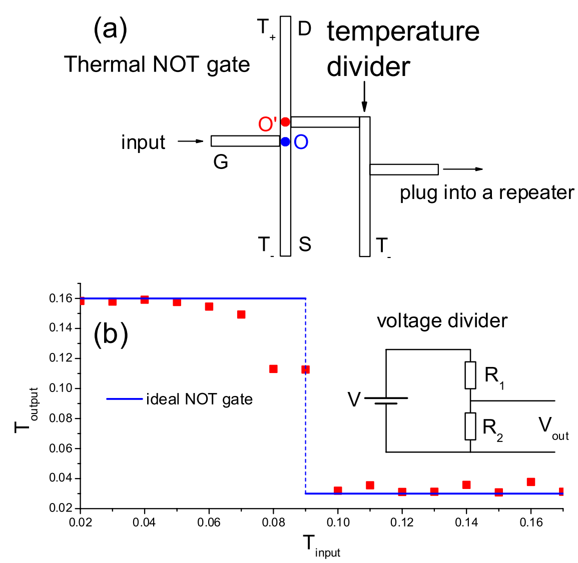

FIG. 4 (color online). (a) Structure of the thermal NOT gate. Through the G segment, the signal is transferred to the O point of the transistor. The output of the transistor (from the O' point) is transferred to the temperature divider. Plug the output of the temperature divider into a repeater; the final output is shown in (b) Function of the thermal NOT gate. It is very close to 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. Without load, the output of the voltage divider is $V_{\text{out}} = VR_2/(R_1 + R_2)$.

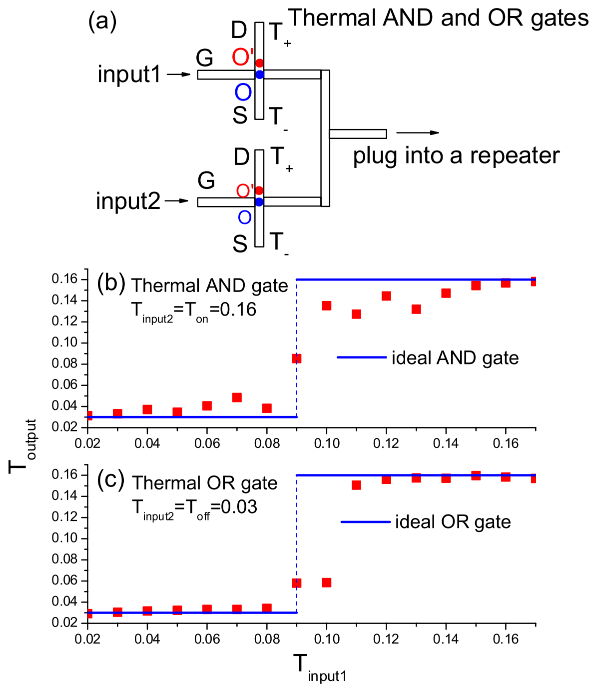

FIG. 5 (color online). (a) Structure of thermal AND and OR gates. Two inputs (after being standardized by repeaters) are transferred to a same repeater. (b) Function of thermal AND gate. We plot T_{output} versus T_{input1} while T_{input2} is fixed to T_{on}. (c) Function of thermal OR gate. We plot T_{output} versus T_{input1} while T_{input2} is fixed to T_{off}.

problem we use a "temperature divider" [counterpart of a voltage divider which is shown in the inset of Fig. 4(b)] whose output is a ratio of its input. By adjusting this ratio, we make its output higher or lower than T_c when the original input T_G is $T_{\mathrm{off}}/T_{\mathrm{on}}$. Then after being standardized by a thermal repeater the final output realizes the function of a NOT gate. See Figs. 4(a) and 4(b) for its structure and function. It is quite a surprising result because high temperature means more entropy or more randomness. Here we demonstrate that one can reduce the randomness of one part of the device by inputting more randomness in another part.

An AND/OR gate is a three-terminal (two inputs and one output) device. If one input is off/on, then the output must be off/on regardless the other input. Otherwise, if one input is on/off, then the output follows the other input. By plugging two inputs (or better, after being standardized by a repeater) to the same repeater, it is clear that when both the inputs are on/off, the output must be on/off. By simply changing some parameters of the repeaters, we can make the final output on/off when the two inputs are different; therefore, an AND/OR gate is realized. See Fig. 5(a) for their structures and Figs. 5(b) and 5(c) for their functions.

In summary, we have presented the feasibility to build up the thermal logic calculation from the thermal transistor model. Although the thermal logical gates given here are only toy models, they may shed light on the study of molecular information technology [24] and smart thermal materials. The study may also be helpful in understanding the complicated heat transport in biological systems.

The FK model we have used here is a very popular model in condensed matter physics and nonlinear physics [22]. It is usually used to describe energy transport in a real solid. We therefore believe that our thermal logic gates can be realized in nanoscale systems experimentally in the foreseeable future, in particular, given the fact that the solid-state thermal rectifier was realized experimentally in 2006 [18], only a few years after the theoretical works.

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