Switchability and controllability of a thermal transistor

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A thermal transistor consists of three segments, the drain, the source, and the gate. We study the influence of the thermal resistance R_G in the gate segment systematically and reveal its key importance. In contrast to the negative differential thermal resistance between the drain and the source that has been studied extensively due to its indispensable function, the role of the gate segment has been neglected for long. It is found that the thermal transistor is switchable, i.e., it can be set exactly to on and off states by setting the control temperature T_G to T_{on} and T_{off} , only when R_G is lower than a critical value. The transistor is controllable, i.e., it can be set to any stable steady state, only when R_G is lower than an even lower critical value. In this case, we are able to build a useful device, a thermal sensor with arbitrarily large temperature sensitivity, by setting a proper value of R_G . However, when these conditions are not satisfied, multiple stable steady states may coexist then the heat currents cannot be exactly determined by the control temperature.

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I. INTRODUCTION

In the past decades, studies on heat conduction in low-dimensional systems have led to impressive theoretical and experimental developments [1,2]. Particularly, much attention has been paid to the field of phononics, a new science and engineering of managing heat flow and processing information with heat. In contrast to electrons, the phonons, the carriers of heat, are bundles of energy that have no mass or charge and are therefore much harder to control. That is why the applications of electronic transistor [3] and other relevant devices that control electric flow have drastically changed many aspects of our daily life, the counterpart technology for heat flow control is, however, still not available for so long.

Productive investigations have been opening the door gradually since the beginning of this century. Shortly after the models of thermal diodes that rectify heat current were proposed [4–6], the finding of negative differential thermal resistance (NDTR) enabled us to propose a model of thermal transistor that switches or modulates heat current [7]. Based on the functions of the thermal transistor, models of thermal logic gates that realize all fundamental logic operations [8] and thermal memory that stores information [9,10] were designed successively. These studies have revealed the theoretical feasibility of completing computation by employing heat rather than electricity [11,12].

Inspired by this theoretical progress, various models of thermal diode [13–16], thermal transistor [17–24], and

thermal memory [25,26] have been worked out based on the same or different underlying mechanisms. In addition, some experimental implementations based on the above theoretical ideas have been reached, including the solid-state thermal diode by using unevenly mass-loaded nanotubes [27], asymmetric cobalt oxides [28], nanotube phonon waveguide [29], and solid-state thermal memory [30–33] as well.

Arguably, among all these thermal devices, the thermal transistor, which can achieve various fundamental thermal control functions, is the most important one. Much effort has been made to realize or improve the NDTR, which builds the kernel of a thermal transistor, in different systems [34–37]. In contrast, the role of the gate (G) segment, is basically ignored. In this paper, we will study systematically the role of the gate segment and reveal the crucial importance of the thermal resistance in it. We will present that the thermal transistor works well as a thermal switch or a thermal modulator only when it is switchable or controllable. These conditions set upper bounds of the thermal resistance in the G segment, beyond which the transistor does not work.

The paper is organized as follows. The model of a thermal transistor will be introduced in Sec. II. Numerical findings are presented in Sec. III. All the findings will be analyzed and explained in Sec. IV. The concepts of switchable and controllable for a thermal transistor will be proposed in this section. Discussions and conclusions are represented finally in Sec. V.

II. MODEL OF THERMAL TRANSISTOR

The model of thermal transistor is depicted in Fig. 1. Analogous to its electric counterpart, the metal-oxide-semiconductor field-effect transistor (MOSFET), a thermal transistor consists of three segments: the drain (D), the source (S), and the gate (G), with particle numbers N_D , N_S and N_G , respectively. Each segment is modeled by a one-dimensional

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FIG. 1. Configuration of the thermal transistor. The ends of the segments S and D are always attached to heat baths with temperatures T_S and T_D , respectively. The positive directions of the heat currents flow through the particle O are illustrated by the arrows.

Frenkel-Kontorova (FK) lattice [38]. Among various phenomenological models, the FK model is one of the most suitable and simple models that describes solid-state systems. The segments S and D are weakly coupled via a linear spring of constant k_{int} , and segment G, the control segment, is coupled to the junction particle O between segments S and D via a linear spring of constant k_{intG} . The weak interface couplings might be realized by the van der Waals forces between molecules, which are typically 1 or 2 orders of magnitude weaker than the chemical bonds.

The Hamiltonian of the whole system takes the same form as we have applied in Ref. [7], i.e.,

$$\begin{aligned}
 H &= H_S + H_D + H_G + H_{\text{int}} + H_{\text{intG}} \\
 &= \sum_{i=1}^{N_S} \frac{1}{2} \dot{x}_{S,i}^2 + \frac{1}{2} k_S (x_{S,i} - x_{S,i-1})^2 - \frac{V_S}{(2\pi)^2} \cos 2\pi x_{S,i} \\
 &\quad + \sum_{i=1}^{N_D} \frac{1}{2} \dot{x}_{D,i}^2 + \frac{1}{2} k_D (x_{D,i} - x_{D,i-1})^2 - \frac{V_D}{(2\pi)^2} \cos 2\pi x_{D,i} \\
 &\quad + \sum_{i=1}^{N_G} \frac{1}{2} \dot{x}_{G,i}^2 + \frac{1}{2} k_G (x_{G,i} - x_{G,i-1})^2 - \frac{V_G}{(2\pi)^2} \cos 2\pi x_{G,i} \\
 &\quad + \frac{1}{2} k_{\text{int}} (x_{S,N_S} - x_{D,N_D})^2 + \frac{1}{2} k_{\text{intG}} (x_{S,N_S} - x_{G,N_G})^2, \quad (1)
 \end{aligned}$$

where $x_{D,i}$, $x_{S,i}$, and $x_{G,i}$ denote the particles' displacements from their equilibrium positions in segments D, S, and G, respectively. We have set the mass of each particle to unity. Fixed boundary conditions (BC) are taken for the D and S segments, i.e., $x_{D,0} = x_{S,0} = 0$; while in contrast to our previous choice [7,9], free BC is applied for the segment G, i.e., $x_{G,0} = x_{G,1}$. Such a choice seems more realistic since the length of this segment will be adjustable in this study. We have confirmed that the change affects the results only very slightly.

The parameters of the thermal transistor are slightly different from those in Ref. [9], i.e., $k_S = 0.42$, $k_D = 0.2$, $k_{\text{int}} = 0.05$, $V_S = 10$, $V_D = 0$, $k_G = k_{\text{intG}} = 1.0$, and $V_G = 10$. We fix $N_D = N_S = 50$ but the length of the G segment N_G is adjustable in order to study its effect. Two Langevin-type heat baths with temperatures $T_S = 0.04$ and $T_D = 0.3$ are always attached to the first particles (labeled $i = 1$) of the segments S and D in all cases.

III. FUNDAMENTAL DIAGRAM AND FINITE TIME TEMPERATURE DISTRIBUTIONS OF A THERMAL TRANSISTOR

A. Fundamental diagram and the control temperature dependence of heat currents

First of all we attach a heat bath to the particle O (the last, i.e., the N_S th particle of the segment S) so as to control its temperature to a desired value T_O . Then after enough long time (typically 10^8 time units), the system approaches the stationary state, which is independent of the initial state. We cannot observe any systematical change of the outputs by further lengthening this time slot. Then the long time (typically 3×10^8 time units) averages of the heat currents J_S and J_D are calculated. J_S denotes the heat current flowing from the particle O to the segment S and J_D denotes the heat current flowing from the segment D to the particle O, see Fig. 1. J_S , J_D , and $\Delta J \equiv J_S - J_D$ versus the temperature T_O are plotted in Fig. 2(a). This figure can be regarded as the fundamental diagram of the thermal transistor. On this basis

FIG. 2. (a) Heat currents J_D , J_S , and $\Delta J \equiv J_S - J_D$ versus the temperature T_O . When $T_O = T_{\text{on}}$ or T_{off} , ΔJ equals exactly zero. (b) Heat currents J_D , J_S , and J_G versus the temperature T_G for $N_G = 50$ (solid lines), 100 (dashed lines), and 200 (dotted lines). In all the cases when $T_G = T_{\text{on}}$ or T_{off} , J_G still keeps exactly zero. (c) Heat currents J_D , J_S , and J_G versus the temperature T_G for $N_G = 800$. No clear on and off states can be observed.

all the findings in this paper can be well explained. ΔJ denotes the net heat current flows from the particle O to the segments S and D. Another heat bath must provide a heat current with the same value that flows into the particle O so as to maintain its temperature constant. In this case the heat bath attached to the particle O plays the role. When T_O increases, the temperature difference in segment S increases, thus not surprisingly J_S increases gradually. However, in a quite wide regime of T_O , J_D also increases despite the decreasing temperature difference in this segment. This counterintuitive phenomenon, the so-called NDTR [7], plays a key role to realize the functions of the thermal transistor. NDTR is possible here because when T_O increases, the power spectrum of the particle O moves leftward to low-frequency regime noticeably thus matches that in the D segment much better. The interface thermal resistance between the D and S segments reduces greatly.

Without NDTR J_D must be a decreasing function of T_O . It can cross J_S , which is an increasing function of T_O , at only one point. We see in Fig. 2(a), however, J_D and J_S cross at three points, which we have named as on, semi-on, and off states [7]. At these three states, $J_D = J_S$ thus the control heat bath does not need to release or absorb any heat current.

Since in practice it is hard to attach the control heat bath directly to the particle O for it is located inside the device, a control heat bath with temperature T_G is attached to the end of the segment G (the first particle $i = 1$, see Fig. 1) instead. Due to the heat resistance R_G in this segment, the resulting temperature T_O does not necessarily equal T_G . Consequently, the dependence of the heat currents on T_G varies with N_G , the length of segment G. The dependence for short N_G is plotted in Fig. 2(b). In all cases when T_G equals $T_{\text{off}} = 0.04$ or $T_{\text{on}} = 0.27$, $J_G = \Delta J$ still keeps zero. It is interesting that for $N_G = 200$, there exists a sudden transition at about $T_G = 0.11$, where the current J_D depends on T_G very sensitively. This feature is quite useful in making a temperature sensor.

When N_G , the length of segment G is too long, things may change quite significantly. In Fig. 2(c), the case for $N_G = 800$ is plotted. Curves become much less smooth, implying very large fluctuations. Furthermore, we cannot see clear on and off states any longer, i.e., $T_G = T_{\text{off}}$ (T_{on}) can no longer guarantee $J_G = 0$. Since the above findings are closely related to those in Sec. III B, they will be discussed and explained altogether in Sec. IV.

B. Finite time temperature distributions

To describe a system in a near-equilibrium state, the concept of the local temperature can be introduced provided that the local thermal equilibrium (LTE) is reached [39,40], i.e., $T_i \equiv \langle \dot{x}_i^2 \rangle$. The value inside the angle brackets can be time dependent and its fluctuation is governed by the fluctuation dissipation theorem in an equilibrium or near-equilibrium state. In a thermal transistor system, which is far from equilibrium, things become much more complicated. In order to understand the state of a thermal transistor we extend the above definition to a finite-time temperature, the average in a finite time window δt [9], i.e.,

$$T_i(t) \equiv \frac{1}{\delta t} \int_{t-\frac{\delta t}{2}}^{t+\frac{\delta t}{2}} \dot{x}_i^2(t') dt'. \quad (2)$$

FIG. 3. (a) The finite time temperature distribution PDF for short N_G . Dotted and solid curves are for $T_G = T_{\text{off}}$ and T_{on} , respectively. Those for the same T_G but different N_G overlap each other very well. (b) PDF for $N_G = 800$. A new peak at about $T_O(t) = 0.07$ appears for $T_G = T_{\text{on}}$. Similarly a new peak, although is not very clearly observed, appears at about $T_O(t) = 0.24$ for $T_G = T_{\text{off}}$.

The best choice of δt depends on the time scale of the relax-to-LTE process thus it may vary for different system size. For simplicity, it is fixed to 10^4 dimensionless time units, which covers about 2000 oscillations of the particles. We have confirmed that it works well in all cases. The probability density function (PDF) of $T_i(t)$ can be defined accordingly. We study the finite time temperature of the particle O only thus PDF always refers to the probability density of this particle hereafter.

The PDF for short N_G , say $N_G = 50, 100, 200$, and 400 are plotted in Fig. 3(a). Two cases are studied, i.e., the terminal G is attached to a control heat bath with temperature $T_G = T_{\text{on}}$ and $T_G = T_{\text{off}}$. We see for $T_G = T_{\text{off}}$ all the curves for various N_G overlap each other very well, and for each curve there exists only one peak at $T_O(t) = T_{\text{off}}$. The case is similar for $T_G = T_{\text{on}}$, i.e., for each curve only one peak is observed at $T_O(t) = T_{\text{on}}$.

However, in long N_G case, say $N_G = 800$, things are quite different. When $T_G = T_{\text{on}}$, besides $T_O = T_{\text{on}}$, there exists another peak located slightly right to T_{off} , see the solid blue curve in Fig. 3(b). Similarly, there also exists one more peak for $T_G = T_{\text{off}}$, see the dashed red curve.

IV. UNDERSTANDING THE FINDINGS

In this section, we analyze and explain the findings revealed in the preceding sections.

A. Switchability of a thermal transistor

First of all we consider the unique and multiple peaks of PDF for short and long segment G presented in Figs. 3(a) and

FIG. 4. The explanations of the single and double peaks observed in Figs. 3(a) and 3(b). The four oblique lines denote $J_G = \kappa(T_G - T_O)/N_G$ for various N_G and T_G . In the short N_G cases the line and the curve can cross at only one point, while in the long N_G cases the line and the curve can cross at more than one points. The blue solid and magenta dashed arrows point at the new crosses that correspond to the SSS for $T_G = T_{\text{on}}$ and $T_G = T_{\text{off}}$, respectively.

3(b). When the temperature of the terminal G is fixed to a value T_G , the dynamics of the temperature T_O reads

$$c_O \frac{dT_O}{dt} = -J_S(T_S, T_O) + J_D(T_D, T_O) + J_G(T_G, T_O), \quad (3)$$

where c_O denotes the heat capacity of the particle O. In a steady state, the left-hand side vanishes thus the conservation equation holds,

$$J_S(T_S, T_O) - J_D(T_D, T_O) = J_G(T_G, T_O), \quad (4)$$

indicating that the heat currents which flow in and out the particle O cancel each other. A steady state is a stable steady state (SSS) if the following stability condition is also satisfied,

$$-\frac{\partial J_S(T_S, T_O)}{\partial T_O} + \frac{\partial J_D(T_D, T_O)}{\partial T_O} + \frac{\partial J_G(T_G, T_O)}{\partial T_O} < 0, \quad (5)$$

indicating that when a small perturbation slightly changes the temperature T_O , the resulting net heat current always pulls T_O back. If T_O falls into a SSS, it will stay there for a long time. Consequently a peak of PDF can be observed there.

Since the segment G is a FK lattice, in which heat conduction is normal, i.e., the Fourier law holds [1,2,41], the right-hand side of the Eq. (4) can be expressed by

$$J_G(T_G, T_O) = \frac{(T_G - T_O)}{R_G} = \frac{\kappa(T_G - T_O)}{N_G}, \quad (6)$$

where κ denotes the heat conductivity in this segment, and $R_G \equiv N_G/\kappa$ is its thermal resistance. Roughly, the temperature dependence of κ is ignored.

We recall the curve for $\Delta J \equiv J_S - J_D$ [the wine solid one in the fundamental diagram Fig. 2(a)] in Fig. 4. The curves J_D and J_S are omitted to avoid confusion. J_G versus T_O that corresponds to the Eq. (6) for $T_G = T_{\text{on}} = 0.27$ with short N_G is expressed by the red dashed line. Equation (4) is satisfied when this line crosses the curve, and the stability condition is satisfied when the slope of the curve is greater than that of the line, i.e., $\frac{\partial \Delta J}{\partial T_O} > \frac{\partial J_G}{\partial T_O}$. Since N_G is short the slope of the line, $\frac{\partial J_G}{\partial T_O} = -\frac{\kappa}{N_G}$, is large and negative. Thus this line can cross

the curve at only one point at $T_O = T_{\text{on}}$, and at this point the stability condition is satisfied. Correspondingly there exists only one SSS and we observe only one peak in Fig. 3(a) (the solid curves). The case for $T_G = T_{\text{off}} = 0.04$ is similar. The unique cross between the line (the green short-dashed one in Fig. 4) and the curve corresponds to a unique SSS, and consequently a unique peak of PDF at $T_O = T_{\text{off}}$ [the dashed curves in Fig. 3(a)]. In conclusion, in the short N_G cases, the unique cross between ΔJ and J_G always locates at $T_O = T_{\text{on}}$ and $T_O = T_{\text{off}}$ for $T_G = T_{\text{on}}$ and $T_G = T_{\text{off}}$, respectively. This explains the facts that (i) the locations of the on and off states, in which $J_G = 0$, do not depend on N_G ; and (ii) the locations of the peaks of PDF do not depend on N_G either.

We call a thermal transistor switchable if for each of the cases $T_G = T_{\text{on}}$ and $T_G = T_{\text{off}}$ there exists only one SSS. The switchability of a thermal transistor guarantees that at each of these two states J_G must be zero and only one peak of PDF exists. Suppose ΔJ gets the most positive and the most negative values ΔJ_{high} and ΔJ_{low} at $T_O = T_{\text{high}}$ and $T_O = T_{\text{low}}$, respectively, then these conditions are roughly

$$\frac{\kappa}{N_G} > \frac{\Delta J_{\text{high}}}{T_{\text{on}} - T_{\text{high}}}, \quad \text{and} \quad (7)$$

$$\frac{\kappa}{N_G} > -\frac{\Delta J_{\text{low}}}{T_{\text{low}} - T_{\text{off}}}. \quad (8)$$

According to Fig. 3(a) we conclude that the thermal transistors for $N_G = 50, 100, 200$, and 400 are switchable.

While when $N_G = 800$, which is too long, the slope for J_G becomes much less negative. The line for J_G with $T_G = T_{\text{on}}$ (the blue dotted line) crosses the curve ΔJ at other two different points. It is easy to confirm that the left cross (indicated by the blue solid arrow) satisfies the stability condition but the right one does not. Likewise the line with $T_G = T_{\text{off}}$ (the magenta short dotted one) also crosses the curve at other two points, and the right one (pointed by the magenta dashed arrow) satisfies the stability condition but the left one does not. Owing to the coexistence of multiple SSS in these two cases, the transistor is no longer switchable. Hence two peaks of PDF are observed [see Fig. 3(b)] and J_G is no longer exactly zero [see Fig. 2(c)]. In the long N_G limit, the right-hand side of Eq. (4) vanishes thus the line for J_G reduces to the horizontal black dashed line. In such a case, the PDF contains two peaks that locate exactly at T_{on} and T_{off} , just like what we have observed in a model of thermal memory [9].

B. Controllability of a thermal transistor

In Fig. 5(a), the fundamental diagram is recalled again and the curve for J_S is omitted. The magenta dashed line that denotes for J_G with $T_G = 0.10$ and $N_G = 200$ crosses the curve for ΔJ at about $T_O = 0.07$, where J_D is basically zero. While when T_G changes a little, say, to $T_G = 0.12$, the line for J_G (the blue solid one) crosses the curve at a much higher value of $T_O > 0.2$, where the value of J_D increases many times. It is then easily understood that when T_G is around 0.11 , T_O [see the inset of Fig. 5(b)] and J_D depend on T_G quite sensitively.

Again, in this figure a cross between the curve and the line corresponds to a SSS and induces a peak in the PDF if the stability condition Eq. (5) holds. Clearly, in the case

FIG. 5. (a) The explanation of the sudden transition around $T_G = T_{\text{semi-on}}$ observed in Fig. 2(b). When T_G changes slightly from 0.10 to 0.12, the cross between the corresponding oblique line and the curve for ΔJ moves largely, and consequently J_D changes greatly. (b) PDF for the same values of T_G . When T_G changes slightly the peaks move largely. Inset: the resulting T_O as a function of T_G .

$T_G = 0.10$, there is only one cross and the stability condition must hold. The case is similar for $T_G = 0.12$. While in the case that $T_G = 0.11$, the line (green dotted) and the curve cross at three points. It is easy to confirm that the stability condition holds for the left and right crosses but does not hold for the middle one. This explains the findings in Fig. 5(b) that there is only one peak for $T_G = 0.10$ and 0.12 , while there are two peaks for the middle case $T_G = 0.11$.

Naturally, we call a thermal transistor globally controllable if for any value of T_G there exists only one corresponding SSS. Because the curve for ΔJ basically reaches the most negative slope at $T_O = T_{\text{semi-on}}$, the controllability condition is then simply

$$\frac{\kappa}{N_G} > -\Delta J', \quad (9)$$

where $\Delta J' \equiv \frac{\partial \Delta J}{\partial T_O} \big|_{T_O=T_{\text{semi-on}}}$. Compared to the switchability conditions, this condition is even more difficult to meet. It is easy to confirm that the transistors for $N_G = 50$ and 100 are controllable but those for longer N_G are not.

If a thermal transistor is not controllable, then for some values of T_G multiple SSS may coexist thus the transistor does not stay in a single SSS. The system may stay at one SSS for a long time, then jumps occasionally to another one due to the thermal fluctuation. The resulting heat currents are then weighted averages of the values in different SSS. Consequently, the fluctuations of the heat currents will be very large. This can be observed for the case $N_G = 800$ in Fig. 2(c). Although the averages of heat currents are taken over much longer time ($\sim 6 \times 10^9$ time unites), the fluctuations are still

very large and the curves look much less smooth than those for the shorter N_G in Fig. 2(b).

On the other hand, the sensitive T_G dependence of J_D provides us a way to build a thermal sensor whose heat current depends sensitively on the control temperature. For a controllable thermal transistor, the sensitivity of the so-built thermal sensor reads

$$S \equiv \frac{\partial J_D}{\partial T_G} \bigg|_{T_G=T_{\text{semi-on}}} = \frac{J'_D}{1 + \frac{N_G}{\kappa} \Delta J'}, \quad (10)$$

where $J'_D \equiv \frac{\partial J_D}{\partial T_O} \big|_{T_O=T_{\text{semi-on}}}$. Based on it, we may build a thermal sensor with any desired large value of sensitivity S by adjusting the length of the control segment G . S diverges to infinity when the denominator equals zero, i.e., $N_G = -\frac{\kappa}{\Delta J'}$. It is worth mentioning that since J_D takes the value within a finite range $[0, J_{D,\text{max}}]$, the above-mentioned sensitive dependence can be observed only in a limited interval of T_G with width proximately $J_{D,\text{max}}/S$, i.e., the higher the sensitivity S the narrower the working region of the thermal sensor.

Another interesting feature is that in the long N_G case the locations of the crosses between the line for J_G and the curve for ΔJ depend on the value of T_G only slightly. Therefore, the resulting currents J_S , J_D , and J_G keep basically constant in a wide regime of T_G . This can be observed in Fig. 2(c).

V. DISCUSSION

In summary, performance of a thermal transistor has been systematically studied. In contrast to the numerous existing studies on the NDTR, we focus on the influence of the heat resistance in the control segment, the G segment. By adjusting the length of the G segment, we observe rich and interesting phenomena, and are able to realize various thermal control functions.

First of all, although the fundamental diagram displays two special states, the on and off states, at which J_G equals zero, the transistor can be set exactly to those states only when the thermal resistance in G segment is lower than a critical value. We call such a transistor switchable. In such a case, PDF, the finite temperature distribution of the key particle O displays a unique peak at each of the on and off states. To make a thermal switch [7], which can realize many functions such as thermal logic gates [8] and thermal memory [9], a thermal transistor must be switchable; otherwise J_G can be nonzero even when the temperature T_G equals T_{on} or T_{off} , and such a switch does not work.

Furthermore, we call a transistor controllable if any value of T_G always induces only one corresponding SSS. In this case only one unique peak of PDF can be observed for each value of T_G . This requires an even lower thermal resistance of the G segment, or equivalently an even shorter length N_G . To make a thermal modulator that controls heat current at will, a thermal transistor must be controllable. In such a case, we are able to design a thermal sensor, whose output heat current depends on the control temperature T_G very sensitively. The sensitivity, i.e., the derivative of heat current J_D with respect to the control temperature T_G , can be set easily to any desired large value. It is also worth mentioning that in all our studies in this paper, the temperature dependence of R_G is always ignored. That is

why J_G versus T_O follows a straight line having a T_G - and T_O -independent slope. The real case is, however, not that simple. By properly designing and utilizing this dependence we may realize even more interesting and useful functions.

If a thermal transistor is not controllable or even not switchable, multiple SSS may coexist. Consequently, the resulting heat current J_D becomes a weighted average of the values for different SSS and the PDF displays not a unique peak but multiple peaks. Things will thus become much more complicated.

These studies deepen our understanding of how a thermal transistor works and help designing thermal devices that

complete desired functions. Possible applications can be reasonably expected.

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