Existence of negative differential thermal conductance in one-dimensional diffusive thermal transport

Jiuning Hu\textsuperscript{1,2,†} and Yong P. Chen\textsuperscript{3,2,1}
\textsuperscript{1}School of Electrical and Computer Engineering, Purdue University, West Lafayette, Indiana 47907, USA
\textsuperscript{2}Birck Nanotechnology Center, Purdue University, West Lafayette, Indiana 47907, USA
\textsuperscript{3}Department of Physics, Purdue University, West Lafayette, Indiana 47907, USA

We show that in a finite one-dimensional system with diffusive thermal transport described by Fourier’s law, negative differential thermal conductance (NDTC) cannot occur when the temperature at one end is fixed. We demonstrate that NDTC requires temperature dependent thermal conductivity and simultaneously varying the temperatures at both ends of the system.

Low dimensional thermal transport is of significant interest from both theoretical and practical perspectives.\textsuperscript{4} In particular, much attention has been devoted to the non-linear thermal transport. For example, thermal rectification has been experimentally and theoretically studied in many nano-structures\textsuperscript{2,5} and heterogeneous bulk materials\textsuperscript{2,4} Negative differential thermal conductance (NDTC), an unusual thermal transport phenomenon where the heat current across a thermal conductor decreases when the temperature bias increases, is an essential element for the construction of thermal transistors\textsuperscript{19} and thermal logic\textsuperscript{13,12} and is shown to exist in many non-linear one-dimensional (1D) systems.\textsuperscript{6,10,11,14} Many studies\textsuperscript{11,14,15,16} suggest that NDTC may vanish as the system length becomes large (approaching diffusive thermal transport). Here, we study the conditions for the existence of NDTC for 1D diffusive thermal transport described by Fourier’s law. We prove that NDTC requires temperature-dependent thermal conductivity and cannot exist when the temperature at one end is fixed. However, we show that NDTC is still possible if the temperatures at both ends are varied, and we demonstrate an example from the study of the non-linear thermal transport in carbon nanotubes (CNTs).

For 1D thermal transport in the diffusive regime and without heat sources or sinks, the steady state thermal transport equation reads

\[ \frac{d}{dx} \left( \kappa(x, T) \frac{dT}{dx} \right) = 0, \]

(1)

where we have assumed in general that the thermal conductivity \( \kappa(x, T) \) is dependent on both the coordinate \( x \) and the local temperature \( T(x) \).

We consider a finite 1D system which lies in the coordinate range \([x_L, x_R]\). Once the temperature at two ends of the system are given, i.e.,

\[ T(x_{L(R)}) = T_{L(R)}, \]

(2)

the temperature profile \( T(x) \) can be calculated from Eq. (1) and boundary conditions Eq. (2), and the resulting heat current \( q \) (independent of \( x \)) flowing in the system can be computed from

\[ q = -\kappa(x, T) \frac{dT}{dx}. \]

(3)

The heat current can also be expressed as

\[ q = \frac{T_L - T_R}{R(T(x))}, \]

(4)

where \( R \) is the thermal resistance of the system

\[ R(T(x)) = \int_{x_L}^{x_R} \frac{1}{\kappa(x, T(x))} dx, \]

(5)

and is a functional of the temperature profile \( T(x) \).

By applying an infinitesimal variation \( \delta T_{L(R)} \) of the boundary temperatures, i.e., \( T_{L(R)} \) is varied to \( T_{L(R)} + \delta T_{L(R)} \) the resulting temperature profile is varied to \( T(x) + \delta T(x) \). We must have

\[ \delta T(x_{L(R)}) = \delta T_{L(R)}. \]

(6)

This temperature profile variation \( \delta T(x) \) can induce a variation \( \delta R \) of the thermal resistance, then the heat current variation is

\[ \delta q = \frac{T_L - T_R + \delta T_L - \delta T_R}{R + \delta R} - \frac{T_L - T_R}{R} = \frac{\delta T_L - \delta T_R - q \delta R}{R + \delta R}. \]

(7)

We define the differential thermal conductance (DTC)

\[ G \equiv \frac{\delta q}{\delta (T_L - T_R)} = \frac{1 - q \frac{\delta R}{R}}{R + \delta R}. \]

(8)

It is clear that \( G \) is dependent on the manner in which \( T_L \) and \( T_R \) are varied, since the heat current \( q \) depends on both \( T_L \) and \( T_R \), and the above definition of \( G \) implicitly depends on \( T_L, T_R, \delta T_L \) and \( \delta T_R \). From Eq. (8) we know that if \( \kappa \) of the system is independent of temperature, the thermal resistance \( R \) is independent of temperature profile, and thus \( q \frac{\delta R}{\delta (T_L - T_R)} \) is independent of temperature, and thus \( q \frac{\delta R}{\delta (T_L - T_R)} = 0 \) and \( G = \frac{1}{R} > 0 \) (no NDTC). We can conclude here that NDTC requires temperature dependent thermal conductivity. On the other hand, if the system is engineered (e.g., by designing the form of \( \kappa \)) in such a way that \( q \frac{\delta R}{\delta (T_L - T_R)} > 1 \), we will have \( G < 0 \), indicating the effect of NDTC. However, as we will show, this can only be achieved when \( T_L \) and \( T_R \) are varied simultaneously.
We start from the expression of the varied heat current:

\[ q + \delta q = -\kappa(x, T + \delta T) \frac{dT}{dx} [T(x) + \delta T(x)] \]

\[ = -\kappa(x, T) \left[ \frac{dT}{dx} + \frac{d\delta T}{dx} \right] - \frac{\partial \kappa}{\partial T} \frac{dT}{dx} \delta T + O(\delta T^2). \]  

(9)

By neglecting the higher order terms \(O(\delta T^2)\) and canceling \(q\) with \(-\kappa(x, T) \frac{dT}{dx}\) (see Eq. 3), we have the heat current variation:

\[ \delta q = -\kappa(x, T) \frac{dT}{dx} \delta T - \frac{\partial \kappa}{\partial T} \frac{dT}{dx} \delta T. \]  

(10)

First, consider the cases that the temperature at only one end is varied: \(T_{L(R)}\) is varied to \(T_{L(R)} + \delta T_{L(R)}\) while \(T_{R(L)}\) is fixed. The DTC now is

\[ G = G_L = \frac{\delta q}{\delta T_L}, \quad \text{when } T_R \text{ is fixed; or} \]

\[ G = G_R = -\frac{\delta q}{\delta T_R}, \quad \text{when } T_L \text{ is fixed.} \]  

(11)

We define

\[ U_{L(R)}(x) = \frac{\delta T(x)}{\delta T_{L(R)}}. \]  

(12)

which according to Eq. 10 satisfies

\[ \frac{d}{dx} U_{L(R)}(x) + \frac{1}{\kappa(x, T)} \frac{\partial \kappa}{\partial T} \frac{dT}{dx} U_{L(R)} + \frac{\eta_{L(R)} G_{L(R)}}{\kappa(x, T)} = 0. \]  

(13)

where \(\eta_L = 1\) and \(\eta_R = -1\). From Eqs. 6 and 12, the boundary conditions for Eq. 13 are

\[ U_L(x_L) = 1, U_L(x_R) = U_R(x_L) = 0, U_R(x_R) = 1. \]  

(14)

Eq. 13 is an inhomogeneous linear ordinary differential equation, and the coefficients \(\frac{1}{\kappa(x, T)} \frac{\partial \kappa}{\partial T} \frac{dT}{dx}\) and \(\frac{\eta_{L(R)} G_{L(R)}}{\kappa(x, T)}\) are functions of \(x\) only, since \(T(x)\) is already solved from Eq. 1 and boundary conditions Eq. 2. The general solution to Eq. 13 is

\[ U_{L(R)}(x) = \frac{U_{L(R)}(x_L)}{F(x)} \frac{\eta_{L(R)} G_{L(R)}}{F(x)} \int_{x_L}^{x} \frac{F(t)}{\kappa(t, T(t))} dt, \]  

where

\[ F(x) \equiv \exp \left( \int_{x_L}^{x} \frac{1}{\kappa(t, T(t))} \frac{\partial \kappa}{\partial T} \frac{dT}{dt} dt \right). \]  

(16)

By evaluating Eq. 15 at \(x = x_R\), we obtain

\[ G_{L(R)} = J \eta_{L(R)} \left[ U_{L(R)}(x_L) - F(x_R) U_{L(R)}(x_R) \right], \]  

(17)

where

\[ J \equiv \left[ \int_{x_L}^{x_R} \frac{F(t)}{\kappa(t, T(t))} dt \right]^{-1}. \]  

(18)

From Eq. 14 and Eq. 17, we have

\[ G_L = J, \quad G_R = F(x_R) J. \]  

(19)

Since \(F(x)\) and \(\kappa\) are positive, we have \(G_L > 0\) and \(G_R > 0\). Namely, if \(T_{R(L)}\) is fixed, the heat current \(q\) will increase as the temperature bias increases by increasing (lowering) \(T_{L(R)}\). Therefore, there is no NDTC in this case where the temperature at one end is fixed.

In general, the heat current \(q = q(T_R, T_L)\) is a function of \(T_R\) and \(T_L\), and its variation is

\[ \delta q = \frac{\partial q}{\partial T_L} \delta T_L + \frac{\partial q}{\partial T_R} \delta T_R = G_L \delta T_L - G_R \delta T_R. \]  

(20)

When both \(T_L\) and \(T_R\) are varied, the corresponding DTC is

\[ G = \frac{\delta q}{\delta T_L - \delta T_R} = \frac{G_L \delta T_L - G_R \delta T_R}{\delta T_L - \delta T_R}. \]  

(21)

Let’s consider the contour lines of constant \(q\) on the quarter plane of \((T_R, T_L) \in [0, \infty) \times [0, \infty)\). These contour lines are described by

\[ \frac{dT_L}{dT_R} = \frac{G_R}{G_L} = F(x_R) \]  

(22)

by assigning \(\delta q = 0\). It is clear that \(\frac{dT_L}{dT_R} > 0\), thus every contour line has a positive slope. Each contour line can be uniquely labeled by the heat current \(q(0, T_L)\) or \(q(T_R, 0)\) at the point where the contour line intersects the \(T_L\) or \(T_R\) axis. From Eq. 14 we already know that \(q(0, T_L)\) \((q(T_R, 0))\) monotonically increases (decreases) with \(T_{L(R)}\). Since each contour line has positive slope at every point along the line, we can conclude that each contour line can intersect with any line of constant \(T_L\) or \(T_R\) at most once. Furthermore, Eq. 22 and the monotonicity of \(q(0, T_L)\) and \(q(T_R, 0)\) ensure the heat current \(q(T_R, T_L)\) is a monotonic function of \(T_{L(R)}\) when \(T_{R(L)}\) is fixed, which implies that NDTC is impossible along lines of constant \(T_L\) or \(T_R\). In other words, Eq. 22 poses a global topological constraint on the contour lines: the heat current at the intersection points of any constant \(T_{R(L)}\) line with all contour lines has the same ordering as that at the intersection points of the \(T_{R(L)}\) axis with all contour lines. This ordering property of the contour lines is a consequence of the mathematical form of Eq. 1, regardless of the choice of \(\kappa(x, T)\). The non-existence of NDTC along lines of constant \(T_L\) or \(T_R\) is a physical consequence of Eq. 1. Namely, it is because of the positivity of the thermal conductivity (i.e., heat always flows from hotter to colder regions) of any physical system obeying the second law of thermodynamics.

On the other hand, a contour line can possibly intersect with curves of non-constant \(T_L\) and \(T_R\) on \((T_R, T_L)\) plane more than once, which provides possibilities of NDTC when temperatures \(T_{L(R)}\) change along these curves. In other words, if we denote \(\beta = \delta T_L / \delta T_R\), we have

\[ G = J \frac{\beta - F(x_R)}{\beta - 1}. \]  

(23)
Since $\kappa$ has no explicit dependence on $x$, from Eqs. (10)- (19) we have
\[
F(x_R) = \frac{\kappa(T_R)}{\kappa(T_L)}
\]
and furthermore
\[
G_L = \frac{\kappa(T_L)}{x_R - x_L}, \quad G_R = \frac{\kappa(T_R)}{x_R - x_L}.
\]
We calculate the heat current $q(T_R, T_L)$, as shown in the colormap of Fig. 1 (a), by integrating Eq. (26):
\[
q(T_R, T_L) = \int_{T_R}^{T_L} G_L(T) dT = \int_{T_R}^{T_L} \frac{\kappa(T)}{x_R - x_L} dT
\]
We plot the heat current as a function of the temperature difference $\Delta T = T_L - T_R$ in Fig. 1 (b) along three lines shown in Fig. 1 (a). These three lines correspond to three different ways to tune the temperatures $T_L$ and $T_R$: (1) $T_L (=300 \text{ K})$ is fixed (solid line), (2) $T_R (=200 \text{ K})$ is fixed (solid line) and (3) $T_L$ and $T_R$ are varied simultaneously according to $T_L = 1.5 T_R$ (dash-dotted line). Only the situation (3) exhibits NDTC.

For the case that $T_L$ is proportional to $T_R$, i.e., $T_L = \beta T_R$, according to Eq. (25) and Eq. (26), the critical temperature ($T_L^c$) of $T_L$ above which NDTC exists satisfies the equation
\[
F(x_R) = \frac{\kappa(T_L^c/\beta)}{\kappa(T_L^c)} = \beta.
\]
We can immediately obtain the critical temperature
\[
T_L^c = \left[\frac{c}{b(\beta^2 + \beta + 1)}\right]^{\frac{1}{3}}.
\]
In the above example $\beta = 1.5$, we have $T_L^c \approx 511 \text{ K}$ which corresponds to the maximum heat current in line (3) of Fig. 1 (b) at $\Delta T \approx 170 \text{ K}$. For the extreme situation that $\beta = \infty$, we have $T_L^c = \infty$ and effectively $T_R = 0$ being fixed, thus NDTC can not be observed for finite $T_L$. It is worth pointing out that if the asymptotic behavior of $\kappa(T)$ in Eq. (24) is changed from $T^{-2}$ to $T^{-1}$, i.e., $b \to 0$, NDTC will not exist along lines of $T_L = \beta T_R$ since $T_L^c \to \infty$ for any positive $\beta$.

In conclusion, we study the steady state 1D thermal transport in the diffusive regime without heat sources or sinks. The Fourier’s law is applied to calculate the differential thermal conductance. We find that the necessary conditions for the existence of NDTC are: 1) thermal conductivity of the system is dependent on temperature and 2) the temperatures at both ends of the system have to be varied simultaneously.

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1 Hu49@purdue.edu
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