Local thermal rectification law

Chuang Zhang,1, ∗ Meng An,2, † Zhaoli Guo,1, ‡ and Songze Chen 1, §

1State Key Laboratory of Coal Combustion, School of Energy and Power Engineering, Huazhong University of Science and Technology, Wuhan 430074, China
2College of Mechanical and Electrical Engineering, Shaanxi University of Science and Technology, 6 Xuefuzhong Road, Weiyang, Xi’an 710021, China

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Thermal rectification which is a diode-like behaviour of heat flux has been studied over several decades. However, a universal and systematic physical description is still lacking. In this letter, a perturbation theory of local thermal rectification is developed, where the terminology ‘local’ requires that the variance of the effective thermal conductivity $\kappa_e(x,T)$ is small in the thermal system. This theory gives a sufficient condition of the local thermal rectification and predicts that the local thermal rectification ratio is proportional to the temperature difference and system size. Furthermore, three dimensionless parameters are identified for the first time and several experimental and numerical observations in literatures are well explained based on these dimensionless parameters. The proposed theory is applicable to any system in which an effective thermal conductivity can be derived, and helpful to unveil general principle for thermal rectification.

Thermal rectification [1–5] is a diode-like behaviour of heat flux. It plays an important role on thermal management and engineering in solid-state devices or materials. In the past decades, much attention has been paid to identify the underline physics and to enhance the thermal rectification ratio [2–4, 6–9]. Many studies show that the thermal rectification between two-segment bulk materials can be realized by selecting materials with suitable properties or different temperature dependent thermal conductivities [10–12]. A simple algebraic expression of the thermal rectification is also given in the common case of low thermal bias and thermal conductivities with power-law temperature dependencies [10]. Meanwhile, a general conclusion was made, i.e., thermal rectification is impossible if the thermal conductivity $\kappa(x,T)$ is separable [13]. For asymmetric nanoscale materials or systems, many accessible strategies have been proposed to realize the thermal rectification, such as asymmetric shape [14–19], mass graded [20, 21], porous or inhomogeneous materials [22–25]. Some physical mechanisms [4, 9, 19] were identified to explain the thermal rectification, such as the different phonon spectra overlap by switching the direction of the temperature gradient [9, 14, 26], asymmetric phonon ballistic or edge scattering [18, 27–29], nonseparable dependence of the thermal conductivity $\kappa(T,x)$ on temperature $T$ and spatial position $x$ [18, 19, 30]. In addition, some theoretical work was also made based on some simplified microscopic models to identify the essential conditions [31–34] for thermal rectification, such as the unusual temperature-dependent potential [2, 3], nonuniform or graded mass distribution [35, 36].

However, to the best of our knowledge, previous studies of thermal rectification are based on specific physical problems or microscopic models. The relationships among them are unclear. In other words, a universal and systematic physical description of the thermal rectification is still lacking.

In this letter, a perturbation theory of local thermal rectification is established and three dimensionless parameters are identified for the first time. The theory is not limited by system size or material properties and presents a clear physical picture of local thermal rectification based on explicit physical assumptions and rigorous theoretical derivations. Numerical simulations are also conducted to verify our theory. In addition, the physical meanings and limitations of this theory are discussed in detail and several experimental and numerical observations in literatures are well explained based on this theory.

First, let’s introduce the main assumptions of this study. For a local effective thermal conductivity $\kappa_e$ can be identified in a thermal system, so that the Fourier law is satisfied formally,

$$ q = -\kappa_e(W,T) \frac{dT}{dx}, \tag{1} $$

where $q$ is heat flux, and $\kappa_e$ is dependent on the temperature $(T)$ and other representative variable $(W)$ of the system. Specifically, $W$ quantifies any physical properties other than the temperature that influences the local effective thermal conductivity, for instance, the local characteristic length [14, 15, 17, 19, 21, 37], mass [6, 20]. The expression, $\kappa_e(W,T)$, also requires assumptions that the representative variable is independent of the temperature, and neglecting the dependence of higher order derivative of temperature. Note that if an effective thermal conductivity could be identified, the Eq. (1) is valid for any thermal conduction systems regardless of system size and material properties.

Consider a one-dimensional thermal conduction system on a small line segment $[x_0 - \Delta x/2, x_0 + \Delta x/2]$, that,

$$ \frac{\partial q}{\partial x} = 0, \tag{2} $$

where $\Delta x$ is the system length. Two temperatures $(T_0 - \Delta T/2, T_0 + \Delta T/2)$ are imposed at the two ends. The terminology, local thermal rectification, refers to the thermal rectification phenomenon on this small region. According to the assumptions we made, the spatial distribution of $W(x)$ is fixed in the system. Therefore, the local effective thermal conductivity can be formally taken as a function of the position and
temperature,
\[
\kappa_e = \kappa_e(W(x), T) = \kappa_e(x, T). \tag{3}
\]
Given that \(\kappa_e(x, T)\) is differentiable in the neighbourhood of \((x_0, T_0)\), it can be approximated by the Taylor expansion [38],
\[
\kappa_e = \kappa_e + \frac{\partial \kappa_e}{\partial x}(x - x_0) + \frac{\partial \kappa_e}{\partial T}(T - T_0) + \frac{1}{2} \frac{\partial^2 \kappa_e}{\partial x^2}(x - x_0)^2
\]
\[
+ \frac{1}{2} \frac{\partial^2 \kappa_e}{\partial T^2}(T - T_0)^2 + \frac{\partial^2 \kappa_e}{\partial x \partial T}(x - x_0)(T - T_0). \tag{4}
\]

The higher order terms are assumed to be negligible in the Taylor expansion. Choosing \(\kappa_0, \Delta x, \Delta T\) as reference variables to normalize the equations (Eqs. (1,2,4)), we can get the dimensionless equations as follows,
\[
\frac{\partial q^*}{\partial x^*} = 0, \quad q^* = -\kappa_e^* \frac{dT^*}{dx^*}, \tag{5}
\]
where,
\[
x^* = \frac{x - x_0}{\Delta x}, \quad T^* = \frac{T - T_0}{\Delta T}, \quad q^* = \frac{q \Delta x}{\kappa_0 \Delta T}, \tag{6}
\]
\[
\kappa_e^* = 1 + \alpha_x x^* + \alpha_T T^* + \alpha_{xT} x^* T^* + \alpha_{xT} x^2 + \alpha_{T} T^2, \tag{7}
\]
and the associated dimensionless parameters are
\[
\alpha_x = \frac{\Delta x}{\kappa_0} \frac{\partial \kappa_e}{\partial x}, \quad \alpha_T = \frac{\Delta T}{\kappa_0} \frac{\partial \kappa_e}{\partial T}, \quad \alpha_{xT} = \frac{\Delta x \Delta T}{\kappa_0^2} \frac{\partial^2 \kappa_e}{\partial x \partial T}, \tag{8}
\]
\[
\alpha_{xT} = \frac{\Delta x^2 \frac{\partial \kappa_e}{\partial x^2}}{2 \kappa_0}, \quad \alpha_T^2 = \frac{\Delta T^2}{2 \kappa_0} \frac{\partial^2 \kappa_e}{\partial T^2}. \tag{9}
\]

Then, the dimensionless equations are solved with two sets of boundary conditions respectively,
\[
\text{forward (‘+‘):} \quad T^*(-\frac{1}{2}) = -\frac{1}{2}, \quad T^*(\frac{1}{2}) = \frac{1}{2}, \tag{10}
\]
\[
\text{backward (‘-‘):} \quad T^*(-\frac{1}{2}) = \frac{1}{2}, \quad T^*(\frac{1}{2}) = -\frac{1}{2}. \tag{11}
\]

With all these assumptions, a local thermal rectification law can be deduced from Eqs. (1,2,3,4) based on perturbation theory [39] or also Direct Taylor expansion [38] (detailed derivations and numerical validations can be found in Supplemental Material),
\[
\beta = \frac{q_+ + q_-}{q_+ - q_-} \approx \beta_p, \tag{12}
\]
\[
\beta_p = \frac{1}{12} \left( \frac{1}{\kappa_0^2} \frac{\partial^2 \kappa_e}{\partial x \partial T} - \frac{1}{\kappa_0} \frac{\partial \kappa_e}{\partial x} \frac{\partial \kappa_e}{\partial T} \right) \Delta x \Delta T
\]
\[
= \frac{1}{12} (\alpha_{xT} - \alpha_x \alpha_T), \tag{13}
\]
where \(\beta\) denotes the local thermal rectification ratio, \(q_+\) is the forward heat flux, \(q_-\) is the backward heat flux, and \(\beta_p\) is the local thermal rectification ratio predicted by perturbation theory.

Equation (13) is the central result of present study, which is a universal and systematic description of the local thermal rectification. It is interesting to find that the leading order term of the local thermal rectification is a cross term \((\Delta x \Delta T)\). It is stemmed from the linear terms and the cross term of the expansion of \(\kappa_e\) (Eq. (4)). And the other second order terms in Eq. (4) have no impact on the leading order term of the local thermal rectification. In fact, the solution can be decomposed into two elementary modes.

**Linear mode:**
\[
\kappa_e^* = 1 + \alpha_x x^* + \alpha_T T^*, \quad \beta_l = -\frac{1}{12} \alpha_x \alpha_T, \tag{14}
\]

**Cross mode:**
\[
\kappa_e^* = 1 + \alpha_{xT} x^* T^*, \quad \beta_l = \frac{1}{12} \alpha_{xT}. \tag{15}
\]

As the theoretical derivations and the numerical simulations (see Supplemental Material) reveal, these two modes affect the thermal rectification ratio independently when \(\alpha_x, \alpha_T\) and \(\alpha_{xT}\) approach zero. Therefore, we introduce their influences to the local thermal rectification separately.

Figure 1 shows the thermal rectification ratio of the linear mode. The dimensionless parameters satisfy \(\alpha_x, \alpha_T \in (0, 2)\), and \(\alpha_x + \alpha_T \leq 2\), so that the thermal conductivity is positive inside the system. The numerical solution \((\beta_l')\) is accurate with at least 4 significant digits. It can be taken as the real thermal rectification ratio. As shown in Fig. 1(c), the predicted \(\beta_l\) (Eq. (14)) is accurate as long as \(\alpha_x \to 0\). Even when \(\alpha_x\) is finite value, say 0.5, the relative error is less than 10%. When \(\alpha_x\) increases beyond 0.5, the theory deviates from the reference solution, becomes inaccurate. It is obvious that \(\beta_l\) is symmetric about the line \((\alpha_x = \alpha_T)\), but \(\beta_l'\) is not. The thermal rectification ratio of the linear mode reaches its maximum \((|\beta_l'| = 0.1573)\) near the point \((\alpha_x = 1.835, \alpha_T = 0.165)\) (Fig. 1(a,d)). It suggests that the thermal rectification ratio is less than 0.1573, if the effective thermal conductivity varies linearly in terms of position and temperature.

The other elementary mode is the cross mode generated from the cross term \((xT)\). As shown in Fig. 2, \(\alpha_{xT}\) varies inside \((0, 4)\) to keep the thermal conductivity positive. \(\beta_l\) in Eq. (15) is a very accurate approximation for the cross mode. Its relative error to the numerical solution \((\beta_l')\) is less than 1% as \(|\alpha_{xT}|\) is smaller than 1.2, and the maximum relative error is less than 15% in all cases. Moreover, the maximum thermal rectification ratio \(|\beta_l'|\) is considerably larger than that of the linear mode, which occurs at \(\alpha_x = 4\) and is about 0.3791.

It is worth noting that the contributions of the linear mode and cross mode are on the same order of magnitude. For instance, if \(\kappa_e\) is separable [13], namely, \(\kappa_e = \kappa_0(x)\kappa_0(T)\), we can derive \(\alpha_x \alpha_T = \alpha_{xT}\). Consequently, the thermal rectification ratio is consistently zero. The linear mode and cross mode cancel each other in this case. In other word, the linear approximation of thermal conductivity is inadequate to feature the local thermal rectification even when \(\alpha_x\) and \(\alpha_T\) (or \(\Delta x\) and \(\Delta T\)) are infinitesimal. It unveils that the thermal rectification is essentially nonlinear phenomenon.

Next, the underlying physical meanings of the theory are
For a practical thermal conduction system, $\Delta x, \Delta T$, are both non-zero. In other word, to realize the thermal rectification, it requires $\alpha_x \alpha_T \neq \alpha_x \alpha_T$, which is a subset of the nonseparable condition. In previous literature[13], the nonseparable condition is only necessary for thermal rectification, but not sufficient. We prove that $\alpha_x \alpha_T \neq \alpha_x \alpha_T$ is a sufficient condition for the local thermal rectification.

Besides, Eq. (13) also predicts linear relationship between the local thermal rectification ratio and $\Delta T$ (and $\Delta x$). However, in previous literature, only the linear dependence of the small temperature difference $\Delta T$ was observed [16, 19, 30, 37]. The other linear dependence of system length $\Delta x$ was rarely reported in the literature although relevant results have been predicted in some previous studies [5, 16, 18]. In fact, figures 1 and 2 imply the reason why $\beta \sim \Delta x$ is difficult to be uncovered. As shown in Fig. 2, $\beta_l$ of the cross mode is very accurate in a wide range. However, the accuracy of $\beta_l$ of the linear mode behaves quite differently with respect to $\alpha_x$ and $\alpha_T$. When $\alpha_x$ is less than 1, the accuracy of $\beta_l$ is nearly independent of $\alpha_T$, which is reflected in Fig. 1(c) that the contour lines of $\beta'_l/\beta_l$ are almost parallel to the $\alpha_x$ axis. Therefore, the thermal rectification ratio can be further approximated by parameterizing the factor in the expression of $\beta_l$,

$$\beta_l = \frac{1 + r(\alpha_x)}{12} \alpha_x \alpha_T,$$

where $1 + r(\alpha_x)$ is actually the ratio between $\beta'_l$ and $\beta_l$, and $r \rightarrow 0$ as $\alpha_x \rightarrow 0$. The real thermal rectification ratio ($\beta$), which is the combination of the linear mode and the cross mode, becomes

$$\beta = \beta_l - \frac{r(\alpha_x)}{12} \frac{1}{\kappa_0} \frac{\partial \kappa_0}{\partial x} \frac{\partial \kappa_0}{\partial T} \Delta x \Delta T.$$

FIG. 2. Thermal rectification ratio ($\beta_l$) of the cross mode. The dash line represents $\beta_l$ predicted by perturbation theory (Eq. (15)); the solid line represents $\beta'_l$ solved by numerical method; the dash dot line represents the ratio between $\beta'_l$ and $\beta_l$. The relative error is less than 1% as $|\alpha_x| \ll 1$, and the maximum relative error is less than 15%. The maximum thermal rectification ratio ($|\beta'_l|$) occurs near $\alpha_x \alpha_T = 0$, is about 0.3791 for the cross mode.
the system due to the temperature change and the heterogeneity of the other physical properties. For more complicated problems, the thermal rectification ratio should be also the function of these dimensionless variables based on dimension analysis, namely, $\beta = \beta(\alpha_x, \alpha_T, \alpha_{\varepsilon T})$.

To show the utility of the dimensionless parameters, we analyse a universal relation between thermal rectification ratio and the geometric parameters and source temperatures in a two-dimensional multiparticle Lorentz gas model [16], i.e.,

$$\frac{q_+ + q_-}{q_+ - q_-} \propto \frac{d}{\tan \theta} \frac{\Delta T}{T_0},$$

where $d$ and $l$ are the system length and width respectively in the 2D homogeneous and asymmetric trapezoidal domain as shown in Fig. 3(a). $T_0 = (T_1 + T_2)/2$ and $\Delta T = |T_1 - T_2|$ are the average temperature and temperature difference between the left and right boundaries, respectively. Based on the numerical results in the literature, these are considerable temperature jumps at the two boundaries, namely, the present theory cannot be used in this system directly. Then we just try to find out the dimensionless parameters for this system.

At first, the two-dimension heat conduction problem is reduced into one-dimensional problem (Fig. 3(b)) and its heat flux along $x$ direction can be described by

$$q = -\int \kappa \frac{dT}{dx} dy,$$

where $\kappa$ is the local thermal conductivity. Fortunately, previous studies have proven that the thermal conductivity almost keeps a constant as the length of the rectangular space changes [16, 40]. Hence we can assume that the leading order term of the local thermal conductivity is only dependent on the local temperature,

$$\kappa = \kappa(T) + \varepsilon,$$

where $\kappa(T) = CT^{1/2}$ [41], $C$ is a constant, $\varepsilon$ represents small deviation from the leading order term. Given that the heat flux is mainly parallel to the $x$ coordinate if $\theta \to \pi/2$, thereby, the variation in $y$ direction can be ignored, so that, $T(x, y) \approx T(x)$. Under these assumptions, a local effective thermal conductivity can be defined,

$$\kappa_s(x, T) = \int \kappa dy = \frac{W(x)}{\kappa} + \varepsilon',$$

$$W(x) = \int dy = l - 2 \frac{x}{\tan \theta},$$

$$\varepsilon' = \int \varepsilon dy, \quad x_0 = d/2,$$

where $W(x)$ is actually the transverse length in $y$ direction. Note that $\varepsilon$ and $\varepsilon'$ are essential to keep $\kappa_s$ nonseparable so that the thermal rectification occurs [13].

After a simple derivation, the dimensionless parameters are obtained by ignoring the small deviation ($\varepsilon, \varepsilon'$),

$$\alpha_x \approx \frac{2d}{l\tan \theta - d}, \quad \alpha_T \approx \frac{\Delta T}{2T_0},$$

$$\alpha_{\varepsilon T} \approx \frac{d}{l\tan \theta - d} \frac{\Delta T}{T_0}.$$

Considering small system assumption, $l\tan \theta \gg d$, Eq. (19) becomes,

$$\frac{q_+ + q_-}{q_+ - q_-} \propto \alpha_{\varepsilon T} \propto \alpha_x \alpha_T.$$

This example demonstrates the significance of $\alpha_x, \alpha_T, \alpha_{\varepsilon T}$ to general thermal rectification. Actually, these three dimensionless parameters are helpful to document the experimental data [5, 18, 19, 37], and to unveil general principle for thermal rectification.

Finally, several notes on the local thermal rectification law are addressed. First, Eq. (13) is only valid for small systems with $\alpha_e \to 0$. In fact, the word "local" literally constrains the system to an infinitesimal region. Second, our theory is unapplicable if the local effective thermal conductivity $\kappa_s(x, T)$ is discontinuous or singular ($\kappa_s = 0$), such as the thermal rectification in phase-change materials [42–44]. Third, the numerical results suggest that the thermal rectification ratio is less than 0.4 if $\kappa_s$ can be described by smooth function with non-zero first and second order derivatives. It implies that, to achieve ideal thermal rectification, we need to find materials or construct system with strongly nonlinear thermal conductivity, for example phase-change materials [43–46].

In conclusion, a systematic and universal theory of the local thermal rectification is established through perturbation theory. Our theory (Eq. (13)) predicts that the local thermal rectification ratio is approximately proportional to the temperature difference and the system size. As a validation, the linear relation of temperature difference has been reported in the literature. Besides, three dimensionless parameters ($\alpha_x, \alpha_T, \alpha_{\varepsilon T}$) are proposed for the first time. We prove that $\alpha_x \alpha_T \neq \alpha_{\varepsilon T}$ is a sufficient condition for the local thermal rectification. And two elementary modes, the linear mode and the cross mode, are identified for the local thermal rectification. These two modes stem from the first order and second order derivatives.
of effective thermal conductivity, but surprisingly have comparative contribution to the overall thermal rectification. Numerical simulations are also conducted to verify our theory. Meanwhile, the upper bound of the local thermal rectification ratio is determined by numerical results for these modes respectively. Several experimental and numerical observations are also well explained based on the theory. We believe that the proposed theory will shed light on the design of the thermal rectifier.

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Local thermal rectification law: Supplemental Material

Chuang Zhang,1,∗ Meng An,2,† Zhaoli Guo,1,‡ and Songze Chen1,§

1State Key Laboratory of Coal Combustion, School of Energy and Power Engineering, Huaizhong University of Science and Technology, Wuhan 430074, China
2College of Mechanical and Electrical Engineering, Shaanxi University of Science and Technology, 6 Xuefuzhong Road, Weiyangdaxueyuan, Xi'an 710021, China
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I. PHYSICAL DESCRIPTIONS

Suppose that a local effective thermal conductivity \( \kappa_e \) can be identified in a thermal system, so that the Fourier law is satisfied formally,

\[
q = -\kappa_e \frac{dT}{dx},
\]

(S1)

where \( q \) is heat flux, \( T \) is the temperature, \( x \) is the position. \( \kappa_e \) is dependent on the temperature \( (T) \) and other representative variable \( (W) \) of the system, i.e.,

\[
\kappa_e = \kappa_e(W(x), T) = \kappa_e(x, T).
\]

(S2)

Consider a one-dimensional thermal conduction system on a small line segment \([x_0 - \Delta x/2, x_0 + \Delta x/2]\), that,

\[
\frac{\partial q}{\partial x} = 0,
\]

(S3)

where \( \Delta x \) is the system length. Two temperatures \((T_0 - \Delta T/2, T_0 + \Delta T/2)\) are imposed at the two ends. The terminology, local thermal rectification, refers to the thermal rectification phenomenon on this small region.

Given that \( \kappa_e(x, T) \) is differentiable in the neighbourhood of \((x_0, T_0)\) [1], it can be approximated by the Taylor expansion,

\[
\kappa_e(x, T) = \kappa_0 + a(T - T_0) + b(x - x_0) + c(x - x_0)(T - T_0) + d(x - x_0)^2 + f(T - T_0)^2,
\]

(S4)

where the high order Taylor expansion terms are assumed to be ignorable in Eq. (S4) and

\[
\begin{align*}
\kappa_0 &= \kappa_e(x_0, T_0) \neq 0, \\
a &= \left. \frac{\partial \kappa_e}{\partial T} \right|_{(x, T) = (x_0, T_0)}, \\
b &= \left. \frac{\partial \kappa_e}{\partial x} \right|_{(x, T) = (x_0, T_0)}, \\
c &= \left. \frac{\partial^2 \kappa_e}{\partial x \partial T} \right|_{(x, T) = (x_0, T_0)}, \\
d &= \frac{1}{2} \left. \frac{\partial^2 \kappa_e}{\partial x^2} \right|_{(x, T) = (x_0, T_0)}, \\
f &= \frac{1}{2} \left. \frac{\partial^2 \kappa_e}{\partial T^2} \right|_{(x, T) = (x_0, T_0)}. \\
\end{align*}
\]

(S5)

In addition, above equations are solved with two sets of boundary conditions respectively,

| Forward (‘+‘) | Backward (‘-‘) |
|---------------|---------------|
| \( T(x_0 - \Delta x/2) = T_0 - \Delta T/2, \) | \( T(x_0 + \Delta x/2) = T_0 + \Delta T/2, \) |
| \( T(x_0 + \Delta x/2) = T_0 + \Delta T/2, \) | \( T(x_0 - \Delta x/2) = T_0 - \Delta T/2. \) |

(S7)

(S8)

For the forward direction (Eq. (S7)), the heat flux \( q \) is denoted by \( q_+ \), and as the temperature gradient is reversed (Eq. (S8)), we denote \( q \) as \( q_- \). In what follows, all variables \( V \) are labeled as \('+\) for the forward direction and \('-\) for the backward direction. The local thermal rectification ratio \( \beta \) is

\[
\beta = \frac{q_+ + q_-}{q_+ - q_-}.
\]

(S9)
II. DIMENSIONLESS TREATMENTS

Before solving above equations analytically, the dimensionless treatment of Eq. (S4) is implemented first, i.e.,

\[ \kappa_e^* = 1 + \alpha_T T^* + \alpha_s x^* + \alpha_{xT} x^* T^* + \alpha_{x^2} x^2 + \alpha_{T^2} T^2, \]  

(S10)

where

\[ \kappa_e^* = \frac{\kappa_e}{\kappa_0}, \quad T^* = \frac{T - T_0}{\Delta T}, \quad x^* = \frac{x - x_0}{\Delta x}, \quad \alpha_s = \frac{b \Delta x}{\kappa_0}, \]  

\[ \alpha_T = \frac{\alpha_s \Delta T}{\kappa_0}, \quad \alpha_{xT} = \frac{c \Delta x \Delta T}{\kappa_0}, \quad \alpha_{x^2} = \frac{d \Delta x^2}{2 \kappa_0}, \quad \alpha_{T^2} = \frac{f \Delta T^2}{2 \kappa_0}. \]  

(S11)

(S12)

Here we assume that

\[ \alpha_s \to 0, \quad \alpha_T \to 0, \quad \alpha_{x^2} \to 0, \quad \alpha_{T^2} \to 0. \]  

(S13)

Similar treatment is implemented on Eq. (S1), i.e.,

\[ q^* = -\kappa_e^* \frac{dT^*}{dx^*}, \]  

(S14)

where the normalized heat flux is \( q^* = (q \Delta x) / (\kappa_0 \Delta T) \). Combining Eqs. (S14) and (S10) leads to

\[ q^* = -\left(1 + \alpha_T T^* + \alpha_s x^* + \alpha_{xT} x^* T^* + \alpha_{x^2} x^2 + \alpha_{T^2} T^2\right) \frac{dT^*}{dx^*}, \]  

(S15)

which is a high-order nonlinear differential equation of \( x^* \) and \( T^* \) [2]. Based on Eqs. (S7) and (S8), we have dimensionless boundary conditions, i.e.,

forward (\( \leftarrow \)) : \( T(-1/2) = -1/2, \quad T(1/2) = 1/2, \)  

(S16)

backward (\( \rightarrow \)) : \( T(-1/2) = 1/2, \quad T(1/2) = -1/2. \)  

(S17)

For the forward direction, the normalized heat flux \( q^* \) is denoted by \( q^*_+ \), and as the temperature gradient is reversed, we denote \( q^* \) as \( q^*_- \). Then Eq. (S9) becomes

\[ \beta = \frac{q^*_+ + q^*_-}{q^*_+ - q^*_-}. \]  

(S18)

First, we consider the forward direction so that \( \left(\frac{1}{2}, \frac{1}{2}\right) \) and \( \left(-\frac{1}{2}, -\frac{1}{2}\right) \) are both the solutions of Eqs. (S10) and (S14). Then similar derivations can be implemented for the backward direction directly.

III. PERTURBATION THEORY OF THE LOCAL THERMAL RECTIFICATION LAW

In order to solve the following equation,

\[ q^* = -\left(1 + \alpha_T T^* + \alpha_s x^* + \alpha_{xT} x^* T^* + \alpha_{x^2} x^2 + \alpha_{T^2} T^2\right) \frac{dT^*}{dx^*}, \]  

(S19)

the perturbation method [3] is used. Firstly, we convert Eq. (S19) into a perturbation problem by introducing a parameter \( \epsilon \) in the right side of the equation, i.e.,

\[ q^* = -\left(1 + \alpha_T T^* + \epsilon \left(\alpha_s x^* + \alpha_{xT} x^* T^* + \alpha_{x^2} x^2 + \alpha_{T^2} T^2\right)\right) \frac{dT^*}{dx^*}. \]  

(S20)

It can be found that Eq. (S20) returns to the original equation (S19) by assigning \( \epsilon = 1 \). We further assume a perturbation series in powers of \( \epsilon \), i.e.,

\[ T^* = T_0^* + \epsilon T_1^* + \epsilon^2 T_2^* + ... = \sum_{i=0}^{\infty} \epsilon^i T_i^*, \]  

(S21)

\[ q^* = q_0^* + \epsilon q_1^* + \epsilon^2 q_2^* + ... = \sum_{i=0}^{\infty} \epsilon^i q_i^*. \]  

(S22)
The zeroth-order problem is obtained by setting $\varepsilon = 0$, i.e.,
\[ q_0^* = - (1 + \alpha_T T_0^*) \frac{dT_0^*}{dx^*}, \]  
(S23)
which is an ordinary differential equation of $x^*$ and $T_0^*$. The constant variation method [2] is used to solve Eq. (S23) and the analytical solution is
\[ x^* = - \frac{T_0^*}{q_0^*} + \frac{\alpha_T}{2} T_0^* + C_0, \]  
(S24)
where $C_0$ is a constant. Combining the boundary conditions (Eqs. (S16) and (S17)), we can determine the heat flux $q_0^*$ and integration constant $C_0$ for the zeroth-order solution,
\[ q_{0+} = -1, \quad C_{0+} = -\frac{\alpha_T}{8}, \]  
(S25)
\[ q_{0-} = 1, \quad C_{0-} = -\frac{\alpha_T}{8}. \]  
(S26)

The first order problem is then obtained by equating the coefficient of $\varepsilon$ on the left and right hand sides of Eq. (S20), i.e.,
\[ q_1^* = -(1 + \alpha_T T_0^*) \frac{dT_1^*}{dx^*} - (\alpha_T T_1^* + \alpha_x x^* + \alpha_{xx} T_0^* + \alpha_{xx} x^* + \alpha_T T_0^*) \frac{dT_0^*}{dx^*}. \]  
(S27)
Substitute Eqs. (S23) into Eq. (S27) to eliminate the derivative of $x^*$, and obtain an ordinary differential equation,
\[ \frac{dT_1^*}{dT_0^*} = - \frac{\alpha_T T_1^*}{1 + \alpha_T T_0^*} + \frac{q_1^*}{q_0^*} \frac{\alpha_x + \alpha_{xx} T_0^* + \alpha_{xx} x^* + \alpha_T T_0^*}{1 + \alpha_T T_0^*}, \]  
(S28)
This equation is solved by the constant variation method [2], and the analytical solution is
\[ T_1^* = \frac{1}{1 + \alpha_T T_0^*} g(T_0^*), \]  
(S29)
where $g(T_0^*)$ is a function of $T_0^*$ and satisfies
\[ \frac{\partial g(T_0^*)}{\partial T_0^*} = \frac{q_1^*}{q_0^*} (1 + \alpha_T T_0^*) - (\alpha_x + \alpha_{xx} T_0^* + \alpha_{xx} x^* + \alpha_T T_0^*). \]  
(S30)
Substitute Eq. (S24) into Eq. (S30) and integrate with respect to $T_0^*$, then $g(T_0^*)$ reads,
\[ g(T_0^*) = A_0 T_0^* + \frac{A_1}{2} T_0^{*2} + \frac{A_2}{3} T_0^{*3} + \frac{A_3}{4} T_0^{*4} + \frac{A_4}{5} T_0^{*5} + C_1, \]  
(S31)
where
\[ A_0 = \frac{q_1^*}{q_0^*} + \frac{\alpha_x \alpha_T}{8} - \frac{\alpha_{xx} \alpha_T}{64}, \]  
(S32)
\[ A_1 = \alpha_T \frac{q_1^*}{q_0^*} + \frac{\alpha_x \alpha_T}{8} + \frac{\alpha_T \alpha_T}{4}, \]  
(S33)
\[ A_2 = -\frac{\alpha_x \alpha_T}{2} - \alpha_{xx} \alpha_T - \alpha_{xx} + \frac{\alpha_T^2 \alpha_T}{8}, \]  
(S34)
\[ A_3 = \frac{\alpha_{xx} \alpha_T}{2} - \alpha_T \alpha_T, \]  
(S35)
\[ A_4 = -\frac{\alpha_T^2 \alpha_T}{4}. \]  
(S36)
$q_1^*$ and $C_1$ are integration constants. And then the boundary conditions for $T_1^*$,
\[ g \left( -\frac{1}{2} \right) = 0, \quad g \left( \frac{1}{2} \right) = 0, \]  
(S37)
are imposed to determine \( q_1^* \) (and \( C_1 \)),

\[
q_1^* = -q_0^* \frac{12}{10} \left( \alpha_x \alpha_T - \alpha_x + \alpha_T \right) - \frac{1}{10} \alpha_T^2 \alpha_x.
\] (S38)

According to Eq. (S22), the heat flux can be approximated as \( q^* \approx q_0^* + \varepsilon q_1^* \) with \( \varepsilon = 1 \). Then the forward and backward heat flux are expressed as follows,

\[
q_+^* = -1 + \frac{1}{12} \left( \alpha_x \alpha_T - \alpha_x - \alpha_T - \frac{1}{10} \alpha_T^2 \right),
\] (S39)

\[
q_-^* = 1 + \frac{1}{12} \left( \alpha_x \alpha_T + \alpha_x + \alpha_T + \frac{1}{10} \alpha_T^2 \right).
\] (S40)

Combining Eqs. (S39) and (S40), the local thermal rectification ratio is approximated as,

\[
\beta = \frac{q_+^* + q_-^*}{q_+^* - q_-^*} \approx \frac{1}{12} \left( \alpha_x \alpha_T - \alpha_x \right) = \frac{1}{12} \left( \frac{\partial^2 \kappa_x}{\partial x \partial T} - \frac{\partial \kappa_x}{\partial x} \frac{\partial \kappa_x}{\partial T} \right) \Delta x \Delta T.
\] (S41)

IV. SOLVING THE LINEAR MODE WITH THE TAYLOR EXPANSION

It is very complex to obtain the thermal rectification ratio of Eq. (S19) through the Taylor expansion. We only show how to solve the linear mode as an illustration. The dimensionless form of the linear mode reads,

\[
\frac{dq^*}{dx^*} = 0, \quad q^* = -\left( 1 + \alpha_T x^* + \frac{\alpha_T}{\alpha_x} \right) \frac{dT^*}{dx^*}.
\] (S42)

Its analytical solution is derived by the constant variation method \cite{2}, i.e.,

\[
x^* = -\frac{\alpha_T}{\alpha_x} x^* + \frac{\alpha_T}{\alpha_x} q^* - \frac{1}{\alpha_x} + C_1 \exp (-\alpha_T x^*/q^*),
\] (S43)

where \( q^* \) and \( C_1 \) are integration constant. For the forward direction, according to boundary conditions (Eqs. (S16) and (S17)), we can get

\[
\frac{1}{2} = \frac{\alpha_T}{\alpha_x} \frac{1}{2} + \frac{\alpha_T}{\alpha_x} q_+^* - \frac{1}{\alpha_x} + C_1 \exp \left( \frac{\alpha_T}{2 q_+^*} \right),
\] (S44)

\[
\frac{1}{2} = -\frac{\alpha_T}{\alpha_x} \frac{1}{2} + \frac{\alpha_T}{\alpha_x} q_+^* - \frac{1}{\alpha_x} + C_1 \exp \left( \frac{-\alpha_T}{2 q_+^*} \right).
\] (S45)

Combining above two equations, we have

\[
\frac{\alpha_T}{\alpha_x} + \alpha_T \frac{\alpha_T}{\alpha_x} = \exp (e_+) - \exp (-e_+) = \tanh (e_+),
\] (S46)

where \( e_+ = \alpha_T / (2 q_+^*) \). According to the solution of Eq. (S23), \( q_+^* \approx -1 \) as long as \( \alpha_T \) is infinitesimal. In another word, if \( \alpha_T \to 0 \), \( e_+ \to 0 \). Then \( \tanh(e_+) \) is expanded under assumption \( \alpha_T \to 0 \),

\[
\tanh(e_+) = e_+ - e_+^3 / 3 + O(e_+^3).
\] (S47)

It is worth noting that no assumption is made on \( \alpha_T \). Then Eq. (S46) becomes

\[
\alpha_T \approx -2 e_+ - \frac{1}{3} (\alpha_T e_+^2 - 2 e_+^3)
\] (S48)

\[
\Rightarrow q_+^* \approx -1 + \frac{\alpha_T}{12} + \frac{\alpha_T^2}{12}.
\] (S49)

Similarly, we can get

\[
q_-^* \approx 1 + \frac{\alpha_T}{12} - \frac{\alpha_T^2}{12}.
\] (S50)
Therefore, the thermal rectification ratio of linear mode is,
\[
\beta_l = \frac{q_+ + q_-}{q_+ - q_-} \approx -\frac{1}{12} \frac{a \alpha T b \Delta x}{\kappa_0} = -\frac{1}{12} \alpha \alpha_T.
\] (S51)

Based on above mathematical derivations, similarly we can get other solutions of the local thermal rectification, i.e.,
\[
\kappa_e^* = 1 + \alpha_T x^T x^*, \quad \beta = \frac{1}{12} \alpha \alpha_T.
\] (S52)
\[
\kappa_e^* = 1 + \alpha_T T^* + \alpha_V x^* + \alpha_T x^T x^*, \quad \beta = \frac{1}{12} (\alpha_T - \alpha_V \alpha_T).
\] (S53)

V. NUMERICAL VALIDATION

In this section, numerical simulations are implemented to validate the local thermal rectification law.

A. Numerical discretization and solutions

Based on Eqs. (S1) and (S3), we can get
\[
\frac{\partial}{\partial x} \left( \kappa_e(x, T(x)) \frac{\partial T}{\partial x} \right) = 0.
\] (S54)

The iterative method is used to solve above equation, i.e.,
\[
\frac{\partial}{\partial x} \left( \kappa_e \frac{\partial \delta T^n}{\partial x} \right) = -\frac{\partial}{\partial x} \left( \kappa_e^* \frac{\partial T^n}{\partial x} \right),
\] (S55)

where \( n \) is the iteration index, \( \delta T^n = T^{n+1} - T^n \) is the temperature variance between two successive iteration steps. When \( n = 0 \), the initial temperature inside the system is \( T^n = T_0 \). To solve it numerically, the finite difference method is used and we discretize the computational domain into \( (M-1) \) uniform cells with \( M \) grid points, i.e.,
\[
x_i = x_0 - \frac{\Delta x}{2} + \frac{(i - 1)\Delta x}{M - 1},
\] (S56)

where \( x_i \) is position of the grid point \( i, i = 1, 2, ..., M \). It can be found that \( x_1 \) and \( x_M \) are two boundaries with fixed temperatures. Then Eq. (S55) becomes
\[
\sum_{j \in N(i)} \kappa_{e,ij} \delta T^n_j - \left( \sum_{j \in N(i)} \kappa_{e,ij} \right) \delta T^n_i
= - \sum_{j \in N(i)} \kappa_{e,ij} T^n_j + \left( \sum_{j \in N(i)} \kappa_{e,ij} \right) T^n_i, \quad i \in [2, M - 1]
\] (S57)

where \( N(i) \) denotes the sets of neighbor grid points of grid point \( i \). In addition,
\[
\delta T^n_i = \delta T^n_M = 0,
\] (S58)
\[
2T_{ij} = T_i + T_j,
\] (S59)
\[
2x_{ij} = x_i + x_j,
\] (S60)
\[
\kappa_{e,ij} = \kappa_e(x_{ij}, T_{ij}).
\] (S61)

Combining the boundary conditions (Eqs. (S7), (S8)), Eq. (S57) can be solved iteratively. Here, the Thomas algorithm [4] is used to solve Eq. (S57) and the iteration converges as
\[
\sqrt{\frac{\sum_{i=1}^{M-1} |\delta T^n_i|^2}{(M - 2)\Delta T^2}} < 10^{-14}.
\] (S62)

For the dimensionless equations (Eqs. (S14) and (S10)), similar iterative method can also be implemented directly. For all numerical simulations, the mesh independence has been tested. Without special statements, we set \( M = 10001 \).
In Eq. (S4), we fix \( x_0 = 1 \), \( T_0 = 1 \). Y axis is \( E_r \) and X axis are eight variables. (a) Change \( a \) and fix \( b = 1, c = 1, d = 0.5, f = 0.2, \kappa_0 = 1, \Delta T = 0.2, \Delta T = 0.2 \). (b) Change \( b \) and fix \( a = 1, c = 1, d = 0.5, f = 0.2, \kappa_0 = 1, \Delta T = 0.2, \Delta T = 0.2 \). (c) Change \( c \) and fix \( a = 1, b = 1, d = 0.5, f = 0.2, \kappa_0 = 1, \Delta T = 0.2, \Delta T = 0.2 \). (d) Change \( d \) and fix \( a = 1, b = 1, c = 0.5, f = 0.2, \kappa_0 = 1, \Delta T = 0.2, \Delta T = 0.2 \). (e) Change \( \Delta T \) and fix \( a = 0.2, b = 1, c = 0.1, d = 0.1, f = 0.01, \kappa_0 = 5, \Delta x = 0.1 \). (f) Change \( \Delta x \) and fix \( a = 1, b = 0.5, c = 1, d = 0.5, f = 0.2, \kappa_0 = 1, \Delta T = 0.2 \). (g) Change \( f \) and fix \( a = 1, b = 1, c = 0.5, d = 0.5, \kappa_0 = 1, \Delta T = 0.2, \Delta T = 0.2 \). (h) Change \( \kappa_0 \) and fix \( a = 1, b = 1, c = 1, d = 0.5, f = 0.2, \Delta x = 0.2, \Delta T = 0.2 \).

### B. Linear mode

Above derivations have given the local thermal rectification of the linear mode, i.e.,

\[
\kappa^* = 1 + \alpha_\epsilon x^* + \alpha_T T^*^*, \quad \beta_r = -\frac{1}{12} \alpha_\epsilon \alpha_T.
\]  

(S63)

In order to validate it, numerical simulations are conducted. For simplicity, the dimensionless parameters satisfy \( \alpha_\epsilon, \alpha_T \in (0, 2) \), and \( \alpha_\epsilon + \alpha_T \leq 2 \), so that the thermal conductivity is positive inside the system. We discrete \( \alpha_\epsilon \in (0, 2) \) into 200 uniform pieces as well as \( \alpha_T \in (0, 2) \). For each discretized piece \( \alpha_\epsilon \) and \( \alpha_T \), the local thermal rectification can be predicted by numerical iterative solutions and the theoretical law (Eq. (S63)). Especially, for the line \( \alpha_\epsilon + \alpha_T = 2 \), we discrete it into 2000 uniform pieces. Detailed numerical results are shown in the article (FIG. 1).

### C. Cross mode

Numerical simulations are conducted to validate the theoretical results of the cross mode, i.e.,

\[
\kappa^* = 1 + \alpha_{\epsilon T} x^* T^*^*, \quad \beta_c = -\frac{1}{12} \alpha_{\epsilon T} \alpha_T.
\]  

(S64)

The dimensionless parameter satisfies \( \alpha_{\epsilon T} \in (0, 4] \), so that the thermal conductivity is positive inside the system. We discrete \( \alpha_{\epsilon T} \in (0, 4] \) into 4000 uniform pieces. For each discretized \( \alpha_{\epsilon T} \), the local thermal rectification can be predicted by numerical iterative solutions and the theoretical law (Eq. (S64)). Detailed numerical results are shown in the article (FIG. 2).

### D. Arbitrary effective thermal conductivity

First, we take Eq. (S4) as an example. We set \( x_0 = 1, T_0 = 1 \). There are eight independent variables in Eq. (S4), i.e., \( a, b, c, d, f, \Delta t, \Delta T, \kappa_0 \). Next, we change one of them and fix others. The predicted thermal rectification ratio \( \beta \) are compared
with our derived analytical solutions, i.e., Eq. (S41). A parameter $E_r$ is introduced to show the relative errors between the numerical ($\beta_{\text{numerical}}$) and theoretical ($\beta_{\text{theory}}$) results, i.e.,

$$E_r = \frac{|\beta_{\text{numerical}} - \beta_{\text{theory}}|}{\beta_{\text{theory}}}.$$  \hfill (S65)

Numerical results are shown in Fig. S1, where Y axis is $E_r$ and X axis are eight variables, respectively. It can be observed that the numerical results are in excellent agreement with our derived theoretical solutions within our assumptions (Eq. (S13)). However, as $\alpha_x$, $\alpha_T$, $\alpha_{xT}$ are large or $|\kappa_e/\kappa_0| \gg 1$, the theoretical results deviate the numerical results significantly.

Actually, our theory is valid for arbitrary effective thermal conductivity $\kappa_e(x,T)$ within our assumptions. For example, we set $\kappa_e = 1 + x^2 + 3T^4$, $x_0 = \Delta x/2$, $T_0 = 1$. Numerical simulations are conducted with different $\Delta x$ (or $\Delta T$), as shown in Fig. S2. It can be observed that as $\Delta x$ and $\Delta T$ are both small, our theory is valid.

FIG. S2. Comparison of the predicted local thermal rectification ratio $\beta$ between the numerical solution and our theory, where $\kappa_e = 1 + x^2 + 3T^4$, $x_0 = \Delta x/2$, $T_0 = 1$. (a) Fix $\Delta x = 5.0$, change $\Delta T \in [0.1, 1.9]$. (b) Fix $\Delta x = 0.2$, change $\Delta T \in [0.1, 1.9]$. (c) Fix $\Delta T = 0.2$, change $\Delta x \in [0.01, 10]$. (d) Fix $\Delta T = 1.8$, change $\Delta x \in [0.01, 10]$.

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