On diffusive non-reciprocity and thermal diode

Ying Li\textsuperscript{1}, Jiaxin Li\textsuperscript{2,1}, Cheng-Wei Qiu\textsuperscript{1}\textsuperscript{*}

\textsuperscript{1}Department of Electrical and Computer Engineering, National University of Singapore, Kent Ridge 117583, Republic of Singapore

\textsuperscript{2}State Key Laboratory of Robotics and System, Harbin Institute of Technology, Harbin 150001, China

Abstract

Wave propagation and diffusion in linear materials preserve local reciprocity in terms of a symmetric Green’s function. For wave propagations, people usually focus on the signals entering and leaving a system, and do not need detailed information about the fields inside it. In such cases, the global reciprocity of the scattering off a system through several ports is more important, which is defined as the symmetric transmission between the scattering channels. When a two-port system supports non-reciprocal (electromagnetic, acoustic) wave propagation, it is a (optical, phonon) diode directly following the definition. However, to date no clear definition or discussion has been made on the global reciprocity of diffusive processes through a system. It thus remains a question whether diffusive non-reciprocity is related with diode for diffusive fields, say, a thermal diode. Here, we provide theoretical analysis based on local reciprocity and define the global reciprocity of diffusion through a two-port system. We further prove the equivalence between a non-reciprocal heat transfer system and a thermal diode, and discuss some methods to realize it. Our results set a general background for future studies on symmetric and asymmetric diffusive processes.

\textsuperscript{*}e-mail: chengwei.qiu@nus.edu.sg
Local reciprocity of diffusion

In processes such as mass transport, thermal conduction, and direct current (DC) transport, the physical fields at macroscale can be described with a diffusion equation. Taking heat transfer as an example, the temperature field $T(r,t)$ ($r$ is the position vector, and $t$ is time) follows

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (\kappa \cdot \nabla T) + \rho c_p v \nabla T + q(r,t)$$  \hspace{1cm} (1)

where $\rho$ is the density, $c_p$ is the specific heat capacity at constant pressure, and $\kappa$ is the thermal conductivity tensor of the material. $q(r,t)$ is the density of heat source in bulk. We also included a convective term for generality, where $v$ is the velocity. In many situations, the steady state or steady oscillatory state is of interest, and it is convenient to study the Fourier transformation of Eq. (1)

$$i\omega \rho c_p T(r, \omega) = \nabla \cdot [\kappa \cdot \nabla T(r, \omega)] + \rho c_p v \cdot \nabla T(r, \omega) + q(r, \omega)$$  \hspace{1cm} (2)

It is well known that when 1) there is no convection; 2) the material properties do not vary with time; 3) the material is temperature independent; and 4) the thermal conductivity tensor is symmetric, Eq. (2) preserves reciprocity in the sense that the Green’s function is symmetric\(^1\) $G(r_1|r_0, \omega) = G(r_0|r_1, \omega)$.

Consider a domain $V$ as in Fig. 1a, where all four conditions are satisfied. The Green’s function follows

$$i\omega \rho c_p G(r | r_0, \omega) = \nabla \cdot [\kappa \cdot \nabla G(r | r_0, \omega)] + Q_0 \delta(r - r_0)$$  \hspace{1cm} (3)

where $\delta(r)$ is the Dirac delta function, $Q_0$ is a constant to ensure correct unit. On the domain boundary $S$ with normal vector $n$, the Green’s function satisfies the Dirichlet ($G(r_S| r_0, \omega) =$
0), Neumann \((\mb{n} \cdot \nabla G(r \mid r_0, \omega)) \cdot \mb{n} = 0\), or mixed \((cG(r \mid r_0, \omega) + \kappa \cdot \nabla G(r \mid r_0, \omega)) \cdot \mb{n} = 0\), \(c\) is a constant) boundary condition. Replacing \(r_0\) with \(r_1\) gives

\[
i\omega pc G(r \mid r_1, \omega) = \nabla \cdot (\kappa \cdot \nabla G(r \mid r_1, \omega)) + Q_0 \delta(r - r_1) \quad (4)
\]

By multiplying Eq. (3) with \(G(r \mid r_1, \omega)\) and Eq. (4) with \(G(r \mid r_0, \omega)\), then integrating their difference over \(V\), we have

\[
\int_V \{G(r \mid r_1, \omega)\nabla \cdot [\kappa \cdot \nabla G(r \mid r_0, \omega)] - G(r \mid r_0, \omega)\nabla \cdot [\kappa \cdot \nabla G(r \mid r_1, \omega)]\} \, dV
\]

\[
= \int_V [G(r \mid r_0, \omega)Q_0 \delta(r - r_1) - G(r \mid r_1, \omega)Q_0 \delta(r - r_0)] \, dV \quad (5)
\]

The Green’s theorem can be applied to the left-hand side

\[
\text{l.h.s} = \int_V \nabla \cdot \left[ G(r \mid r_1, \omega)\kappa \cdot \nabla G(r \mid r_0, \omega) - G(r \mid r_0, \omega)\kappa \cdot \nabla G(r \mid r_1, \omega) \right] \, dV
\]

\[
= \int_S \left[ G(r_s \mid r_1, \omega)\kappa \cdot \nabla G(r_s \mid r_0, \omega) - G(r_s \mid r_0, \omega)\kappa \cdot \nabla G(r_s \mid r_1, \omega) \right] \cdot \mb{n} \, dS \quad (6)
\]

We have used the property that \(\kappa\) is symmetric, which is satisfied for common materials thanks to the Onsager reciprocity relation\(^2\). It is easy to see that the integrand is zero for all kinds of boundary conditions. The right-hand side of Eq. (5) is simplified using the sifting property of the Dirac delta function and gives

\[
\text{r.h.s} = Q_0 [G(r_1 \mid r_0, \omega) - G(r_0 \mid r_1, \omega)] = 0 \quad (7)
\]

The local reciprocity of Eq. (2) is thus proved.

**Global reciprocity of diffusion through ports**

The above definition of reciprocity does not directly apply to transportation through a system with several ports. For wave propagation, the reciprocity of such processes is often defined as the symmetry of the scattering matrix\(^3\). Similarly, we can study the reciprocity in terms of the relation between field amplitudes at different ports of a diffusive system. Consider a two-port heat transfer system as in Fig. 1b, the region \(V\) is thermally insulted,
except for two channels $C_1$ and $C_2$ that have uniform and linear material properties. It is also assumed that both channels are long, narrow, and aligned in the lateral $x$ direction, with their upper and lower boundaries insulated. At oscillatory frequency $\omega$, the supported modes are

$$T_c(x, \omega) = e^{\pm ik_c x}, \quad k_c = (1 - i)\sqrt{\omega / 2D_c}$$

where $D_c$ is the diffusivity of the channels. If the interfaces between the left and right ports and the system are at $x_1$ and $x_2$, we can define the fields in the channels as

$$T_c(x, \omega) = \begin{cases} 
A_1 e^{-ik_c (x-x_1)} + B_1 e^{ik_c (x-x_1)}, & x \leq x_1 \\
A_2 e^{ik_c (x-x_2)} + B_2 e^{-ik_c (x-x_2)}, & x \geq x_2 
\end{cases}$$

Note that the field evolution is obtained by multiplying $T(x, \omega)$ with $e^{i\omega t}$, so $A_1$ and $A_2$ are the amplitudes of the incident fields, while $B_1$ and $B_2$ are the amplitudes of the outgoing fields. They are related through the scattering matrix $S$

$$\begin{pmatrix} B_1 \\ B_2 \end{pmatrix} = S \begin{pmatrix} A_1 \\ A_2 \end{pmatrix} = \begin{pmatrix} r_{11} & t_{12} \\ t_{21} & r_{22} \end{pmatrix} \begin{pmatrix} A_1 \\ A_2 \end{pmatrix}$$

where $r_{11}$ and $r_{22}$ ($t_{12}$ and $t_{21}$) are the reflection (transmission) coefficients. Reciprocity of scattering processes through the system is defined as a symmetric $S$, or $t_{12} = t_{21}$.

Assuming that we already have the Green’s function for the entire system plus the two channels $(V \cup C_1 \cup C_2)$. It satisfies the Neumann boundary condition, and must have the similar form as Eq. (9) in the two channels.
\[
G(x | x_a, \omega) = \begin{cases} 
A_1(x_a, \omega) \frac{e^{-ik_c(x-x_1)} - e^{ik_c(x_1-x)}}{1 - e^{-ik_cx_1}} + B_1(x_a, \omega) \frac{e^{ik_c(x_1-x)} - e^{-ik_cx}}{1 - e^{-ik_cx}}, & x_a \leq x \leq x_1 \\
B_2(x_a, \omega) \frac{e^{-ik_c(x_1-x_2)} - e^{-ik_c(L-x_2)}}{1 - e^{-ik_c(L-x_2)}}, & x \geq x_2 \\
B_1(x_b, \omega) \frac{e^{ik_c(x-x_2)} - e^{-ik_c(L+x_2)}}{1 - e^{-ik_c(L+x_2)}}, & x \leq x_1 \\
A_2(x_b, \omega) \frac{e^{ik_c(x-x_2)} - e^{-ik_cx_2}}{1 - e^{-ik_cx_2}} + B_2(x_b, \omega) \frac{e^{-ik_c(x_2-x)} - e^{ik_cx}}{1 - e^{-ik_cx}}, & x_2 \leq x \leq x_b 
\end{cases}
\]

(11)

where \(x_a \leq x_1\) and \(x_b \geq x_2\). We adopt this special form in order to ensure a meaningful linear distribution in the limit of \(\omega (k_c) \rightarrow 0\), instead of the zero fields in Eq. (9). The boundary condition is \(G(\pm L | x_a, \omega) = G(\pm L | x_b, \omega) = 0\) for \(L \rightarrow \infty\). Therefore

\[
t_{12} = \frac{B_1(x_b, \omega)}{A_2(x_b, \omega)} = \frac{G(x | x_1, \omega)}{A_2(x_a, \omega)}, \\
t_{21} = \frac{B_2(x_a, \omega)}{A_1(x_a, \omega)} = \frac{G(x | x_2, \omega)}{A_1(x_b, \omega)}
\]

(12)

When the sources are close to the interfaces: \(x_a \rightarrow x_1\) and \(x_b \rightarrow x_2\), Eq. (12) is

\[
t_{12} = \frac{G(x | x_1, \omega)}{A_2(x_2, \omega)}, \\
t_{21} = \frac{G(x | x_2, \omega)}{A_1(x_1, \omega)}
\]

(13)

Clearly, the amplitude of an incident field only depends on the source, since the reflections at \(x = \pm L \rightarrow \pm \infty\) are negligible. It turns out that \(A_1(x_1, \omega) = A_2(x_2, \omega) = A(\omega)\), and the reciprocity of the two-port system is equivalent to

\[
G(x | x_1, \omega) = G(x | x_2, \omega)
\]

(14)

We note that in the limit of \(\omega (k_c) \rightarrow 0\), one cannot distinguish the incident, reflected, and transmitted parts of a field, since there is no directionality of field propagation. However, the definition of reciprocity in Eq. (14) is still meaningful as an extension from the cases with nonzero frequency.

**Non-reciprocity and diode**
For wave propagation, a non-reciprocal two-port system is almost the same thing as a diode, both refer to an asymmetric transmission. It is worth noting that for a diode, the incident and outgoing waves under consideration are generally required to be at equal frequency, while it is correct to state that the transmission between two modes at different frequencies is non-reciprocal. Here, we focus on the equal-frequency transmission.

In diffusive processes, a diode is usually defined differently. For example, a thermal diode refers to a system in contact with two thermal reservoirs at temperatures $T_1$ and $T_2$, and the heat fluxes passing through it must be asymmetric after swapping the values of $T_1$ and $T_2$, as shown in Fig. 1c. Naturally, one would ask whether a non-reciprocal heat transfer system is still equivalent to a thermal diode. We could answer the question by fixing the temperatures of the interfaces $S_1$ and $S_2$ at $T_1$ ($T_2$).

For such setups, only the fields at zero frequency or steady state are of interest, so we consider the steady-state Green’s function first. It must be linear in the channels, thus

$$G(x \mid x_a, 0) = \begin{cases} C_1(x_a)(x + L), & -L \leq x \leq x_a \\ D_1(x_a)(x - x_a) + C_1(x_a)(x_a + L), & x_a \leq x \leq x_1 \\ C_2(x_a)(x - L), & x_2 \leq x \leq L \end{cases}$$

$$G(x \mid x_b, 0) = \begin{cases} C_1(x_b)(x + L), & -L \leq x \leq x_1 \\ D_2(x_b)(x - x_b) + C_2(x_b)(x_b - L), & x_2 \leq x \leq x_b \\ C_2(x_b)(x - L), & x_b \leq x \leq L \end{cases}$$

where $x = \pm L$ are the positions of the left and right ends of the channels. Again $x_a \leq x_1$ and $x_b \geq x_2$. The function satisfies Dirichlet boundary condition $G(\pm L \mid x_a, 0) = G(\pm L \mid x_b, 0) = 0$. Assuming that the total energy generation $H$ in $V$ is independent of the conditions outside, the energy conservation requires that
\[
\kappa_c D_1(x_a) \sigma = \kappa_c C_2(x_a) \sigma + H
\]
\[
\kappa_c C_1(x_b) \sigma = \kappa_c D_2(x_b) \sigma + H
\]
\[
\kappa_c [C_1(x_a) - C_2(x_a)] \sigma = \kappa_c [C_1(x_b) - C_2(x_b)] \sigma = Q_0 + H
\]  

(16)

where \( \kappa_c \) is the thermal conductivity, and \( \sigma \) is the cross-section area of the channels. If the differential operator on the field in region \( V \) is linear, the linear combination \( F(x) = f_a G(x|x_a,0) + f_b G(x|x_b,0) \) is also a solution to the equation in region \( V \). If we require \( F(x_a) = T_1 \) and \( F(x_b) = T_2 \), the coefficients satisfy

\[
G \begin{pmatrix} f_a \\ f_b \end{pmatrix} = \begin{pmatrix} G(x_a | x_a) & G(x_a | x_b) \\ G(x_b | x_a) & G(x_b | x_b) \end{pmatrix} \begin{pmatrix} f_a \\ f_b \end{pmatrix} = \begin{pmatrix} T_1 \\ T_2 \end{pmatrix}
\]

(17)

The heat fluxes \( q_1 \) and \( q_2 \) in \( C_1 \) and \( C_2 \) near the interfaces \( S_1 \) and \( S_2 \) are

\[
\begin{pmatrix} q_1 \\ q_2 \end{pmatrix} = \kappa_c \begin{pmatrix} D_1(x_a) & C_1(x_b) \\ C_2(x_a) & D_2(x_b) \end{pmatrix} \begin{pmatrix} f_a \\ f_b \end{pmatrix} = Q \begin{pmatrix} f_a \\ f_b \end{pmatrix}
\]

(18)

By letting \( x_a \to x_1 \) and \( x_b \to x_2 \), we approach the desired setup. Now we can swap the values of \( T_1 \) and \( T_2 \) to solve another set of coefficients

\[
G \begin{pmatrix} \tilde{f}_a \\ \tilde{f}_b \end{pmatrix} = \begin{pmatrix} T_2 \\ T_1 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} T_1 \\ T_2 \end{pmatrix}
\]

(19)

Therefore,

\[
\begin{pmatrix} \tilde{f}_a \\ \tilde{f}_b \end{pmatrix} = G^{-1} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} G \begin{pmatrix} f_a \\ f_b \end{pmatrix}
\]

(20)

The corresponding heat fluxes are

\[
\begin{pmatrix} \tilde{q}_1 \\ \tilde{q}_2 \end{pmatrix} = Q \begin{pmatrix} \tilde{f}_a \\ \tilde{f}_b \end{pmatrix} = Q G^{-1} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} G Q^{-1} \begin{pmatrix} q_1 \\ q_2 \end{pmatrix}
\]

(21)

Note that when \( H = 0 \), \( Q \) is singular, but the following results can be similarly obtained.

If the system is not a diode, it is required that
\[
\begin{pmatrix}
\tilde{q}_1 \\
\tilde{q}_2
\end{pmatrix}
= -
\begin{pmatrix}
q_2 \\
q_1
\end{pmatrix}
= -
\begin{pmatrix}
0 & 1 \\
1 & 0
\end{pmatrix}
\begin{pmatrix}
q_1 \\
q_2
\end{pmatrix}
\] (22)

Substituting into Eq. (21) and considering that the temperature values are arbitrarily chosen, we have

\[
QG^{-1}
\begin{pmatrix}
0 & 1 \\
1 & 0
\end{pmatrix}
GQ^{-1} +
\begin{pmatrix}
0 & 1 \\
1 & 0
\end{pmatrix}
= 0
\] (23)

Assuming that the system is reciprocal, namely \( G = G^T \), it is easy to check that \( Q \) is anti-symmetric in the limit \( L \to \infty \). Combining with Eq. (16) gives that \( \text{tr}(Q) = 0 \) and \( G_{11} = G_{22} \) in the limit \( L \to \infty \). Using all the properties, we found that Eq. (23) is satisfied and the system is not a diode. On the other hand, if the system is non-reciprocal \( G \neq G^T \), Eq. (23) is not satisfied and the system is a diode.

**Discussions**

Based on our analysis, it is noticed that there are several methods to break the reciprocity and make a thermal diode. First, if the governing differential equation is nonlinear, \( e.g. \) because of a temperature dependent thermal conductivity, its solution cannot be obtained through the Green’s function. In such cases, nonlinearity can lead to asymmetric Green’s functions as well as diode effect\(^7\), but they do not necessarily imply each other. Second, when the thermal conductivity tensor is asymmetric, such as the thermal Hall effect in magnetic fields\(^8\), an additional term appears in Eq. (6)

\[
\int_V \nabla G(r \mid r_1, \omega) \cdot (\kappa - \kappa^T) \cdot \nabla G(r \mid r_0, \omega) \, dV
\] (24)

which could, but not necessarily be nonzero. Similarly, if thermal convection is present, an additional term appears that could possibly break the reciprocity

\[
-\int_V \left[ G(r \mid r_1, \omega) \rho c_p v \cdot \nabla G(r \mid r_0, \omega) - G(r \mid r_0, \omega) \rho c_p v \cdot \nabla G(r \mid r_1, \omega) \right] \, dV
\] (25)
In addition, if the energy generation $H$ in the system depends on the direction of heat transfer: $H \neq \tilde{H}$, the additional term is

$$\int_{V} [G(r \mid r_1, \omega)H - G(r \mid r_0, \omega)\tilde{H}]dV$$

(26)

which indicates non-reciprocity. In fact, the convective term can be regarded as an energy source with directionality. Another example is a system that is in contact with a temperature gradient. Therefore, we may conclude that directional mass or energy flux will break the reciprocity and thereby make a thermal diode. Finally, dynamic materials whose parameters are temporally modulated have attracted great interests as a potential tool to induce diffusive non-reciprocity$^{9,10}$. We will discuss about it elsewhere.

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Fig. 1. a, Local reciprocity in heat transfer; b, global reciprocity of heat transfer through a two-port system; c, thermal diode.