Ballistic thermal rectification in asymmetric three-terminal mesoscopic dielectric systems

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Abstract. By coupling a temperature probe to the asymmetric three-terminal mesoscopic dielectric system, ballistic thermal rectification at low temperature is analytically studied based on the Landauer formulation of transport theory. It is seen that thermal rectification is a purely quantum effect and the quantum statistics of phonons in thermal reservoirs is necessary. Moreover, when the phonon re-emits into the system from the temperature probe, energy changing is necessary to realize thermal rectification. Another necessary condition is the different asymmetries for phonons with different frequencies, which is reflected by the dependence of the ratio \( \tau_{RC}(\omega)/\tau_{RL}(\omega) \) on \( \omega \), the phonon’s frequency, where \( \tau_{RC}(\omega) \) and \( \tau_{RL}(\omega) \) are respectively the transmission coefficients from two asymmetric terminals to the temperature probe. The analytical results are confirmed by extensive numerical simulations.

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1. Introduction

The control of heat transport in various applications in electronics and biotechnology has attracted much attention. As the basic device for controlling heat transport, the thermal rectifier allows heat current to flow mainly in one direction and only weakly in the opposite one when it is pushed out of equilibrium. By using the property that effective phonon bands of different segments of a one-dimensional nonlinear chain will change from matching to non-matching when the heat baths are reversed, the first nanoscale model for the thermal rectifier was proposed in 2002 \[1]. Since then, much theoretical work has been performed to study thermal rectification \[2]–\[10], and two experimental works that demonstrate thermal rectification have also been reported \[11, 12]. Recently, based on one-dimensional nonlinear chains, models of thermal logic gates \[13] and thermal memory \[14] have been theoretically proposed to demonstrate that phonons can be used to carry information and processed accordingly.

However, with the development of modern nanotechnology, the sizes of nanoscale materials are comparable with the phonon mean-free path at low temperature. The inherent nonlinearity is then insignificant and thermal transport is dominated by the transmission of ballistic phonons at low temperature \[15]–\[17]. Much work has been performed to study thermal rectification in these harmonic systems, and it is seen that there is no thermal rectification in a two-terminal harmonic system at low temperature \[6]. This absence of thermal rectification in a harmonic system is also found in classical models: the harmonic chain with self-consistent reservoirs \[18, 19] and the harmonic $N$-terminal junction \[20]. Only recently, motivated by work on the voltage probe in mesoscopic electronic systems \[21]–\[28], by asymmetric coupling with an additional probe connected to a self-consistent reservoir (denoted as the temperature probe in the following), has ballistic thermal rectification been obtained in quantum harmonic systems in the nonlinear regime \[29, 30]. From the numerical results, in \[29], two necessary conditions to realize ballistic thermal rectification have been obtained: phonon incoherence or phase braking and asymmetry, which is reflected by the difference of $\tau_{RC} - \tau_{RL}$, where $\tau_{RC}$ and $\tau_{RL}$ are respectively the transmission coefficients from two asymmetric terminals to the temperature probe. In \[30], the necessity of asymmetry is confirmed by the graded mass quantum chain of harmonic oscillators.

Similar to the voltage probe in mesoscopic electronic systems \[23]–\[27], the temperature probe will lead some coherent phonons to transmit into the self-consistent reservoir. After scattering in the reservoir, the phonons re-emit into the harmonic system with their phase coherence being lost and their energies changing. It is not very clear whether phase incoherence or energy changing is necessary to realize ballistic thermal rectification. In this work, we theoretically study ballistic thermal rectification in the harmonic system similar to the system.
in [29]. By coupling a temperature probe to the asymmetric three-terminal mesoscopic dielectric system, in the nonlinear response regime, the leading term of ballistic thermal rectification is analytically obtained at low temperature. Our analytical results explicitly indicate that the phase incoherence is not enough to induce ballistic thermal rectification even with the asymmetry. The energy changing when the phonons re-emit into the system is necessary to realize ballistic thermal rectification. On the other hand, our analytical results also indicate that realization of ballistic thermal rectification is determined by the dependence of the ratio \( \tau_{RC}(\omega)/\tau_{RL}(\omega) \) on the frequency \( \omega \). This means that the asymmetry is reflected not by \( \tau_{RC} - \tau_{RL} \), but by \( \tau_{RC}/\tau_{RL} \). Different asymmetries for phonons with different frequencies are necessary to realize thermal rectification. Besides these, the influence of the quantum statistics of phonons in the thermal reservoir has explicitly appeared in the analytical results. The analytical results are confirmed by extensive numerical simulations.

The rest of the paper is organized as follows. In section 2, the model and the analytical formulae and results are presented. The numerical results are presented in section 3. Section 4 is devoted to a summary.

2. Model and formalism

The asymmetric three-terminal junction is sketched in the inset of figure 1. Through terminals L and C, the junction is coupled to two thermal reservoirs at temperatures \( T_L \) and \( T_C \). The steady-state heat flux \( \dot{Q} = \dot{Q}_C = -\dot{Q}_L \) is passed through the junction via terminals C and L. A third terminal R is connected to another thermal reservoir at temperature \( T_R \). This third terminal is a temperature probe; it means that \( T_R \) is adjusted at such a way that no heat flux passes through terminal R. The ballistic regime is considered in this work. The heat flux \( \dot{Q}_i \) from terminal \( i \) \( (i = L, R, C) \) flowing into the midsection J can be expressed as

\[
\dot{Q}_i = \sum_{j(j \neq i)} \int_{0}^{+\infty} [n(T_i, \omega) - n(T_j, \omega)] \hbar \omega \tau_{ji}(\omega) \frac{d\omega}{2\pi}, \tag{1}
\]

where \( n(T_i, \omega) = [\exp(\hbar \omega/k_B T_i) - 1]^{-1} \) is the Bose–Einstein distribution function of phonons in the \( i \)th reservoir, \( T_i \) is the equilibrium temperature of thermal reservoir \( i \), \( \tau_{ji}(\omega) = \sum_m \theta(\omega - \omega_{jm}) \) is the transmission coefficient, \( \tau_{ji,m}(\omega) = \sum_{m,n} \theta(\omega - \omega_{jn}) \theta(\omega - \omega_{im}) \) is the total transmission coefficient, \( \tau_{ji,mn}(\omega) \) is the transmission coefficient from mode \( m \) of terminal \( i \) at frequency \( \omega \) across all the interface into mode \( n \) of terminal \( j \), and \( \omega_{im} \) is the cut-off frequency of mode \( m \) in terminal \( i \). By time-reversal symmetry, we have \( \tau_{ji}(\omega) = \tau_{ij}(\omega) \). The influence of the temperature probe R on the steady-state heat flux \( \dot{Q} \) is determined by the transmission coefficients \( \tau_{RC}(\omega) \) and \( \tau_{RL}(\omega) \).

Firstly, the reservoir L is set at temperature \( T_L = T_{\text{hot}} \), which is higher than the temperature \( T_C = T_{\text{cold}} \) of reservoir C. The temperature of reservoir R is adjusted at \( T_R \). The heat flux flowing through the system is \( \dot{Q}_- \equiv \dot{Q}_C \). Evidently, the heat flux flows into reservoir C and hence \( \dot{Q}_- < 0 \). By reversing the temperature bias, i.e. let \( T_L = T_{\text{cold}} \) and \( T_C = T_{\text{hot}} \), the temperature of reservoir R is adjusted at \( T'_R \), and the heat flux is equal to \( \dot{Q}_+ \equiv \dot{Q}_C > 0 \).

To study ballistic thermal rectification, \( \dot{Q}_- \) is added to \( \dot{Q}_+ \):

\[
\Delta \dot{Q} \equiv \dot{Q}_- + \dot{Q}_+ = \int_{0}^{+\infty} [n(T_{\text{cold}}, \omega) - n(T_R, \omega) + n(T_{\text{hot}}, \omega) - n(T'_R, \omega)] \tau_{RC}(\omega) \hbar \omega \frac{d\omega}{2\pi}, \tag{2}
\]
where $T_R$ and $T'_R$ are determined by $\dot{Q}_R = 0$. Obviously, $T_R$ and $T'_R$ are determined by the transmission coefficients $\tau_{RC}(\omega)$ and $\tau_{RL}(\omega)$, which are temperature independent. Therefore, whether rectification can be attained depends critically on the transmission coefficients $\tau_{RC}(\omega)$ and $\tau_{RL}(\omega)$. In the linear response regime, by using $\dot{Q}_i = \sum_{j \neq i} G_{ji}(T_i - T_j)$ [17, 31], where $G_{ji}$ is the two-terminal thermal conductance from reservoir $i$ to $j$, one can easily find that $n(T_{\text{cold}}, \omega) - n(T_R, \omega) + n(T_{\text{hot}}, \omega) - n(T'_R, \omega) = 0$ for any $\omega$. Thus, $\Delta \dot{Q} = 0$, which means there is no rectification in the linear response regime. This corresponds to what was obtained in [32] for thermoelectric transport in a chain of quantum dots with self-consistent reservoirs. On the other hand, if the ratio $\tau_{RC}(\omega)/\tau_{RL}(\omega)$ is a constant for any frequency $\omega$, by using $\dot{Q}_R = 0$, one can easily find that $\Delta \dot{Q} = 0$ and rectification is absent even in the nonlinear response regime. Therefore, even in the nonlinear regime, thermal rectification is absent in the symmetric three-terminal junctions with $\tau_{RC}(\omega) = \tau_{RL}(\omega)$.

In a more general situation where the ratio $\tau_{RC}(\omega)/\tau_{RL}(\omega)$ for any frequency is not a constant, the fact that $\tau_{RC}(\omega)/\tau_{RL}(\omega)$ varies with $\omega$ means there are different asymmetries for transmission of phonons in different frequencies. One can certainly expect that $\Delta \dot{Q}$ is not zero in the nonlinear response regime and it is determined by the dependence of the ratio $\tau_{RC}(\omega)/\tau_{RL}(\omega)$ on $\omega$. We start by letting $T_0 = (T_{\text{hot}} + T_{\text{cold}})/2$ and $\Delta T = (T_{\text{hot}} - T_{\text{cold}})/2$, where $T_0$ can be regarded as the working temperature according to the following text. When $\Delta T$ is a small value, by using the Taylor expansion of the Bose–Einstein distribution function $n(T, \omega)$ as well as the results of $T_R$ and $T'_R$ in [33] for the asymmetric three-terminal junctions, one can find

$$\Delta \dot{Q} = (1 - \beta^2) \frac{F_2(\tau_{RC}) F_1(\tau_{RL}) - F_2(\tau_{RL}) F_1(\tau_{RC})}{F_1(\tau_{RC}) + F_1(\tau_{RL})} (\Delta T)^2 + O[(\Delta T)^4]$$

$$\equiv \alpha (\Delta T)^2 + O[(\Delta T)^4],$$

(3)

where

$$F_k(\tau_{RL}) = \int_0^{+\infty} \left( \frac{\partial^k n}{\partial T^k} \right)_{\tau_{RL}} \frac{\hbar \omega \tau_{RL}}{2\pi} d\omega,$$

(4)

$$\beta = \frac{F_1(\tau_{RL}) - F_1(\tau_{RC})}{F_1(\tau_{RC}) + F_1(\tau_{RL})}.$$

(5)

By simple algebra, $F_2(\tau_{RC}) F_1(\tau_{RL}) - F_2(\tau_{RL}) F_1(\tau_{RC})$ can be re-expressed as

$$\int_0^{+\infty} d\omega_1 \int_{-\omega_2}^{+\omega_2} d\omega_2 N(\omega_1, \omega_2, T_0) T(\omega_1, \omega_2) \hbar \omega_1 \hbar \omega_2 / (2\pi)^2,$$

(6)

where

$$N(\omega_1, \omega_2, T_0) = \left[ \frac{\partial^2 n(\omega_1)}{\partial T^2} \frac{\partial n(\omega_2)}{\partial T} - \frac{\partial^2 n(\omega_2)}{\partial T^2} \frac{\partial n(\omega_1)}{\partial T} \right]_{T_0}$$

$$= \left\{ \frac{\hbar \omega_1}{k_B T_0} [1 + 2n(\omega_1)] - \frac{\hbar \omega_2}{k_B T_0} [1 + 2n(\omega_2)] \right\} \frac{1}{T_0} \left[ \frac{\partial n(\omega_1)}{\partial T} \frac{\partial n(\omega_2)}{\partial T} \right]_{T_0},$$

(7)

$$T(\omega_1, \omega_2) = \tau_{RC}(\omega_1) \tau_{RL}(\omega_2) - \tau_{RC}(\omega_2) \tau_{RL}(\omega_1).$$

(8)

This is the main result of this work. In (7), $\partial^2 n / \partial T^2 = [(1 + 2n) \hbar \omega / (k_B T^2) - 2 / T] \partial n / \partial T$ is used. From (3), one can find that the linear term of $\Delta T$ is absent, which means that thermal rectification is absent in the linear response regime as shown in the preceding text.

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Obviously, $N(\omega_1, \omega_2, T_0)$ is $T_0$ dependent and can only be non-zero when the phonons in the thermal reservoirs obey quantum statistics. In the high-temperature limit, the Bose–Einstein distribution function is transformed as $n(T, \omega) = k_B T / (\hbar \omega)$. Then $\partial^2 n / \partial T^2 = 0$ and the thermal rectification vanishes as shown in [18]–[20]. Therefore, ballistic thermal rectification is a purely quantum effect at low temperature.

The other factor $T(\omega_1, \omega_2)$ originates from the inelastic scattering of phonons in the temperature probe. The first term of $T(\omega_1, \omega_2)$ in (8) can be understood as the process in which the ballistic phonon with frequency $\omega_1$ transports from reservoir C into reservoir R through the temperature probe with transmission coefficient $\tau_{RC}(\omega_1)$. After being inelastically scattered into the different frequency $\omega_2$, the ballistic phonon transports from reservoir R into reservoir L with the transmission coefficient $\tau_{RL}(\omega_2)$. The second term presents a similar process, but in the opposite direction. If $\omega_1 = \omega_2$, from the temperature probe, the phonon re-emits into the system without the energy changing. This energy conserving scattering only induces the phase breaking of phonons and is not enough to induce thermal rectification because $T(\omega_1, \omega_1) = 0$. Thus, the energy changing of phonons with $\omega_1 \neq \omega_2$ after scattering in reservoir R is necessary to realize the ballistic thermal rectification.

To study the sign of $N(\omega_1, \omega_2, T_0)$, $\partial [x(1 + 2n(x))] / \partial x$ is studied, where $x = \hbar \omega / k_B T_0$.

$$\frac{\partial [x(1 + 2n(x))] \partial x}{(\varepsilon^2 - 2x \varepsilon^1 - 1)/(\varepsilon^1 - 1)^2} = \frac{1}{(\varepsilon^1 - 1)^2} \sum_{l=0}^{\infty} 2^l l - 1 (l + 1)! 2x^{l+1} > 0 \quad (9)$$

for all $x > 0$. Hence, $N(\omega_1, \omega_2, T_0) > 0$ for all $\omega_1 > \omega_2 > 0$. Thus, the inelastic scattering factor, $T(\omega_1, \omega_2)$, determines the sign of $\alpha$ due to $0 \leq \beta^2 < 1$. By re-expressing $T(\omega_1, \omega_2)$ as $[\tau_{RC}(\omega_1)/\tau_{RL}(\omega_1) - \tau_{RC}(\omega_2)/\tau_{RL}(\omega_2)] \tau_{RL}(\omega_1) / \tau_{RL}(\omega_2)$ when $\tau_{RL}(\omega) \neq 0$ for all $\omega$, one can easily find that the sign of $\alpha$ is determined by the dependence of the ratio $\tau_{RC}(\omega)/\tau_{RL}(\omega)$ on $\omega$. Obviously, $\tau_{RC}(\omega_1)/\tau_{RL}(\omega_1) \neq \tau_{RC}(\omega_2)/\tau_{RL}(\omega_2)$ is required to realize ballistic thermal rectification. $\Delta \dot{Q} > 0$ when $\tau_{RC}(\omega)/\tau_{RL}(\omega)$ increases with $\omega$.

3. Numerical results

To obtain the exact $\Delta \dot{Q}$, we carry out numerical calculations for (2) with the scattering matrix method used in [33]. In the calculation, the geometrical parameters of the system are chosen as $W_L = W_R = W_C = D_j = 10$ nm, while $W_T$ can be varied. We limit the temperature $T_{\text{hot}}$ of the thermal reservoir at the higher temperature to be lower than $T_{\text{ph}} = \hbar \pi v / W_i k_B \approx 7.61$ K ($v$ is the sound velocity) [33] to ensure that phonon relaxation can be neglected [17], and heat conduction is determined by the ballistic transmission of acoustic phonons.

Figure 1 shows the results of $\Delta \dot{Q}$ versus $2\Delta T$ for different $T_0$ with $W_T = 21$ nm. Firstly, at small but finite $\Delta T$, $\Delta \dot{Q}$ shows a quadratic dependence on $\Delta T$, in agreement with (3). Secondly, corresponding to the factor $N(\omega_1, \omega_2, T_0)$, $\Delta \dot{Q}$ decreases with increasing $T_0$ for a system with a certain $W_T$. Thirdly, when the temperature difference $2\Delta T = T_{\text{hot}} - T_{\text{cold}}$ is finite, thermal rectification is obtained with $\Delta \dot{Q} > 0$ in figure 1. This means that $T(\omega_1, \omega_2) > 0$ at these $T_0$; hence there is a greater heat flux in the direction from reservoir C to reservoir L than the heat flux in the inverse direction when the temperature bias is reversed. This indicates that by undergoing inelastic scattering introduced by the temperature probe, the ballistic phonon has more probability to transport from reservoir C into reservoir L than transport in the inverse direction. To understand this, one must recall that $\Delta \dot{Q}$ is determined by the factors $N(\omega_1, \omega_2, T_0)$ and $T(\omega_1, \omega_2)$, as shown in (6). Because phonons in reservoirs
Figure 1. Difference of heat flux $\Delta \dot{Q} = \dot{Q}_- + \dot{Q}_+$ (in units of $k_B T_{ph}$) versus $2\Delta T = T_{hot} - T_{cold}$ at different $T_0$ values, where $W_T = 21$ nm. Inset: schematic illustration of an asymmetric three-terminal mesoscopic dielectric system coupled with a temperature probe by the R terminal.

Figure 2. Dependence of the ratio $\tau_{RC}/\tau_{RL}$ on frequency $\omega$ (in units of $k_B T_{ph}/\hbar$). Inset: $\Delta \dot{Q}$ versus $2\Delta T$ for different $W_T$ at average temperatures of $T_0 = 0.1 T_{ph}$.

obey the Bose–Einstein statistics, and $\partial \{x [1 + 2n(x)] \}/\partial x \to 0$ when $x \to 0$ as shown in (9), phonons with frequencies in the region $0 < \omega < 3 T_0/T_{ph}$ (where the unit $k_B T_{ph}/\hbar$ is omitted) dominate $N(\omega_1, \omega_2, T_0)$ when $\Delta T$ is a small finite value and the phonon with lower frequency is more dominant. Thus, for $W_T = 21$ nm, at $T_0 = 0.3 T_{ph}$, phonons with frequencies $0 < \omega < 0.9$ dominate $N(\omega_1, \omega_2, T_0)$. Phonons with frequencies $0 < \omega < 0.25$ are more dominant to $N(\omega_1, \omega_2, T_0)$, but as shown in figure 2, $\tau_{RC}/\tau_{RL}$ decreases slowly in this region and increases faster in the region $0.25 < \omega < 0.58$. Hence, by considering contributions from both $N(\omega_1, \omega_2, T_0)$ and $T(\omega_1, \omega_2)$, phonons with frequencies $0.25 < \omega < 0.58$ determine $\Delta \dot{Q} > 0$.
Figure 3. Efficiency of rectification versus temperature difference $2\Delta T$ ($= T_{\text{hot}} - T_{\text{cold}}$) for different $W_T$ at average temperatures of $T_0 = 0.3T_{ph}$ and $0.4T_{ph}$.

Figure 4. Efficiency of rectification versus temperature difference $2\Delta T$ ($= T_{\text{hot}} - T_{\text{cold}}$) for different $W_T$ at average temperatures of $T_0 = 0.5T_{ph}$ and $0.6T_{ph}$.

because $\mathcal{T}(\omega_1, \omega_2) > 0$ in this region. A similar analysis can be applied to other $T_0$. One can expect that at very low $T_0$ values, $\Delta \hat{Q} < 0$ because $\mathcal{T}(\omega_1, \omega_2) < 0$ is in the dominant region of frequency. This is confirmed by the inset of figure 2. Thermal rectification can be studied by efficiency, which is defined as $\eta = |\Delta \hat{Q}| / |\hat{Q}_-| \times 100\%$. The numerical results of efficiency are shown in figures 3 and 4 for different $T_0$ and different $W_T$. The efficiency can achieve about 5.5%, as shown in the two figures. In the system with $W_T = 27$ nm, at $T_0 = 0.3T_{ph}$, $0.4T_{ph}$ and $0.5T_{ph}$, the highest efficiencies are achieved. As shown in figure 2, the region of frequency in
which $\tau_{RC}/\tau_{RL}$ slowly decreases is the shortest; thus there are more phonons with frequencies in the increasing region contributing to the heat flux. However, at $T_0 = 0.6T_{ph}$, the system with $W_T = 13$ nm has the highest efficiency. This is because, for higher $T_0$, more phonons with higher frequencies are populated in reservoirs and contribute to the heat flux. For the system with $W_T = 13$ nm, the region $0.35 < \omega < 0.7$ in which $\tau_{RC}/\tau_{RL}$ increases is the widest.

4. Summary

In summary, we have analytically and numerically studied ballistic thermal rectification in asymmetric three-terminal systems. The leading term of thermal rectification is analytically obtained. From the analytical results, it is seen that when phonons re-emit into the system from the temperature probe, not the incoherence but the energy changing is necessary to realize ballistic thermal rectification. The quantum statistics of phonons in thermal reservoirs is also necessary, and thus rectification is purely a quantum effect. The other necessary condition is the different dependence of the ratios $\tau_{RC}(\omega)/\tau_{RL}(\omega)$ on different $\omega$’s. Thermal rectification can change sign when the ratio $\tau_{RC}(\omega)/\tau_{RL}(\omega)$ changes from decreasing with $\omega$ to increasing with $\omega$. $\tau_{RC}(\omega)/\tau_{RL}(\omega)$ is determined by the inelastic scattering of phonons through the temperature probe. Therefore, one can attain and control ballistic thermal rectification by asymmetrically introducing the inelastic scattering of phonons into mesoscopic systems.

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