Superlattice nanowire heat engines with direction-dependent power output and heat current

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Heat engines (HEs) made of low dimensional structures offer promising applications in energy harvesting due to their reduced phonon thermal conductance. Many efforts have been devoted to the design of HEs made of quantum-dot (QD) superlattice nanowire (SLNW), but only SLNWs with uniform energy levels in QDs were considered. Here we propose a HE made of SLNW with staircase-like QD energy levels. The power output and efficiency of such a SLNW are better than SLNWs with uniform QD energy levels. With a staircase-like distribution for QD energy levels and nonlinear Seebeck effect, the SLNW HE has direction-dependent power output and heat current. In addition, the HE has the functionality of a heat diode with impressive negative differential thermal conductance under open circuit condition.

Recently, many efforts were devoted to the studies of the nonlinear thermoelectric properties of low dimension systems.\(^{1,2}\) The figure of merit (ZT) of quantum dots (QDs) junction system approaches infinity (corresponding to Carnot efficiency) in the limit of vanishingly small phonon thermal conductance. However, their electrical power output is extremely weak.\(^{1}\) A remarkable thermoelectric device needs not only a high efficiency but also significant power output.\(^{3,4}\) Therefore, how to design a heat engine with near Carnot efficiency and optimized power output is under hot pursuit.\(^{1,2,4}\) It is expected that the efficiency of SLNW heat engines (HEs) is relatively high when compared with other low dimensional systems. Nevertheless, theoretical studies of SLNW HEs reported so far are based on the assumption of uniform energy levels in QDs\(^{5,8,17}\) without considering the effect of nonlinear Seebeck voltage.\(^{1,10}\)

In this paper, the effect of Seebeck voltage on the power output and TE efficiency of SLNW HEs are revealed. Furthermore, we also demonstrate that electron heat diodes can be implemented by using nonlinear Seebeck voltage of a QD SLNW with staircase-like energy levels. The design structure is shown in Fig. 1(a). Although the staircase-like energy levels of QDs in a SLNW make it difficult for the electron transport under a small temperature bias, a suitable alignment of QD energy levels can be designed to allow resonant electron transport under large forward temperature bias, while the system is in off-resonant regime under reverse bias. This mechanism can give rise to a high efficiency and optimized power output for SLNW HEs.

To study the direction-dependent nonlinear thermoelectric properties of QD SLNW connected to metallic electrodes shown in Fig. 1(a), we start with the system Hamiltonian given by an extended Anderson model

\[ H = H_0 + H_{QD}, \]

where

\[ H_0 = \sum_{k,\sigma} c_k^\dagger a_{k,\sigma} + \sum_{k,\sigma} c_k b_{k,\sigma}^\dagger \]

\[ + \sum_{k,s} V_{k,L}^L a_{k,\sigma}^\dagger + \sum_{k,s} V_{k,R}^R b_{k,\sigma}^\dagger + \text{c.c.} \]

The first two terms of Eq. (1) are for free electrons in the left and right electrodes.\(^{1,12}\) The QD superlattice nanowires (SLNWs) offer high potential to realize significantly reduced phonon thermal conductance.\(^{1,8,15}\) It is expected that the efficiency of SLNW heat engines (HEs) is relatively high when compared with other low dimensional systems. Nevertheless, theoretical studies of SLNW HEs reported so far are based on the assumption of uniform energy levels in QDs\(^{5,8,17}\) without considering the effect of nonlinear Seebeck voltage.\(^{1,10}\)

\[ H_{QD} = \sum_{\ell,s} E_{\ell,s} n_{\ell,s} + \sum_{\ell\neq j} t_{\ell,j} d_{\ell,s}^\dagger d_{j,s} + \text{c.c.} \]

where \(E_{\ell}\) denotes the energy of the level of the \(\ell\)-th QD, and \(t_{\ell,j}\) describes the electron hopping strength between the \(\ell\)-th QD and its nearest neighbor QD labeled by \(j\). For the SLNW depicted in Fig. 1(a), \(E_{\ell}\) depends on the location of QD. Here, we assume the QD energy levels have a staircase-like distribution as shown in Fig. 1(b) in which \(E_N = E_R\), and \(E_{\ell} = E_R + (N-\ell)\Delta E\), where \(\Delta E\) denotes the energy level separation. Such a variation in QD levels can be engineered by considering suitable size variation of QDs in the SLNW. The electron Coulomb interactions have been neglected in Eq. (2). The electron Coulomb interactions are weak under the resonant tunneling condition, since the electron wavefunction in SLNW becomes delocalized. The electron current from electrode to the QD SLNW can be derived by using the Meir-Wingreen formula.\(^{20}\)

We have

\[ J = \frac{se}{\hbar} \int \frac{d\epsilon}{2\pi} \mathcal{T}_{LR}(\epsilon)[f_L(\epsilon) - f_R(\epsilon)], \]
Fermi distribution function for the $\alpha$ constant, respectively.
tron charge, the Planck's constant, and the Boltzmann $\alpha$ coefficient of QD SLNW connected to electrodes.

is the one-particle retarded Green function of the leftmost (rightmost) QD with energy level $E_L$ ($E_R$).

where $f_{\alpha}(\epsilon) = 1/[\exp((\epsilon - \mu_{\alpha})/k_BT_{\alpha}) + 1]$ denotes the Fermi distribution function for the $\alpha$-th electrode, where $\mu_{\alpha}$ and $T_{\alpha}$ are the chemical potential and the temperature of the $\alpha$ electrode, $e$, $h$, and $k_B$ denote the electron charge, the Planck's constant, and the Boltzmann constant, respectively. $\mathcal{T}_{L,R}(\epsilon)$ denotes the transmission coefficient of QD SLNW connected to electrodes.

The transmission function has the following form

$$\mathcal{T}_{L,R}(\epsilon) = \frac{4\Gamma_L(\epsilon)\Gamma_{R}^{fj}(\epsilon)}{\Gamma_L(\epsilon) + \Gamma_{R}^{fj}(\epsilon)} (-Im(G_L^{f}(\epsilon))),$$

(4)

where the tunneling rate $\Gamma_L(\epsilon) = \sum_{k} |V_{k,L}(\epsilon)|^2 \delta(\epsilon - \epsilon_k)$. In the wide band limit of electrodes, the energy-dependent $\Gamma_L(\epsilon)$ can be neglected. The notation $Im$ means taking the imaginary part of the function that follows, and

$$G_L^{f}(\epsilon) = 1/(\epsilon - E_1 + i\Gamma_L - \Sigma_{1,N})$$

(5)

is the one-particle retarded Green function of the leftmost QD with the energy level of $E_1$. The self energy $\Sigma_{1,N}(\epsilon)$ results from electron tunneling from the leftmost QD to the right electrode mediated by $N-1$ QDs, which is given by

$$\Sigma_{1,N} = \frac{t_{1,2}}{\epsilon - E_2 - \sum_{n=1}^{N} \frac{t_{n+1,n}^2}{\epsilon - E_{n+1} - \sum_{n=1}^{N-1} \frac{t_{n+1,n}^2}{\epsilon - E_{n+1} - \sum_{n=1}^{N-2} \frac{t_{n+1,n}^2}{\epsilon - E_{n+1} - \sum_{n=1}^{N-3} \frac{t_{n+1,n}^2}{\epsilon - E_{n+1}}}}}}$$

(6)

where $N$ denotes the total number of QDs. The rightmost QD is the $N$th QD. The effective tunneling rate $\Gamma_{L,R}^{fj}(\epsilon) = - Im(\Sigma_{1,N}(\epsilon))$. For simplicity, we assume $t_{\ell,j} = t_c$ for all $\ell$ and $j$ being the nearest neighbor of $\ell$, and $\Gamma_L = \Gamma_R = \Gamma$.

The heat current for electrons leaving from the left (right) electrode is given by

$$Q_{e,L(R)} = \frac{s}{h} \int \frac{d\epsilon}{2\pi} \mathcal{T}_{L,R}(\epsilon)(\epsilon - \mu_{L(R)})(f_L(\epsilon) - f_R(\epsilon)).$$

(7)

We note that $Q_{e,L} + Q_{e,R} = -(\mu_L - \mu_R)J/e$, which describes the Joule heating.

To the phonon heat current ($Q_{ph}$), which coexists with the electron heat current, we adopted an empirical formula $Q_{ph} = F_s Q_{La}$. $Q_{La}$ is the lattice heat current of silicon nanowire given in Ref.\[22]. $F_s = 0.1$ is a reduction factor for phonon transport due to scatterings from QDs embedded in a nanowire.\[23]. Due to the low electron density considered here and weak electron phonon interactions (EPI) in Si/Ge, the electron mean free path $(\lambda)$ of Si/Ge QD SLNWs is longer than 170 nm at room temperature. The length of QD SLNW considered here is around 127 nm, which is smaller than $\lambda$ reported in Ref.\[24]. Therefore, the neglect of EPIs is justified.

To design a heat engine driven by a high temperature-bias $\Delta T = T_L - T_R$, the Seebeck voltage $(V_{th} = \mu_L - \mu_R)$ across the external load with conductance $G_{ext} = 1/R_{ext}$ needs to be calculated. Meanwhile, the energy levels $E_{\ell}$ for all $\ell$ should be readjusted according to $V_{th}$. As a consequence, $\mathcal{T}_{L,R}(\epsilon)$ will depend on $V_{th}$. The electron heat current satisfies the condition $Q_{L} + Q_{R} = -J V_{th} = P_{gen}$, which denotes the work done by the heat engine per unit time. The efficiency of heat engine is defined as the power output divided by the power input. The power input is the heat current out of the hot side and the power output is the electrical power generated $P_{gen}$. Thus, the direction-dependent efficiency of heat engine is given by ($\beta$ = forward, reverse)

$$\eta_\beta = -J V_{th}/Q_{e,\beta}.$$  

(8)

We consider an $N = 25$ SLNW with a staircase alignment of energy levels. Namely, we have $E_L = E_1 = E_R + 24\Delta E$, $E_2 = E_R + 23\Delta E$, and $E_N = E_R$. With an induced Seebeck voltage, $V_{th}$, the energy levels $E_{\ell}$ are modified according to $\epsilon_{\ell} = E_{\ell} + \eta e V_{th}$. In a simple approximation where the electric field is uniformly distributed in spacer layers in the SLNW, the level modulation factor is expressed as $\eta = -(L_s - L/2)/L$ with $\mu_{L,R}(\epsilon) = E_F \pm eV_{th}/2$. The pair length (that of one QD plus one spacer layer) adopted is $L_s = 5$ nm and the length of SLNW is $L = 127$ nm. The Seebeck voltage can be evaluated by Eq. (3) under the condition $G_{ext} V_{th} + J(V_{th}, \Delta T) = 0$. Once $V_{th}$ is obtained, the electron current $J$ and electron heat current $Q_{e,L(R)}$ can be evaluated by Eq.(3) and Eq. (7), respectively. The resulting output power, $P_{gen}$ and $V_{th}$ as functions of temperature bias for various values of $\Delta E$ at $t_c = R_L = R_R = 1\Omega$, $G_{ext} = 0.04G_0$ and $E_R = E_F + 4\Gamma_0$.
are plotted in Fig. 2. \( G_0 = e^2/h \) denotes the quantum conductance and \( E_F \) is the Fermi energy of electrodes. All energy scales are in units of \( G_0 \) throughout this article. The value of \( G_0 \) depends on the desired temperature range considered in the design. In typical designs considered, \( G_0 = 1 \text{meV} \).

Figure 2(a) shows the asymmetrical behavior of output power, \( P_{gen} \). It is found that \( P_{gen} \) under reverse temperature bias (\( \Delta T < 0 \)) is always smaller than that under forward bias (\( \Delta T > 0 \)). The asymmetry ratio, \( R_{asy} = \frac{P_{gen}(\Delta T)}{P_{gen}(-\Delta T)} \) is found to be 1, 1.43, and 2.81 for \( \Delta E = 0 \), 0.05 \( G_0 \), and 0.1 \( G_0 \), respectively. To understand the asymmetrical behavior of \( P_{gen} \), it is important to examine the relation between \( V_{th} \) and \( \Delta T \). (See inset in Fig. 2(a))

The Seebeck coefficient, \( \sigma_{ch} \), is proportional to \( \Delta T \), which counter balances the electron flow from the hot side to the cold side, but also influences the alignment of energy levels. With forward temperature bias, the QD levels are tilted toward alignment, allowing resonant tunneling of electrons from the left electrode to the right electrode, while under reverse bias the QD levels are further misaligned, leading to an off-resonance condition. (See insets in Fig. 2(a)) In the limit of \( \Delta T \to 0 \), we have \( G_{ext} V_{th} + e^2 \mathcal{L}_0 V_{th} + L_n \Delta \frac{T}{eT} = 0 \), where \( \mathcal{L}_n = \frac{k_B T}{e} \int d\epsilon \mathcal{L}_{LR}(\epsilon) (\epsilon - \epsilon_F)^\alpha \). Note that transmission coefficient \( \mathcal{T}_{LR}(\epsilon) \) is independent of \( V_{th} \). The Seebeck voltage is then given by \( V_{th} = \frac{e(k_B T)}{(e^2 \mathcal{L}_0 + e^2 \mathcal{L}_n + e^2 \mathcal{L}_n)} \), which explains that \( V_{th} \) and \( \Delta T \) always have opposite signs, if \( E_R > E_F \) and \( P_{gen} \) is proportional to \( \Delta T^2 \). In the nonlinear response region, \( \mathcal{T}_{LR}(\epsilon) \) involves \( V_{th} \), the relation between \( V_{th} \) and \( \Delta T \) can be rather complicated.

To further investigate the thermoelectric properties of SLNW HEs, we show the electron heat current \( Q_L \) and efficiency \( \eta \) as functions of forward temperature bias in Fig. 3(a) and 3(b), respectively. Like \( P_{gen} \), the electron heat current \( Q_L \) at \( \Delta E = 0 \) is smaller than that at \( \Delta E = 0.1 \) \( G_0 \). In particular, the maximum efficiency of HEs (\( \eta_{max} \)) at \( \Delta E = 0.1 \) \( G_0 \) is better than the case of \( \Delta E = 0 \). From the results of Fig. 2(a) and Fig. 3(b), we have demonstrated that the \( P_{gen} \) and \( \eta \) of SLNW HEs with staircase-like energy levels have better performance. Fig. 3(c) shows the dependence of \( \eta \) on the external load resistance, \( R_{ext} \). The dotted curve includes the phonon heat current \( Q_{ph} \) [17], where a silicon nanowire with diameter \( D = 3 \) \( \text{nm} \) and surface roughness width \( \delta = 3 \) \( \text{nm} \) is considered. The suppression of \( \eta = \frac{P_{gen}}{Q_{ph} + Q_{ph}} \) due to finite \( Q_{ph} \) is expected. The maximum \( \eta \) occurs at \( R_{ext} \approx 20 \) \( R_0 \), where \( R_0 = \frac{1}{G_0} \). Note that when \( R_{ext} \to 0 \), we have \( V_{th} \to 0 \), which leads to vanishingly small \( P_{gen} \). On the other hand, as \( R_{ext} \to \infty \) we have \( J \to 0 \) and \( P_{gen} \to 0 \). Fig. 3(d) shows \( \eta \) as a function of \( E_R \) at \( \Delta E = 0.1 \) \( G_0 \). The maximum \( \eta \) occurs near \( E_R = E_F + 0.1 \) \( G_0 \). In this case, all QD energy levels are above \( E_F \), and the electron transport is mainly due to thermionic process.

Heat diodes (HDs) play an important role in applications of energy harvesting [23-31]. Those designs considered three kinds of heat carriers: phonons [23-27], photons [28], and electrons [11-16]. To investigate the behavior of SLNW HDs, we consider the open-circuit condition (\( J = 0 \)) with \( Q_{e.L} = -Q_{e,R} = Q_e \). The rectification ratio of HDs is defined as \( \eta_R = \frac{Q_{e,F}}{Q_{e,R}} \), where \( Q_{e,F} \) and \( Q_{e,B} \) are the heat currents in the forward and reverse temperature bias, respectively. Fig. 4(a) shows the calculated electron heat current as a function of temperature bias, and the behavior of the direction-dependent

\[ \begin{align*}
\eta_R & = \frac{Q_{e,F}}{Q_{e,R}} \\
\Delta T & = T_F - T_L
\end{align*} \]
electron heat current (heat rectification) is apparent. Under forward bias, a negative differential thermal conductance (NDTC) is observed. To analyze the behavior of NDTC, we examine the Seebeck voltage ($V_{th}$) as a function of $\Delta T$ in Fig. 4(b). For simplicity, let’s consider $t_c = 2 \Gamma_0$, which corresponds to a narrow bandwidth case. For this case, the QD energy levels are aligned (the resonant-tunneling condition) when $\Delta T = 2.5 \Gamma_0$, which corresponds to $eV_{th} = -10 \Gamma_0$ for $\Delta E = 0.4 \Gamma_0$. When $K_B \Delta T$ deviates from $2.5 \Gamma_0$, the system is driven away from the resonant condition. This explains why the electron heat current has a peak near $K_B \Delta T = 2.5 \Gamma_0$, which leads to NDTC as $K_B \Delta T$ exceeds $2.5 \Gamma_0$. In Fig. 4(c), we show the electron heat rectification ratio ($\eta_R$) as a function of $\Delta T$. Although the maximum $\eta_R$ reaches a very high value near 60 at $t_c = 2 \Gamma_0$, the heat current is very small. Good thermal diodes also require large heat current. Thus, the cases with $t_c = 3 \Gamma_0$ (red) and $4 \Gamma_0$ (blue) are better designs than the $t_c = 2 \Gamma_0$ case, since the heat current is significantly higher even though the maximum $\eta_R$ is somewhat lower. The differential thermal conductances (DTC) corresponding to the curves shown in Fig. 4(a) are given in Fig. 4(d) in which very robust NDTC behavior is observed. The feature of NDTC plays a remarkable role in the design of thermal transistors.\cite{29, 31} So far, little literature has reported NDTC resulting from electron carriers.

For further optimization we calculate $Q_e$ and $\eta_R$ as functions of $\Delta T$ for various values of $E_R$ at $t_c = \Gamma_L = \Gamma_R$, $K_B T = 3 \Gamma_0$ and $E_R = E_F + 6 \Gamma_0$. The results are shown in Fig. 5. At a given value of positive $\Delta T$, $Q_{e,F}$ is suppressed with increasing $E_R$ due to the reduction of electron population at high energy levels in the thermionic process. In the thermal-assisted transport process, $V_{th}$ increases significantly with increasing $E_R$ (not shown). In the cases of $E_R = E_F + 4 \Gamma_0$ and $E_R = E_F + 6 \Gamma_0$, the magnitude of $V_{th}$ is not enough to create the resonant-tunneling condition for electron transport under forward bias. Therefore, no NDTC is observed in these two cases. In Fig. 5(b), it is seen that $\eta_R$ for $E_R = E_F + 4 \Gamma_0$ reaches a very impressive value of 100. However, the maximum $\eta_R$ for this case is reduced to near 10 when $Q_{ph}$ is included (dotted curve). It is expected that the effect of phonon heat current can be reduced in the future with the advances in nanotechnology.\cite{29}

In conclusion, we have theoretically investigated the direction-dependent electrical power output and electron heat rectification of a QD SLNW. The alignment of energy levels of QDs in the nanowire can be altered by the temperature-bias induced Seebeck voltage which leads to resonant tunneling for electrons in forward bias but off-resonance in reverse bias for properly designed distribution of QD energy levels in SLNW. This provides a physical mechanism for achieving direction-dependent $P_{gen}$ and $Q_e$. We found that the maximum efficiency and optimized $P_{gen}$ of SLNW with staircase-like QD energy levels are better than those of SLNW with uniform QD energy levels. In addition, we have demonstrated that such SLNWs have unique behavior not only in electron heat rectification but also in NDTC, which is a key ingredient for the implementation of thermal logical gates and transistors.

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FIG. 4: (a) Electron heat current $Q_e$, (b) Seebeck voltage $V_{th}$, (c) heat rectification ratio $\eta_R$ and (d) differential thermal conductance (DTC) as functions of temperature bias for different electron hopping strengths. $G_{ext} = 0, t_c = \Gamma_L = \Gamma_R, K_B T = 3 \Gamma_0$ and $E_R = E_F + 6 \Gamma_0$.

FIG. 5: (a) Electron heat current $Q_e$, and (b) heat rectification ratio as function of temperature bias for different $E_R$ values at $t_c = \Gamma_L = \Gamma_R = 4 \Gamma_0$, $K_B T = 3 \Gamma_0$, and $\Delta E = 0.4 \Gamma_0$.

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