Thermoelectric effects of quantum dot arrays embedded in nanowires

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The thermoelectric properties of quantum dot arrays (QDAs) embedded in nanowires connected to electrodes are studied theoretically in the Coulomb blockade regime. An extended Hubbard model and Anderson model is used to simulate the electronic contribution to thermoelectric properties of a QDA junction system. The electrical conductance, Seebeck coefficient, and electron thermal conductance are calculated in the Keldysh Green function technique. The phonon thermal conductivities are calculated by using the equation of phonon radiative transfer method. In the Coulomb blockade regime the electron thermal conductance is much smaller than the phonon thermal conductance. Therefore, the optimal figure of merit (ZT) can be enhanced by increasing thermal power and decreasing phonon thermal conductance simultaneously. We found that it is possible to obtain ZT value of InGaAs/GaAs QDAs embedded in nanowires larger than one at room temperature.

I. INTRODUCTION

To design solid-state coolers and power generators,[1-7] many efforts seek efficient thermoelectric materials with the figure of merit (ZT) larger than 3. The optimization of $ZT = S^2G_eT/\kappa$ depends on the electrical conductance ($G_e$), Seebeck coefficient (S), and thermal conductance ($\kappa$). $T$ is the equilibrium temperature. These physical quantities are usually related to one another. Mechanisms leading to the enhancement of power factor ($PF = S^2G_e$) would also enhance the thermal conductance. Consequently, it is difficult to obtain ZT above one in conventional bulk materials.[1]

Recently, the ZT values of quantum dot superlattice nanowires with impressive values (larger than one) have been experimentally demonstrated.[8] The power factor and thermal conductance become independent thermoelectric variables under the condition $\kappa_c/\kappa_{La} \ll 1$, where $\kappa_c$ and $\kappa_{La}$ denote, respectively, the electron thermal conductance and lattice thermal conductance.[8] In the Coulomb blockade regime, electron transport process is seriously suppressed by the electron Coulomb interactions, therefore $\kappa_c$ as well as $G_e$ are reduced seriously.[9] Under the condition $\kappa_c/\kappa_{La} \ll 1$, one can increase the power factor and decrease the phonon thermal conductance simultaneously to optimize ZT.[9]

Thermoelectric properties of quantum dots (QDs) embedded in a matrix connected to metallic electrodes were studied by several groups in the absence of phonon thermal conductivity.[10-16] For the applications of solid state coolers and power generators at room temperature, one needs to consider a large number of serially coupled QDs, otherwise it is not easy to maintain a large temperature difference across the QD junction, which was pointed out to be crucial in the implementation of high-efficiency thermoelectric devices.[1,2] In addition, the phonon thermal conductivity plays a significant role in the optimization of ZT at high temperatures. In this paper, we carry out theoretical analysis of ZT of QD arrays embedded in nanowires, including the phonon conductance, which is calculated by using the phonon radiative transfer method as introduced in Ref. [17]. Although the method does not take into account the microscopic mechanisms associated with quantum confinement of acoustic phonons, it gives reasonable agreement with the lattice-dynamics model and experiments for nanowires by merely considering the boundary scattering effect of phonons.

II. FORMALISM

A QDA embedded in a nanowire connected to the metallic electrodes can be described by the extended Hubbard model and Anderson model. Here we consider nanoscale semiconductor QDs, in which the energy level separations are much larger than their on-site Coulomb interactions and thermal energies. Thus, only one energy level for each quantum dot needs to be considered. The Hamiltonian of the system is given by $H = H_0 + H_{QD}$:

$$H_0 = \sum_{k,\sigma} \epsilon_k a_{k,\sigma}^\dagger a_{k,\sigma} + \sum_{k,\sigma} \epsilon_k b_{k,\sigma}^\dagger b_{k,\sigma} + \sum_{k,\sigma} V_{k,L} d_{L,\sigma}^\dagger a_{k,\sigma} + \sum_{k,\sigma} V_{k,R} d_{R,\sigma}^\dagger b_{k,\sigma} + c.c$$

where the first two terms describe the free electron gas of left and right electrodes. $a_{k,\sigma}^\dagger$ (b$_{k,\sigma}^\dagger$) creates an electron of momentum $k$ and spin $\sigma$ with energy $\epsilon_k$ in the left (right) electrode. $V_{k,\ell}$ ($\ell = L, R$) describes the coupling between the electrodes and the left (right) QD. $d_{\ell,\sigma}^\dagger$ ($d_{\ell,\sigma}$) creates (destroys) an electron in the $\ell$-th dot.
\[ H_{QD} = \sum_{\ell,\sigma} E_{\ell} n_{\ell,\sigma} + \sum_{\ell} U_{\ell} n_{\ell,\sigma} n_{\ell,\sigma} \]
\[
+ \frac{1}{2} \sum_{\ell,\sigma,\sigma'} U_{\ell,\sigma} n_{\ell,\sigma} n_{\ell,\sigma'} + \sum_{\ell,j} t_{\ell,j} d_{\ell,\sigma} d_{j,\sigma'},
\]
where \( E_{\ell} \) is the spin-independent QD energy level, and \( n_{\ell,\sigma} = d_{\ell,\sigma}^\dagger d_{\ell,\sigma} \). Notations \( U_{\ell} \) and \( U_{\ell,j} \) describe the intradot and interdot Coulomb interactions, respectively. \( t_{\ell,j} \) describes the electron interdot hopping. Noting that the interdot Coulomb interactions as well as intradot Coulomb interactions play a significant role on the charge transport for semiconductor QD array.

Using the Keldysh-Green’s function technique \[18\], the charge and heat currents of electrons leaving electrodes are expressed as

\[ J = \frac{2e}{h} \int d\mathcal{T}(\epsilon) [f_L(\epsilon) - f_R(\epsilon)], \]
\[ Q_{L(R)} = \pm \frac{2e}{h} \int d\mathcal{T}(\epsilon) (\epsilon - \mu_{L(R)}) [f_L(\epsilon) - f_R(\epsilon)], \]

where \( \mathcal{T}(\epsilon) \) is the transmission coefficient. \( f_L(\epsilon) = \frac{1}{e^{(\epsilon - \mu_L) / k_B T_L} + 1} \) denotes the Fermi distribution function for the left (right) electrode. \( \mu_L \) and \( \mu_R \) denote the chemical potentials of the left and right leads, respectively, with their average denoted by \( \mu_E = (\mu_L + \mu_R)/2 \). \( \mu_L - \mu_R = e\Delta V \) is the voltage across the QDA junction. \( T_{L(R)} \) denotes the equilibrium temperature of the left (right) electrode. \( e \) and \( h \) denote the electron charge and Planck’s constant, respectively. \( Q_{L(R)} \) denotes the heat current leaving from the left (right) electrode.

In the linear response regime, Eqs. (3) and (4) can be rewritten as

\[ J = \mathcal{L}_{11} \frac{\Delta V}{T} + \mathcal{L}_{12} \frac{\Delta T}{T^2}, \]
\[ Q = \mathcal{L}_{21} \frac{\Delta V}{T} + \mathcal{L}_{22} \frac{\Delta T}{T^2}, \]

where there are two sources of driving force to yield the charge and heat currents. \( \Delta T = T_L - T_R \) is the temperature difference across the junction. The thermoelectric coefficients in equations (5) and (6) (\( \mathcal{L}_{11}, \mathcal{L}_{12}, \mathcal{L}_{21}, \) and \( \mathcal{L}_{22} \)) are evaluated by

\[ \mathcal{L}_{11} = \frac{2e^2 T}{h} \int d\mathcal{T}(\epsilon) (\frac{\partial f(\epsilon)}{\partial E_F})_T, \]
\[ \mathcal{L}_{12} = \frac{2eT^2}{h} \int d\mathcal{T}(\epsilon) (\frac{\partial f(\epsilon)}{\partial T})_{E_F}, \]
\[ \mathcal{L}_{21} = \frac{2eT}{h} \int d\mathcal{T}(\epsilon) (\epsilon - E_F) (\frac{\partial f(\epsilon)}{\partial E_F})_T, \]

and

\[ \mathcal{L}_{22} = \frac{2T^2}{\hbar} \int d\mathcal{T}(\epsilon) (\epsilon - E_F) (\frac{\partial f(\epsilon)}{\partial T})_{E_F}. \]

Here \( \mathcal{T}(\epsilon) \) and \( f(\epsilon) = 1/[e^{(\epsilon - E_F)/k_B T} + 1] \) are evaluated under the equilibrium condition. The detailed expression of \( \mathcal{T}(\epsilon) \) can be found in ref. [19].

If the system is in an open circuit, the electrochemical potential will be established in response to a temperature gradient; this electrochemical potential is known as the Seebeck voltage (Seebeck effect). The Seebeck coefficient (amount of voltage generated per unit temperature gradient) is defined as \( S = \Delta V/\Delta T = -\mathcal{L}_{12}/(T\mathcal{L}_{11}) \). To judge whether the system is able to generate or extract heat efficiently, we need to consider the figure of merit [1]

\[ ZT = \frac{S^2 G_{\epsilon} T}{\kappa_{\epsilon} + \kappa_{La}} = \frac{(ZT)_0}{1 + \kappa_{La}/\kappa_{\epsilon}}, \]

Here, \( G_{\epsilon} = \mathcal{L}_{11}/T \) is the electrical conductance and \( \kappa_{\epsilon} = ((\mathcal{L}_{22}/T^2) - \mathcal{L}_{11}S^2) \) is the electron thermal conductance. \( (ZT)_0 \) represents the ZT value in the absence of phonon thermal conductance, \( \kappa_{La} \). In the Hamiltonian \( H \), the term (\( H_{\epsilon,ph} \)) describing the interactions between electrons and phonons is ignored. For simplicity, we adopt \( \kappa_{La} = \kappa_{wire} F_s \) to describe the phonon thermal conductance of QD array (QDA) embedded a nanowire. The dimensionless scattering factor \( F_s \) is used to include the phonon scattering effect arising from surface boundary of QDs.\[1\] It is possible to reduce phonon thermal conductance by one order of magnitude when a quantum wire filled with QDA as phonon scatterers.\[20\] Therefore, the maximum \( F_s \) is assumed to be 0.1 in this study. For example, Ref. \[20\] pointed out that the phonon thermal conductance reduction of QDA nanowires in a high temperature regime arises from the filtering of high frequency phonons.\[2\] However, the method considered in Ref. \[20\] requires a heavily numerical calculation of \( \kappa_{La} \) in the optimization of ZT.

Based on Holland’s model \[21,22\] in which the longitudinal and transverse acoustical phonon branches are treated separately, we calculate \( \kappa_{wire} \) of a rectangular nanowire with cross sectional area \( A \) and length \( L_x \). The thermal conductance \( \kappa_{wire} \) is related to the phonon thermal conductivity by \( \kappa_{wire} = K_{ph}/L_x \), where \( K_{ph} = K_{T_0} + K_{T_u} + K_L \) denotes the thermal conductivity with

\[ K_{T_0} = \frac{2}{3} T^3 \int_{0}^{\theta_1/T} \frac{C_{Tu} x^4 e^x (e^x - 1)^{-2} dx}{\tau_b^{-1} + \tau_f^{-1} + \beta x T^3}, \]
\[ K_{T_u} = \frac{2}{3} T^3 \int_{\theta_1/T}^{\theta_2/T} \frac{C_{Tu} x^4 e^x (e^x - 1)^{-2} dx}{\tau_b^{-1} + \tau_f^{-1} + \beta T_x T^2/\sinh(x)}, \]

and

\[ K_L = \frac{1}{3} T^3 \int_{0}^{\theta_3/T} \frac{C_L x^4 e^x (e^x - 1)^{-2} dx}{\tau_b^{-1} + \tau_f^{-1} + \beta x T^3}. \]
The phonon thermal conductivities $K_{T_0}$, $K_{Tu}$ and $K_L$ result from the low-frequency transverse branch, high-frequency transverse branch and longitudinal acoustical phonon branch, respectively. In equations (12)-(14), we have $C_j = T_0, Tu, L = (k_B/2\pi^2 v_j)(k_B/h)^3$, where $v_j$ is the phonon group velocity for the $j^{th}$-branch. $\tau_b^{-1}$ is the phonon boundary scattering rate, and $\tau_i^{-1} = \alpha x^4 T^4$ is the phonon-impurity scattering rate. $\beta_T x T^5$, $\beta_{Tu} x^2 T^3$/$\sin(x)$, and $\beta_L x^2 T^3$ arise from three-phonon scattering rates. $\alpha$ and $\beta$ are the fitting parameters from experimental data. $\theta_i(h\omega_i/k_B)(i = 1, 2, 3)$ denotes the Debye temperature. The frequencies of $\omega_i$ for $T_0$, $Tu$ and $L$ modes can be found in Ref. [17]. The $\alpha$, $\beta$, $v_j$ and $\theta_i$ for Si and GaAs can be adopted from Ref. 17 and Ref. 22, respectively. Eqs. (12)-(14) can well describe the phonon thermal conductivity of semiconductor materials when $\tau_b = v_b/L$. The notation $v_b = [(2v_T^{-1} + v_L^{-1})/3]^{-1}$ is the average phonon group velocity, where $v_T$ and $v_L$ are corresponding to the group velocity of the transverse and longitudinal branches. $L$ denotes the sample size. Chen and Tien [21] extended the Holland model to illustrate the phonon thermal conductivity of quantum wells by considering geometry effect on $\tau_b$. Based on the formalism of ref.[21], the phonon-boundary scattering rate ($\tau_b^{-1}$) of quantum wire is derived and determined by

$$\tau_b^{-1} = (1/G - 1) \cdot \tau_i^{-1},$$

where $\tau_i = (A \omega^4 + (B_1 + B_2) T^3 \omega^2 + v_b/L_c)^{-1}$ is the total internal relaxation time of the bulk which includes normal process and umklapp process. $A = \alpha (h/k_B)^4$, and $B_j = \beta_j (h/k_B)^2$. $L_c$ denotes the sample length.

The factor of $G = G^{++} + G^{+-} + G^{-+} + G^{--}$ illustrates the boundary effects on the phonon thermal conductivity of nanowires. The expression of $G$ is given by

(i) $0 < \theta < \pi/2$ and $0 < \phi < \pi$

$$G^{++}/\Pi = \int d\Omega \frac{(e^{-\xi_s} - 1)(e^{-\xi_z} - 1)}{e^{-\xi_s} e^{-\xi_z} - 1},$$

(ii) $0 < \theta < \pi/2$ and $\pi < \phi < 2\pi$

$$G^{+-}/\Pi = \int d\Omega \frac{(e^{-\xi_s} - 1)(e^{-\xi_z} - 1)}{e^{-\xi_s} e^{-\xi_z} - 1},$$

(iii) $\pi/2 < \theta < \pi$ and $0 < \phi < \pi$

$$G^{-+}/\Pi = \int d\Omega \frac{(e^{-\xi_s} - 1)(e^{-\xi_z} - 1)}{e^{-\xi_s} e^{-\xi_z} - 1},$$

(iv) $\pi/2 < \theta < \pi$ and $\pi < \phi < 2\pi$

$$G^{--}/\Pi = \int d\Omega \frac{(e^{-\xi_s} - 1)(e^{-\xi_z} - 1)}{e^{-\xi_s} e^{-\xi_z} - 1}.$$

We have the notations $\Pi = \frac{3}{2\pi L_c L_z}$ and $d\Omega = dy dz d\theta d\phi \sin^3(\theta) \cos^2(\phi)$ in equations (16)-(19), where $L_y(z)$ is the lateral size of rectangular wire in the $y(z)$ direction.

III. RESULTS AND DISCUSSION

Before investigating the thermoelectric properties of QDAs with large number of coupled dots, we first consider the simplest structure of QDA, which consists of serially coupled triple QDs (SCTQD). The full solution for SCTQD in the Coulomb blockade regime has been reported.[28] The electrical conductance ($G_e$), Seebeck coefficient ($S$) and electrical thermal conductance ($\kappa_e$) of SCTQD calculated by using the full solution of Ref. [28] has been carried out and will be reported.
elsewhere.\textsuperscript{29} Due to many-body effects, the full solution to charge transport through QDAs with more than three dots is very complicated. Many efforts attempted to solve such a difficult problem with some approximation scheme.\textsuperscript{[9,29,30]} The results based on the procedure of Ref. \textsuperscript{[9]} can achieve good agreement with those calculated by full solution of Ref. \textsuperscript{[29]} in the high temperature regime. Because we have a closed-form solution for the thermoelectric coefficients of Eqs. (7)-(10), the procedure of Ref. \textsuperscript{9} is very efficient in the optimization of ZT at high temperatures. Therefore, we illustrate the thermoelectric properties of QDAs by considering the procedure of Ref. \textsuperscript{9} instead of using the full solution of Ref. \textsuperscript{[28]}, which requires much heavier numerical calculation.

Because the optimization of power factor (PF) prefers identical QDs, size-independent electron hopping strength, and symmetrical tunneling rates,\textsuperscript{9} in Fig. 2 we plot \(G_c, S, \kappa_c\) and PF of SCTQD as functions of gate voltage \((eV_g)\) for two different temperatures by considering the homogenous electron interdot hopping (with \(t_{ij} = t_e = 3t_0\)), tunneling rates (with \(\Gamma_L = \Gamma_R = 1t_0\)), and intradot Coulomb interaction (with \(U_l = U_0 = 30t_0\)). All energy scales are in units of \(\Gamma_0\), which is taken to be 1 meV. Here, the interdot Coulomb interactions are ignored for simplicity. The solid lines and dot-dashed lines are calculated according to the procedure of Ref. \textsuperscript{9} and the mean-field theory of Ref.\textsuperscript{[30,31]}, respectively. For simplicity, the procedure of Ref.\textsuperscript{[9]} neglecting interdot correlation functions is called the on-site Coulomb approximation (OCA), while the mean-field theory corresponds to the Hartree-Fock approximation (HFA) which was adopted in Refs. \textsuperscript{[30-32]}. Both OCA and HFA are efficient tools for studying the charge transport through molecular junctions. It is interesting to examine the difference between two approaches.

For all four physical quantities \((G_c, S, \kappa_c\) and PF) of SCTQD, the spectra consist two main groups of features, which are mirror image of each other with respect to the mid point \((eV_g = 45\Gamma_0)\). This is a consequence of the electron-hole symmetry possessed by the SCTQD structures. At low temperature \((k_B T = 0.1\Gamma_0)\), there is a gap between the two groups, which is related to on-site Coulomb interaction, \(U_0\). The first three peaks of \(G_c\) (shown by the solid line) correspond to three resonant channels at \(E_0 - \sqrt{2t_c}, E_0\), and \(E_0 + \sqrt{2t_c}\). For the higher-energy group, there are also three peaks arising from resonant channels at \(E_0 + U_0 - \sqrt{2t_c}, E_0 + U_0\) and \(E_c + U_0 + \sqrt{2t_c}\). We find that the behaviors of \(G_c, S\) and \(\kappa_c\) calculated by HFA (dot-dashed lines) are quite different from those calculated by OCA (solid lines). For example, the maximum \(G_c\) of dot-dashed lines is larger than \(e^2/h\) (quantum conductance), but not for OCA. This is due to the inability of HFA to include electron correlation. The energy positions of resonant channels within HFA depend on the average occupation number in each QD.\textsuperscript{[30-32]} which can be a fractional number. In contrast, within OCA the energy positions of resonant channels are determined by integral charges, while electron correlation functions and fractional occupation numbers only appear in the probability weights of quantum paths.\textsuperscript{[9]} In addition, we observe an unphysical enhancement of \(S\) at the mid point of Coulomb gap \((eV_g = 45\Gamma_0)\) for HFA results (dot-dashed line). This illustrates the drawback of HFA calculation for thermoelectric coefficients of QDs at low temperatures when the charging process plays a significant role. At high temperatures (for example, \(k_B T = 0.1\Gamma_0\)), the detailed resonant structures are washed out, and the unphysical enhancement of \(S\) in the middle of Coulomb gap also disappears. These two approaches give qualitatively similar results at high temperatures. However, the HFA approach tends to overestimate \(G_c, \kappa_c,\) and PF. If we include the interdot Coulomb interactions, the interdot correlation effects become crucial. The symmetrical behavior of thermoelectric coefficients will be lost. In general, we will obtain smaller PF for QD energy levels below \(E_F\) than that for QD energy levels above \(E_F\) at high temperatures.\textsuperscript{[9,29]}

For thermoelectric devices operated at room temperature, it is important to optimize their ZT values at high temperatures. To further clarify the differences between these two approaches, Fig. 3 shows the \(G_c, S, \kappa_c\) and PF as functions of the detuning energy \((\Delta = E_0 - E_F > 0)\) for various temperatures. The other physical parameters are the same as those of Fig. 2. From the results of \(S\) and PF, these two approaches agree well with each other when QD energy levels are far above \(E_F\). This is expected, because the electron Coulomb interactions become unimportant for large \(\Delta\) values. The maximum PF value decreases with increasing temperature. For \(k_B T = 1\Gamma_0, k_B T = 5\Gamma_0\) and \(k_B T = 13\Gamma_0\), the maximum PF occur, respectively, at near \(\Delta = 5\Gamma_0, \Delta = 15\Gamma_0,\) and \(\Delta = 35\Gamma_0\). When \(k_B T = 26\Gamma_0\), the maximum PF occurs at near \(\Delta = 50\Gamma_0\).

From results of Fig. 3, we see that HFA is a reasonably good approximation for analyzing the thermoelectric coefficients of QDAs with QD energy levels above \(E_F\). Thus, we can use HFA to investigate thermoelectric coefficients of QDA nanowire with large number of dots. Here, we use the HFA (instead of OCA) of Ref. \textsuperscript{30} to study QDA nanowire with \(N=10\) because of its simplicity. Fig. 4 shows \(G_c, S\) and \((ZT)_0\) as functions of temperature for various detuning energies \((\Delta)\). The other physical parameters are the same as those of Fig. 2. The behavior of \(G_c\) with respect to temperature can be roughly understood by considering \(G_c \approx 1/(k_B T \cosh^2(\Delta/2k_B T))\) for \(U_t = 0\) (see the curve with triangle marks). \(S\) is proportional to \(T\) when temperature approaches zero (not shown here), whereas \(S \approx \Delta/k_B T\) at high temperatures and \(\Delta/T \gg 1\) (see the curves with triangle marks). In the absence of \(\kappa_{\ell\alpha}\), a very large \((ZT)_0\) appears in the low temperature regime. The maximum \((ZT)_0\) is beyond three, which is a critical value for the realization of solid state coolers and power generators. \((ZT)_0\) larger than 3 is a direct consequence of the ratio of \(G_c/\kappa_c \gg 1\) (\(\kappa_c\) not shown here) and highly enhancement of \(S^2\) in the Coulomb blockade regime. Using smaller nanowires
in quantum conductance limit and vacuum surrounding to blockade phonon heat current was proposed to yield a vanish small phonon thermal conductivity.\cite{Minnich2009} However, such a design requires advanced nanotechnology. The results of Fig. 4(c) also imply that the on-site electron Coulomb interactions can be ignored only when $U_E/k_B T \gg 1$. ($ZT)_0$ is highly overestimated at high temperatures in the absence of $U_E$.

Fig. 5(a) shows $ZT$ in the presence of $\kappa_{La} = F_s \kappa_{ph}(A/L_z)$ for the case of a GaAs nanowire with $L_z = L_y = 5$ nm and $L_x = 250$ nm. $F_s$ is assumed to be 0.1 in the calculation. The curves of Fig. 5(a) have one-to-one correspondence to those of Fig. 4(c). The maximum $ZT$ is seriously reduced in the presence of $\kappa_{La}$. This reduction of $ZT$ results from $\kappa_{La}/\kappa_e \gg 1$ [see Eq. (11)], which implies that the optimization of $ZT$ can be achieved by reducing $\kappa_{ph}$ and increasing power factor $PF = S^2 G_e$ simultaneously. The maximum $ZT$ depends on the detuning energy, $\Delta$. This behavior can be understood by the results of Fig. 3(d). The $ZT$ value is almost independent on temperature for $\Delta = 40\Gamma_0$, when $k_B T \geq 20\Gamma_0$. This is because the ratio of $G_e/(T\kappa_{La})$ is nearly constant. In the high temperature regime we have $K_{ph} \approx 1/T$ and $G_e$ decays very slowly with increasing temperature.

Fig. 5(b) shows $(ZT)$ as a function of temperature for various electron hopping strengths at $\Delta = 40\Gamma_0$. $(ZT)$ is enhanced with increasing $t_c$. Under the condition $\kappa_{La}/\kappa_e \gg 1$, the behavior of $ZT$ with respect to $t_c$ can be analyzed by the power factor $PF = S^2 G_e$. When the QD energy is far above $E_F$ ($\Delta = 40\Gamma_0$), the behavior of $S = \Delta/k_B T$ is independent of $t_c$ in the Coulomb blockade regime once $k_B T \geq 10\Gamma_0$. Therefore, the enhancement of $ZT$ is completely determined by the increase of $G_e$ with respect to $t_c$. When $t_c$ is smaller than tunneling rate ($\Gamma_0 = \Gamma_{ph} = \Gamma$), $G_e$ increases quickly with increasing $t_c$, and it becomes insensitive to $t_c$ when $t_c \geq 2\Gamma_0$. This demonstrates that the optimization of $ZT$ can be realized by the enhancement of $PF$ for a given $\kappa_{La}$.

In Fig. 5, we consider square nanowires with a small cross section with $L_y = L_z = 5$ nm. To understand the dependence on QDA cross-sectional area, we show in Fig. 6 $ZT$ as a function of temperature for various values of $L_z$ with $L_y = 5$ nm. We adopt $\Gamma_L = \Gamma_R = \Gamma = 3\Gamma_0$, $t_c = 3.5\Gamma_0$, $U_E = 30\Gamma_0$ and $\Delta = 40\Gamma_0$. In our model, we keep a large separation between QDAs along the $z$ direction ($D_s = 25$ nm), this allow us to avoid the electron hopping effects and electron Coulomb interactions between QDAs along that direction. Fig. 6 shows the maximum $ZT$ of QDA with $L_z = 7L_y$ can be larger than one. This is due to the enhancement of $G_e$ with increased tunneling rates ($\Gamma = 3\Gamma_0$). The $ZT$ value reduces significantly for the cases with large $L_z \geq 13L_y$. This $ZT$ reduction comes from the increased value of $\kappa_{La}$ [see Fig. 1(b)]. If we reduce the separation, $D_s$ between QDAs to increase the density of QDAs, the proximity effect arising from electron Coulomb interactions between QDAs should be included.\cite{Minnich2009} In general, the proximity effect from electron Coulomb interactions will suppress the $G_e$ values.

IV. SUMMARY AND CONCLUSIONS

We have theoretically investigated the thermoelectric properties of QDAs embedded in nanowires connected to metallic electrodes in the Coulomb blockade regime. Both OCA and HFA calculations were examined. It was shown that while HFA gives unphysical results for the Seebeck coefficient at low temperature when the QDs are nearly half filled, it gives reasonable results at high temperatures and when the QD energy level is far above the Fermi level (low filling condition). Under the condition $\kappa_{La} \gg \kappa_e$, the optimization of $ZT$ can be achieved by reducing $K_{ph}$ and increasing the power factor $PF = S^2 G_e$, simultaneously. We found that for various design parameters, $ZT > 1$ can be achieved. In our simulation, we assumed that the presence of QDs reduces the phonon conductivity in nanowires by a factor $F_s = 0.1$. It is conceivable that a smart nanostructure design which reduces the value of $F_s$ further can increase the maximum $ZT$ even more. The maximum $ZT$ value of a QDA nanowire with small cross section is found insensitive to temperature variation [see Figs. 5(b) and 6]. Such a feature is quite different from that of conventional thermoelectric materials.\cite{Zebarjadi2012,Mahan1997} The ability of QDAs to maintain $ZT$ near its maximum value for a wide range of temperatures is an important feature in the realization of useful thermoelectric devices.\cite{Zebarjadi2012}

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FIG. 1: (a) Phonon thermal conductivity of a silicon nanowire as a function of temperature for the different cross sections. The square cross section is defined as $A = L_y \times L_z$, where $L_y$ and $L_z$ are lateral sizes, and (b) phonon thermal conductivity of a GaAs nanowire with rectangular cross section $A = L_y \times L_z$ as a function of temperature for different $L_z$ values at fixed $L_y = 5 \text{ nm}$.

FIG. 2: (a) Electrical conductance ($G_e$), (b) Seebeck coefficient ($S$), (c) electron thermal conductance ($\kappa_e$), and (d) power factor $PF = S^2G_e$ of triple QDs junction systems as a function of gate voltage for two different temperatures. Solid line and dot-dashed line are calculated by OCA and HFA, respectively.
FIG. 3: (a) Electrical conductance ($G_e$), (b) Seebeck coefficient ($S$), (c) electron thermal conductance ($\kappa_e$), and (d) power factor $PF = S^2 G_e$ of triple QDs junction systems as a function of detuning energy $\Delta = E_0 - E_F$ for different temperatures. The other physical parameters are the same as those of Fig. 2.

FIG. 4: (a) Electrical conductance, (b) Seebeck coefficient and (c) $(ZT)_0$ of a QDA system with dot number $N=10$ in the absence of $\kappa_{ph}$ as a function of temperature for different detuned energies. Other physical parameters are the same as those of Fig. 2.
FIG. 5: Figure of merit of a QDA system with dot number $N=10$ in the presence of $\kappa_{ph}$ as a function of temperature. The curves of diagram (a) correspond to those of Fig. 4. Diagram (b) shows $ZT$ for various electron hopping strengths.

FIG. 6: $(ZT)$ as a function of temperature for different $L_z$ values. The physical parameters are $t_c = 3.5\Gamma_0$ and $\Gamma_L = \Gamma_R = 3\Gamma_0$. Solid line ($L_z = 7L_y$), dashed line ($L_z = 13L_y$), dotted line ($L_z = 19L_y$) and dot-dashed line ($L_z = 25L_y$). Other physical parameters are the same as those of Fig. 5(b).