Current Applied Physics 14 (2014) 34–45

Contents lists available at ScienceDirect

Current Applied Physics

journal homepage: www.elsevier.com/locate/cap

# Impurities-contributed abnormal thermoelectric effect in a parallel double quantum dot structure

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ARTICLE INFO

*Article history:*
Received 3 August 2013
Accepted 5 October 2013
Available online 12 October 2013

*Keywords:*
Thermoelectric properties
Quantum dot
Fano effect
Impurity

ABSTRACT

We discuss the influence of local impurities on the thermoelectric effect in a parallel double quantum dot (QD) structure. It is first found that in this structure, the Fano effect contributes significantly to the enhancement of thermoelectric efficiency, especially in the case of $\phi = \pi$. Next, impurities are introduced to couple to the QDs, respectively. We readily find that regardless of which QD is coupled to a local impurity, the thermoelectric efficiency can be enhanced by the strengthening of impurity–QD coupling. This means that the destruction of the Fano interference is not the necessary condition to suppress the thermoelectric effect. Accordingly, we hope that the numerical results can help to understand the role of impurities in adjusting the thermoelectric properties of the QD structure.

## 1. Introduction

The field of thermoelectricity and solid-state thermionics has recently received renewed attention, due to advances in growth and fabrication of complex compounds, mesoscopic devices and nanostructures [1,2]. The main purpose is to enhance the efficiency of solid-state thermoelectric devices at a mesoscopic or nanoscopic scale [3]. The thermoelectric efficiency of a solid-state device is described by the figure of merit *ZT*, which is defined as,

$$ZT = S^2 \square T/\kappa. \tag{1}$$

*S*, *G*, and *T* are thermopower, electronic conductance, and absolute temperature, respectively. $\kappa = \kappa_e + \kappa_p$ is the thermal conductance, in which $\kappa_e$ is the electron and $\kappa_p$ the phonon thermal conductance [4]. The thermal and electronic conductances for most macroscopic metals at very low or room temperatures are constrained by the Wiedemann–Franz law $\kappa/GT = L_0$, where $L_0 = k_B^2\pi^3/3e^2$ is the Lorentz number with $k_B$ the Boltzmann constant and *e* the electron charge [5]. Because of the relationship between these parameters, it is difficult to achieve the increment of thermoelectric efficiency in bulk materials.

The succession in the field of mesoscopic physics motivates scientists to decrease the dimension of the traditional thermoelectric materials to improve the thermoelectric efficiency. A number of interesting experimental results have been reported, and the barrier of $ZT = 1$ has been overcome at high temperatures. For instance, Harman et al. observed $ZT \simeq 1.6$ in a PbSeTe based QD superlattice. Venkatasubramanian et al. achieved $ZT \approx 2.4$ in a p-type $Bi_2Te_3/Sb_2Te_3$ superlattice [6]. More recently, Kanatzidis and co-workers found that bulk $AgPb_{18}SbTe_{20}$ with internal nanostructures has $ZT \approx 2$ at $T = 800$ K [7]. In nanocrystalline BiSbTe bulk alloys *ZT* reached the value 1.4 at $T = 373$ K [8]. Albeit these existed works, it is still desirable to explore new low-dimensional thermoelectric materials. Now, there have reported some important results. For instance, a 100-fold improvement of *ZT* compared to the bulk value has been reported lately in Si nanowires [9,10]. Lyeo et al. measured the Seebeck coefficient across a junction formed by a semiconducting substrate and the tip of a scanning transmission microscope. The consensus is that finding a material with a thermoelectric figure of merit $ZT \geq 4$ would mark a major technological breakthrough [11]. In addition, the experimental results were well explained by theoretical workers. Interpretively, the enhanced *ZT* in nanostructures is attributed to the decrease of the thermal conductance produced by the scattering of phonons off the structure [12,13], or due to the increase of thermopower induced by the presence of enhanced densities of states at the Fermi level. [14–16].

QD systems are typical nanostructures, since they contain a variety of interesting quantum transport properties with potential applications. Furthermore, basing on the work of Mahan and Sofo [16], it can be anticipated that QDs and molecular junctions are good candidates to explore the thermoelectric properties of low-

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http://dx.doi.org/10.1016/j.cap.2013.10.005

dimensional structures, since the $\delta$-like density of states and small phonon contribution to thermal conductance in these systems [12,16,17]. Consequently, many experimental and theoretical groups have devoted themselves to the thermoelectric properties of QDs and molecules, as a result, some interesting phenomena were reported [17–31]. First, it was found that in these systems, the characteristics of level quantization and Coulomb blockade effects indeed lead to novel thermoelectric features, such as oscillations of the thermopower and oscillations of the thermal conductance [19,20,23,24]. On the other hand, the Coulomb interactions in QD devices have a significant influence on thermoelectric transport coefficients, and lead to strong violation of the Wiedeman–Franz law [22,32]. Experiments performed on QDs in the Kondo regime reveal a strong influence of spin correlations on the thermopower [29]. Also, Murphy et al. demonstrated that violation of the Wiedeman–Franz law is the main mechanism of an enhanced thermoelectric efficiency in molecular junctions, which can be important for possible applications in energy conversion devices [33]. Then, the above results confirm that the peculiar properties of QDs play important roles in the change of thermoelectric properties.

As is known, QDs have important characteristics that some QDs can be coupled to form coupled-QD systems. In comparison with single-QD system, coupled QDs present more intricate quantum transport behaviors, because of the tunable structure parameters and abundant quantum interference mechanisms. Recently, the thermoelectric properties of the coupled-QD structures have received much attention [34–37]. Calculations based on the density-functional formalism indicate that the thermoelectric efficiency of molecules which exhibit the Fano resonance can be significantly enhanced [38]. And, Yoshida et al. illustrated that in the structure of a QD side coupled to a quantum wire, the interplay between the quantum interference and Kondo effect makes nontrivial contributions to thermoelectric properties [30]. Apart from the T-shaped QD system, thermoelectric effects of the parallel coupled QDs were also studied extensively. Very recently, Liu et al. have investigated thermoelectric effects in parallel double QDs attached to two metallic leads, and with a magnetic flux threading the QD device. [39] They arrived at the conclusion that the figure of merit $ZT$ can be enhanced in the vicinity of the Fano resonance. Similar conclusion also follows from a recent paper, where the influence of electron interference in a two-level system on the maximum thermoelectric power is analyzed [40,41].

Note that it is still a formidable challenge to fabricate two clean QDs in experiment due to irregularities and defects in the QD system. Some localized states often appear in QD systems, which are hybridized with the QD levels. However they are not coupled directly to the leads, which, thereby, are called the impurity states. The presence of impurity state is certain to modify the Fano interference and then destroy the Fano-induced thermoelectric effect. Motivated by this idea, we aim to discuss the influence of local impurities on the thermoelectric effect in a parallel QD structure. Consequently, we find that the thermoelectric efficiency can be enhanced by the strengthening of impurity–QD coupling. This means that the destruction of the Fano interference is not the necessary condition to suppress the thermoelectric effect.

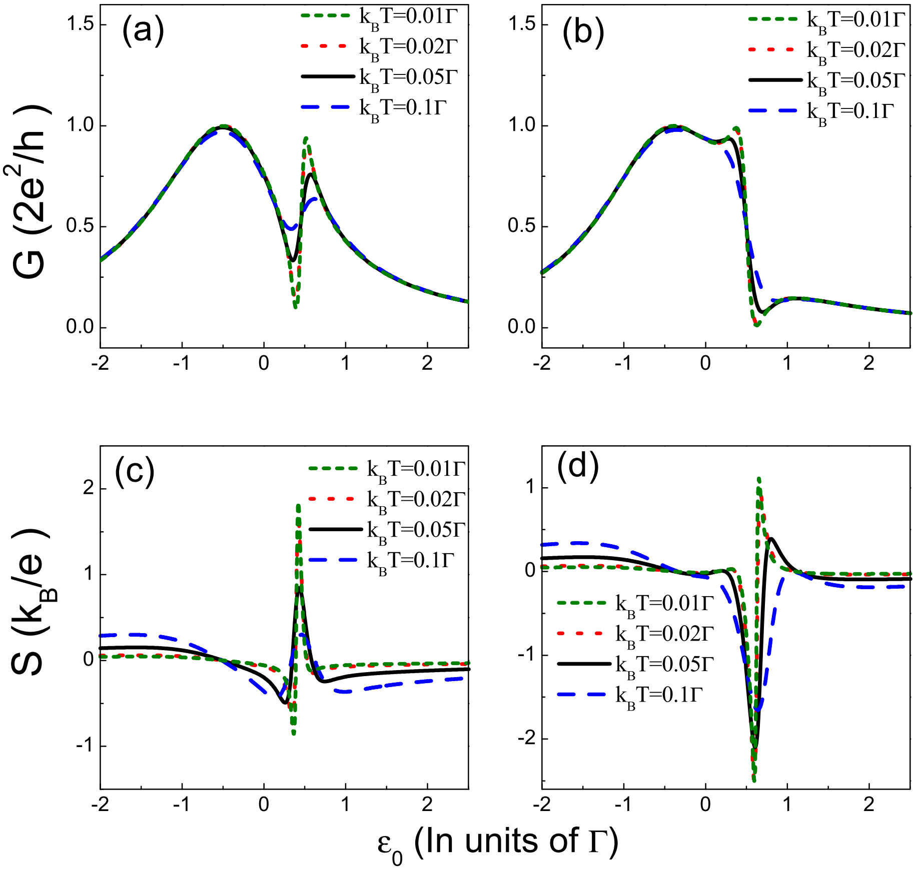

**Fig. 1.** (a) and (b), The electronic conductances with the increase of temperature, in the cases of $\phi = 0$ and $\phi = \pi$, respectively. The corresponding thermopowers are shown in (c) and (d).