Fractal lattice as an efficient thermoelectric device

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Abstract. Figure of merit is an essential quantity to describe the efficiency of a thermoelectric device and asymmetry in transmission probability is the main requirement to increase the efficiency. Keeping this fact in the mind, here we choose a Sierpinski Gasket (SPG) triangle, a nice example of fractal lattice, as the functional element since it has peculiar energy spectrum compared to the traditional elements. In the framework of tight binding (TB) model we calculate all the thermoelectric quantities using Landauer’s prescription. The atypical and strange behavior of transmission function can be further modified by incorporating asymmetry in the hopping integrals of the SPG network. Here, we acquire a remarkably large value of thermoelectric efficiency from the system and we strongly believe that our work can be verified by a suitable experimental setup. The present analysis can easily be generalized in other similar kind of fractal lattices having multiple loops.

1. Introduction

For the last many years, people are relentlessly searching for a renewable and unconventional energy sources as the limited amount traditional energy resources in the nature are gradually reducing. Thermoelectric energy is one of those unconventional energy sources, whose function is basically to convert ‘waste-heat’ energy into usable electrical one. In the aspect of energy accumulation issue, its demand in the energy market is moderately increasing. The key reasons are the eco friendly behavior and at the same time the devices can be maintained quite easily. Though, this prescription is still not at that usable stage as the efficiency of present thermoelectric devices is too small.

The efficiency of a thermoelectric machine is defined through a quantity, namely, figure of merit (ZT) which is expressed as

\[ ZT = GS^2 T/K \]  

where, \( T \), \( G \) and \( S \) represent equilibrium temperature, electrical conductance and thermopower of the machine respectively and \( K \) stands for thermal conductance consisting of two parts – electronic (\( K_{el} \)) and phononic (\( K_{ph} \)). A substantial amount of work has been done so far on thermoelectric behavior of the bulk samples but no satisfactory result has come out. Restricted by the Widemann-Franz (WF) law, due to its higher value of \( K \) and lower value of \( G \), the magnitude of \( ZT \) of a bulk material cannot go above the unity. On the other hand it is revealed that nano materials offer better thermoelectric response as there is no such restriction by WF law and an extensive amount of theoretical studies
show that molecular junctions can be efficient thermoelectric device but when these are experimentally verified, their performances are still not up to the mark.

So, our aim is to look for a quantum system which can exhibit a reasonable value of ZT in an experimentally viable way and from all the proposals of the above mentioned studies it is known that asymmetry in transmission function is the key factor behind the enhancement of ZT. Now, due to fractal eccentricity and gapped nature of energy spectrum, fractal lattice acts like a bridging material between a perfect lattice and completely random ones, shows an anomalous transmission spectrum which can provide an appreciable value of ZT. So, in this paper we consider a very well known fractal lattice – Sierpinski Gasket Triangle as our quantum system to study the thermoelectric behavior. Here, we introduce the asymmetry in its two kinds of hopping integrals – horizontal and non-horizontal and it is observed that the value of ZT is enhanced when horizontal hopping integral is different from the non-horizontal one.

Fig.1: The schematic diagram of SPG triangle connected in between two semi-infinite leads kept at two different temperatures.

2. Tight binding model and Theoretical formulation

We consider a 3rd generation Sierpinski Gasket triangle (schematically shown in Fig.1) as our model quantum system containing 15 atomic sites which is connected with two heat reservoirs kept at two different temperatures. In this paper, two kinds of hopping integrals – horizontal ($t_x$) and non-horizontal ($t_y$) are considered to examine the asymmetry effect on its thermoelectric behavior. The coupling integrals between the system and the reservoirs are denoted by $t_c$. Now, considering the linear response regime, all the essential thermoelectric quantities are evaluated by the Landauer’s integrals –

$$G = 2 e^2 L_0, \quad S = \frac{L_1}{e \tau L_0} \quad \text{and} \quad K_{el} = \left(\frac{L_2}{L_0}\right)^{\frac{1}{2}}$$

and the general form of the Landauer’s integrals is given by

$$L_n = \frac{1}{\hbar} \int dE T(E)(E - E_F)^n \frac{\partial f}{\partial E} \quad \quad (2)$$

where, $\hbar$, $f$ and $E_F$ are used to indicate Planck’s constant, equilibrium Fermi-Dirac occupation probability and Fermi energy respectively and $T(E)$ is the transmission probability of the system. Now, we use the non-equilibrium green’s functions technique to calculate the energy dependent $T(E)$ where

$$T(E) = \Gamma^r L \Gamma^a \quad \quad (3)$$

The $\Gamma_{L(R)}$ are energy broadening matrices for left (right) leads, which are the imaginary parts of the self energy matrices ($\Sigma_{L(R)}$). Here, $G^r$ and $G^a$ are used for retarded and advanced green’s functions.
respectively and the relation between them is given by \( -G^a = (G^r)^f \). The mathematical form of the retarded green’s function is expressed as

\[
G^r = (E I_n - H_S - \sum_I - \sum_R)^{-1}
\]

where \( I_n \) is the identity matrix of order \( n \) (number of atomic sites) and \( H_S \) is the matrix for SPG triangle. Now, we use the tight binding framework considering only the nearest neighbor interactions to describe all kind of Hamiltonians for the system. The Hamiltonian of SPG triangle is like

\[
H_S = \varepsilon_0 \sum_i^n b_i^\dagger b_i + \sum_{i,j} t_{ij} (b_i^\dagger b_j + \text{h.c.})
\]

where, \( \varepsilon_0 \) is atomic site potential, the value of ‘\( j \)’ and whether the hopping integral \( t_{ij} \) taking \( t_x \) or \( t_y \) depends on the site ‘\( i \)’. Here, the \( b_i^\dagger \) (\( b_i \)) denote the creation (annihilation) operator. The similar mathematical form is used for the Hamiltonians of the left and right leads where the creation (annihilation) operator take the form \( a_i^\dagger \) (\( a_i \)) and \( c_i^\dagger \) (\( c_i \)) respectively and the hoping integrals are denoted by \( t_0 \). The coupling Hamiltonians between the SPG triangle and the leads are expressed as,

\[
H_{L/R} = t_c (b_p^\dagger a_1 t_p^\dagger c_1 + \text{h.c.})
\]

where, \( p \) is pth atomic site of the SPG triangle, \( t_c \) is the coupling integral and \( \text{h.c.} \) is the abbreviation of hermitian conjugate.

3. Numerical results

In the entire work, the site potentials both for the system and the leads are chosen to be 0. The value of \( t_c \) and \( t_0 \) are taken as 1 and 2 respectively whereas the values for the \( t_x \) and \( t_y \) are considered either 1.2 or 1.5 depending on the conditions mentioned below. All kinds of energies are taken in unit of electron-volt (eV).

![Variations of electrical conductance with the Fermi energy at a temperature T = 300K](image)

Here, we focus on the behaviors of all the thermoelectric quantities with respect to \( E_F \) at a temperature \( T = 300K \) for three different hopping integral conditions:
1. Symmetric Condition: horizontal hopping = non-horizontal hopping ($t_x = t_y = 1.2$)
2. Asymmetric condition: horizontal hopping > non-horizontal hopping ($t_x = 1.5$ and $t_y = 1.2$)
3. Asymmetric condition: horizontal hopping < non-horizontal hopping ($t_x = 1.2$ and $t_y = 1.5$)

Now, it is seen from the variation of electrical conductance with Fermi energy (Fig.2) that in a small energy range (varied by the temperature dependent thermal broadening function) difference between two peaks adjacent to the dotted line set at a Fermi energy is much more atypical in two asymmetric cases compared to the symmetric one i.e. $T(E)$ as well as $G$ is more asymmetric when $t_x \neq t_y$.

Therefore, it is expected that a reasonable value of thermopower will be obtained in these two asymmetric cases and it is clearly visible from the Fig.3 that the magnitudes of thermopower in those two cases (400 μV for $t_x > t_y$ and almost 900 μV for $t_x < t_y$) are much higher which can lead to a high value of $ZT$ whereas its value is 300 μV/K for the symmetric case.

Now, if we look at the dependence of the electronic thermal conductance on Fermi energy (Fig.4) it is observed that the value of $K_{el}$ is much lower (300 pW/K) for the case ($t_x = t_y$) and it takes a moderate number (500 pW/K) when horizontal hopping integral is not equal to the vertical one. Here, the impact of $K_{ph}$ is safely ignored because the contribution of $K_{ph}$ is very less compared to $K_{el}$ due to having small number of lattice sites.

So, from the results of higher value of thermopower and some moderate value of the electronic thermal conductivity, it can be assumed that a large value of $ZT$ can be achieved in these two asymmetric cases of hopping integrals.

Now, if we concentrate on the behavior of $ZT$ with the Fermi energy in each of these three cases (Fig.5), the results obtained here will fit with our assumption. The value of $ZT$ is close to 2 for the symmetric case, while for $t_x < t_y$ its value gets enhanced up to 5, and the best thermoelectric performance is obtained in the other asymmetric case ($t_x > t_y$) where the value of $ZT$ goes beyond 30.
which is quite large. This larger figure of merit is well above that obtained for many other proposed quantum systems available in the literature.

Fig.4: Dependence of electronic thermal conductivity on Fermi energy for a temperature $T = 300K$

Fig.5: For a temperature $T = 300K$, the variation of figure of merit with Fermi energy
4. Summary
From our analysis, it can be concluded that the SPG triangle can be utilized as an efficient thermoelectric device due to its gapped nature of energy spectra and peculiar transmission function. The thermoelectric response is enhanced drastically when asymmetry is included in its two different types of hopping integrals. These results are not confined for a particular set of values, rather applicable for wide range of parameters which indicates the robustness of our work. In our forthcoming work, we want to focus on how to estimate the degree of efficiency of any higher generation SPG network getting the results of few lower generations. This might be possible due to the strange self-similar feature of this system. Our analysis can also be generalized in any other similar kind of fractal lattices.

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