



## FIGURE OF MERIT OF ONE-DIMENSIONAL RESONANT TRANSMISSION SYSTEMS IN THE QUANTUM REGIME

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**Abstract-** The figure of merit,  $ZT$ , for a one-dimensional conductor displaying a Lorentzian resonant transmission probability is calculated. The optimum working conditions for largest  $ZT$  values are determined. It is found that, the resonance energy has to be adjusted to be several resonance widths away from the Fermi level. Similarly it is better for the temperature to be equal to several resonance widths. The approximate relationships, which can be a fairly good guide for designing devices, between different parameters under optimum working conditions are given.

**Key Words-** Figure of Merit, Thermoelectric Effects, Quantum Conductance, Ballistic Transport, Quantum Point Contacts.

### 1. INTRODUCTION

Recent advances in fabrication and material growth technologies have made possible the production of devices whose dimensions are order of a few nanometers. The thermoelectric power, thermal and electrical conductivities of these mesoscopic scale materials are of interest for thermoelectric device applications [1], such as heat pumps [2] and power generators. The performance of a thermoelectric device is usually quantified by a dimensionless number called as figure of merit,  $ZT$ , which measures the efficiency of thermoelectric energy conversion. Higher values of  $ZT$  correspond to higher thermoelectric energy conversion efficiency so that, for example, if  $ZT$  tends to infinity, the efficiency approaches to that of an ideal Carnot engine. Recent work on superlattice semiconducting devices demonstrated  $ZT \approx 2.5$  at room temperature [3] and  $ZT \approx 1.4$  at high temperatures [4], breaking the long-standing limit of  $ZT \approx 1$  for most of best known thermoelectric materials.

In 1D nanoscale systems, the increase of  $ZT$  might be further enhanced by the quantum confining of electrons and phonons in low dimensions [5]. In the recent experimental study, for instance,  $ZT$  could be increased by embedding nanoparticles in crystalline semiconductors [6]. High values of  $ZT$  can also be obtained for one-

dimensional structures displaying resonant transmission. In this case, the transmission probabilities are very sensitive to the electron energies leading to large values of the thermopower and hence of the figure of merit. In this contribution, relationships between different thermoelectric coefficients are calculated, and probably the first,  $ZT$  values of a resonant tunneling device is computed and its dependence on device parameters is investigated. We are expecting that our calculations will be a good guide to researchers studying on thermoelectric devices.

## 2. TRANSPORT COEFFICIENTS

In here a one-dimensional mesoscopic device is considered. It is assumed that there is only one transverse mode that is occupied by the electrons. The thermoelectric currents in such a device under linear regime can be expressed in terms of the energy dependent transmission probability  $T(E)$  of the electrons [7]. The electric current,  $I$ , and the heat current,  $\dot{Q}$ , under a potential difference  $\phi V$  and a temperature difference  $\phi T$  can be expressed as [8]

$$I = \frac{2e^2}{h} g_0 \Delta V + \frac{2(-e)k_B}{h} g_1 \Delta T, \quad (1)$$

$$\dot{Q} = \frac{2(-e)k_B T}{h} g_1 \Delta V + \frac{2k_B^2 T}{h} g_2 \Delta T, \quad (2)$$

where  $g_n$  are

$$g_n = \int_{-\mu/k_B T}^{\infty} dx x^n (-f'(x)) \mathfrak{I}(\mu + x k_B T), \quad (3)$$

$\mu$  is the chemical potential and  $f(x) = 1/(1 + e^x)$  is the Fermi-Dirac distribution function.

Frequently measured transport coefficients, the electrical conductance  $G_{el}$ , the thermal conductance  $G_{th}$ , the Seebeck coefficient  $S$ , and the dimensionless thermoelectric figure of merit  $ZT$  can be expressed as

$$G_{el} = \frac{2e^2}{h} g_0, \quad (4)$$

$$G_{th} = \frac{2k_B^2}{h} T \left( g_2 - \frac{g_1^2}{g_0} \right), \quad (5)$$

$$S = \frac{k_B}{(-e)} \frac{g_1}{g_0}, \quad (6)$$

$$ZT = \frac{S^2 G_{el} T}{G_{th}} = \frac{g_1^2}{g_0 g_2 - g_1^2}. \quad (7)$$

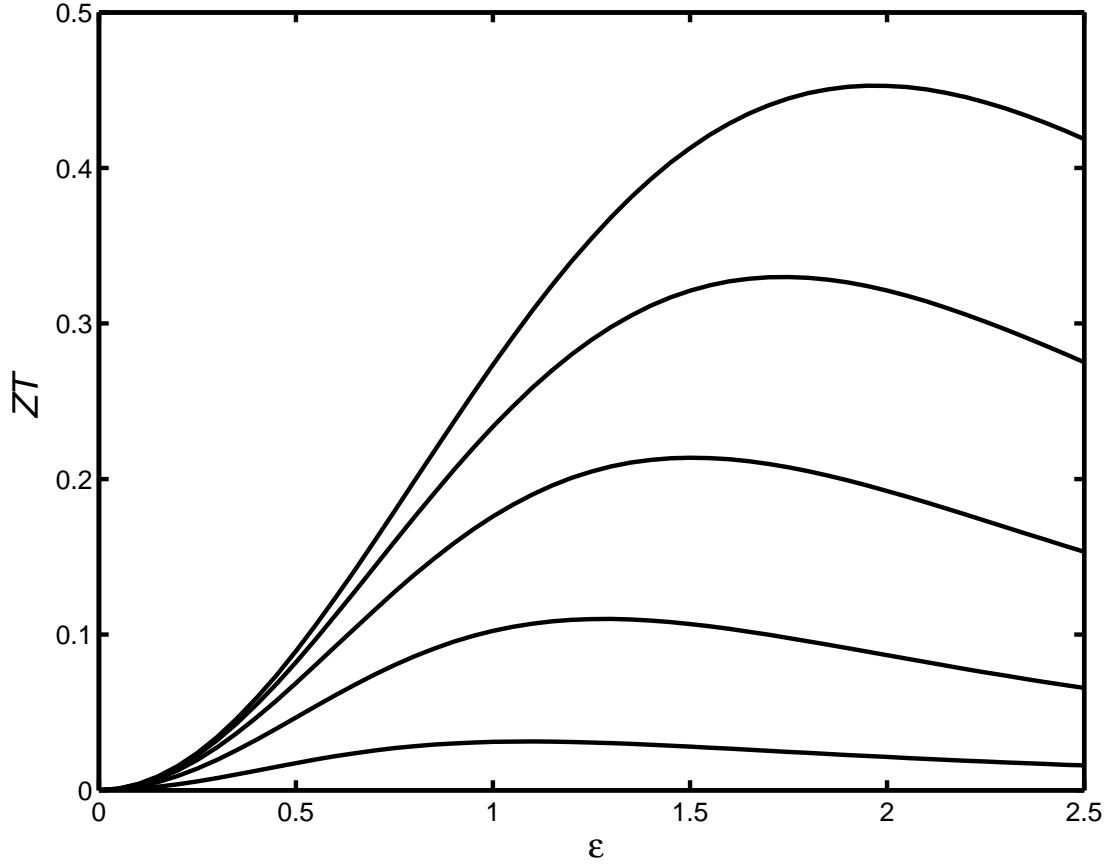
It can be seen that, to obtain large values of  $ZT$ , the factor  $g_1$ , which also appears in the Seebeck coefficient, has to be large. Equation (3) implies that at low temperatures,  $g_1$  is basically proportional to the first derivative of  $\mathfrak{I}(E)$ . For this reason, large values of  $g_1$  can be achieved when  $\mathfrak{I}(E)$  is strongly energy dependent, and the fastest change in it occurs around the Fermi level. In this contribution we investigate a probability is assumed to have a Lorentzian form

$$\mathfrak{I}(E) = \frac{\mathfrak{I}_{\max}}{1 + (E - E_o)^2 / \Gamma^2}, \quad (8)$$

where  $E_o$  is the resonance energy and  $\Gamma$  is the half width. The factor  $g_1$  and the Seebeck coefficient  $S$  changes sign when the Fermi energy crosses the resonance energy  $E_o$ . However, when  $\mu$  differs from  $E_o$  by an energy of the order of  $\Gamma$ , both of these quantities attain large values and this is the region where we should look for large values of  $ZT$ . It is assumed that the Fermi level is very large compared to the temperature so that the lower limit of the integral in Eq. (3) is extended to minus infinity.

### 3. RESULTS AND DISCUSSION

It can be seen that the values of  $ZT$  depend on two dimensionless parameters. One of them,  $\varepsilon = (\mu - E_o)/\Gamma$ , indicates the distance of the Fermi level from the resonance energy in units of the half width  $\Gamma$ , and the other,  $\theta = k_B T / \Gamma$  gives the temperature compared to the resonance width.



**Fig. 1** Variation of  $ZT$  for different values of temperature ( $\theta=0.1, 0.2, 0.3, 0.4, 0.5$  from bottom to top) as a function of  $\varepsilon$

The values of  $ZT$  as a function of dimensionless Fermi level,  $\varepsilon$ , for different temperatures is shown in Fig. 1. The Seebeck coefficient is zero at  $\varepsilon=0$  and has different signs at different sides of this point. Since  $ZT$  is an even function of  $\varepsilon$ , only the positive values of  $\varepsilon$  is shown in the figure. It can be seen that when  $\varepsilon$  is varied,  $ZT$  values increase, reach a maximum and then start to decrease. The place and the value of the maxima depends on the temperature.

The maximum attainable value of figure of merit,  $ZT_{\max}$  and the best place of Fermi level,  $\varepsilon_{\max}$  for each temperature are plotted in Fig. (2). For low temperatures,  $\delta$  0.1, the best place of the Fermi level is approximately one resonance width above or below of the resonance energy ( $\varepsilon \approx \pm 1$ ), but the maximum attainable figure of merit value is very low. For high temperatures however, both of these parameters have a linear dependence on temperature which are approximately given as

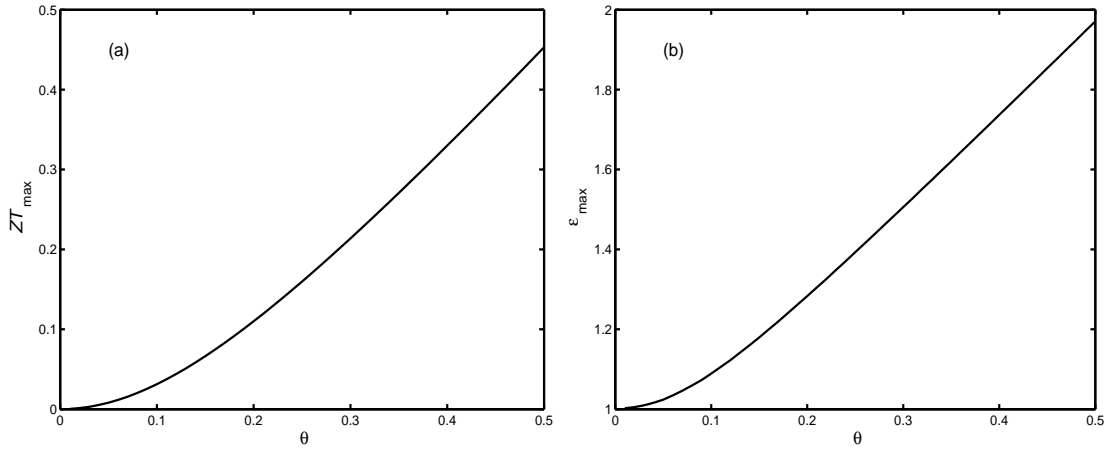
$$\varepsilon_{\max} \approx 0.8 + 2.4\theta, \quad (9)$$

$$ZT_{\max} \approx 1.4\theta - 0.3. \quad (10)$$

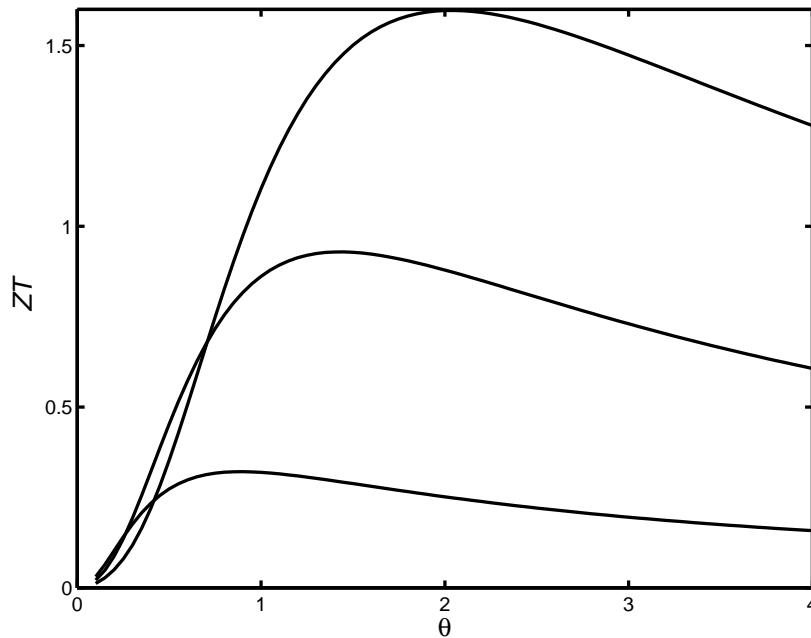
It can be seen that, in each case the optimum value of the figure of merit is obtained when  $|\varepsilon| > 1$ , i.e., the Fermi level should be more than one half-width away

from the resonance energy. If the Lorentzian form of the resonance in Eq. (8) remains valid for a large energy interval, sufficiently large  $ZT$  values can be obtained in this domain.

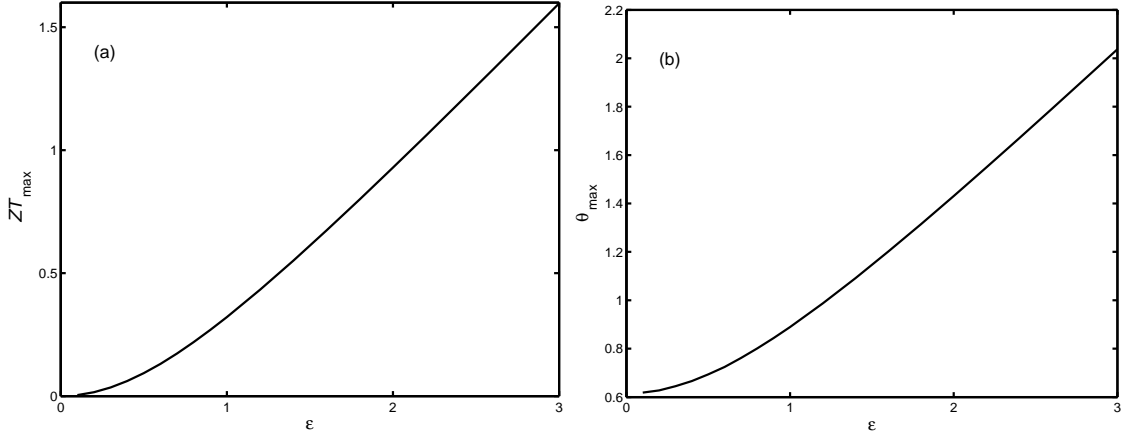
The values of  $ZT$  as a function of  $\theta$  for different places of the Fermi level is shown in Fig. 3. The figure of merit reaches a maximum for a certain temperature in this case as well. The maximum attainable value



**Fig. 2** (a) The maximum values of  $ZT$  as a function of  $\mu$  is plotted for different values of  $\theta$ . (b) The value of  $\epsilon$  at maxima is plotted for different values of  $\theta$ .



**Fig. 3** Variation of  $ZT$  for different placements of the Fermi level ( $\epsilon = 1, 2, 3$  from bottom to top) as a function of  $\theta$ .



**Fig. 4** (a) The maximum values of  $ZT$  as temperature is varied is plotted as a function of  $\varepsilon$ . (b) The value of  $\theta$  at maxima is plotted as a function of  $\varepsilon$ .

of figure of merit,  $ZT_{\max}$  and the optimum temperature,  $\theta_{\max}$  are shown in Fig. (4) as a function of  $\varepsilon$ . When the Fermi level is almost coincident with the resonance energy ( $\varepsilon \approx 1$ ), the temperature at which maximum attained is around  $\theta \approx 0.6$ . However, in this region,  $ZT$  values are low. In the opposite case, for  $\varepsilon \gg 1$ , the optimum temperature and the best value of  $ZT$  appear to be linear in  $\varepsilon$  with the following numerical relationships

$$\theta_{\max} \approx 0.6\varepsilon + 0.2, \quad (11)$$

$$ZT_{\max} \approx 0.7\varepsilon - 0.4. \quad (12)$$

The approximate relation  $\theta_{\max} \approx 0.9ZT_{\max} + 0.6$  seems to hold over the whole range investigated in this study.

It is seen that for one-dimensional systems displaying resonant transmission, it is possible to obtain large values of the figure of merit  $ZT$  by fine-tuning the device parameters, the resonance width and the place of the resonance energy relative to the Fermi level. The optimum working conditions for the largest values of  $ZT$  appears to be far away from the resonance: Fermi level is several  $\Gamma$  away from the resonance energy  $E_o$  and  $k_B T$  is several times  $\Gamma$ . It can be argued that, under such extreme cases, the validity of Lorentzian form in Eq. (8) is questionable and some of the results obtained in here can be changed. However, the crucial feature leading to these results is the strong energy dependence of the transmission probability. Specifically, the transmission probability should continue decreasing at the Fermi level and not reach to a minimum. For this reason, similar results can be expected for realistic devices. Numerical computations for a double barrier system displaying resonances indicate that when the half width  $\Gamma$  is much smaller than the distance between the resonances, results obtained are roughly in agreement with the ones in here. For this reason Lorentzian form can be used as a fairly good guide for designing devices.

An important problem, connected with being far away from the resonance, is the smallness of the electrical and thermal conductances. For this reason, efficient devices can only work with very small power. Moreover, precautions should be taken to make

the phonon contribution to the heat conductance to be very small as this will always decrease the  $ZT$  value.

#### 4. CONCLUSIONS

The figure of merit has been computed for a system whose transmission probability displays a Lorentzian peak. By adjusting the resonance width to be small and carefully placing the Fermi level for the working temperatures of interest, significantly high values of  $ZT$  can be obtained. Approximate numerical relationships, which can be a guide for designing thermoelectric devices, for the optimum values of the parameters are also given.

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