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Exact Solution of a Constrained Optimization Problem in Thermoelectric Cooling

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Abstract

We consider an optimization problem in thermoelectric cooling. The maximum achievable cooling temperature in thermoelectric cooling is, among other things, affected by the Seebeck coefficient profile of the inhomogeneous materials. Mathematically, the maximum cooling temperature is a non-linear functional of the Seebeck coefficient function. In this study, we solve this optimization problem exactly.

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1 Introduction

In 1822 Thomas Seebeck [6] observed that if two different metals kept at different temperatures were joined, a current would flow. In 1834 Jean Peltier [4] discovered that there is a heating or cooling effect when electric current passes through two conductors. It was not until 1851 that William Thomson (Lord Kelvin) [8] drew the connection between the Seebeck and Peltier effects, which was the first significant contribution to the understanding of thermoelectric phenomena. He predicted and subsequently observed experimentally that in the presence of a temperature gradient, a single conductor with current flow, will have reversible heating and cooling. With these principles of thermoelectrics in mind and the rapid developments of semiconductor materials in the late 1950's, thermoelectric cooling has become a viable technology in microelectronics with applications in many areas including flight vehicles and military equipments.

In thermoelectric cooling using inhomogeneous materials, the maximum achievable cooling temperature is mathematically given by [1]:

$$\frac{\Delta T_{max}}{T} = \frac{1}{2} ZT \frac{\int_0^L S(x) \int_0^x S(x')dx'dx}{\int_0^L \int_0^x S^2(x')dx'dx} \tag{1}$$

where L is the length of the thermoelectric cooling element, and ZT is the dimensionless "figure of merit" [5] which puts a limit on the maximum achievable cooling temperature when a single stage of uniform material is used. Since 1990s, nanostructured materials have drawn a lot of attention because they can achieve ZT values up to 2.4 at room temperature [7], [3], [9]. In a parallel direction, a much larger cooling temperature beyond that of uniform materials can be achieved by using graded thermoelectric materials

In equation (1), x is the length coordinate along the thermoelectric cooling element, and function $S(x)$ is the Seebeck coefficient profile of the inhomogeneous element. The Seebeck coefficient of a material can be varied by changing the level of doping. In semiconductor production, doping refers to the process of intentionally introducing impurities into an extremely pure semiconductor in order to change its electrical properties.

Without loss of generality, we take $L = 1$, or equivalently we normalize all lengths by introducing $\tilde{x} = \frac{x}{L}$ and using the dimensionless $\tilde{x}$ as the independent variable. We introduce functional $F[S(x)]$ as

$$F[S(x)] \equiv \frac{\int_0^1 S(x) \int_0^x S(x')dx'dx}{\int_0^1 \int_0^x S^2(x')dx'dx} \tag{2}$$

In terms of functional $F[S(x)]$, the maximum achievable cooling temperature has the form

$$\frac{\Delta T_{max}}{T} = \frac{1}{2} ZTF[S(x)] \tag{3}$$

In the expression of $F[S(x)]$ defined in (2), the Seebeck coefficient profile $S(x)$ is not allowed to be any arbitrary positive function. Due to the limitations in manufacturing, an acceptable Seebeck coefficient profile $S(x)$ must be between S_1 and S_2 ($S_2 > S_1$). Mathematically, $S(x)$ is restricted by

$$S_1 \le S(x) \le S_2, \quad \text{for all } x \text{ in } [0,1] \tag{4}$$

The goal of the current study is to find an acceptable Seebeck coefficient profile that will yield the largest maximum achievable cooling temperature. From a mathematical point of view, that is, to optimize functional $F[S(x)]$ with respect to function $S(x)$ subject to constraint (4).

2 Exact solution of the constrained optimization problem

To optimize functional $F[S(x)]$ defined in (2) subject to constraint $S_1 \le S(x) \le S_2$, we rewrite the integral in the numerator and the integral in the denominator of $F[S(x)]$, respectively, as

$$\begin{aligned}
\int_0^1 S(x) \int_0^x S(x')dx'dx &= \int_0^1 \int_0^x S(x)S(x')dx'dx \\
&= \frac{1}{2}\left(\int_0^1 \int_0^x S(x)S(x')dx'dx + \int_0^1 \int_0^x S(x)S(x')dx'dx\right) \\
&= \frac{1}{2}\left(\int_0^1 \int_0^x S(x)S(x')dx'dx + \int_0^1 \int_{x'}^1 S(x)S(x')dxdx'\right) \\
&= \frac{1}{2}\int_0^1 \int_0^1 S(x)S(x')dx'dx \\
&= \frac{1}{2}\left(\int_0^1 S(x)dx\right)^2
\end{aligned} \tag{5}$$

$$\begin{aligned}
\int_0^1 \int_0^x S^2(x')dx'dx &= \int_0^1 S^2(x') \int_{x'}^1 dxdx' \\
&= \int_0^1 S^2(x)(1-x)dx
\end{aligned} \tag{6}$$

Thus, the optimization problem becomes

$$\underset{S_1 \le S(x) \le S_2}{\arg\max} \; F[S(x)] \tag{7}$$

where

$$F[S(x)] \equiv \frac{1}{2} \frac{\left(\int_0^1 S(x) dx \right)^2}{\int_0^1 S^2(x)(1-x) dx} \tag{8}$$

In [2], based on intuitions, a Seebeck coefficient profile was guessed as the solution of optimization problem (7). The conjectured optimal Seebeck coefficient profile is given by [2]

$$Q(x) = \begin{cases} S_1, & 0 \le x \le x_1 \\ \dfrac{q}{1-x}, & x_1 \le x \le x_2 \\ S_2, & x_2 \le x \le 1 \end{cases} \tag{9}$$

where q, x_1 and x_2 are given by

$$\begin{aligned} q &\equiv \frac{S_1}{2} \\ x_1 &\equiv 1 - \frac{q}{S_1} = \frac{1}{2} \\ x_2 &\equiv 1 - \frac{q}{S_2} = 1 - \frac{S_1}{2S_2} \end{aligned} \tag{10}$$

Below, we will show rigorously that the conjectured optimal Seebeck coefficient profile $Q(x)$ is indeed the exact solution of the optimization problem (7). That is,

$$Q(x) = \arg \max_{S_1 \le S(x) \le S_2} F[S(x)] \tag{11}$$

To proceed, we do it in two steps:

- Step 1: we calculate the value of functional $F[Q(x)]$ and at the same time derive two properties of function $Q(x)$.

- Step 2: we use the two properties derived in Step 1 to prove that $Q(x)$ is indeed the exact solution of problem (7). Mathematically, we will show

  $$F[S(x)] \le F[Q(x)] \tag{12}$$

  for all functions $S(x)$ satisfying $S_1 \le S(x) \le S_2$.

Step 1: The integral in the numerator and the integral in the denominator of $F[Q(x)]$ are respectively

$$\begin{aligned}\int_0^1 Q(x)dx &= \int_0^{x_1} S_1 dx + \int_{x_1}^{x_2} \frac{q}{1-x}dx + \int_{x_2}^1 S_2 dx \\ &= S_1 x_1 - q\ln\left(\frac{1-x_2}{1-x_1}\right) + S_2(1-x_2) \\ &= S_1\left(1-\frac{q}{S_1}\right) - q\ln\left(\frac{1-\left(1-\frac{q}{S_2}\right)}{1-\left(1-\frac{q}{S_1}\right)}\right) + S_2\frac{q}{S_2} \\ &= S_1 + q\ln\left(\frac{S_2}{S_1}\right) \\ &= q\left(2+\ln\left(\frac{S_2}{S_1}\right)\right) \end{aligned} \tag{13}$$

$$\begin{aligned}&\int_0^1 Q^2(x)(1-x)dx \\ &= \int_0^{x_1} S_1^2(1-x)dx + \int_{x_1}^{x_2}\left(\frac{q}{1-x}\right)(1-x)dx + \int_{x_2}^1 S_2^2(1-x)dx \\ &= \frac{S_1^2}{2}\left(1-(1-x_1)^2\right) - q^2\ln\left(\frac{1-x_2}{1-x_1}\right) + \frac{S_2^2}{2}(1-x_2)^2 \\ &= \frac{S_1^2}{2}\left(1-\frac{q^2}{S_1^2}\right) + q^2\ln\left(\frac{S_2}{S_1}\right) + \frac{S_2^2}{2}\frac{q^2}{S_2^2} \\ &= \frac{S_1^2}{2} + q^2\ln\left(\frac{S_2}{S_1}\right) \\ &= q^2\left(2+\ln\left(\frac{S_2}{S_1}\right)\right)\end{aligned} \tag{14}$$

Substituting (13) and (14) into (8) yields

$$\begin{aligned}F[Q(x)] &\equiv \frac{1}{2}\frac{\left(\int_0^1 Q(x)dx\right)^2}{\int_0^1 Q^2(x)(1-x)dx} \\ &= \frac{1}{2}\frac{q^2\left(2+\ln\left(\frac{S_2}{S_1}\right)\right)^2}{q^2\left(2+\ln\left(\frac{S_2}{S_1}\right)\right)} = \frac{1}{2}\left(2+\ln\left(\frac{S_2}{S_1}\right)\right)\end{aligned} \tag{15}$$

Multiplying by the denominator $\int_0^1 Q^2(x)(1-x)dx$, we obtain

$$\left(2+\ln\left(\frac{S_2}{S_1}\right)\right)\int_0^1 Q(x)^2(1-x)dx - \left(\int_0^1 Q(x)dx\right)^2 = 0 \tag{16}$$

Properties (13) and (16) will play a key role in Step 2 below.
Step 2: In this step we shall show

$$F[S(x)] \equiv \frac{1}{2}\frac{\left(\int_0^1 S(x)dx\right)^2}{\int_0^1 S^2(x)(1-x)dx} \leq \frac{1}{2}\left(2+\ln\left(\frac{S_2}{S_1}\right)\right) \tag{17}$$

for all functions $S(x)$ satisfying $S_1 \leq S(x) \leq S_2$. For mathematical convenience, we write $S(x)$ as $Q(x)$ plus perturbation:

$$S(x) = Q(x) + P(x) \tag{18}$$

Constraint $S_1 \leq S(x) \leq S_2$ on function $S(x)$ implies the constraint below on function $P(x)$.

$$\begin{cases} 0 \leq P(x) \leq S_2 - S_1, & 0 \leq x \leq x_1 \\ -(S_2 - S_1) \leq P(x) \leq 0, & x_2 \leq x \leq 1 \end{cases} \tag{19}$$

Note that condition (19) is a consequence of condition (4) but (19) is not equivalent to (4). More specifically, (19) is weaker than (4). To prove (17), we only need to show that

$$\begin{aligned} G[P(x)] \;\; \equiv \;\; & \left(2+\ln\left(\frac{S_2}{S_1}\right)\right)\int_0^1 (Q(x)+P(x))^2\,(1-x)dx \\ & -\left(\int_0^1 Q(x)+P(x)dx\right)^2 \geq 0 \end{aligned} \tag{20}$$

for all functions $P(x)$ constrained by condition (19). Expanding the squares in (20) and using property (16), we have

$$\begin{aligned} G[P(x)] \;\; = \;\; & \left(2+\ln\left(\frac{S_2}{S_1}\right)\right)\left(2\int_0^1 Q(x)(1-x)P(x)dx + \int_0^1 P^2(x)(1-x)dx\right) \\ & -2\int_0^1 Q(x)dx\int_0^1 P(x)dx - \left(\int_0^1 P(x)dx\right)^2 \end{aligned} \tag{21}$$

To further simplify $G[P(x)]$, we write $Q(x)(1-x)$ as

$$Q(x)(1-x) = Q(x)(1-x) - q + q \tag{22}$$

Substituting (22) into (21) and using property (13) of $Q(x)$, we arrive at

$$G[P(x)]$$

$$= \left(2+\ln\left(\frac{S_2}{S_1}\right)\right)\left(2\int_0^1 \left(Q(x)(1-x)-q\right)P(x)dx + \int_0^1 P^2(x)(1-x)dx\right) - \left(\int_0^1 P(x)dx\right)^2 \quad (23)$$

It is straightforward to verify that $Q(x)(1-x)-q$ satisfies

$$Q(x)(1-x)-q = \begin{cases} S_1(1-x)-q \geq 0, & 0 \leq x \leq x_1 \\ 0, & x_1 \leq x \leq x_2 \\ S_2(1-x)-q \leq 0, & x_2 \leq x \leq 1 \end{cases} \quad (24)$$

Combining result (24) and constraint (19) yields

$$\left(Q(x)(1-x)-q\right)P(x) = \begin{cases} \geq 0, & 0 \leq x \leq x_1 \\ 0, & x_1 \leq x \leq x_2 \\ \geq 0, & x_2 \leq x \leq 1 \end{cases} \quad (25)$$

Using result (25) and the fact that $-S_2 \leq P(x) \leq 0$ for $x \in [x_2, 1]$, we write the first term in (23) as

$$\begin{aligned} & 2\int_0^1 \left(Q(x)(1-x)-q\right)P(x)dx + \int_0^1 P^2(x)(1-x)dx \\ & \quad \geq \int_{x_2}^1 \left(S_2(1-x)-q\right)P(x)dx + \int_0^1 P^2(x)(1-x)dx \\ & \quad = \int_{x_2}^1 \left(\frac{q}{S_2}-(1-x)\right)S_2(-P(x))dx + \int_0^1 P^2(x)(1-x)dx \\ & \quad \geq \int_{x_2}^1 \left(\frac{q}{S_2}-(1-x)\right)P^2(x)dx + \int_0^1 P^2(x)(1-x)dx \\ & \quad = \int_0^{x_2} (1-x)P^2(x)dx + \int_{x_2}^1 \frac{q}{S_2}P^2(x)dx \end{aligned} \quad (26)$$

Let us introduce a new function:

$$R(x) = \begin{cases} \dfrac{1}{1-x}, & 0 \leq x \leq x_2 \\ \dfrac{S_2}{q}, & x_2 \leq x \leq 1 \end{cases} \quad (27)$$

We notice that $R(x)$ is a positive function in $[0,1]$, and satisfies

$$\int_0^1 R(x)dx = \int_0^{x_2} \frac{1}{1-x}dx + \int_{x_2}^1 \frac{S_2}{q}dx$$

$$\begin{aligned} &= -\ln(1-x_2) + \frac{S_2}{q}(1-x_2) \\ &= 1 + \ln(2) + \ln\left(\frac{S_2}{S_1}\right) \end{aligned} \tag{28}$$

Combining (23) and (26), and expressing the result in terms of function $R(x)$, we are led to

$$G[P(x)] \;\geq\; \left(2 + \ln\left(\frac{S_2}{S_1}\right)\right) \int_0^1 \frac{P^2(x)}{R(x)} - \left(\int_0^1 P(x)dx\right)^2 \tag{29}$$

To finish the proof, we apply the Cauchy-Schwartz inequality to $\left(\int_0^1 P(x)dx\right)^2$:

$$\begin{aligned} \left(\int_0^1 P(x)dx\right)^2 &= \left(\int_0^1 \sqrt{R(x)} \cdot \frac{P(x)}{\sqrt{R(x)}} dx\right)^2 \\ &\leq \left(\int_0^1 R(x)dx\right) \cdot \left(\int_0^1 \frac{P^2(x)}{R(x)} dx\right) \\ &= \left(1 + \ln(2) + \ln\left(\frac{S_2}{S_1}\right)\right) \cdot \left(\int_0^1 \frac{P^2(x)}{R(x)} dx\right) \end{aligned} \tag{30}$$

Finally, substituting (30) into (29), we conclude

$$G[P(x)] \geq (1 - \ln(2)) \int_0^1 \frac{P^2(x)}{R(x)} dx \geq 0 \tag{31}$$

for all functions $P(x)$ constrained by condition (19). It follows immediately that function $Q(x)$ is indeed the optimal Seebeck coefficient profile for maximizing the cooling temperature.

3 Conclusions

In thermoelectric cooling, the maximum achievable cooling temperature is expressed as a nonlinear functional of the Seebeck coefficient profile of the inhomogeneous materials used. One challenge in thermoelectric cooling applications is to design an optimal Seebeck coefficient profile so that the cooling temperature is maximized. In manufacturing, the Seebeck coefficient is varied by changing the level of doping on a piece of semi-conductor material. The range of the Seebeck coefficient is limited so the Seebeck coefficient profile is constrained between two values. In the study presented, we solved exactly this constrained optimization problem arised in thermoelectric cooling. Specifically, we proved rigorously that a previously conjectured optimal Seebeck coefficient profile is indeed the exact solution of the optimization problem. The methods and techniques employed in the current study may also be useful for other constrained functional optimization problem.

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