Topic area: **CMMSP**

Efficiency of Ideally Filtered Thermionic Devices

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Introduction

It has long been known that thermionic devices may be used for power generation [1–3]. Thermionic refrigeration was first suggested by Mahan using vacuum based devices, however, it was stated that such devices would not be useful for room temperature applications due to the low work functions required [4]. It was then suggested that such small barrier heights may be achieved using semiconductor heterostructures [5, 6] and later, that highly-efficient devices could be constructed using multilayer structures [7, 8]. Successful thermionic cooling has been reported by Shakouri *et al.* using a single barrier InGaAsP based structure [9] and by LaBounty *et al.* using a 25-barrier InGaAsP based multilayer system [10]. The reported cooling in both instances was about one degree.

A thermionic device consists of two electron reservoirs separated by a barrier system, such as a single-barrier or multiple-barrier semiconductor nanostructure. Electrons may travel from one reservoir to the other due to thermal excitation. The system will behave as either a heat engine or refrigerator depending on the bias on the system. If the mean free path of an electron in the system is greater than the separation of the reservoirs then electron transit will be ballistic. For such ballistic travel a quantum-mechanical transmission probability function may be calculated which defines the probability of an electron with a particular energy traversing the system between the reservoirs. Thus, the system between the reservoirs forms an energy filter which may be designed so as to favourably engineer the energy spectrum of transmitted electrons. In a general semiconductor thermionic device, which is translationally invariant in the y and z directions, electron energies will be filtered in the direction of transport, x, only [11]. We shall denote this as a 'k_x filtered thermionic device'. We shall compare this to a theoretical one-dimensional thermionic device which has been previously investigated.

In this paper we shall examine the 'electronic efficiency', which is the efficiency due to electronic processes only. It has been shown for a one-dimensional system that the Carnot efficiency may be achieved with ideal filtering, that is, when electrons of only a single energy are transmitted between the reservoirs [12]. Here it is shown that a three-dimensional k_x filtered thermionic device does not achieve Carnot efficiency for arbitrary reservoir electrochemical potentials.

Theory

Since transport is ballistic we may use the Landauer equation to calculate the electric and heat currents between the reservoirs. For a one-dimensional thermionic device the transmission probability is a function of the total electron energy $E = \hbar^2 k^2/2m^*$. The net electrical current from the cold to hot reservoir is given by [12]

$$I^{1D} = \frac{2e}{h}\int_{U_C}^{\infty}\left[f(E,T_C,\mu_C) - f(E,T_H,\mu_H)\right]\tau(E)dE \tag{1}$$

where

$$f(E,T_{C/H},\mu_{C/H}) = \left[1+\exp\left(\frac{E-\mu_{C/H}}{k_B T_{C/H}}\right)\right]^{-1} \tag{2}$$

is the Fermi-Dirac occupation function, U_C is the bottom energy of the cold reservoir, $\tau(E)$ the transmission probability and $T_{C/H}$ and $\mu_{C/H}$ are the temperatures and electrochemical potentials of the cold/hot reservoirs respectively. It is assumed that the cold reservoir electrochemical potential is greater than that of the hot reservoir.

The heat flux in the cold and hot reservoirs may by calculated by noting that an electron which enters or leaves the cold or hot reservoirs will add or remove energy equal to the difference between the energy of the electron and the average energy of the electrons in the C(old)/H(ot) reservoir, $E-\mu_{C/H}$ [12]. Introducing this inside the number current integral we obtain expressions for the net heat flux out of the cold/hot reservoirs

$$\dot{Q}^{1D}_{C/H} = \pm\int_{U_C}^{\infty}(E-\mu_{C/H})\left[f(E,T_C,\mu_C) - f(E,T_H,\mu_H)\right]\tau(E)dE. \tag{3}$$

In a k_x device, the transmission probability is a function of what may be loosely defined as the 'kinetic energy of electrons in the x direction', $E_x = \hbar^2 k_x^2/2m^*$. It is therefore useful to write the electrical and heat current equations in terms of E_x. Doing so, the electrical current density is given by [13]

$$I^x = e\int_{U_C}^{\infty}\left[N^x(E_x,T_C,\mu_C) - N^x(E_x,T_H,\mu_H)\right]\tau(E_x)dE_x \tag{4}$$

where

$$N^x(E_x,T_{C/H},\mu_{C/H}) = \frac{m^* k_B T_{C/H}}{2\pi^2\hbar^3}\ln\left[1+\exp\left(-\frac{E_x-\mu_{C/H}}{k_B T_{C/H}}\right)\right] \tag{5}$$

is the number of electrons with kinetic energy in the x direction E_x arriving at the reservoir interface per unit area per unit time. In a k_x filtered thermionic device the electron energy components in the y and z directions are unfiltered and the amount of heat removed from a reservoir by a leaving electron is not equal to the amount of heat added when an electron arrives at the reservoir. The energy in the y and z directions may take any value and, assuming Maxwell-Boltzmann statistics, will contribute $k_B T_{C/H}$ to the energy of electrons emitted from the cold/hot reservoir. Thus, the heat current density out of the cold/hot reservoir for a k_x filtered device is given by

$$\dot{Q}^{x}_{C/H} = \pm\int_{U_C}^{\infty}\left[(E_x+k_B T_C-\mu_{C/H})N^x(E_x,T_C,\mu_C) - (E_x+k_B T_H-\mu_{C/H})N^x(E_x,T_H,\mu_H)\right]\tau(E_x)dE_x. \tag{6}$$

The efficiency of the system, under bias V, acting as a heat engine is given by

$$\eta^{1D/x}_{HE} = VI^{1D/x}/\dot{Q}^{1D/x}_{H} \tag{7}$$

and the coefficient of performance (COP) of the system acting as a refrigerator is given by

$$\eta^{1D/x}_{R} = \dot{Q}^{1D/x}_{C}/VI^{1D/x}. \tag{8}$$

For the case of ideal filtering, the transmission probabilities for the k_x and 1D systems are both equal to one for a particular x or total energy value, respectively, and zero elsewhere. Here we may simply evaluate the electric and heat current equation at this energy, removing the integral.

It may be undesirable to use Maxwell-Boltzmann statistics if the energy region of interest is less than $3k_BT$ above the Fermi energy. Using only Fermi-Dirac statistics, the following equation may be found by integrating the Landauer equation over energies in the y and z directions and evaluating for a filter at E_x of intfinitesimal width δE_x

$$\dot{Q}^x_{C_{out/in}} = \frac{4\pi m^*}{h^3}\left((\mu_C - E_x)k_BT_{C/H}\ln\theta - (k_BT_{C/H})^2\left((ln\theta)^2 - PolyLog[2, 1-\theta]\right)\right)\delta E_x \qquad (9)$$

where $\theta = \exp[\alpha]/(exp[\alpha]+1)$, $\alpha = (E_x - \mu_{C/H})/k_BT_{C/H}$, $\text{PolyLog}[n,t] = \sum_{k=1}^{\infty} t^k/k^n$ and the net heat current is given by the difference between the heat currents out of and into the cold reservoir. A similar equation exists for the hot reservoir heat currents. The results given by Equations (6) and (9) differ at low energies, but converge for energies greater than $3k_BT$, as expected.

Efficiency with ideal filtering

The heat-engine efficiency and refrigerator COP relative to the Carnot value have been evaluated for both the one-dimensional and k_x filtered thermionic systems for cold/hot reservoir temperatures and chemical potentials of 270K/300K and 1eV/0.98eV, respectively, as shown in Figure 1.

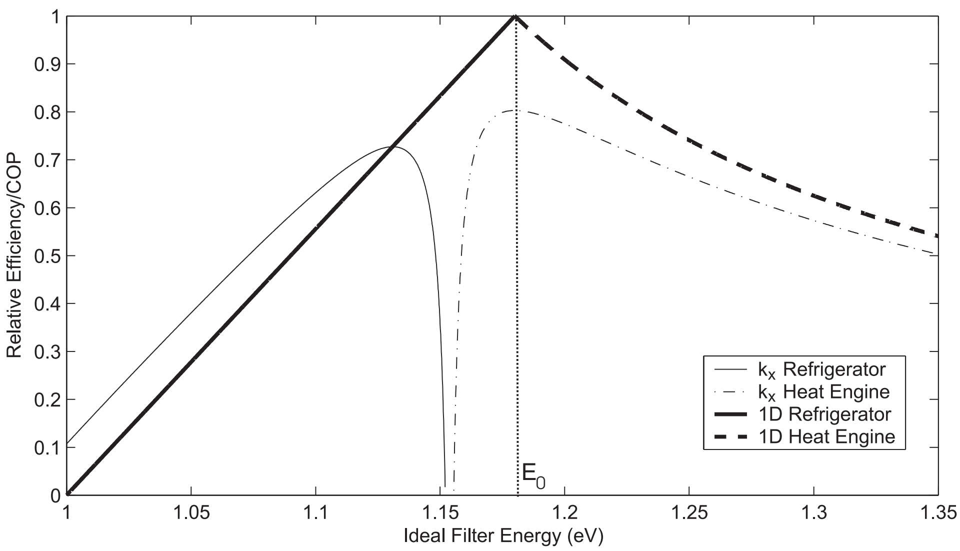

Figure 1: Heat-engine efficiency and refrigerator COP relative to the Carnot value for ideally filtered one-dimensional and k_x thermionic systems versus the energy of the ideal filter.

With ideal filtering the one-dimensional efficiency and COP equations may be reduced to [12]

$$\eta^{1D}_{HE} = (\mu_C - \mu_H)/(E' - \mu_H), \qquad (10)$$

$$\eta^{1D}_{R} = (E' - \mu_C)/(\mu_C - \mu_H). \qquad (11)$$

Both of these are equal to their Carnot values at $E_0 = (\mu_C T_H - \mu_H T_C)/(T_H - T_C)$, as shown on Figure 1. At this energy the reservoirs are in equilibrium and there is no net electric or heat current flow. The k_x ideally filtered thermionic system does not reach the Carnot value, however, for arbitrary chemical potentials. The k_x filtered thermionic system does not filter the energies in the y and z directions which means that reversibility is not achieved.

If we consider the case where $E_x - \mu_{C/H} \gg k_B T_H$, the $k_B T_{C/H}$ terms in Equation (6) may be ignored. In this case the efficiency/COP equations reduce to those above for the one-dimensional ideally filtered system which give the Carnot efficiency at E_0. In order for this condition to be true, we require that

$$eV \gg k_B T_H/\eta^{Carnot}. \tag{12}$$

There are clear energy positions of the ideal k_x energy filter where maximum efficiency or COP is achieved. We may analytically determine the maximum efficiency of the ideally filtered k_x thermionic heat-engine by noting from Figure 1 that this occurs at E_0. It may be shown that the heat engine efficiency will be a maximum at E_0 for $(\mu_C - \mu_H)/(T_H - T_C) \gg 0$, which is generally the case. In this limit the efficiency is given by

$$\eta^x_{HE} = \eta^{Carnot}[1 + \eta^{Carnot} k_B(T_H + T_C)/eV]^{-1}. \tag{13}$$

Conclusions

It has been shown that, unlike an ideally filtered one-dimensional thermionic device, an ideally filtered k_x thermionic device does not achieve Carnot efficiency for arbitrary electrochemical potentials. We therefore conclude, from a theoretical view point with ideal filtering, that a system which filters the total electron energy (such as the one-dimensional thermionic system) may achieve higher efficiency than a k_x filtered device.

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