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Power optimization in thermionic devices

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Abstract
Conventional thermionic power generators and refrigerators utilize a barrier in the direction of transport to selectively transmit high-energy electrons, resulting in an energy spectrum of electrons that is not optimal for high efficiency or high power. Here, we derive the ideal energy spectrum for achieving maximum power in thermionic refrigerators and power generators. By using energy barriers that block or transmit electrons according to their total momentum rather than their momentum in the direction of transport, the power of thermionic devices can, in principle, be doubled and the electronic efficiency improved by 25%.

Thermionic power generators [1] utilize a temperature difference between two reservoirs of electrons to transport high-energy electrons against an electrochemical potential gradient. By increasing the applied voltage between the reservoirs, the same device can operate in reverse as a refrigerator [2–7], using the electrochemical potential difference to remove high-energy ('hot') electrons from the colder reservoir. The required energy selectivity is conventionally achieved by a barrier between the hot and cold reservoirs (figure 1), which may be the work function of the emitter in vacuum devices [1] or a wide bandgap material in solid-state heterostructure devices [8]. Thermionic devices may be distinguished from thermoelectric devices by the use of a barrier that is narrower than the electron mean free path (ballistic transport) [9]. For the purposes of this paper, it is important to note that the 'energy barriers' used in conventional devices may more precisely be called 'k_x-barriers', as they actually constrain the momentum of electrons in the direction of transport only, so that $k_x \geqslant k'_x$. While all electrons with energies less than $E_B = (\hbar k'_x)^2/2m$ are blocked by such a barrier, this conventional design has the drawback that not all electrons with $E \geqslant E_B$ are transmitted [10–12]. The term 'k_r-filter' will be used here to denote a mechanism that selectively transmits electrons in a particular range of $E = (\hbar k_r)^2/2m$, where $k_r^2 = k_x^2 + k_y^2 + k_z^2$. Such a filter could be realized, for instance, via a resonance in a quantum dot [13, 14] or a super-lattice in which there is non-conservation of the lateral momentum of electrons [11, 12]. The difference between the energy spectrum of electrons transmitted in a k_x- and a k_r-filtered device is illustrated in figures 1(*b*) and 2(*b*).

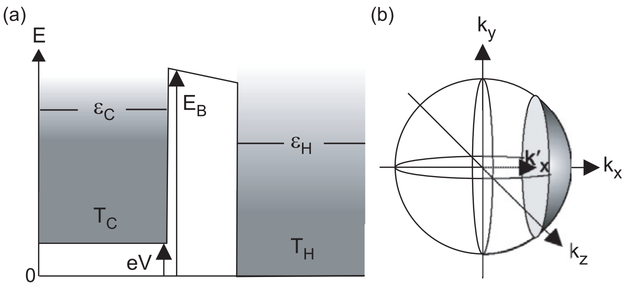

Figure 1. (*a*) Schematic of a conventional thermionic device, consisting of two electron reservoirs with different temperatures and electrochemical potentials. An intervening energy barrier of height $E_B = (\hbar k'_x)^2/2m$ constrains the momentum of electrons in the direction of transport to those with $k_x \geqslant k'_x$. For relatively low voltages, there are more high-energy electrons on the hot side of the barrier, and power is generated by a net electron flow from the hot to the cold reservoirs. If the voltage is increased, the number of high-energy electrons on the cold side of the barrier increases. At the open-circuit voltage, the net current direction reverses, and for higher voltages the device cools the cold reservoir by removing 'hot' electrons. (*b*) The fermi sphere where the segment transmitted for a k_x-barrier ($k_x \geqslant k'_x$) has been shaded.

It was recently shown that an infinitely sharp energy filter can be used to achieve an electronic efficiency (defined as the efficiency in the absence of radiative or phononic heat leaks [1]) equal to the Carnot limit in ballistic electron heat engines [14]. However, devices operating at Carnot efficiency have zero power output, a limit which is not of interest for practical applications. It is a separate optimization problem to find the conditions under which a heat engine

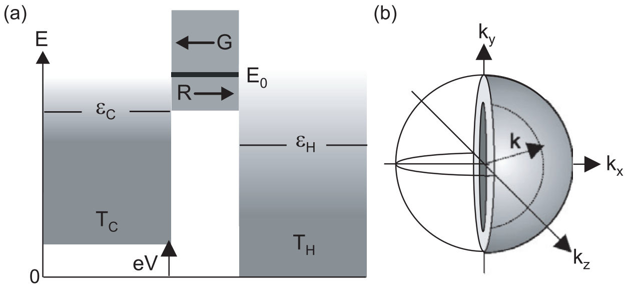

Figure 2. (*a*) At the energy E_0, defined by equation (1), the Fermi distributions in the two reservoirs are equal, $f_C(E_0) = f_H(E_0)$. The letter G indicates the energy range ($E_0 < E < \infty$) for which electrons flow spontaneously from hot to cold, and where power generation occurs. In the range R ($\varepsilon_C < E < E_0$) electrons flow from cold to hot and remove heat from the cold reservoir. (*b*) Fermi sphere showing the thin shell of electrons transmitted by a k_r-filter.

has maximum power output, and to establish the efficiency of the device in this maximum power regime [15]. Here, we derive the energy spectrum of electrons that must be transmitted in thermionic devices to achieve maximum power, and obtain expressions for the theoretical maximum power of thermionic power generators and refrigerators. We find that over a wide temperature range, maximum power is obtained for a barrier height of $1.7kT_H$ for an idealized k_r-filtered device and $1.1kT_H$ for a similarly idealized k_x-filtered device, with the k_r-filtered thermionic power generator having double the maximum power output and a 25% higher efficiency than the k_x-filtered device.

Hot carrier solar cells [16, 17], quantum dot cryogenic refrigerators [13, 18] and quantum Brownian heat engines [10, 14] that employ sharp energy filters have been proposed. It has been shown that ballistic transport of electrons between two reservoirs of free electron gas is an isentropic process at the energy

$$E_0 = \frac{\varepsilon_C T_H - \varepsilon_H T_C}{T_H - T_C}, \qquad (1)$$

where the Fermi distributions, $f_{H/C}(E_0) = [1 + \exp([E_0 - \varepsilon_{H/C}]/kT_{H/C})]^{-1}$, in the hot (H) and cold (C) reservoirs are equal [10, 14]. Measuring energy from the Fermi energy in the hot reservoir (i.e. setting $\varepsilon_H = 0$ for convenience), equation (1) can be written as $E_0 = eV/(1 - T_C/T_H)$, where $eV = (\varepsilon_C - \varepsilon_H)$. For power generation, E_0 satisfies $W = \eta Q_{in}$ [16, 17], where $W = eV$ is the work done by each electron transported from the hot to the cold reservoirs against the electrochemical potential difference, $Q_{in} = (E_0 - \varepsilon_H)$ is the heat removed from the hot reservoir by an electron with energy E_0 and $\eta = (1 - T_C/T_H)$ is the 'Carnot factor', the maximum fraction of heat that may be transformed into useful work by a heat engine working between temperatures T_H and T_C. For refrigeration, E_0 fulfils the condition $Q_{out} = W[T_C/(T_H - T_C)]$, where $[T_C/(T_H - T_C)]$ is the coefficient of performance of a reversible refrigerator and $Q_{out} = (E_0 - \varepsilon_C)$ is the heat removed by an electron with energy E_0 from the cold reservoir.

At E_0, transport of electrons is reversible and there is no thermodynamically spontaneous direction for current to flow. It follows that a ballistic electron heat engine which only transmitted electrons with energy E_0 would produce no power. In this paper, we are interested in the energy spectrum of electrons that should be transmitted for maximum power. We note that electrical power is generated whenever electrons flow from the hot to the cold reservoir. On the other hand, the cold reservoir is refrigerated when electrons from above the electrochemical potential in the cold reservoir flow to the hot reservoir. Over what energy ranges is it a thermodynamically spontaneous process for electrons to flow from the hot to the cold reservoirs and vice-versa?

To proceed, we assume the availability of an idealized energy filter, which transmits all electrons in a desired energy range, which arrive at the interface between reservoirs, and we neglect phonon heat leaks. Using spherical polar coordinates and working in k-space, the particle current density, $\mathrm{d}j_{H/C}(k_r)\delta k_r$, of electrons with momentum in the infinitesimal range δk_r around k_r arriving at the reservoir interface from the hot/cold reservoir is given by

$$\mathrm{d}j_{H/C}(k_r)\delta k_r = 2\int_0^{\pi}\int_{-\pi/2}^{\pi/2} g(\theta, \phi, k_r)v_x(\theta, \phi, k_r) \times f_{H/C}(k)\mathrm{d}\theta\,\mathrm{d}\phi\,\delta k_r, \qquad (2)$$

where the density of states (DOS) of a three-dimensional reservoir is $g = (2\pi)^{-3}k_r^2 \sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi\,\delta k_r$, the velocity of electrons in the x direction (perpendicular to the reservoir interface) is $v_x = \hbar m^{-1}k_r \sin\phi\cos\theta$ and the factor of 2 accounts for degeneracy due to electron spin. The net particle current density of electrons from the hot to the cold reservoirs is then given by $j(k_r)\delta k_r = [j_H(k_r) - j_C(k_r)]\delta k_r$. Evaluating the integral over ϕ and θ, and changing variables to $E = (\hbar k_r)^2/2m$, we obtain

$$j(E)\delta E = \frac{mE}{2\pi^2\hbar^3}[f_H(E) - f_C(E)]\delta E. \qquad (3)$$

Assuming that $T_H > T_C$ and $\varepsilon_C > \varepsilon_H$, then $[f_H(E) - f_C(E)]$ is positive for $E > E_0$, and $j(E)\delta E > 0$. This means that electrons in the range $E_0 < E < \infty$ flow from the hot to the cold reservoirs and do work $W = eV$ each, while electrons transmitted below E_0 actually reduce the power, each consuming work eV as they flow in the 'wrong' direction from the cold to the hot reservoirs. The theoretical maximum power density that can be obtained from a ballistic electron power generator operating at a voltage V is, therefore,

$$P_r^G = eV\int_{E_0}^{\infty} j(E)\delta E. \qquad (4)$$

Below E_0, $f_H(E) < f_C(E)$ and $j(E)\delta E < 0$, so electrons flow from the cold to the hot reservoirs. In order to refrigerate the cold reservoir, transmitted electrons must satisfy $E > \varepsilon_C$ as well, as the heat change δQ_C in the cold reservoir upon removing an electron with energy E is given by $\delta Q_C = (E - \varepsilon_C) = (E - eV)$ (as $\varepsilon_C - \varepsilon_H = eV$ and $\varepsilon_H = 0$). Electrons with $E > E_0$ flow from hot to cold, heating the cold reservoir. The theoretical maximum cooling power density that can be obtained from a ballistic electron refrigerator operating at a voltage V, is therefore,

$$P_r^R = -\int_{\varepsilon_C}^{E_0} (E - eV)j(E)\,\mathrm{d}E. \qquad (5)$$

We now compare these theoretical limits to the maximum power density that may be obtained from an idealized, conventional thermionic device, which utilizes a k_x-barrier.

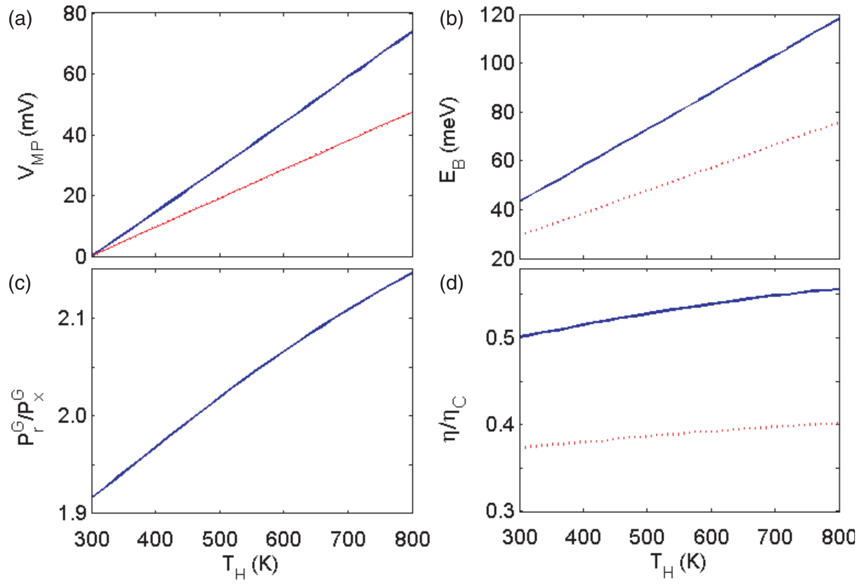

Figure 3. (*a*) The voltage at which maximum power is obtained in a k_r (blue, solid line) and k_x (red, dotted line) filtered thermionic power generator as a function of the temperature of the hot reservoir for $T_C = 300$ K. The gradient of the line for the k_r-filtered device is $1.7 \pm 1\%$ and that for the k_x-filtered device is $1.1 \pm 1\%$. (*b*) The barrier height E_B for which the power is maximised in a k_r (blue, solid line) and k_x (red, dotted line) filtered thermionic device. (*c*) The ratio of P_r^G/P_x^G, showing that an idealized k_r-filtered device produces twice as much power as an idealized k_x-filtered device. (*d*) The electronic efficiency of a k_r (blue, solid line) and k_x (red, dotted line) filtered thermionic power generator operating at maximum power.

(This figure is in colour only in the electronic version)

We assume complete transmission for all available electrons with $k_x > k'_x$ (see figure 1) and zero transmission for electrons with $k_x < k'_x$, and find

$$P_x^G = eV \int_{E_B}^{\infty} \left(\frac{1 - E_B}{E}\right) j(E)\mathrm{d}E, \tag{6}$$

$$P_x^R = -\int_{E_B}^{\infty} \left(\frac{1 - E_B}{E}\right) (E - eV) j(E)\mathrm{d}E, \tag{7}$$

where $E_B \equiv (\hbar k'_x)^2/2m$ ($= E_0$ for maximum power). The multiplicative term $(1 - E_B/E)$ is a geometrical factor giving the fraction of all electrons with energy greater than E_B that are transmitted by devices utilizing a k_x-barrier. This factor makes the integrand in equations (6) and (7) smaller than that in equations (4) and (5), respectively, for all electron energies, so $P_G^{Con} < P_G$ and $P_R^{Con} < P_R$. For the refrigeration regime there is an additional source of non-ideality in the use of a k_x-barrier, which is noticeable when $eV \lesssim kT$. In this case, there is substantial occupation of states above E_0, and transmission of electrons with $E > E_0$ by a k_x-barrier results in a 'backcurrent' of hot electrons flowing from the hot to the cold reservoirs, reducing the refrigerating power below the theoretical maximum, given by equation (5). However, this is not a consideration at the high voltages where the heat current density is maximized ('saturation' [19]) because as $f_H(E_B) \to 0$, $E_0 \to \infty$.

While there is no well defined maximum in the cooling power density as a function of voltage in the refrigeration regime, in the power generation regime there is a particular value of voltage at which the power produced is maximized. In special cases, such as in low-dimensional ballistic electron heat engines, e.g. [13, 14] where the product of the DOS and velocity in equation (2) is independent of energy, the voltage that maximizes the power may be found analytically [10], and, if Maxwell–Boltzmann statistics are assumed, then it can be shown that the power of such a k_r-filtered device is maximized when $eV/(kT_H - kT_C) = 1$ precisely. However, for three-dimensional electron reservoirs with simple DOS as considered here, the voltage at maximum power is most simply found by numerically maximizing equations (4) and (6) with respect to eV. We find that the ratio of the voltage to the temperature difference at maximum power shows very little variation with temperature ($\pm 1\%$ over the range $T_H = 301$–800 K, with $T_C = 300$ K), and is given by $eV/(kT_H - kT_C) \approx 1.7$ for k_r-filtered devices and $eV/(kT_H - kT_C) \approx 1.1$ for k_x-filtered devices. The numerically calculated voltage at maximum power, V_{MP}, is shown in figure 3(*a*) as a function of the temperature in the hot reservoir T_H, for a cold reservoir temperature of $T_C = 300$ K. There is a very simple relationship between this voltage and the optimum barrier height for maximum power, shown in figure 3(*b*), $E_B = T_H e V_{MP}/(kT_H - kT_C)$. These values for the optimum barrier height and voltage at maximum power are unaffected by non-idealities such as radiative or phonon heat leaks, but are influenced by Joule heating in the contacts and leads, which is proportional to the square of the current, and reduces the available power produced by the generator. Ulrich *et al* [20] have shown that finite contact resistance can have a significant impact upon the maximum temperature difference that can be achieved in solid-state refrigerators. It is expected that in practical solid-state thermionic generators with finite contact resistance, the barrier height that yields maximum power will be shifted to higher energies than those calculated above for an idealized generator.

Figure 3(*c*) shows that the power produced by an idealized k_r-filtered thermionic device operating at V_{MP} is double that produced by a similarly optimized k_x-filtered device, while figure 3(*d*) shows that the electronic efficiency of a k_r-filtered thermionic device optimized for power production is about 25% higher than that of a k_x-filtered device. This quite significant increase in power and efficiency is due to the fact that in a k_r-filtered device many more electrons with total energies close to E_0 contribute to the current than in a k_x-filtered device. Such electrons not only contribute to the power produced, but they also do this with a higher-than-average efficiency (up to the Carnot limit for electrons with $E = E_0$). Increasing the fraction of electrons with energies close to E_0, which contribute to the current, will always increase the efficiency of thermionic and thermoelectric [21] devices.

The above results provide design criteria for achieving maximum power in thermionic power generators, and demonstrate that devices that utilize k_r- rather than k_x-barriers offer significant gains in both power and efficiency. Such an improvement would be useful in practical solid-state thermionic devices, where phonon heat leaks are a substantial loss mechanism. In principle, suitable energy filtering for electrons could be implemented in solid-state devices via resonant tunnelling through quantum dots [13], heterostructure nanowires [22], or in materials such as semiconductor/metallic super-lattices in which there is non-conservation of the lateral momentum of electrons [11, 12].

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