

# Local Electron Heating in Nanoscale Conductors

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## ABSTRACT

The electron current density in nanoscale junctions is typically several orders of magnitude larger than the corresponding one in bulk electrodes. Consequently, the electron–electron scattering rate increases substantially in the junction. This leads to local electron heating of the underlying Fermi sea in analogy to the local ionic heating that is due to the increased electron–phonon scattering rates. We predict the bias dependence of local electron heating in quasi-ballistic nanoscale conductors and its effect on ionic heating and discuss possible experimental tests of our results.

In the process of electrical charge transport, the dissipation of energy via heat production plays a significant role. This effect is of particular importance in nanoscale systems, like, e.g., atomic or molecular structures between bulk electrodes,<sup>1</sup> since it determines their structural stability under current flow. It is now understood that the large current densities in nanojunctions, compared to their bulk counterparts, may lead to substantial heating of the nanostructure ions.<sup>2–4</sup> This effect is directly related to the consequent increase of the electron–phonon scattering rates in the junction. In quasi-ballistic systems, i.e., when the mean free path is much longer than the dimensions of the nanostructure, by assuming a bulk lattice heat conduction mechanism, the local ionic temperature is predicted to be  $T_{\text{ion}} \propto V^{1/2}$ , where  $V$  is the applied bias.<sup>2–4</sup> For the same reasons, and due to the viscous nature of the electron liquid,<sup>5</sup> we here suggest that the local increase of the electron–electron scattering rate in the junction gives rise to local heating of the *underlying Fermi sea*, whether the system has one or many conducting channels. This local electronic temperature would also affect the electron–phonon scattering rates and, consequently, the bias dependence of the ionic temperature.

In this Letter, we first estimate the bias dependence of the local electron temperature in quasi-ballistic systems, assuming no ionic heating is produced. We will then determine the effect of the electron heating on the bias dependence of the ionic temperature. We finally discuss possible experiments to test our predictions.

Let us start from a simple argument on the expected bias dependence of the electron heating. Assume first no electron–phonon scattering is present in the system. The power generated in the nanostructure due to exchange of energy

between the current-carrying electrons and the underlying Fermi sea has to be a small fraction of the total power of the circuit  $V^2/R$  ( $R$  is the resistance). Let us define this fraction as  $P = \alpha V^2/R$ , with  $\alpha$  a positive constant to be determined from a microscopic theory. At steady state this power has to balance the thermal current  $I_{\text{th}}$  (heat per unit time) carried away into the bulk electrodes by the electrons. Let us first assume that the electron thermal conductivity  $k$  follows a bulk law; i.e., it is related to the specific heat per unit volume  $c_V$  via the relation  $k = v_F \lambda_e c_V/d$ , where  $v_F$  is the Fermi velocity,  $\lambda_e$  is the electron mean free path, and  $d$  is the dimensionality of the system.<sup>6</sup> We will later give a general argument to justify the form of this law in quasi-ballistic systems away from electronic resonances. We know that at small temperatures the specific heat of an electron liquid is proportional to the electronic temperature  $T_e$  so that

$$k = \gamma T_e \quad (1)$$

where  $\gamma = k_F^2 k_B^2 \lambda_e / 9\hbar$  in three dimensions and  $\gamma = \pi k_F k_B^2 \lambda_e / 6\hbar$  in two dimensions.  $k_F$  is the Fermi momentum and  $k_B$  the Boltzmann constant. The thermal current,  $I_{\text{th}} \propto k T_e$ , is then given by  $I_{\text{th}} = \gamma' T_e^2$ , where  $\gamma'$  has to be determined from microscopic theory. At steady state the condition  $P = I_{\text{th}}$  implies a linear increase of the electronic temperature with bias

$$T_e = \gamma_{e-e} V \quad (2)$$

if the coefficient  $\gamma_{e-e}$  does not vary appreciably with bias. In macroscopic electrical contacts this result is known as the “ $\varphi$ – $\Theta$  relation”.<sup>7</sup> Here, we will rederive it from a microscopic theory and determine the quantity  $\gamma_{e-e}$  in terms

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of the properties of the junction and of the electron liquid. This theory needs to take into account the influence of electron–electron interactions on both the heat production and dissipation. Two of the authors (R.D’A. and M.D.V.) have recently shown that the dynamics of the electron liquid in nanojunctions can be described using a hydrodynamic approach<sup>8</sup> (see ref 9 for a different hydrodynamical approach to the electron liquid flow) so that the equations of motion for the electron density  $n(r,t)$  and velocity field  $v(r,t)$  can be written in the Navier–Stokes form<sup>8,10</sup>

$$Dn(r,t) = -n(r,t)\nabla\cdot v(r,t)$$

$$mn(r,t)D_t v_i(r,t) = -\nabla_i P(r,t) + \nabla_j \sigma_{ij}(r,t) - n(r,t)\nabla_i V_{\text{ext}}(r,t) \quad (3)$$

where  $P$  is the pressure,  $D_t = \partial_t + v\cdot\nabla$  is the convective derivative operator, and  $V_{\text{ext}}$  is an external potential (like the electron-ion potential). The stress tensor  $\sigma_{ij}$  is<sup>5,8,11,12</sup>

$$\sigma_{ij} = \eta\left(\partial_i v_j(r,t) + \partial_j v_i(r,t) - \frac{2}{d}\delta_{ij}\nabla\cdot v\right) + \zeta\delta_{ij}\nabla\cdot v \quad (4)$$

where  $\eta$  and  $\zeta$  are positive parameters which correspond to the shear and bulk viscosity of the liquid, respectively. They have been determined for the electron liquid using linear response theory.<sup>5</sup> Since in the dc limit (the regime of interest here)  $\zeta \ll \eta$ ,<sup>5</sup> in what follows we will consider the shear viscosity only. This term is the one responsible for the heating of the Fermi sea: electrons crossing the junction experience an internal “friction” with the electrons of the underlying Fermi gas, thus creating electron–hole pairs and generating heat. In keeping with this hydrodynamic picture, we supplement eqs 3 for the particle densities and velocity field with an equation which describes the energy dissipation and diffusion. Since the quantity  $\nabla_i \sigma_{ij}$  gives the force acting on the electron liquid caused by viscosity, the equation for the heat transfer reads<sup>10</sup>

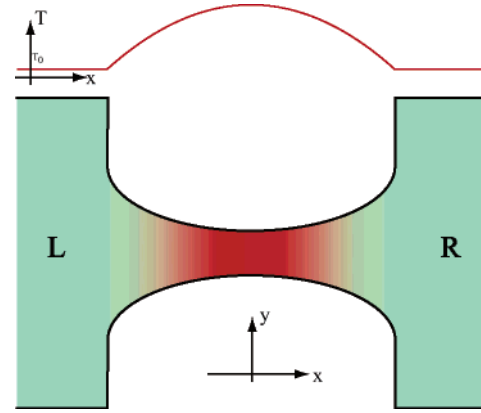
$$T_c(r,t)D_t s(r,t) = \sigma_{ij}(r,t)\partial_j v_i(r,t) + \nabla\cdot[k(r,t)\nabla T_c(r,t)] \quad (5)$$

where  $k$  is again the thermal conductivity and  $s$  is the local entropy per unit volume.<sup>13</sup>

For metallic quantum point contacts (QPCs) of interest here the electron liquid can be assumed incompressible.<sup>14</sup> At steady state eq 5 therefore becomes

$$\sigma_{ij}(r)\partial_j v_i(r) + \nabla\cdot[k(r)\nabla T_c(r)] = c_V(T_c)v(r)\cdot\nabla T_c(r) \quad (6)$$

where we used  $T(r)\nabla s(r) = c_P\nabla T(r)$ ,  $c_P$  being the specific heat per unit volume at constant pressure.<sup>15</sup> For an electron liquid at low temperatures  $c_V \sim c_P$ .<sup>16</sup> Equations 3 and 6, with all quantities time independent, together with the definition of the stress tensor 4, constitute a set of equations that describes the charge and heat flow at steady state. In this effective theory, quantum mechanics enters explicitly in the electron liquid constants  $\eta$ ,  $k$ , and  $c_V$ .<sup>17</sup>



**Figure 1.** Schematic of the local electronic temperature profile of a nanojunction.

Before proceeding with the calculation of the temperature from eq 6, we need to know the form of the thermal conductivity  $k$ . We give here a simple argument to justify the use of the bulk form, eq 1 in quasi-ballistic systems at low temperatures (and bias) and in the absence of electronic resonances. Following the Landauer approach,<sup>18</sup> let us assume the electrons tunnel across the junction from the right electrode which is in local equilibrium with temperature  $T_R$  and chemical potential  $\mu_R$  to the left electrode in local equilibrium with temperature  $T_L$  and chemical potential  $\mu_L$ . If the transmission coefficient for electrons to move elastically from right to left is  $\mathcal{T}(E)$ , the energy current transported by the charge is of the form

$$I_{\text{th}} \propto \int dE E \mathcal{T}(E)[f_{\text{R}}(E, T_{\text{R}}) - f_{\text{L}}(E, T_{\text{L}})] \quad (7)$$

where  $f_{\text{R(L)}}$  is the local Fermi–Dirac distribution function of the right (left) electrode at its own local temperature and chemical potential. Let us set  $T_L = 0$  and consider a small right electrode temperature  $T_R \equiv T_e$ . For small biases, in the absence of electronic resonances, the transmission coefficient  $\mathcal{T}(E)$  can be assumed independent of energy,  $\mathcal{T}(E) \equiv \mathcal{T}$ . From eq 7 we therefore see that  $I_{\text{th}} \propto T_e^2$ , i.e., the thermal conductivity, must be of the form of eq 1. In the following we will assume  $\mathcal{T} \sim 1$ , typical of metallic QPCs, and therefore assume the form of eq 1 for  $k$  with the same coefficients.

In order to obtain the temperature profile of the electron gas inside the nanojunction and evaluate the relation between  $T_e$  and  $V$ , we need to solve eq 6 together with Navier–Stokes equations 3 with the boundary conditions imposed by the geometry of the junction. For an arbitrary system, this is obviously an impossible task. Since we are only interested in the analytical dependence of the temperature on bias, and the estimate of the coefficients in this relation, we proceed as follows. Let us assume a given profile for the velocity of the fluid and solve eq 6 with the boundary condition that the temperature reaches the constant bulk value far away from the constriction. We choose a reference frame in which the direction of the current flow is along the  $x$  axis and the constriction, whose length is  $L$ , is centered at  $x = 0$  (see

Figure 1). Let us also assume that the velocity varies negligibly in the  $(y, z)$  directions compared to the much larger variation along the  $x$  direction.

Since the system has a variable cross section and the total current  $I$  has to be constant throughout the device, the fluid velocity and the cross section of the system are approximately related via

$$I = env_x(x)A(x) \quad (8)$$

The cross-section profile  $A(x)$  contains the information about the geometry of the device. In the following we assume the simplest profile possible which allows an analytical solution: the adiabatic model (see Figure 1)

$$A(x) = (A_c + rx^2)\theta\left(\frac{L^2}{4} - x^2\right) + \left(A_c + r\frac{L^2}{4}\right)\theta\left(x^2 - \frac{L^2}{4}\right) \quad (9)$$

with  $A_c$  and  $r$  positive parameters describing the minimal cross section of the junction and the “rate” at which it opens, respectively, and  $\theta(x)$  is the Heaviside step function.<sup>19</sup> With this choice of the profile  $A(x)$  we get the velocity profile we need to supply in eq 6 to obtain the temperature profile

$$v_x(x) = \frac{I}{ne} \left[ \frac{1}{A_c + rx^2} \theta\left(\frac{L^2}{4} - x^2\right) + \frac{1}{A_c + rL^2/4} \theta\left(x^2 - \frac{L^2}{4}\right) \right] \quad (10)$$

The total electron velocity  $u(x)$  is the sum of the Fermi velocity and the fluid velocity,  $u = v_F + v_x$ . In the bulk where the heating can be considered negligible,  $u$  is related to the applied bias voltage via  $mu^2 = 2(E_F + eV)$ , and since, in general,  $v_x \ll v_F$  we get  $v_x = eV/mv_F$  for the fluid velocity in the bulk.<sup>20</sup> This is the boundary condition that eq 10 has to satisfy for  $|x| \geq L/2$ , i.e.,  $A_c + rL^2/4 = mv_F I / ne^2 V$ . This condition implies  $rL^2/4A_c \sim 1$ , which simply reflects the physical fact that, due to screening, the electron velocity approaches the bulk value very fast away from the junction.

In the following we assume that deep inside the electrodes the electron gas is in equilibrium with a zero-temperature thermal bath, i.e.,  $\lim_{|x| \rightarrow \infty} T_e(x) = 0$ .<sup>21</sup> The solution to eq 6 can be calculated analytically and expressed in terms of a combination of rational, trigonometric, and hypergeometric functions. From this solution we can estimate that the contribution of the advection term  $c_V v \cdot \nabla T$  is controlled by the dimensionless quantity  $\Gamma \equiv (Id/v_F \lambda_c ne A_c)(A_c/r)^{1/2}$ . Due to the quasi-ballistic assumption, we find  $\Gamma \ll 1$  so that the advection term can be neglected.

In the absence of the advection term the solution to eq 6 inside the constriction ( $|x| < L/2$ ) is given by

$$T_e^2(x) = \left(\frac{I}{neA_c}\right)^2 \left[ \frac{(d-1)\eta}{3d\gamma} \right] \left\{ \frac{1 - rL^2/4A_c}{(1 + rL^2/4A_c)^2} - \frac{1 - rx^2/A_c}{(1 + rx^2/A_c)^2} + 3\left(\frac{r}{A_c}\right)^{1/2} \left[ \frac{L}{2} \tan^{-1}\left(\left(\frac{r}{A_c}\right)^{1/2} \frac{L}{2}\right) - x \tan^{-1}\left(\left(\frac{r}{A_c}\right)^{1/2} x\right) \right] \right\} \quad (11)$$

Let us then estimate the maximum temperature which, in the absence of the advection term, occurs at  $x = 0$

$$T_M = \left(\frac{I}{neA_c}\right) \left(\frac{d-1}{3d} \frac{\eta}{\gamma}\right)^{1/2} \left( 3\left(\frac{r}{A_c}\right)^{1/2} \frac{L}{2} \tan^{-1}\left(\left(\frac{r}{A_c}\right)^{1/2} \frac{L}{2}\right) + \frac{1 - rL^2/4A_c}{(1 + rL^2/4A_c)^2} - 1 \right)^{1/2} \quad (12)$$

In the linear transport regime and for  $\mathcal{T} \sim 1$ ,  $I = G_0 V$  with  $G_0 = 2e^2/h$ . As we have anticipated in eq 2, the relation between the temperature and the bias then simplifies to  $T_M = \gamma_{e-e} V$ , where  $\gamma_{e-e}$  is a constant that can be read from eq 12. It is interesting to note that a similar expression has been found in the case of superconducting junctions, where, however, the maximum temperature inside the junction is found to be independent of both the junction geometry and the electron properties.<sup>22</sup>

By using the expression of  $\eta$  as a function of the particle density given in ref 5, we can estimate the value of the constant  $\gamma_{e-e}$  for various systems. We consider here both a three-dimensional (3D) gold point contact and a two-dimensional (2D) electron gas (2DEG). For a 3D gold ( $r_s = 3$ ) QPC with effective cross section  $A_c = 7.0 \text{ \AA}^2$ , by assuming a typical inelastic mean free path in quasi-ballistic systems of  $\lambda_e \sim 100 \text{ nm}$ , we get  $\gamma_{e-e}(\text{QPC}) \approx 65 \text{ K/V}$ . For a 2DEG, assuming  $r_s = 10$ ,  $\lambda_e \approx 10 \text{ \mu m}$ , and  $A_c = 20 \text{ nm}$ , we get  $\gamma_{e-e}(\text{2DEG}) \approx 1.2 \times 10^2 \text{ K/V}$ .

Let us now discuss the effect of local electron heating on the ionic heating. In the 2DEG we expect a negligible heating of the ions. In atomic-scale junctions, instead, the ions may heat up substantially due to electron–phonon scattering. As discussed at the beginning of the paper, the ionic temperature in quasi-ballistic systems is predicted to be  $T_{\text{ion}} = \gamma_{e-p} V^{1/2}$ , if no electron heating is taken into account. The constant  $\gamma_{e-p}$  has been estimated in refs 2 and 3 for atomic and molecular systems. If we now allow for the electron heating, then part of the ionic heating is lost in favor of the local electron temperature. Since the source of energy is the same for both processes (the kinetic energy of the electron), the ionic temperature must be *lower* in the presence of the electron heating than without it. To first order we can assume the electron–electron and electron–phonon processes independent and occurring with equal probability. Let us also suppose that, for a given bias, the local electron temperature in the absence of electron–phonon scattering,  $T_e$ , is smaller than the ionic temperature in the absence of electron heating,  $T_{\text{ion}}$ . The energy lost by an electron due to heating is “seen” by the phonons as a “sink” of energy at the electron temperature  $T_e$ . This energy however is “lost” by the phonons at their own rate. The balance between the power absorbed by the phonons in the junction and the power dissipated away at steady state therefore gives the new ionic temperature

$$T_w = [\gamma_{e-p}^4 V^2 - \gamma_{e-e}^4 V^4]^{1/4} \quad (13)$$

If  $T_{\text{ion}} \approx T_e$ , the processes of energy release from current-carrying electrons to the phonon gas or to the Fermi sea cannot be considered independent and a microscopic theory that considers them on equal footing is needed.

We point out that for metallic QPCs the theoretical values for  $\gamma_{e-p}$  are of the order of hundreds of  $K/V^{1/2}$  while our estimate for  $\gamma_{e-e}$  is of the order of tens of  $K/V$ .<sup>2,3</sup> We thus expect that, for these systems, the electron heating contribution to the ionic temperature is small for a wide range of biases. In the case of a 2DEG, on the other hand, either the ionic heating is not present or it is very small and it may be possible to measure the effects of the electron temperature directly. In the case of organic molecules between metallic electrodes, it is known that  $\gamma_{e-p}$  decreases exponentially with the length of the molecules.<sup>3</sup> For such systems, we thus expect the two effects to be of similar importance and one should therefore be able to observe deviations from the  $V^{1/2}$  dependence of the ionic temperature due to electron heating as predicted in eq 13. However, the exact value of the parameter  $\gamma_{e-e}$  requires generalization of the present theory to the case of nonideal conductance, i.e., for a transmission coefficient  $\mathcal{T}$  less than 1. This can, in principle, be done, but no general analytical solution can be derived. The reason is that one needs to know both the thermal conductivity dependence on the transmission coefficient and the junction profile that leads to such a coefficient. For  $\mathcal{T} \ll 1$  this may even lead to a nonlinear dependence of  $T_e$  as a function of  $V$ . We can however comment that if one works at fixed current while varying  $\mathcal{T}$ , for example, by acting with a gate voltage or by stretching the chemical bonds of the molecule, an increase of electron temperature due to reduced thermal conductivity is expected. We finally suggest that the local increase of the electron temperature in a nanojunction may be extracted by measuring the Johnson–Nyquist noise.<sup>23</sup> Any deviation of this noise compared to the expected one in the absence of electron heating may give direct evidence of this effect.

In conclusion, we have discussed the phenomenon of local electron heating in nanoscale junctions. We have predicted its bias dependence and estimated, using a hydrodynamic approach, its magnitude in quasi-ballistic systems. We have also discussed its role on the local ionic heating and suggested systems where this effect is most likely to be observed.

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- (15) In eq 8 we are assuming that the temperature variations are small so that the density fluctuations due to temperature can be neglected.
- (16) We assume that the system is in local thermal equilibrium; thus local thermodynamic quantities such as energy and entropy densities can be defined.
- (17) It is well-known that for a translationally invariant electron, liquid  $\eta(\omega=0)$  diverges for small temperatures as  $1/T_e^2$ . (See: Abrikosov, A. A.; Khalatnikov, I. M. *Rep. Prog. Phys.* **1959**, *22*, 330.) The presence of the nanojunction breaks translational invariance thus putting an effective cut-off to this divergence. We can see this as follows. In an ideal electron liquid the divergence of  $\eta$  can be understood by bearing in mind that  $\eta$  is related via a Kramers–Kronig relation to the value of the shear modulus  $\mu_\infty$ . We thus have  $\mu_\infty = \int d\omega \eta(\omega)/\pi \propto \eta(\omega=0)/\tau$  where  $\tau$  is the quasi-particle lifetime, which in an ideal electron liquid diverges as  $1/T_e^2$ . However, the constriction introduces another lifetime  $\tau_c$  due to the elastic scattering with the junction<sup>8</sup> which cuts-off the divergence of  $\eta(\omega=0)$  via the relation  $\eta(\omega=0) = \mu_\infty \tau_c$ . (See also: Di Ventra, M.; Todorov, T. N. *J. Phys.: Condens. Matter* **2004**, *16*, 8025. Bushong, N.; Sai, N.; Di Ventra, M. *Nano Lett.* **2005**, *5*, 2569.)
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- (19)  $\theta(x) = 1$  if  $x > 0$ ,  $\theta(0) = 1/2$ , and 0 otherwise.
- (20) In this hydrodynamic picture, the Fermi velocity does not contribute to the fluid velocity, the former being an “incoherent” part of the electron motion.
- (21) If the electron temperature inside the electrodes,  $T_0$ , is not zero, the electron temperature is  $T^2(x) = T_0^2 + T_e^2(x)$ , with  $T_e^2(x)$  given in eq 11.
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