

# Effect of electron-phonon scattering on shot noise in nanoscale junctions

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We investigate the effect of electron-phonon inelastic scattering on shot noise in nanoscale junctions in the regime of quasi-ballistic transport. We predict that when the local temperature of the junction is larger than its lowest vibrational mode energy  $eV_c$ , the inelastic contribution to shot noise (conductance) increases (decreases) with bias as  $V$  ( $\sqrt{V}$ ). The corresponding Fano factor thus increases as  $\sqrt{V}$ . We also show that the inelastic contribution to the Fano factor saturates with increasing thermal current exchanged between the junction and the bulk electrodes to a value which, for  $V \gg V_c$ , is independent of bias. A measurement of shot noise may thus provide information about the local temperature and heat dissipation in nanoscale conductors.

It is an established fact that for systems with dimensions much longer than the inelastic mean free path  $\lambda_{ph}$  (e.g. a macroscopic sample) steady-state zero temperature current fluctuations (shot noise) are suppressed by electron-phonon scattering [1, 2, 3]. Similarly, for metallic diffusive wires with length much smaller than  $\lambda_{ph}$  (and smaller than the electron-electron scattering length), the Fano factor (i.e. the ratio between shot noise and its Poisson value,  $2eI$ , where  $e$  is the electron charge and  $I$  is the current of the system) equals 1/3 and is not affected by inelastic processes [4]. Systems of nanoscale dimensions may not fall in either one of the above cases. In this instance each electron, on average, releases only a small fraction of its energy to the underlying atomic structure during the time it spends in the junction, making transport quasi-ballistic [5, 6, 7, 8, 9, 10, 11]. However, the current density and, consequently, the power per atom are much larger in the junction compared to the bulk. This leads to heating and inelastic features in the differential conduction which are indeed observed in experiments with metallic quantum point contacts [12, 13, 14, 15] and molecular structures [8, 10, 16, 17, 18] as a direct consequence of the interplay between electron and phonon statistics [19]. For these systems it is therefore not obvious what is the effect of inelastic scattering on shot noise.

In this Letter we show analytically that shot noise in quasi-ballistic nanoscale junctions is enhanced by inelastic scattering whenever electrons have enough energy to excite the phonon modes of the junction. The current instead decreases. As a consequence, the Fano factor increases. We find it increases with bias as  $\sqrt{V}$  when the local temperature of the junction is larger than its lowest vibrational mode energy  $eV_c$ . We also show that with increasing thermal current carried away from the junction to the bulk electrodes, the inelastic contribution to the Fano factor converges to a minimum value independent of bias for  $V \gg V_c$ . A measurement of the Fano factor may thus provide information about the local temperature and heat dissipation in nanoscale conductors.

Transport in a model atomic gold point contact will be used to illustrate these findings.

Since the dimensions of the junction are much smaller than  $\lambda_{ph}$  (and the observed inelastic features in quasi-ballistic systems are very small [12, 16, 17]) first-order perturbation theory in the electron-phonon coupling captures the dominant contribution to inelastic scattering. This is the contribution we calculate in this paper.

Let us assume that the junction is connected to two biased bulk electrodes. The electronic states of the full system are thus described by the field operator  $\hat{\Psi} = \sum_{E,\alpha=L,R} a_E^\alpha \Psi_E^\alpha(\mathbf{r}, \mathbf{K}_\parallel)$ , constructed from the single-particle wave functions  $\Psi_E^{L(R)}(\mathbf{r}, \mathbf{K}_\parallel)$  and annihilation operators  $a_E^{L(R)}$  corresponding to electrons propagating from the left (right) electrode at energy  $E$ .  $\mathbf{K}_\parallel$  is the transverse component of the momentum [21]. We also assume that the electrons rapidly thermalize into the bulk electrodes so that their statistics are given by the equilibrium Fermi-Dirac distribution,  $f_E^{L(R)} = 1/(\exp[(E - E_{FL(R)})/k_B T_e] + 1)$  in the left (right) electrodes with local chemical potential  $E_{FL(R)}$ , where  $T_e$  is the electronic temperature. In the following we will assume that  $T_e = 0$  K [20], and the left electrode is positively biased so that  $E_{FL} < E_{FR}$ . The stationary scattering states  $\Psi_E^{L(R)}(\mathbf{r}, \mathbf{K}_\parallel)$  are eigenstates of an effective single-particle Hamiltonian  $H_e$  which may be computed, e.g., using a scattering approach within the static density-functional theory of many-electron systems [21]. The combined dynamics of electrons and phonons is described by the Hamiltonian (atomic units will be used throughout this paper) [8]

$$H = H_e + H_{ph} + H_{e-ph}, \quad (1)$$

where  $H_{ph} = \frac{1}{2} \sum_{i,\mu \in vib} \dot{q}_{i\mu}^2 + \frac{1}{2} \sum_{i,\mu \in vib} \omega_{i\mu}^2 q_{i\mu}^2$  is the phonon contribution, with  $q_{i\mu}$  the normal coordinate and  $\omega_{i\mu}$  the normal frequency of the vibration labeled by the  $\mu$ -th component of the  $i$ -th ion.  $H_{e-ph}$  describes the electron-phonon interaction and has the following form [8]

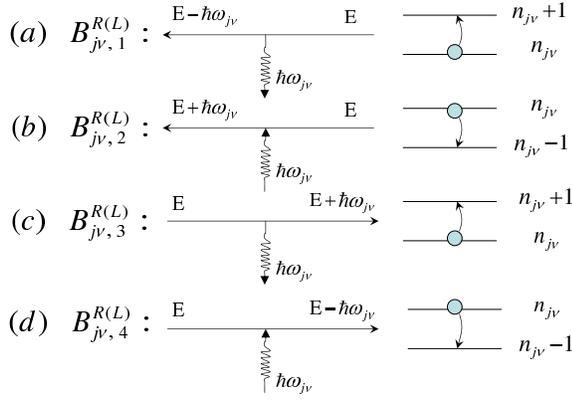


FIG. 1: Feynman diagrams and corresponding amplitudes (see text) of the main electron-phonon scattering mechanisms contributing to the correction of the current and noise.

$$H_{e-ph} = \sum_{\alpha,\beta} \sum_{E_1, E_2} \sum_{i\mu, j\nu \in vib} \sqrt{\frac{1}{2\omega_{j\nu}}} A_{i\mu, j\nu} J_{E_1, E_2}^{i\mu, \alpha\beta} a_{E_1}^{\alpha\dagger} a_{E_2}^{\beta} (b_{j\nu} + b_{j\nu}^{\dagger}), \quad (2)$$

where  $\alpha = L, R$  and  $b_{j\nu}$  is the phonon annihilation operator.  $\{A_{i\mu, j\nu}\}$  is the transformation matrix that relates Cartesian coordinates to normal coordinates, and  $J_{E_1, E_2}^{i\mu, \alpha\beta}$  is the electron-phonon coupling constant which can be directly calculated from the scattering wave-functions

$$J_{E_1, E_2}^{i\mu, \alpha\beta} = \int d\mathbf{r} \int d\mathbf{K}_{\parallel} \Psi_{E_1}^{\alpha*}(\mathbf{r}, \mathbf{K}_{\parallel}) \partial_{\mu} V^{ps}(\mathbf{r}, \mathbf{R}_i) \Psi_{E_2}^{\beta}(\mathbf{r}, \mathbf{K}_{\parallel}), \quad (3)$$

where we have chosen to describe the electron-ion interaction with pseudopotentials  $V^{ps}(\mathbf{r}, \mathbf{R}_i)$  for each  $i$ -th ion [21].

We use as unperturbed states of the full system (electron plus phonon) the states  $|\Psi_E^{L(R)}; n_{j\nu}\rangle = |\Psi_E^{L(R)}(\mathbf{r}, \mathbf{K}_{\parallel})\rangle \otimes |n_{j\nu}\rangle$ , where  $n_{j\nu}$  is the occupation number of the  $j\nu$ -th normal mode. The first-order perturbation to the wave functions is thus

$$|\Phi_E^{L(R)}; n_{j\nu}\rangle = |\Psi_E^{L(R)}; n_{j\nu}\rangle + |\delta\Psi_E^{L(R)}; n_{j\nu}\rangle, \quad (4)$$

where the first-order correction term is

$$|\delta\Psi_E^{\alpha}; n_{j\nu}\rangle = \lim_{\epsilon \rightarrow 0^+} \sum_{\alpha'=L, R} \sum_{j'\nu'} \int dE' D_{E'}^{\alpha'} \frac{\langle \Psi_{E'}^{\alpha'}; n_{j'\nu'} | H_{el-vib} | \Psi_E^{\alpha}; n_{j\nu} \rangle \langle \Psi_{E'}^{\alpha'}; n_{j'\nu'} |}{\varepsilon(E, n_{j\nu}) - \varepsilon(E', n_{j'\nu'}) - i\epsilon}, \quad (5)$$

with  $D_E^{R(L)}$  the partial density of states of left (right) moving electrons, and  $\varepsilon(E, n_{j\nu}) = E + (n_{j\nu} + 1/2)\omega_{j\nu}$  the energy of state  $|\Psi_E^{\alpha}; n_{j\nu}\rangle$ . Carrying out explicitly the integrals in Eq. (5), the nonvanishing corrections to the wave function can be written as

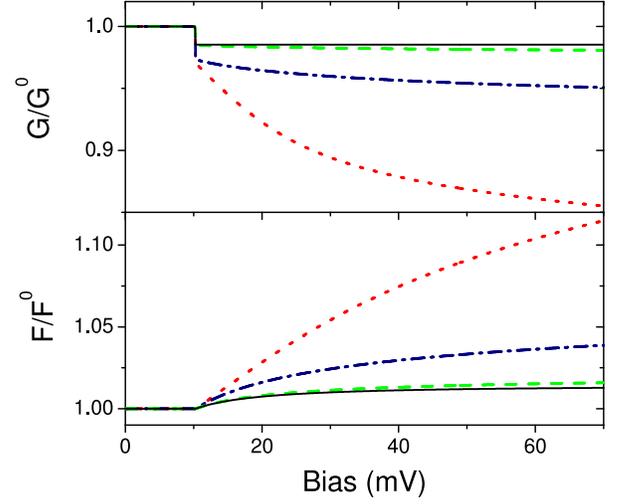


FIG. 2: Top panel: ratio of the total conductance  $G$  of an atomic gold point contact and its value in the absence of inelastic effects  $G^0$  as a function of bias for different values of thermal current coefficient (see text):  $A_{th} = 10^{-19}$  (dot),  $10^{-17}$  (dot-dashed),  $10^{-15}$  (dashed), and  $\infty$  (solid)  $\text{dyn}/(\text{sK}^4)$ . Bottom panel: corresponding Fano factor ratio.

$$|\delta\Psi_E^{\alpha}; n_{j\nu}\rangle = (B_{j\nu,1}^{\alpha} + B_{j\nu,3}^{\alpha}) |\Psi_{E+\omega_{j\nu}}^{\alpha}; n_{j\nu} + 1\rangle + (B_{j\nu,2}^{\alpha} + B_{j\nu,4}^{\alpha}) |\Psi_{E-\omega_{j\nu}}^{\alpha}; n_{j\nu} - 1\rangle, \quad (6)$$

where  $B_{j\nu,1}^{\alpha}$ ,  $B_{j\nu,2}^{\alpha}$ ,  $B_{j\nu,3}^{\alpha}$  and  $B_{j\nu,4}^{\alpha}$  correspond to the diagrams depicted in Fig. 1. For  $|\delta\Psi_E^R; n_{j\nu}\rangle$ , the coefficients are given by:

$$B_{j\nu,1(2)}^R = i\pi \sum_{i\mu} \sqrt{\frac{1}{2\omega_{j\nu}}} A_{i\mu, j\nu} J_{E\pm\omega_{j\nu}, E}^{i\mu, LR} D_{E\pm\omega_{j\nu}}^L \cdot \sqrt{(\delta + \langle n_{j\nu} \rangle) f_E^R (1 - f_{E\pm\omega_{j\nu}}^L)}, \quad (7)$$

and

$$B_{j\nu,3(4)}^R = -i\pi \sum_{i\mu} \sqrt{\frac{1}{2\omega_{j\nu}}} A_{i\mu, j\nu} J_{E\pm\omega_{j\nu}, E}^{i\mu, RL} D_{E\pm\omega_{j\nu}}^L \cdot \sqrt{(\delta + \langle n_{j\nu} \rangle) f_E^L (1 - f_{E\pm\omega_{j\nu}}^R)}, \quad (8)$$

where  $\delta = 1$  and "−" sign are for the scattering diagrams (a) and (c);  $\delta = 0$  and "+" sign for diagrams (b) and (d). The average number of phonons is given by  $\langle n_{j\nu} \rangle = 1/[\exp(\omega_{j\nu}/k_B T_w) - 1]$  where  $T_w$  is the local temperature of the junction [8, 10]. Similarly, the coefficients in  $|\delta\Psi_E^L; n_{j\nu}\rangle$  have the forms

$$B_{j\nu, k}^L = B_{j\nu, k}^R (L \Leftrightarrow R), \quad (9)$$

where  $k = 1, \dots, 4$ ; the notation  $(L \Leftrightarrow R)$  means interchange of labels R and L.

At  $T_e = 0$  K the first-order correction to the current is thus:

$$I = -i \int_{E_{FL}}^{E_{FR}} dE \int d\mathbf{R} \int d\mathbf{K}_{\parallel} \tilde{I}_{E,E}^{RR} \cdot \left[ 1 - \sum_{j\nu} (|B_{j\nu,1}^R|^2 + |B_{j\nu,2}^R|^2) \right], \quad (10)$$

with  $\tilde{I}_{E,E}^{\alpha\beta} \equiv (\Psi_E^\alpha)^* \partial_z (\Psi_E^\beta) - \partial_z (\Psi_E^\alpha) (\Psi_E^\beta)$ . Equation (10) has been simplified by using (i)  $\tilde{I}_{E\pm\omega_{j\nu}, E\pm\omega_{j\nu}}^{RR} \simeq \tilde{I}_{E,E}^{RR}$ , valid for energies close to the chemical potentials; and (ii)  $\tilde{I}_{E,E}^{RR} = -\tilde{I}_{E,E}^{LL}$ , a direct consequence of time-reversal symmetry. The current is therefore reduced by inelastic effects.

Let us now calculate the corresponding correction to shot noise. We have previously shown that shot noise can be written in terms of single-particle scattering states as [22, 23]

$$S = \int_{E_{FL}}^{E_{FR}} dE \left| \int d\mathbf{R} \int d\mathbf{K} \tilde{I}_{E,E}^{LR} \right|^2, \quad (11)$$

which reduces to the well-known formula  $S \propto \sum_i T_i (1 - T_i)$  when the eigenchannels transmission probabilities  $T_i$  are extracted from the single-particle states with independent transverse momenta [1, 22, 23]. Replacing (4) into (11) we get

$$S = \int_{E_{FL}}^{E_{FR}} dE \left| \int d\mathbf{R} \int d\mathbf{K} \tilde{I}_{E,E}^{LR} \right|^2 \cdot [1 + \sum_{j\nu; k=1,2} (|B_{j\nu,k}^R \cdot B_{j\nu,k}^{L*}|^2)]. \quad (12)$$

Since the summation over vibrational modes contains only positive terms, shot noise is *enhanced* by electron-phonon inelastic effects in the quasi-ballistic regime. Therefore, the Fano factor  $F$  normalized to the corresponding value in the absence of electron-phonon interactions ( $F^0$ ) is

$$F/F^0 = \frac{\int_{E_{FL}}^{E_{FR}} dE \left[ 1 + \sum_{j\nu, k=1,2} (|B_{j\nu,k}^R \cdot B_{j\nu,k}^{L*}|^2) \right]}{\int_{E_{FL}}^{E_{FR}} dE \left[ 1 - \sum_{j\nu, k=1,2} |B_{j\nu,k}^R|^2 \right]}, \quad (13)$$

which *increases* with electron-phonon scattering.

Note that due to the orthogonality of phonon states, the absolute value of the correction to shot noise is smaller than that to the current (cf. Eq. (10) and Eq. (12)). Note also that conservation of energy and the Pauli exclusion principle play an important role. The former dictates an onset bias  $V_c$  for inelastic contributions;

the latter prohibits the scattering processes depicted in Fig. 1(c) and (d) at  $T_e = 0$  K.

These results are illustrated in Fig. 2 where the inelastic contribution to the conductance and shot noise are plotted for a gold atom placed in the middle of two bulk gold electrodes (represented with ideal metals, jellium model,  $r_s \approx 3$ ). Details of the calculations of both the scattering wavefunctions within static density-functional theory and the vibrational modes for this system can be found in Refs. [8, 21]. In the absence of electron-phonon interactions, the unperturbed differential conductance  $G^0$  is about 1.1 (in units of  $2e^2/h$ ) and the Fano factor is  $F^0 \simeq 0.14$  [22] in the bias range of Fig. 2. Inelastic effects cause a discontinuity in the conductance, and a variation of the Fano factor ratio (Eqs. (13)), at a bias  $V_c \approx 11$  mV, corresponding to the energy of the lowest longitudinal mode of the system. In addition, the above inelastic corrections depend on the local temperature of the junction  $T_w$  (see Eqs. (7) through (9)) which, in turn, is the result of the competition between the rate of heat generated locally in the nanostructure and the thermal current  $I_{th}$  carried away into the bulk electrodes [5, 6, 7, 8, 10, 11]. The latter has a temperature dependence of  $I_{th} = A_{th} T^4$  [24], where the constant  $A_{th}$  depends on the details of the coupling between the local modes of the junction and the modes of the bulk electrodes. At steady state this thermal current has to balance the power generated in the nanostructure, which is a small fraction of the total power of the circuit  $\frac{V^2}{R}$  ( $V$  is the bias,  $R$  is the resistance) [5, 8].

The larger  $A_{th}$ , the larger the heat dissipated into the bulk and, thus, the lower the local temperature  $T_w$  [25]. In the limit of infinite  $A_{th}$ , i.e.  $T_w = 0$ , at any given bias larger than  $V_c$ , electrons can only emit phonons [ $\langle n_{j\nu} \rangle = 0$  in Eqs. (7) and (8)]. The inelastic contribution to the conductance and Fano factor, therefore, saturate to a specific value (see Fig. 2). We can derive both the bias dependence and this saturation value, to first order in the bias, as follows.

By equating the thermal current  $I_{th}$  to the power generated in the junction, it is easy to show that  $T_w = \alpha \sqrt{V}$  [7, 26], where the constant  $\alpha$  depends on the details of the thermal contacts between the junction and electrodes. Let us assume for simplicity a single phonon mode of frequency  $\omega$ . For  $T_w > \omega/k_B$ , we expand  $\langle n_{j\nu} \rangle \approx k_B T_w / \omega$  in Eqs. (7) and (8). From Eq. (10) we then get

$$\frac{G}{G^0} \simeq 1 - \alpha \frac{3 k_B}{2 \omega} \gamma_I \theta(V - V_c) \sqrt{V}, \quad (14)$$

where  $\theta(V - V_c)$  is the Heaviside function;  $\gamma_I = |(dI/dV) / (dI^0/dV)|$  is the relative change in conductance due to inelastic effects at  $V_c$  (its value is about 1% for the specific case, in agreement with experiments on similar systems [8, 12]). The inelastic contribution to

the conductance thus decreases with bias as  $\sqrt{V}$ . This square-root dependence is clear in Fig. 2 for  $A_{th} < 10^{-15}$  dyn/(sK<sup>4</sup>) which corresponds to temperatures for which the condition  $T_w > \omega/k_B$  is satisfied [27].

The same analysis applied to shot noise leads to

$$\frac{S}{S^0} \simeq 1 + \alpha^2 \left( \frac{k_B}{\omega} \right)^2 \gamma_S \theta(V - V_c)(V - V_c), \quad (15)$$

where  $\gamma_S = |(dS/dV) / (dS^0/dV)|$  is the relative change of shot noise due to inelastic effects at  $V = V_c$  (it is about 0.04 % for the specific gold quantum point contact). The inelastic correction to shot noise thus increases linearly with bias for  $T_w > \omega/k_B$ . Consequently,  $F/F^0 \propto \sqrt{V}$  as it is also evident from Fig. 2.

In the opposite limit of perfect heat dissipation in the bulk electrodes, i.e. for  $T_w \rightarrow 0$  [see Fig. 2,  $A_{th} \rightarrow \infty$  dyn/(sK<sup>4</sup>)], then from Eqs. (7) and (8) it is easy to prove that  $I/I_0 = 1 - \theta(V - V_c)\gamma_I(V - V_c)/V$  and  $S/S_0 = 1 + \gamma_S [(V - V_c)/V]\theta(V - V_c)$ . Therefore,

$$F/F^0 = \frac{1 + \gamma_S \frac{V - V_c}{V} \theta(V - V_c)}{1 - \gamma_I \frac{V - V_c}{V} \theta(V - V_c)}, \quad (16)$$

which tends to the constant value  $F/F^0 \rightarrow (1 + \gamma_S)/(1 - \gamma_I)$  as  $V \gg V_c$ .

We have thus shown that the Fano factor depends sensitively on the efficiency of heat dissipation in nanoscale junctions. It therefore provides a tool to probe local temperatures and heat transport mechanisms in these systems. The predictions reported here should be readily tested experimentally.

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<sup>26</sup> The thermal current scales as  $l^{-2}$  with wire length  $l$  (Ref. [24]). On the other hand, the power dissipated in the junction has weak length dependence for metallic wires [7, 8, 11]; instead it scales as  $\exp(-\beta l)$  for insulating junctions, where  $\beta$  is a characteristic inverse length of the wire [10]. The local temperature of the wire thus scales with length as  $\sqrt{l}$  [5, 15] and  $\exp(-\frac{\beta l}{4})$  [8, 10] for metallic and insulating wires, respectively.

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