

LETTER TO THE EDITOR

Injection statistics simulator for dynamic analysis of noise in mesoscopic devices

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Abstract. We present a model for electron injection from thermal reservoirs, which is applied to particle simulations of one-dimensional mesoscopic conductors. The statistics of injected carriers is correctly described from non-degenerate to completely degenerate conditions. The model is validated by comparing Monte Carlo simulations with existing analytical results for the case of ballistic conductors. An excellent agreement is found for the average and noise characteristics, in particular, the fundamental unities of electrical and thermal conductances are exactly reproduced.

The systematic trend of the reduction in the size of electronic devices has led to the appearance of new phenomena that require special attention and need to be properly investigated. In particular, mesoscopic conductors are attracting increasing interest in recent years [1, 2]. Here, the microscopic interpretation of carrier transport and fluctuations demand approaches which differ from those typically used in macroscopic devices. Several techniques have been used to this end. Accordingly, to account for phase coherence the scattering matrix theory originally proposed by Landauer [3] has been further elaborated [4–6]. A Wigner function formalism has also been used for the analysis of ballistic and diffusive conductors [7–10]. When phase coherence does not play an essential role, semiclassical methods based on the Boltzmann–Langevin equation have shown to provide viable solutions [11–13]. In all of these theoretical approaches, the modelling of the contacts has proven to be crucial. The active region of the devices is considered to be surrounded by leads, which are usually treated as ideal thermal reservoirs. In other words, contacts are assumed to be always at thermal equilibrium; absorbed carriers are thermalized immediately, thus any correlation is destroyed, and the emitted carriers obey a Fermi–Dirac distribution.

Recently, particle simulations, mainly based on the Monte Carlo method, have been used to study fluctuations in mesoscopic structures [14–18]. This technique, which is

widespread for the analysis of macroscopic electronic devices [19, 20], has the advantage of being applicable under physical conditions which can be very far from thermal equilibrium, and often cannot be studied analytically. Moreover, it can provide detailed microscopic information about the physical processes and the time scales associated with the transport and the fluctuations in electronic devices. This last feature makes particle simulations quite attractive for the study of mesoscopic conductors. In the case of macroscopic devices, the presence of energy dissipation and diffusive regions inside the structures washes out the influence of the contact injecting statistics on the output currents and voltages, and the simulation of contacts does not require very detailed models [21, 22]. In contrast, when dealing with mesoscopic structures, the modelling of carrier injection from thermal reservoirs is a delicate problem. In particular, the statistics of electron injection associated with a Fermi–Dirac distribution at the electrodes is essential for the correct analysis of the fluctuations and the effects related to the Pauli exclusion principle. For a classical injector, the statistics of transmitted charge is Poissonian [1], and can be easily accounted [15]. In contrast, under degenerate conditions one should use a binomial distribution [23, 24], and to our knowledge this issue has not been addressed so far.

The aim of this Letter is to present a model for particle injection from ideal thermal reservoirs into one-dimensional mesoscopic conductors, which takes into account the fluctuating occupancy of the incoming electron

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states associated with a Fermi–Dirac distribution. The model can be continuously applied from non-degenerate to degenerate statistics at the contacts. The results obtained with a Monte Carlo simulation of a one-dimensional, two-terminal ballistic conductor implementing the present contact model are compared with the existing analytical results to validate the injection scheme.

Let us consider a one-dimensional conductor connected to leads which act as perfect thermal reservoirs. The density (in k -space) of the incoming electron states with wave vector k impinging per unit time upon the boundary between the leads and the conductor, ζ_k , is given by the product of the density of states n_k and the velocity v_k normal to the boundary, $\zeta_k = n_k v_k = (1/\pi)(\hbar k/m)$, where we have taken a parabolic isotropic $\varepsilon - k$ relation. These n_k states obey Fermi–Dirac statistics, thus only a fraction of them $f(\varepsilon_k) = \{1 + \exp[(\varepsilon_k - \varepsilon_F)/k_B T]\}^{-1}$ will be occupied and eventually will inject a carrier into the conductor, with ε_F the Fermi level. Therefore, the injection rate density of carriers with momentum k , Γ_k , is given by $\Gamma_k = \zeta_k f(\varepsilon_k)$. While ζ_k does not depend on time, the instantaneous occupancy of an incoming k -state $\hat{f}(\varepsilon_k, t)$, of which $f(\varepsilon_k)$ is the average, fluctuates in time obeying a binomial distribution [23, 24] with a probability of success $f(\varepsilon_k)$. The injecting statistics imposed by this binomial distribution is determined by the Fermi–Dirac statistics electrons obey, i.e., ultimately, by the Pauli exclusion principle. When $\varepsilon_k - \varepsilon_F \ll -k_B T$, $f(\varepsilon_k) \cong 1$ and the injecting statistics of the corresponding k -state becomes uniform in time. On the contrary, when $\varepsilon_k - \varepsilon_F \gg k_B T$, $f(\varepsilon_k) \ll 1$ and the injecting statistics of the corresponding k -state becomes Poissonian in time. In a completely degenerate (quantum) reservoir, the former condition is fulfilled for any incoming k -state and the injection is uniform in time for all the k values up to the Fermi wave vector k_F . On the contrary, in a non-degenerate (classical) reservoir, the latter condition applies for all k values.

To reproduce the injecting statistics imposed by the Pauli exclusion principle in a particle simulation, it is necessary to discretize the momentum space into a certain number of meshes of width Δk around discrete values of k , k_i . For each of these meshes, the number of incoming electron states per unit time with wave vector k_i is given by $\zeta_{k_i, \Delta k} = \zeta_{k_i} \Delta k$, with a probability of occupancy given by $f(\varepsilon_{k_i})$. In the simulation, at each time interval of duration $1/\zeta_{k_i, \Delta k}$ an attempt to introduce an incoming electron with wave vector k_i takes place. At this point a random number r uniformly distributed between zero and one is generated, and the attempt is considered successful only if $r < f(\varepsilon_{k_i})$. This rejection-technique scheme properly accounts for the injection statistics at each mesh in k -space.

For a completely degenerate reservoir, in every mesh up to k_F an electron is injected every time interval $1/\zeta_{k_i, \Delta k}$ † and there is no need of the rejection technique. This is the case of the simple contact modelling used in [14]. For a non-degenerate reservoir, since $f(\varepsilon_{k_i}) \ll 1$ for all k_i -states, it is possible to use global Poissonian statistics characterized

† In this sense the injection is uniform in time, since electrons are injected equally spaced in time, which can also be interpreted as an injection *periodic* in time, with period $1/\zeta_{k_i, \Delta k}$.

by an injection rate $\Gamma_{clas} = \int_0^{+\infty} \Gamma_k dk$. Accordingly, the time between two consecutive electron injections is generated with a probability per unit time $P(t) = \Gamma_{clas} e^{-\Gamma_{clas} t}$. Then, the electron wave vector is randomly picked from a Maxwell–Boltzmann distribution, and there is no need of using a mesh in k -space. This is the scheme used in [15–18]. For any intermediate level of degeneracy, to account for the proper statistics at each value of k_i , it is necessary to use the scheme explained above, which of course is also valid in the classical and degenerate limits, but less efficient from the point of view of computation time. The accuracy of the proposed scheme depends on the number of meshes in k -space used to inject the carriers. In any case, it is not necessary to use a very large number of meshes. Indeed, it is well known that the noise of an electrical system depends only on the kinetics of the electron states in a small energy range around the Fermi level. We have checked that very satisfactory noise results can be obtained by simulating just an energy range of $3k_B T$ above and below ε_F , and dividing it into 50 meshes. Below and above this range all k -states can be respectively considered to be completely occupied and empty. Therefore, they do not contribute to current fluctuations and can be ignored.

In the following we will report the results of a Monte Carlo simulation of a one-dimensional, two-terminal ballistic conductor of length L connected with two thermal reservoirs modelled according to the above scheme. The temperature is taken to be 300 K and the effective mass $m = 0.25 m_0$, m_0 being the free electron mass. Carriers are considered to move ballistically into the conductor following the classical equations of motion, and when a voltage U is applied to the leads, electrons are accelerated by an electric field $E = U/L$. When a carrier inside the conductor reaches a contact, it is considered to be immediately thermalized and it is cancelled from the simulation. For simplicity, the cross sectional area of the conductor is assumed to be sufficiently small so that only the lowest sub-band is occupied. We remark that Coulomb interactions are ignored and the Pauli exclusion principle is taken into account only at the contact injection. Under these conditions, the literature provides several analytical results which will be used to validate the model.

Figure 1 shows the low-frequency value of the current spectral density $S_I(0)$ at equilibrium normalized to $2qI_S$ as a function of the degeneracy factor $\varepsilon_F/k_B T$, with ε_F measured with respect to the bottom of the conduction band. $I_S = q \int_0^{+\infty} v_k n_k f(\varepsilon_k) dk$ is the saturation current, i.e. the maximum current a contact can provide. In the classical limit, corresponding to large negative values of the degeneracy factor, $S_I(0) = 4qI_S$. Here all carriers contribute to the current noise and $S_I(0)$ is just the sum of the full shot noise related to the two opposing currents I_S injected by the contacts [7, 9, 15, 18]. Under degenerate conditions, corresponding to positive values of the degeneracy factor, $S_I(0)$ decreases with respect to $4qI_S$ in accordance with the suppression factor $\varepsilon_F/k_B T$ related to Fermi correlations at the reservoirs [6, 7]. Here, as known, only carriers around the Fermi level contribute to the noise. As shown by the figure, the agreement between the results of the Monte Carlo simulation and the analytical expectations in the non-degenerate and degenerate limits is excellent, thus indicating

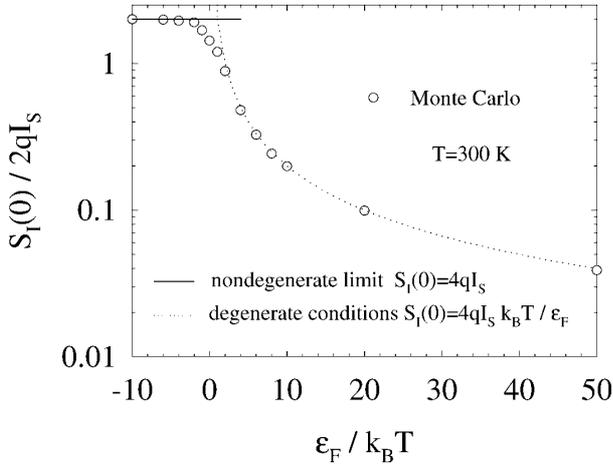


Figure 1. Low-frequency current spectral density at equilibrium normalized to $2qI_S$ as a function of the degeneracy factor $\varepsilon_F/k_B T$, at $T = 300$ K. Symbols correspond to Monte Carlo calculations and full line and broken curve to non-degenerate and degenerate conditions, respectively.

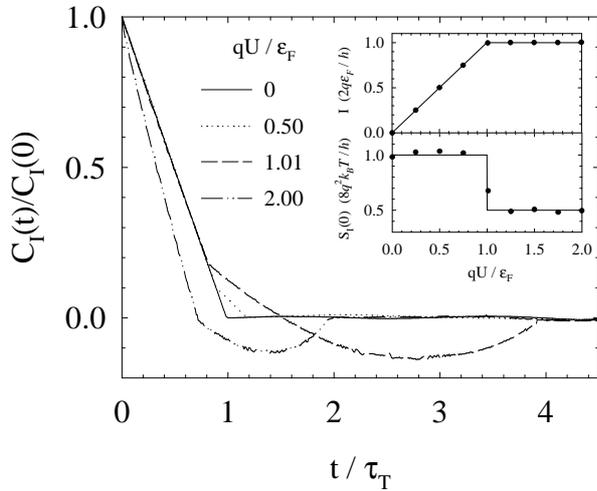


Figure 2. Current autocorrelation function normalized to the zero-time value for several applied voltages. The calculations correspond to degenerate conditions with $\varepsilon_F/k_B T = 100$. The upper inset reports the $I-U$ characteristic of the structure, while the lower inset shows the $S_I(0)-U$ characteristic. Results are normalized to appropriate units. Full lines in the insets correspond to analytical results and full circles to the Monte Carlo calculations.

that the carrier injecting statistics achieved with the proposed model are valid in both regimes.

Figure 2 reports the current autocorrelation function $C_I(t)$ in the same structure as figure 1 when $\varepsilon_F/k_B T = 100$ for several applied voltages as a function of time normalized to the transit time at the Fermi level $\tau_T = L(m/2\varepsilon_F)^{1/2}$. The corresponding $I-U$ curve is shown in the upper inset of figure 2. Due to the imbalance in the number of carriers reaching the opposite contact, the current increases linearly with the applied voltage until $qU = \varepsilon_F$, when the current reaches the saturation value $I_S = 2q\varepsilon_F/h$. For higher U all of the carriers injected at the left lead reach the opposite contact, while no electron injected at

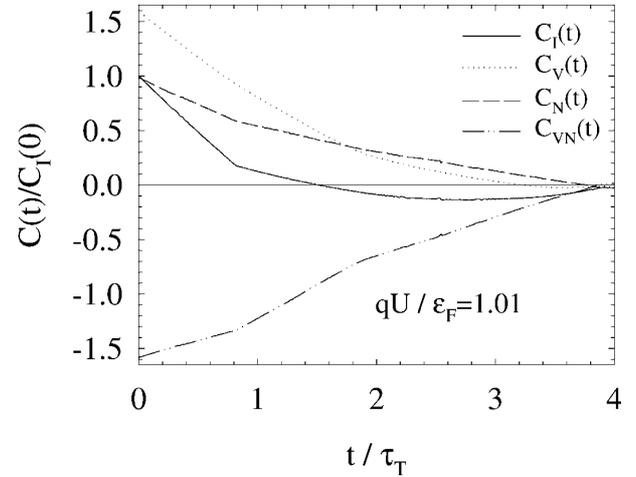


Figure 3. Decomposition of the current autocorrelation function into velocity, number and velocity-number contributions for the case of $qU/\varepsilon_F = 1.01$ and $\varepsilon_F/k_B T = 100$.

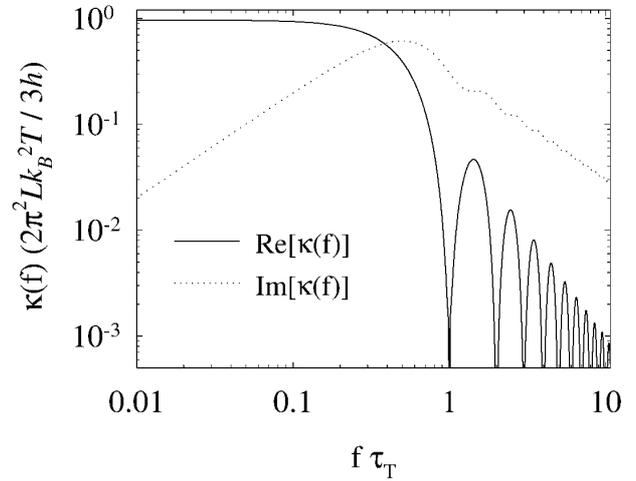


Figure 4. Spectrum of thermal conductivity at equilibrium normalized to the theoretically predicted zero-frequency value. Solid and broken curves correspond to the real and imaginary parts, respectively. Calculations are performed for $\varepsilon_F/k_B T = 100$.

the anode reaches the cathode, and therefore the current saturates. The conductance in the linear region corresponds to the value of the fundamental unit $2q^2/h$ [3]. The current autocorrelation function $C_I(t)$ exhibits the following features. At equilibrium it shows the typical triangular shape, vanishing at $t = \tau_T$ since the contributions of carriers moving in both directions are symmetrical. This shape parallels that of a vacuum tube with a constant velocity emitter. Here, the same shape comes from the Pauli exclusion principle, which allows only carriers in a small range around the Fermi energy, and therefore moving with practically the same velocity, to contribute to the noise. When a voltage below ε_F/q is applied to the structure, $C_I(t)$ exhibits a two-slope behaviour because now the transit times of carriers moving in opposite directions are different. At voltages higher than ε_F/q a negative part appears in $C_I(t)$ since the carriers injected against the electric field no longer reach the cathode and return to the anode. At further increases of voltage the negative part appears sooner due to the shorter time it takes to the carriers to return back to

the right contact [7]. The low-frequency spectral density $S_I(0)$ as a function of U is shown in the lower inset of figure 2. At equilibrium the value obtained corresponds to $S_I(0) = 8q^2k_B T/h$, which, when compared with the Nyquist formula, $S_I(0) = 4k_B T G$, again provides for the static conductance $G = 2q^2/h$. The fact that in our model the conductance obtained from the $I-U$ curve reproduces the fundamental unit value is a valid check of the correct use of the one-dimensional density of states at the contacts. Furthermore, the same value $2q^2/h$ is also obtained from noise results at equilibrium, which proves that the injecting statistics model under degenerate conditions proposed here is also correct. The voltage dependence of $S_I(0)$ exhibits a step-like behaviour, taking the equilibrium value up to $U = \varepsilon_F/q$ and half this value for higher U . This behaviour is understood as follows. For $U < \varepsilon_F/q$, carriers around the Fermi level which are injected at both contacts reach the opposite side and therefore both contribute to the low-frequency noise. On the contrary, for $U > \varepsilon_F/q$ only carriers injected at the cathode reach the anode and thus the value of $S_I(0)$ is halved. We remark that all of the results shown in figure 2 are in excellent agreement with previous analytical results in degenerate systems [7–9].

One of the advantages of using particle simulations for the noise analysis is the possibility to interpret the time and frequency behaviour of the fluctuations in terms of different contributions. Thus, in figure 3, in the case of degenerate conditions and $qU/\varepsilon_F = 1.01$, $C_I(t)$ is decomposed into velocity $C_V(t)$, number $C_N(t)$ and velocity–number $C_{VN}(t)$ contributions [15]. Here it can be observed that the origin of the negative part in $C_I(t)$ comes from the velocity–number correlation, which at zero time exactly compensates the velocity contribution. Furthermore, from the time dependence of the fluctuations three different characteristic times can be identified. The shortest time corresponds to the transit of carriers injected from the left contact, as better evidenced in C_N and C_{VN} . It is close to the transit time at equilibrium τ_T , but slightly shorter due to the acceleration of the field. A second time is the time taken by the carrier injected at the anode to reverse its velocity, and is reflected mainly in C_{VN} . Finally, the longest time is the time at which all correlation functions vanish. It corresponds to the time spent by the electrons injected at the anode to return back to the same contact.

As final result, in figure 4 we report the spectrum of the thermal conductivity $\kappa(f)$ at equilibrium, calculated according to [10]. Here, we remark that not only the correlations of the electrical current fluctuations are involved, but also those of the heat flux and the cross-correlations between both. The oscillatory structure of $\text{Re}[\kappa(f)]$, with geometrical resonances at the inverse of τ_T , is associated with the fact that all the involved correlation functions exhibit the triangular shape already found in the case of the current (see figure 2). A corresponding structure is also detectable in the imaginary part $\text{Im}[\kappa(f)]$. Again, the results of the Monte Carlo simulation are in excellent agreement with analytical results. In particular, they reproduce with great accuracy the fundamental unit of thermal conductance $K = 2\pi^2k_B^2 T/3h$ inferred in [10], which again confirms the validity of the proposed model for the injection statistics at the reservoirs.

In summary, we have presented an injection scheme of electrons at thermal reservoirs for particle simulations of mesoscopic conductors which takes into account the binomial distribution of the injected electrons imposed by Fermi statistics. The model has been validated for the case of ballistic transport in quasi one-dimensional degenerate conductors. In particular, at thermal equilibrium we have reproduced the fundamental units of electrical and thermal conductances, analytically calculated from the correlation-function formalism. The scheme can be applied continuously from classical to completely degenerate conditions, and it can be extended to two and three dimensions, and multi-sub-band systems. The proposed scheme is open to applications involving degenerate diffusive conductors.

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