Shot noise at hopping via two sites

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The average current and the shot noise at correlated sequential tunneling via two localized sites are studied. At zero temperature the Fano factor averaged over the positions and energies of sites is shown to be 0.707. The noise dependence on temperature and frequency is analyzed numerically.

Shot noise in mesoscopic structures has been the subject of thorough studies in the recent past.[1–3] In particular, a theory of shot noise at tunneling of single electrons correlated due to Coulomb blockade effects[4] has been well developed[5–10] and verified experimentally.[11] Recently, attempts have been made[12,13] to extend this theory to hopping transport,[14] which can be formally considered as a special case of correlated single-electron tunneling.

In a typical hopping situation there is a considerable $1/f$ contribution at low frequencies (see Ref. 15, and references therein), so one can discuss the shot noise only at sufficiently high frequencies. The $1/f$ noise at hopping is mainly due to electron-electron interaction: the slowly evolving trapped charge configurations can significantly affect the current through nearby channels. The $1/f$ component is absent at hopping through noninteracting one-dimensional (1D) chains of sites[12] (while the slow fluctuations of the chain parameters due to external traps can restore this component). In the present paper we consider hopping through very short chains which are just pairs of sites, and assume that the parameters of these pairs do not fluctuate in time, so that the noise does not have $1/f$ contribution.

For two-site hopping we basically follow the model introduced by Glazman and Matveev.[16] The only difference is that we take into account the correlation between tunneling events neglected in Ref. 16 (in this respect our model is closer to the model of Ref. 22). Using the methods developed in Ref. 6 we calculate the current I and the current spectral density $S_I(\omega)$ for an individual two-site channel. The summation over many parallel channels with random parameters is done similar to Ref. 16. The main object of our study is the Fano factor F (the low frequency noise normalized by the Schottky value $S_I=2eI$). We will show that at zero temperature the Fano factors for individual two-site channels range from 5/14 to 1, while after averaging we get $\overline{F}=0.707$ (the similar problem for one-site channels has been considered in Ref. 17 with the result $\overline{F}=3/4$). For a finite temperature T the Fano factor can be calculated numerically; after the averaging we obtain $\overline{F}$ as a function of the ratio T/eV where V is the voltage between electrodes.

The schematic of a two-site channel is shown in Fig. 1. The thickness d of an insulating layer between two metallic electrodes is assumed to be much greater than the electron localization radius a, and we use the model of sequential (incoherent) hops of single electrons. The lengths of the left and right hops are x_1 and x_3, respectively, while the hop between two sites has the length $r_2=(x_2^2+y^2)^{1/2}$, where $x_2=d-x_1-x_3$ and y is the shift of site positions in the plane parallel to electrodes. Each site can be occupied by at most one electron and the effect of electron spin is neglected (the case of double degeneracy due to spin will be discussed later). The tunneling rates from electrodes to empty sites (tunneling to nearest neighbor only, see Fig. 1) are assumed to be

$$\Gamma_1^+=\Gamma_0\exp(-2x_1/a)f(-eV+\varepsilon_1),$$
$$\Gamma_3^-=\Gamma_0\exp(-2x_3/a)f(\varepsilon_2), \qquad (1)$$

where superscripts indicate the direction of tunneling, ε_1 and ε_2 are the site energies counted from the Fermi level of the right electrode, and $f(\varepsilon)=[1+\exp(\varepsilon/T)]^{-1}$ is the Fermi function. Similarly, the rates of tunneling from occupied sites to neighboring electrodes are

$$\Gamma_1^-=\Gamma_0\exp(-2x_1/a)f(eV-\varepsilon_1),$$
$$\Gamma_3^+=\Gamma_0\exp(-2x_3/a)f(-\varepsilon_2). \qquad (2)$$

Notice that we have neglected the Coulomb interaction of electrons on different sites (energies $\varepsilon_{1,2}$ do not depend on the occupation of neighboring site). The rate of inelastic tunneling between the sites depends on the energy difference $\Delta\varepsilon=\varepsilon_1-\varepsilon_2$, and for $|\Delta\varepsilon|$ much smaller than $\hbar s/a$ (where s is the sound velocity) can be calculated as[14]

$$\Gamma_2^{\pm}=\alpha\Gamma_0\exp(-2r_2/a)\,\frac{\pm\Delta\varepsilon}{1-\exp(\mp\Delta\varepsilon/T)}, \qquad (3)$$

where the dimensional factor α describes the relative strength of phonon-assisted tunneling compared to ''resonant'' tunneling assumed in Eqs. (1) and (2).

Let us start with the zero-temperature case. Then the transport is possible only if $eV>\varepsilon_1>\varepsilon_2>0$, and electrons move only in one direction, $\Gamma_1^-=\Gamma_2^-=\Gamma_3^-=0$ (for simplicity we omit the superscript ''+,'' $\Gamma_i\equiv\Gamma_i^+$). The kinetic (''mas-

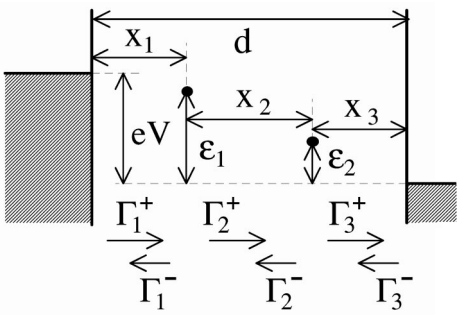

FIG. 1. Schematic of two-site tunneling channel.

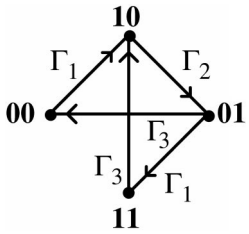

FIG. 2. Graphical representation of the master equation for zero temperature.

ter'') equation in this case can be represented graphically by Fig. 2. The configuration space consists of four charge states of the two-site system which are denoted as 00, 01, 10, and 11, while arrows show transitions between them. The graphical representation of the master equation in a relatively small configuration space is a very convenient tool and often allows straightforward calculation of the average current and zero-frequency spectral density (see, e.g., Ref. 18).

The basic idea of the method[6] is to consider the random ''travel'' of the system state within the configuration space and divide the duration of this stochastic process into blocks which start and end in a specific charge state. Because of the Markovian property of the process (absence of memory) these blocks are mutually uncorrelated, so the averaging over the blocks is rather simple. In the case of Fig. 2 let us choose the charge state 01 as the block divider. Then there are two types of blocks: $01\to00\to10\to01$ (type 1) and $01\to11\to10\to01$ (type 2), while the blocks are additionally characterized by the time spent in each charge state.

The average current can be calculated[6] as

$$I=e\overline{k}/\overline{\tau}, \tag{4}$$

where $\overline{\tau}$ is the average block duration and $\overline{k}$ is the average number of electrons transferred between electrodes per block (the averaging is taken over a large number of blocks). To calculate these average magnitudes let us notice that the blocks of type 1 and type 2 have probabilities

$$p_1=\Gamma_3/(\Gamma_1+\Gamma_3), \quad p_2=\Gamma_1/(\Gamma_1+\Gamma_3), \tag{5}$$

and the average durations $\overline{\tau_1}$ and $\overline{\tau_2}$ of the blocks of each type can be calculated as

$$\overline{\tau_1}=(\Gamma_1+\Gamma_3)^{-1}+\Gamma_1^{-1}+\Gamma_2^{-1},$$
$$\overline{\tau_2}=(\Gamma_1+\Gamma_3)^{-1}+\Gamma_3^{-1}+\Gamma_2^{-1} \tag{6}$$

[notice that the average waiting time $(\Gamma_1+\Gamma_3)^{-1}$ of the first hop is equal for both types]. Taking into account that each block corresponds to the transfer of one electron, $k_1=k_2=\overline{k}=1$, and calculating the average block duration

$$\overline{\tau}=p_1\overline{\tau_1}+p_2\overline{\tau_2}, \tag{7}$$

we finally obtain the formula for the average current:[19]

$$I=e\left(\frac{1}{\Gamma_2}+\frac{1+\Gamma_1/\Gamma_3+\Gamma_3/\Gamma_1}{\Gamma_1+\Gamma_3}\right)^{-1}. \tag{8}$$

This equation differs from the result of Ref. 16 because the correlation between the occupations of two sites was neglected in Ref. 16. The correct equation for the current which coincides with Eq. (8) was obtained later in Ref. 22.

The same method as above can be used for the calculation of the low-frequency limit $S_I(0)$ of the current spectral density which is given by the general equation[6]

$$S_I(0)=(2/\overline{\tau})(e^2\overline{k^2}+I^2\overline{\tau^2}-2eI\overline{k\tau}) \tag{9}$$

(averaging is again over blocks) which in our case at zero temperature simplifies to

$$S_I(0)=2eI[(\overline{\tau^2}/\overline{\tau^2})-1]. \tag{10}$$

So, besides Eqs. (4)–(7) we also need to calculate $\overline{\tau^2}$:

$$\overline{\tau^2}=p_1\overline{\tau_1^2}+p_2\overline{\tau_2^2}, \tag{11}$$

where because of Poissonian statistics of each tunneling event we have

$$\overline{\tau_1^2}-\overline{\tau_1}^2=(\Gamma_1+\Gamma_3)^{-2}+\Gamma_1^{-2}+\Gamma_2^{-2},$$
$$\overline{\tau_2^2}-\overline{\tau_2}^2=(\Gamma_1+\Gamma_3)^{-2}+\Gamma_3^{-2}+\Gamma_2^{-2}. \tag{12}$$

Combining these equations we finally obtain

$$S_I(0)=2eI\left(\frac{1}{\Gamma_2^2}+\frac{(1+R+R^{-1})^2-4}{(\Gamma_1+\Gamma_3)^2}\right)\times\left(\frac{1}{\Gamma_2}+\frac{1+R+R^{-1}}{\Gamma_1+\Gamma_3}\right)^{-2}, \tag{13}$$

where $R\equiv\Gamma_1/\Gamma_3$. Analyzing the Fano factor $F\equiv S_I(0)/2eI$ one can see that the uniform case $\Gamma_1=\Gamma_2=\Gamma_3$ provides $F=9/25$ which is not the minimum possible value. The minimum Fano factor is achieved at $\Gamma_1=\Gamma_3=5/6\times\Gamma_2$ and equal to $F_{min}=5/14$ (it is still noticeably larger than the naive estimate $F=1/3$). The maximal value $F_{max}=1$ is obviously achieved when one of the rates Γ_i is much smaller than two other rates.

Following Ref. 16 let us assume many two-site channels ''in parallel'' and find the total current I_Σ and spectral density $S_{I,\Sigma}(0)$ integrating over channels with different site positions x_1, x_3, y and different energies ε_1 and ε_2. Assuming a sufficiently thick insulating layer we may approximate the distance between sites as $r_2\simeq x_2+y^2/2\tilde{x}_2$, where $\tilde{x}_2$ corresponds to the channel with the maximum current. For such a channel $y=0$ and $\Gamma_1=\Gamma_2=\Gamma_3=\Gamma_0\exp(-2d/3a)(\alpha eV)^{1/3}$ [see Eqs. (8) and (1)–(3)] which gives $\tilde{x}_2=(d/3)+(a/3)\ln(\alpha eV)$. At zero temperature the total current can be calculated as

$$I_\Sigma=n^2A\int_{-\infty}^{\infty}d\xi_1\int_{-\infty}^{\infty}d\xi_3\int_0^{\infty}2\pi y\,dy\times\int_0^{eV}d\Delta\varepsilon\;(eV-\Delta\varepsilon)\,I(\xi_1,\xi_3,y,\Delta\varepsilon), \tag{14}$$

where n is the density of states, A is the area [$A\gg d^2$, $A\gg n^{-2}a^{-3}d^{-1}(eV)^{-2}$], the x-positions of the sites are measured from the optimal values, $\xi_i=x_i-\tilde{x}_i$, $\tilde{x}_1=\tilde{x}_3=(d-\tilde{x}_2)/2$ (the integration is extended to infinity since $d\gg a$), and the current I is given by Eq. (8).

Using the relation $I(\xi_1,\xi_3,y,\Delta\varepsilon)=\exp(-2\delta/a)\,I(\xi_1-\delta,\xi_3-\delta,0,\Delta\varepsilon)$ where $\delta=y^2/6\tilde{x}_2$, it is easy to show that the

integration $\int_0^\infty 2\pi y\,dy$ gives the factor $3\pi a\tilde{x}_2$. Calculating the integral over $\Delta\varepsilon$ analytically and integrals over ξ_1 and ξ_3 numerically, we get the result

$$I_\Sigma = 5.237\, e\Gamma_0\, n^2 A a^3 \tilde{x}_2 \exp(-2d/3a)\, \alpha^{1/3} (eV)^{7/3}. \tag{15}$$

Notice that the scaling $I_\Sigma \propto V^{7/3}$ is the same as in the model which neglects correlations.[16]

A similar sum over different two-site channels can be calculated for the current spectral density at zero frequency [just replacing I in Eq. (14) with $S_I(0)$ given by Eq. (13)]. Integrating analytically over y and $\Delta\varepsilon$ and numerically over the two remaining variables we obtain the following average Fano factor at zero temperature:

$$\overline{F} \equiv S_{I,\Sigma}(0)/2eI_\Sigma = 0.7074. \tag{16}$$

Let us now consider the finite-temperature case. Our method for calculation of I and $S_I(0)$ based on the analysis of blocks can still be easily applied if $\Gamma_2^- \neq 0$ while $\Gamma_1^- = \Gamma_3^- = 0$ (this situation occurs when ε_1 and ε_2 are well inside the energy strip defined by the Fermi levels of the electrodes). In this case the current I and the spectral density $S_I(0)$ are given by Eqs. (4) and (9), where[21]

$$\overline{\tau} = p_1\overline{\tau_1} + p_2\overline{\tau_2} + p_3\overline{\tau_3}, \quad \overline{k} = \overline{k^2} = p_1 + p_2,$$
$$p_1 = \Gamma_3^+/\Gamma_\Sigma,\ p_2 = \Gamma_1^+/\Gamma_\Sigma, \quad p_3 = \Gamma_2^-/\Gamma_\Sigma,$$
$$\overline{\tau_1} = 1/\Gamma_\Sigma + 1/\Gamma_1^+ + 1/\Gamma_2^+, \quad \overline{\tau_3} = 1/\Gamma_\Sigma + 1/\Gamma_2^+,$$
$$\overline{\tau_2} = 1/\Gamma_\Sigma + 1/\Gamma_3^+ + 1/\Gamma_2^+, \quad \Gamma_\Sigma = \Gamma_3^+ + \Gamma_1^+ + \Gamma_2^-,$$
$$\overline{\tau^2} = p_1\overline{\tau_1^2} + p_2\overline{\tau_2^2} + p_3\overline{\tau_3^2},\ \overline{k\tau} = p_1\overline{\tau_1} + p_2\overline{\tau_2},$$
$$\overline{\tau_1^2} - \overline{\tau_1}^2 = (\Gamma_\Sigma)^{-2} + (\Gamma_1^+)^{-2} + (\Gamma_2^+)^{-2},$$
$$\overline{\tau_2^2} - \overline{\tau_2}^2 = (\Gamma_\Sigma)^{-2} + (\Gamma_3^+)^{-2} + (\Gamma_2^+)^{-2}.$$
$$\overline{\tau_3^2} - \overline{\tau_3}^2 = (\Gamma_\Sigma)^{-2} + (\Gamma_2^+)^{-2}. \tag{17}$$

In the case when all Γ_i^- are nonzero, it is more natural to use the general master-equation formalism for the average current[4] and spectral density.[6] We have developed a numerical code and integrated over different two-site channels in the same way as above, just using the numerical results for I and $S_I(0)$ instead of Eqs. (8) and (13). (One more difference from the zero-temperature case is the separate integration over ε_1 and ε_2.) The dashed line in Fig. 3 shows the dependence of the ratio $g \equiv I_\Sigma(T)/I_\Sigma(0)$ on the normalized temperature T/eV. [We neglect the weak temperature dependence of $\tilde{x}_2$ and actually calculate the dependence of the numerical factor in Eq. (15).] The asymptote at $T \gg eV$ is $g = 21.7\,(T/eV)^{4/3}$, so the conductance G is equal to $G = 113.6\, e^2\Gamma_0\, n^2 A a^3 \tilde{x}_2 \exp(-2d/3a)\, \alpha^{1/3} T^{4/3}$, where $\tilde{x}_2$ can be approximated as $(d/3) + (a/3)\ln(\alpha T)$ (the scaling $T^{4/3}$ is the same as in the model without correlations[16]).

The Fano factor averaged over different channels, as a function of T/eV, is shown in Fig. 3 by the thick solid line. The low-temperature value is given by Eq. (16), while the high-temperature asymptote $\overline{F} = 2T/eV$ (lower dotted line) can be easily derived from the Nyquist formula.

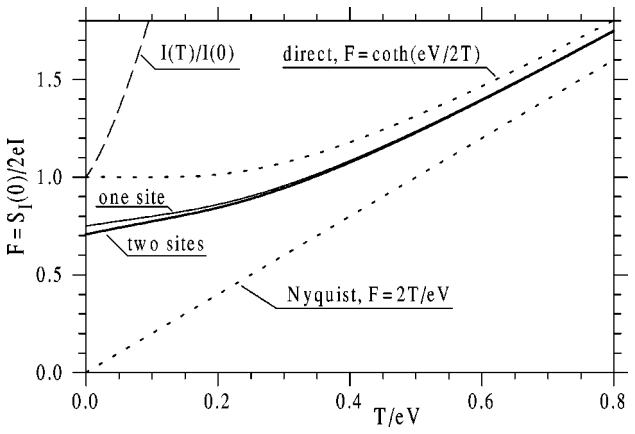

FIG. 3. The Fano factor $\overline{F}$ averaged over two-site (thick solid line) and one-site (thin solid line) channels, as a function of temperature. Dotted lines show $F(T)$ for direct tunneling and Ohmic conduction. Dashed line shows the averaged two-site current $I(T)$ normalized by $I(0)$.

It is interesting to compare the temperature dependence of $\overline{F}$ for two-site and one-site channels. In the latter case we still use Eqs. (1) and (2) for the tunneling rates similar to Ref. 17. The thin solid line in Fig. 3 shows the average Fano factor for one-site channels, as a function of T/eV (this curve in other coordinates has been calculated in Ref. 17). The low-temperature value is $\overline{F} = 3/4$, while the high-temperature asymptote $\overline{F} = 2T/eV$ is the same as for two-site channels and direct-tunneling case. [The result for the direct tunneling, $F = \coth(eV/2T)$, is shown for comparison by the upper dotted line.] Obviously, with the increase of the number N of sites in the channel the average Fano factor decreases. However, its dependence on N seems to saturate rapidly, as indicated by the small difference between the results for one-site and two-site channels. So, even for large N one should expect the dependence $\overline{F}(T)$ to deviate significantly at $T \lesssim eV$ from the result for an Ohmic conductor, $F = 2T/eV$. This can be explained by the fact that the 1D chains of sites with ''soft'' (not strong) bottlenecks still give considerable contribution to the total current, while the Fano factor for such chains is comparable to unity. (The situation is different[13] for 2D or 3D hopping because the percolation cluster does not have bottlenecks at the size scale much larger than the correlation length of the cluster. As a consequence, for sufficiently large samples we expect $F = 2T/eV$.)

So far we have discussed only the current spectral density at zero frequency. Our computer code can also treat the finite-frequency case. At finite frequency ω it is necessary to specify where the current is measured. We have considered the current in the electrodes and assumed natural electrostatics when the electron hop through the ith gap transfers charge $q_i = ex_i/d$ in the electrodes. The spectral density at finite ω depends not only on tunneling rates $\Gamma_i^\pm$ but also on q_i and thus on the positions of sites. For averaging over the two-site channels we have used the approximation $q_i \simeq e\tilde{x}_i/d \simeq e/3$. The solid line in Fig. 4 shows the frequency dependence $S_{I,\Sigma}(\omega)/2eI_\Sigma$ for $T = 0$. The frequency scale is determined by tunneling rates, so for normalization we have used $\Gamma_n \equiv \Gamma_0 \exp(-2d/3a)(\alpha eV)^{1/3}$. For comparison, we also show $S_I(\omega)/2eI$ for the uniform channel, $\Gamma_1 = \Gamma_2 = \Gamma_3$

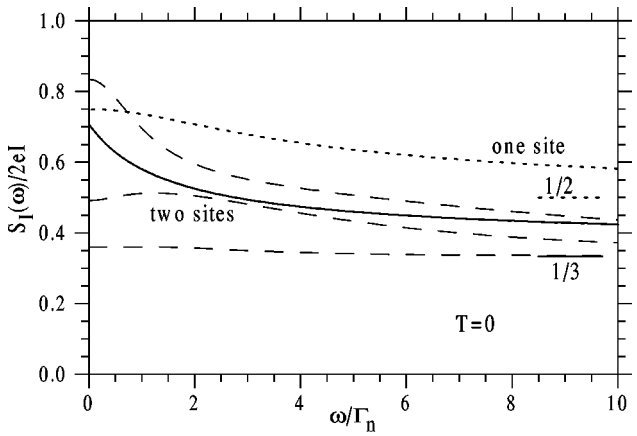

FIG. 4. Solid line: the frequency dependence of the normalized current spectral density $S_I(\omega)/2eI$ averaged over two-site channels. Dashed lines correspond to particular channels (see text). The dotted line shows $S_I(\omega)/2eI$ averaged over one-site channels.

(lower dashed line) and for two nonuniform channels: $\Gamma_1 = \Gamma_2 = 0.1\Gamma_3$ (middle dashed line) and $10\Gamma_1 = \Gamma_2 = 0.1\Gamma_3$ (upper dashed line) at $\Delta\varepsilon = eV$. Notice that the solid line (averaged noise) has a finite slope at $\omega = 0$ (even though the slope is zero for each individual channel) and approaches the high-ω asymptote of 1/3 as $\omega^{-1/2}$. The dotted line in Fig. 4 shows the ratio $S_I(\omega)/2eI$ averaged over one-site channels [then $\Gamma_n \equiv \Gamma_0 \exp(-d/a)$], which can be calculated analytically: $1/2 + [(\omega^2\Gamma_n^{-2}+4)^{1/2} - 2]\,\Gamma_n^2/\omega^2$.

Finally, let us briefly consider the effect of electron spin using a simple model. Assuming the double degeneracy due to spin (but still allowing at most one electron per site), we should double the tunneling rates Γ_1^+ and Γ_3^- [see Eq. (1)], while leaving all other rates unchanged. At zero temperature this will lead to a trivial extra factor $2^{1/3}$ in Eq. (15) and a very small change of $\tilde{x}_2$, while the average Fano factor given by Eq. (16) does not change. The calculations at finite temperature show that $\overline{F}$ is a little larger in the case of double degeneracy compared to the spinless case, however, the difference is so small that the corresponding curves in Fig. 3 cannot be distinguished. The maximum difference $\Delta\overline{F} \approx 5 \times 10^{-4}$ is achieved at $T/eV \approx 0.3$, while at $T \gg eV$ the difference approaches zero. A similar very weak dependence on the spin degeneracy for one-site channels has been reported in Ref. 17 (we have found the maximum difference $\Delta\overline{F} = 1.12 \times 10^{-3}$ at $T/eV \approx 0.33$).

In conclusion, we have studied the shot noise of two-site hopping channels. The different average Fano factor and different frequency dependence of the noise in comparison with one-site channels and direct tunneling can, in principle, be verified experimentally (using the difference of the temperature dependence of the average current).

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