Efficient algorithm for current spectral density calculation in single-electron tunneling and hopping

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This write-up describes an efficient numerical method for the Monte Carlo calculation of the spectral density of current in the multi-junction single-electron devices and hopping structures. In future we plan to expand this write-up into a full-size paper.

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In this paper we describe an algorithm for the Monte Carlo calculation of the spectral density $S_I(\omega)$ of tunneling current in multi-junction single-electron devices.[1] The same algorithm is applicable to calculation of the noise at hopping[2] because of the problem similarity. This algorithm has been used in several of our earlier papers;[3,4,5,6,7] however, it has not yet been described explicitly (except for revised versions of unpublished paper 6).

The first spectral calculations of the electron transport in single-electron devices using the Monte Carlo technique have been performed in Refs. 8 and 9; in these papers the spectral density has been calculated as a Fourier transform of the correlation function. However, this method is rather slow in the case when the current $I(t)$ is a sequence of δ-functions, corresponding to tunneling events:

$$I(t) = \sum_n q_n \delta(t - t_n), \tag{1}$$

where t_n is a (random) time of the n-th tunneling event and q_n is the corresponding charge transfer. (The sequence $\{q_n\}$ is also random and reflects the path in the space of charge configurations.)

A significantly faster "standard" algorithm[10] (embedded, for example, into the simulation package MOSES[11]) is based on the definition of the spectral density $S_I(\omega)$ of the current $I(t)$ via the square of the Fourier transform $|I(\omega)|^2$. More specifically, for the rectangular time window (natural in simulations) there is a relation

$$\frac{2}{T}\left\langle \left| \int_{t_0}^{t_0+T} I(t) \exp(i\omega t)\, dt \right|^2 \right\rangle = \int_{-\infty}^{+\infty} S_I(\omega+\Omega)\, \frac{1-\cos(\Omega T)}{\pi T \Omega^2}\, d\Omega \tag{2}$$

(here $\langle ... \rangle$ denotes ensemble averaging and i is the imaginary unit), whose right hand side tends to $S_I(\omega)$ in the limit $T \to \infty$. Therefore,

$$\tilde{S}_I(\omega) \equiv \frac{2}{T}\left\langle \left| \sum_n q_n \exp(i\omega t_n) \right|^2 \right\rangle \tag{3}$$

is a good approximation for the true spectral density $S_I(\omega)$ even for a finite, but large enough time interval T. (Summation in Eq. (3) is over the tunneling events within the interval $t_0 < t_n < t_0 + T$). In the standard method[10,11] the ensemble averaging in Eq. (3) is replaced by averaging over K sequential time segments (each of duration T) of the Monte Carlo realization, so that t_0 becomes jT, where $j = 1, 2, ... K$. It is natural to calculate simultaneously the spectral density for a set of frequency points (the set of harmonics of a certain low frequency is most convenient), and it is useful to choose $\omega/2\pi$ equal to integer multiples of T^{-1} to avoid "poisoning" of the right hand side of Eq. (2) by the δ-function contribution from $S_I(0)$ due to dc current $\overline{I}$. (Other ways of subtracting the effect of $\overline{I}$ are also possible.)

A major disadvantage of this standard method is that the relative accuracy of the spectral density calculation cannot be better than approximately $K^{-1/2}$, because the right hand side of Eq. (3) before averaging over K segments has the rms fluctuation comparable to the mean value. It is easy to increase K (without increasing the total simulation time) by decreasing T; however, besides increasing the smoothing of $S_I(\omega)$ [which is $\Delta\omega \sim T^{-1}$ – see Eq. (2)], this may lead to incorrect results when T becomes comparable or less than the longest correlation time of the simulated process, and therefore the T-segments are no longer statistically independent. Since the correlation time is not known in advance (it may be estimated as the lowest frequency at which the spectral density levels off), the choice of T is not a trivial task and requires some intuition that complicates the use of the standard method.

Here we describe the advanced algorithm of spectral density calculation which eliminates this problem and also makes calculation significantly faster (for the same

accuracy of the result). The method is somewhat similar to the "reduced" method for dc current calculation[10] and basically treats the randomness of tunneling times t_n analytically, while the path in the charge configuration space is still simulated[8] by the Monte Carlo technique.

Let us consider a T-long realization of the process assuming for simplicity $t_0 = 0$, so that $t_n = \sum_{k=1}^{n} \tau_k$ where τ_k is the time between the adjacent tunneling events, i.e. time spent in a particular charge state. In the case when the system parameters (external voltage, etc.) do not change with time, the random time τ_k has the Poisson distribution with the average value $\langle \tau_k \rangle = 1/\Gamma_{k,\Sigma}$, where $\Gamma_{k,\Sigma}$ is the sum of all tunneling rates for the corresponding charge state. The quantity $s \equiv \left| \sum_n q_n \exp\left(i\omega t_n\right) \right|^2$, which is related to the spectral density via Eq. (3), may be easily expressed as

$$\begin{aligned} s &= \sum_{n,m} q_n q_m \exp\left[i\omega \left(\sum_{k=1}^{n} \tau_k - \sum_{k=1}^{m} \tau_k \right) \right] \\ &= \sum_n q_n^2 + 2\,\mathrm{Re} \sum_{n>m} q_n q_m \exp\left[i\omega \sum_{k=m+1}^{n} \tau_k \right]. \end{aligned} \quad (4)$$

For the ensemble averaging of s let us first average Eq. (4) over random τ_k, leaving averaging over paths in charge space for later. Using the mutual independence of τ_k fluctuations, we can average each exponent independently:

$$\left\langle e^{i\omega\tau_k} \right\rangle = \int_0^\infty \frac{e^{-\tau/\langle\tau_k\rangle}}{\langle \tau_k \rangle} e^{i\omega\tau} d\tau = \frac{1}{1 - i\omega \langle \tau_k \rangle}, \quad (5)$$

thus obtaining the expression

$$\langle s \rangle = \sum_n q_n^2 + 2\,\mathrm{Re} \left(\sum_{n>m} q_n q_m \prod_{k=m+1}^{n} \frac{1}{1 - i\omega \langle \tau_k \rangle} \right). \quad (6)$$

This expression can be calculated iteratively introducing complex variables

$$A_p \equiv \sum_{n=1}^{p} q_n^2 + 2 \sum_{n>m}^{p} q_n q_m \prod_{k=m+1}^{n} \frac{1}{1 - i\omega\langle\tau_k\rangle}, \quad (7)$$

$$B_p \equiv \sum_{m=1}^{p} q_m \prod_{k=m+1}^{p} \frac{1}{1 - i\omega \langle \tau_k \rangle}, \quad (8)$$

that satisfy recurrent equations

$$A_{p+1} = A_p + q_{p+1}^2 + 2 q_{p+1} B_p \frac{1}{1 - i\omega \langle \tau_{p+1} \rangle}, \quad (9)$$

$$B_{p+1} = q_{p+1} + B_p \frac{1}{1 - i\omega \langle \tau_{p+1} \rangle}, \quad (10)$$

with initial condition $A_0 = B_0 = 0$, while $\langle s \rangle = \mathrm{Re} A_p$ at the end of realization.

It is important to notice that $\mathrm{Re}A_p$ accumulates with the length of realization (in contrast to s before averaging, which is a strongly fluctuating variable), so that $(2/\langle t_p \rangle)\,\mathrm{Re}A_p$ (where $\langle t_p \rangle = \sum_k^p \langle \tau_k \rangle$) tends to some limit at $p \to \infty$. This is the reason why, in contrast to the standard method, the numerical averaging over many T-segments is not necessary now, and the ensemble averaging of the segments over different realizations can be replaced by the natural "time" averaging over the length of a realization. This eliminates the problem of choosing T, discussed above, and now T can be treated as a running variable $T_p = \langle t_p \rangle$ during the whole simulation run. Similarly, s can also be treated as a running variable s_p. (Strictly speaking, averaging over τ_k in the segments with a fixed time T and/or a fixed charge path is different; however, the difference vanishes at large T).

Thus, the basic algorithm is the following. The Monte Carlo technique is used to simulate one long realization of the random path in the configuration (charge) space, while the time is treated deterministically as $\sum_k \langle \tau_k \rangle$; the variables A_p and B_p are updated after each tunneling event using Eqs. (9)–(10), and the current spectral density $S_I(\omega)$ is calculated as

$$S_I(\omega) \approx \frac{2}{\langle t_p \rangle} \mathrm{Re} A_p. \quad (11)$$

Even though breaking the simulation into segments is not needed in the new method, the calculation and comparison of partial results for $S_I(\omega)$ on some time segments is useful for run-time estimates of the calculation accuracy.

Actually, this basic algorithm still requires several improvements to become faster than the standard method, especially at low frequencies. First, the accuracy can be significantly improved by explicitly calculating the spectral density for the function $I(t) - \overline{I}$ instead of $I(t)$. (The average current $\overline{I}$ can be calculated as $\sum_k q_k / \sum_k \langle \tau_k \rangle$, which is the same as in the reduced method.[10,11]) For this purpose the definition of quantity s_p should be modified to $s_p = \left| [\sum_n^p q_n \exp(i\omega t_n)] - \overline{I}\,[\exp(i\omega t_p) - 1]/i\omega \right|^2 = \left| \sum_n^p \exp(i\omega t_n) \left[q_n - \overline{I}\,(1 - \exp(-i\omega\tau_n))/i\omega \right] \right|^2$. From this point, the derivation is similar to that discussed above, though is now significantly lengthier. The final result is that the only change in the algorithm is a different set of recurrent equations replacing Eqs. (9)–(10):

$$\begin{aligned} A_{p+1} &= A_p + q_{p+1}^2 - 2\overline{I}\,\langle \tau_{p+1} \rangle \frac{q_{p+1} - \overline{I}\langle\tau_{p+1}\rangle}{1 + (\omega \langle \tau_{p+1} \rangle)^2} \\ &\quad + 2 \frac{q_{p+1} - \overline{I}\,\langle \tau_{p+1} \rangle}{1 - i\omega \langle \tau_{p+1} \rangle} B_p, \end{aligned} \quad (12)$$

$$B_{p+1} = q_{p+1} - \frac{\overline{I}\,\langle \tau_{p+1} \rangle}{1 - i\omega \langle \tau_{p+1} \rangle} + B_p \frac{1}{1 - i\omega \langle \tau_{p+1} \rangle}. \quad (13)$$

(The initial conditions are still $A_0 = B_0 = 0$).

However, this improvement still does not solve the problem of relatively poor convergence of the algorithm, especially at low frequencies. The origin of the problem is hinted at by Eq. (2). Since we eliminated the T-segmentation used in the standard method, and now T is much longer (the whole simulation period), we are

calculating $S_I(\omega)$ with a much smaller degree of spectral smoothing. The price for a better spectral resolution $\Delta\omega$ is the longer simulation time for the same accuracy. Therefore, to improve convergence, we have to re-introduce some time constant T_0 that would define the spectral smoothing $\Delta\omega \sim 1/T_0$. In principle, there are many ways to do this. For example, we can periodically (with period T_0) set to zero the value of B_p (in this case the algorithm becomes somewhat similar to the standard method). Alternatively, we can introduce a gradual cutoff of B_p, for example, multiplying the last term in Eq. (13) by $\exp(-\langle\tau_{p+1}\rangle/T_0)$, and so on.

We have used the following way of introducing T_0, which is the best among those we had tried. For simplicity, let us consider first the algorithm without subtraction of $\overline{I}$, and average Eq. (6) over frequency (from $\omega=-\infty$ to $\omega=\infty$) with the Lorentzian weight factor $(T_0/\pi)/\left[1+(\omega-\tilde{\omega})^2 T_0^2\right]$. The integral can be easily calculated using the residue theorem since all the poles of Eq. (6) are in the lower half of the complex plane; therefore, closing the integration contour in the upper half-plane, we will have only one pole at $\omega=\tilde{\omega}+i/T_0$. As a result, the only change in Eq. (6) after integration is that ω is replaced by $\omega+i/T_0$ (more correctly, by $\tilde{\omega}+i/T_0$, but for simplicity we change the notation from $\tilde{\omega}$ back to ω). Therefore, the Lorentzian averaging over frequency in our algorithm exactly corresponds to replacing ω with $\omega+i/T_0$ in the iteration equations (9)–(10).

For the algorithm with $\overline{I}$ subtraction, the Lorentzian averaging is a little more difficult, because of the extra poles in the equation for $\langle s\rangle$ at $\omega=i/\langle\tau_k\rangle$ (upper half-plane) and at $\omega=0$. However, as seen from Eqs. (12)–(13), the pole at $\omega=0$ is eventually canceled, while the poles at $\omega=i/\langle\tau_k\rangle$ remain only in the simple additive term in Eq. (12). Therefore, the recipe of replacing ω with $\omega+i/T_0$ still works for B_{p+1}, and the extra residue of the upper-half-plane pole should be simply added to A_{p+1}. As a result, Eqs. (12)–(13) are replaced with

$$A_{p+1}=A_p+q_{p+1}^2+2\frac{q_{p+1}-\overline{I}\langle\tau_{p+1}\rangle}{1-i\left(\omega+i/T_0\right)\langle\tau_{p+1}\rangle}B_p$$
$$-\frac{2\overline{I}\langle\tau_{p+1}\rangle\left(q_{p+1}-\overline{I}\langle\tau_{p+1}\rangle\right)\left(1+\langle\tau_{p+1}\rangle/T_0\right)}{1+\left(\omega\langle\tau_{p+1}\rangle\right)^2+2\langle\tau_{p+1}\rangle/T_0+\left(\langle\tau_{p+1}\rangle/T_0\right)^2}, \quad (14)$$
$$B_{p+1}=q_{p+1}-\frac{\overline{I}\langle\tau_{p+1}\rangle}{1-i\left(\omega+i/T_0\right)\langle\tau_{p+1}\rangle}$$
$$+B_p\frac{1}{1-i\left(\omega+i/T_0\right)\langle\tau_{p+1}\rangle}, \quad (15)$$

while the rest of the algorithm does not change.

The introduction of Lorentzian smoothing greatly improves the convergence of the algorithm. However, it gives rise to another difficulty. The problem is that the averaging over frequency increases the δ-function contribution from $S_I(0)$ due to average current, and the trick of the standard method, discussed above, is impossible for Lorentzian averaging [in contrast to Eq. (2), in which the convolution function contains zeros]. Formally, our algorithm subtracts $\overline{I}$ beforehand; however, in a real simulation $\overline{I}$ is not known exactly (note that the estimated value of $\overline{I}$ improves during the course of simulation). It can be shown that the inaccuracy ΔI in the average current estimate used in Eqs. (14)–(15) brings to $S_I(\omega)$ the extra contribution

$$\Delta S_I(\omega)=4T_0(\Delta I)^2/\left(1+\omega^2T_0^2\right). \quad (16)$$

This contribution can be subtracted from $S_I(\omega)$ at the end of the simulation run, when a better estimate of $\overline{I}$ is known and the difference from the initially used estimate can be calculated. Actually, the value of $\overline{I}$ used in Eqs. (14)–(15) can be periodically (sufficiently rare) updated during the simulation run; in this case $(\Delta I)^2$ in Eq. (16) can naturally be replaced with the time-weighted value.

With these modifications, the advanced algorithm becomes significantly faster and more convenient than the standard algorithm. Accurate comparison of their efficiencies is not straightforward because both methods have adjustable parameters. (T in the standard method and T_0 in the new method both affect the smoothing of the spectral density and the convergence speed; the choice of too short T could also lead to incorrect results.) Crudely, the speed-up factor (the ratio of CPU times for the same accuracy using the two methods) for our typical simulation runs is two to three orders of magnitude.

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