Coulomb-correlations in the electric power of nanoscale open systems

G.Albareda and X.Oriols
Departament d'Enginyeria Electrònica, Universitat Autònoma de Barcelona, 08193 Bellaterra, Spain
guillem.albareda@uab.cat

Due to computational limitations, one necessary strategy to study nanoscale structures is to reduce, as much as possible, the simulated degrees of freedom. This procedure is always traumatic because, in general, a subcomponent of the whole system cannot be described independently of the rest (See Fig. 1). The openness of classical and quantum systems has been studied extensively in the literature, but few works are devoted to discuss its effect on the computation of electric power. Here, we provide a novel expression for accurate estimation of the electric power in nanoscale open systems using a many-particle electron transport formalism that goes beyond the standard "mean field" approximation [1]. Surprisingly, we show that the usual expression of the electric power, as the product of the (time-averaged) current $\langle I \rangle_T$ and the applied voltage ΔV, is not correct in nanoscale systems.

In order to provide a common classical and quantum language for our argumentation, we formulate the problem in terms of the de Broglie–Bohm approach of quantum mechanics for an open system of non-relativistic (spinless) Coulomb-interacting electrons [1,2]. Then, it can be shown that the mean electric power, P, for the *N(t)* electrons inside the open system (see Fig. 1b) is:

$$P = \left\langle \sum_{i=1}^{N(t)} q\vec{v}_i(t)\vec{E}_i\left(\vec{r}_i(t)\right) \right\rangle_B = \lim_{T\to\infty} \frac{1}{T} \sum_{i=1}^{M(T)} q\left(K_i(L) - K_i(0)\right), \qquad (1)$$

where $\vec{v}_i(t)$ is the (Bohm) velocity of the *i* electron, $q\vec{E}_i(t)$ is the electrostatic force made by the rest of electrons of the whole (closed) system on it, and $K_i(L)$ and $K_i(0)$ are its (Bohm) kinetic energies at the final and initial positions respectively. Here, $\langle ... \rangle_B$ is the de Broglie-Bohm averaging that can be converted into time averaging $\langle ... \rangle_T$ under standard ergodic argumentations. After some straightforward development, the final value of the mean electric power P of expression (1) can be written as:

$$P = \langle I \rangle_T \cdot \Delta V - \left\langle \frac{q}{2} \sum_{i=1}^{N(t)} \sum_{\substack{j=1 \\ j\neq i}}^{N(t)} \left(\vec{v}_j - \vec{v}_i\right) \cdot \frac{\left(\vec{r}_i - \vec{r}_j\right)}{4\pi\varepsilon \left|\vec{r}_i - \vec{r}_j\right|^3} \right\rangle_T , \qquad (2)$$

where $W_i\left(\vec{r}_1,..,\vec{r}_j,..,\vec{r}_i(t),..,\vec{r}_M\right)$ is the *i-th* electrostatic potential defined in Ref. [1] that depends on the *M* electrons present in the close (whole) system (see Fig. 1a) and $\vec{R}_i(t) = \left(\vec{r}_1(t),..,\vec{r}_j(t),..,\vec{r}_{i-1}(t),\vec{r}_{i+1}(t),..,\vec{r}_M(t)\right)$. The first term on the right side of (2) is the standard $\langle I \rangle_T \cdot \Delta V$ power expression, while the second term represents the effects of the many-particle coulomb correlations on the electric power.

In order to show the relevance of the many-particle power correlations, we have simulated a nanoscale resistance using, both, a standard single-particle semiconductor Monte Carlo simulator and a many-particle electron transport approach explained in

Ref. [1]. In fig. 2a, we have represented the current-voltage characteristic for a nanoscale resistance using a single-particle (i.e. time-independent electric-field) electron transport approach. We define the correlation power factor as the following (dimensionless) parameter, $G = \left(\langle I \rangle_T \cdot \Delta V\right) / P$. As expected, the value of G reduces to unit, i.e. $P \approx \langle I \rangle_T \cdot \Delta V$, indicating that many-particle Coulomb-interaction effects in the power computation are not accessible with single-particle electron transport simulations. On the contrary, when the many-particle electron transport formalism explained in Ref. [1] is used, then, the relevance of correlations in the average power becomes evident (at low bias) in the correlation power factor G depicted in Fig. 3b.

The physical explanation of our "unexpected" many-particle corrections on the electric power is that the computation of power in numerical simulators has to account only for the (non-conservative) energy associated to the *N(t)* electrons inside the open system rather than the (conservative) energy of the M electrons inside the whole system (see Fig. 1).

References:

[1] G. Albareda, J. Suñé and X. Oriols, Physical Review B, **79** (2009) 075315.
[2] X. Oriols, Physical Review Letters, **98** (2007) 066803.

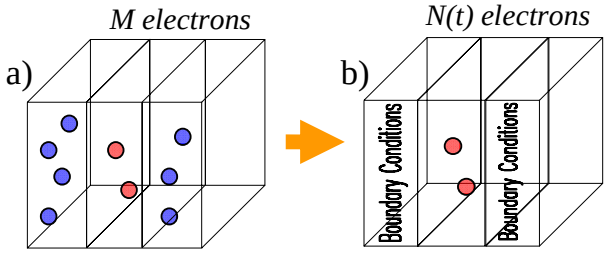

Fig.1. Schematic representation of the electrons in an electron device. a) A closed (whole) system of *M* electrons in the active region and the reservoirs and b) the open system of *N(t)* electrons in the active region.

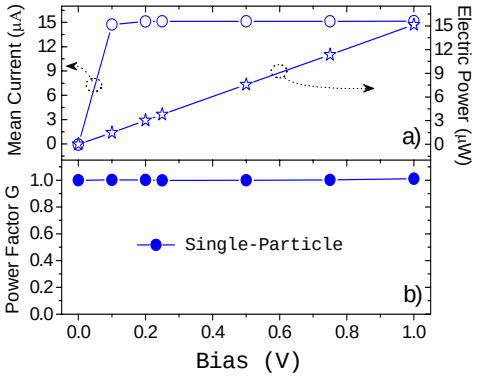

Fig.2. a) Average current, electric power, and b) correlation power factor, G, defined in the text as a function of bias. Electron transport is computed from a single-particle approach.

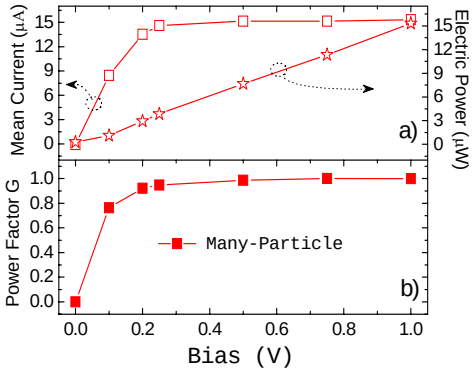

Fig.3. a) Average current, electric power, and b) correlation power factor, G, defined in the text as a function of bias. Electron transport is computed from the many-particle approach described in [1].