# Analytic solution for the current-voltage characteristic of two mesoscopic tunnel junctions coupled in series

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We present a theoretical analysis for a system composed of two mesoscopic tunnel junctions coupled in series. We show that the current-voltage characteristic for this system can be obtained analytically. The usefulness of the model is demonstrated through the fit of experimental data acquired with a cryogenic (4.2 K) scanning tunneling microscope. A simple extension of the model predicts additional structure in the system characteristics when discrete middle electrode states are present.

Recently, considerable interest has been directed toward tunnel-junction systems where the discreteness of the electronic charge plays a prominent and observable role. These systems involve at least one ultra-small conductive element with a capacitance, $C$, such that its capacitive charging energy, $E_c$, is greater than the thermal energy: $E_c=e^2/2C>k_BT$, where $e$ is the fundamental charge unit and $k_B$ is the Boltzmann's constant. One of the simplest such systems consists of two mesoscopic tunnel junctions coupled in series, with the shared electrode having dimensions on the order of 100 Å. Applying an external voltage, the small capacitances (typically $10^{-18}$ F) of the junctions must first charge up to certain "threshold" voltages before an electron can tunnel through the system. The result is, for a range of junction parameters, the occurrence of current steps in the current-voltage ($I$-$V$) characteristics of the two-junction system. This "Coulomb staircase" arises from the incremental increase in the current at voltages where it is energetically favorable for an additional electron to sit on the middle electrode.

Early work[1,2] studying capacitive charging effects predict these current steps, though their experimental geometries only allowed measurements of ensemble phenomena. Later theoretical treatments[3,4] have quantified this prediction, describing the details of the expected step structure in the $I$-$V$ characteristics of small two junction systems. Recent experiments[5-9] on systems consisting of two mesoscopic junctions coupled in series have exhibited the expected staircase structure. The experiment of Wilkins *et al.*[8] show striking quantitative agreement with stochastic calculations based on a semiclassical model[4] of mesoscopic junctions. Equivalently, the solution of the appropriate master equation can be calculated numerically.[10,11] Because of their numerical nature, both methods make fitting of data laborious. In this Brief Report we present a theoretical treatment of the two-junction system from which an exact analytic form for the $I$-$V$ characteristics can be obtained. The simple result for the calculated $I$-$V$ characteristics provides an efficient means to compare theory and experiment. As an example, we fit data obtained with a cryogenic scanning tunneling microscope (CSTM). We also consider briefly an extension of the simple two-junction system where an external bias can be applied to the shared electrode. This extension has possible relevance to other experimental mesoscopic systems.[12] Lastly, we show that allowing the electronic energy levels of the shared electrode to be discrete can give additional structure in the $I$-$V$ characteristics.

Consider one possible two-junction system, as shown in Fig. 1. Here we have two junctions driven by an ideal (no internal resistance) constant voltage source $V$. We use the semiclassical model to describe the two-junction system.[11] In this model the state of each junction is fully characterized by the voltage dropped across the junction, a classical variable. The state of the system is then given by $V_1$ and $V_2$, the voltage dropped across the first and second junctions, respectively. Using charge conservation for the middle electrode and Kirchoff's voltage law for the circuit loop, the junction voltages are written in terms of the number of extra electrons (as supplied by the external circuit) on the middle electrode, $N$:

 

$$V_1=\frac{C_2}{C_1+C_2}V-\frac{Ne}{C_1+C_2}-V_p\ ,$$
$$V_2=\frac{C_1}{C_1+C_2}V+\frac{Ne}{C_1+C_2}+V_p\ , \tag{1}$$

where the capacitance of the $i$th junction is $C_i$. An additional voltage, $V_p$, is added to account for any misalignment of the middle electrode Fermi level with the Fermi levels of the outer electrodes when $N$ and $V$ are zero.[2] From the voltage equations (1), it is clear that the state of the system is equivalently defined by $N$ and $V$.

Ensemble-averaged dynamics for the two-junction system are obtained from the master equation for $\rho(N,V,t)$, the probability that there are $N$ extra electrons on the middle electrode at time $t$ with applied voltage $V$:[3,10,11]

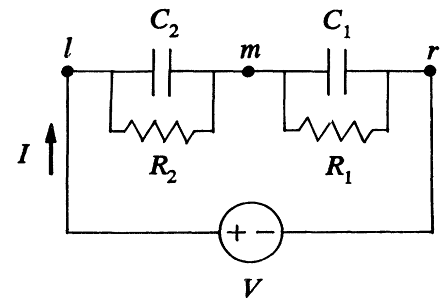


FIG. 1. Schematic representation of one possible system composed of two mesoscopic tunnel junctions coupled in series. The two junctions of capacitances $C_1$ and $C_2$, and normal state resistances $R_1$ and $R_2$, are driven by the ideal voltage source $V$.

$$\frac{\partial\rho(N,V,t)}{\partial t}=[r_1(N-1,\,V)+l_2(N-1,\,V)]\rho(N-1,\,V,t)+[l_1(N+1,\,V)+r_2(N+1,\,V)]\rho(N+1,\,V,t)$$
$$-[r_1(N,V)+l_1(N,V)+r_2(N,V)+l_2(N,V)]\rho(N,V,t)\ , \tag{2}$$

where $r_i(N,V)$ and $l_i(N,V)$ are the electron tunneling rates from the right and left, respectively, on the $i$th junction. This equation describes how $\rho(N,V,t)$ changes in time as a result of single electron tunneling events. Alternatively, the actual charge transfer can be modeled from a stochastic process written for $N$.[4]

Here we are interested in the dc characteristics of the two-junction system, therefore the steady-state solution of Eq. (2) is desired. The steady-state master equation is found by setting the time derivative of the probability distribution function equal to zero in Eq. (2). This equation describing the steady state, for fixed $V$, states that the net probability of making a transition between the state $N$ and the adjacent states $N+1$ and $N-1$ must be zero. A considerable simplification can be achieved by noting that the steady state is equivalently obtained by requiring that, for fixed $V$, the net probability of making a transition between any two adjacent states (say, $N$ and $N+1$) must be zero. Therefore, the following simplified equation describes the steady state:

$$x(N,V)\rho(N,V)-y(N+1,\,V)\rho(N+1,\,V)=0\ , \tag{3}$$

where $x(N,V)\equiv r_1(N,V)+l_2(N,V)$ and $y(N,V)\equiv l_1(N,V)+r_2(N,V)$. Equation (3) is a linear first-order difference equation that can be solved subject to the normalization condition on $\rho(N,V)$:

$$\sum_{N=-\infty}^{+\infty}\rho(N,V)=1\ . \tag{4}$$

The result is

$$\rho(N,V)=\frac{\left[\prod_{i=-\infty}^{N-1}x(i,V)\right]\left[\prod_{i=N+1}^{+\infty}y(i,V)\right]}{\sum_{j=-\infty}^{+\infty}\left[\prod_{i=-\infty}^{j-1}x(i,V)\right]\left[\prod_{i=j+1}^{+\infty}y(i,V)\right]}\ . \tag{5}$$

The average current is calculated using

$$I=\sum_{N=-\infty}^{+\infty}e[r_2(N,V)-l_2(N,V)]\rho(N,V)$$
$$=\sum_{N=-\infty}^{+\infty}e[r_1(N,V)-l_1(N,V)]\rho(N,V)\ . \tag{6}$$

The $I$-$V$ characteristic may then be calculated if the rates are known as functions of $N$ and $V$. The electron tunneling rates may be determined from a "golden-rule" calculation. For example, $r_1(N,V)$ is calculated by integrating, over energy, the square of the tunneling matrix element coupling the initial and final states at energy $E$, $|T(E)|^2$, with the number of occupied initial states and the number of unoccupied final states:

$$r_1(N,V)=\int_{-\infty}^{+\infty}\frac{2\pi}{\hbar}|T(E)|^2D_r(E-E_r)f(E-E_r)D_m(E-E_m)[1-f(E-E_m)]dE\ , \tag{7}$$

where $f(E)$ is the Fermi distribution function, $D_r(E)$ and $D_m(E)$ are the density of states of the right and middle electrode, respectively, and similarly $E_r$ and $E_m$ are their Fermi energies. For simplicity assume that $D_r(E)$, $D_m(E)$, and $|T(E)|^2$ are energy independent, so that $D_r(E)=D_{r0}$, $D_m(E)=D_{m0}$, and $|T(E)|^2=|T_0|^2$. Equation (7) integrates to[13]

$$r_1(N,V)=\frac{1}{e^2R_1}\frac{E_r-E_m}{1-e^{-(E_r-E_m)/k_BT}}\ , \tag{8}$$

where $R_1\equiv\hbar/(2\pi e^2D_{r0}D_{m0}|T_0|^2)$ is the normal-state resistance of the first junction. The difference between the right electrode Fermi energy before a tunneling event and the middle electrode Fermi energy after the event,

$E_r - E_m$, is the energy the electron gains during the tunneling event. This energy is dependent on the amount of charge that is transferred from the external system to the junction during the tunneling event. If we assume that the charge distribution completely relaxes during the tunneling event (the time of tunneling is much longer than the relaxation time of the system but shorter than the time between tunneling events), the energy difference is given by

$$E_r - E_m = -\frac{(2N+1)e^2}{2(C_1+C_2)} + \frac{eC_2V}{C_1+C_2} = eV_1(N,V) - E_c \;, \tag{9}$$

where $(2N+1)e^2/2(C_1+C_2)$ is the change in the electrostatic energy of the system, $eC_2V/(C_1+C_2)$ is the work done by the voltage source, and $E_c \equiv e^2/2(C_1+C_2)$ is the junction charging energy. The resultant electron tunneling rate is

$$r_1(N,V) = \frac{1}{e^2R_1}\frac{eV_1(N,V)-E_c}{1-e^{[-eV_1(N,V)+E_c]/k_BT}} \;. \tag{10}$$

The other tunneling rates can be determined in a similar manner. From Eq. (10) it is clear that at $T = 0.0$ K tunneling is suppressed for $eV_1 < E_c$. The value $E_c/e$ is the junction voltage at which the individual junctions will first be able to transfer charge, the junction threshold voltage. The applied voltage at which the system will pass charge (system threshold voltage, $V_t$) occurs when either junction reaches its threshold. The applied voltage at this point is, $V_t = e/2\max\{C_1, C_2\}$. For $T > 0.0$ K the thresholds are thermally rounded with a voltage width proportional to $k_BT/e$.

In Fig. 2, curve $A$, we show experimental data for a two-junction system taken with a CSTM. The data was obtained by bringing the tip of the STM near a small (approx 100 Å diameter) indium droplet that is sitting on an oxidized conducting substrate. One junction is formed between the tip and the droplet and the other between the droplet and the substrate. The experimental setup and procedure have been described in detail elsewhere.[8] To demonstrate the usefulness of the theory presented here, we show a fit to experimental data in Fig. 2, curve $B$. The data was fit using a least squares technique, which would be difficult without an analytic form for the $I$-$V$ characteristic. It should be noted that in addition to the linear term in the rates a cubic term was added to account for the nonlinear background conductance in the data.[8]

The two-junction system analysis presented above applies to systems other than the simple one chosen. Another system in which the theory applies is composed of two junctions driven by a constant voltage source $V$ with an additional voltage, $V_{ex}$, applied to the middle electrode through a capacitance $C_{ex}$, forming a three-terminal transistorlike device. The voltage equations describing that system are

$$\begin{aligned} V_1 &= \frac{C_2}{C_1+C_2+C_{ex}}V - \frac{Ne}{C_1+C_2+C_{ex}} - V_p + \frac{C_{ex}}{C_1+C_2+C_{ex}}V_{ex} \;, \\ V_2 &= \frac{C_1+C_{ex}}{C_1+C_2+C_{ex}}V + \frac{Ne}{C_1+C_2+C_{ex}} + V_p - \frac{C_{ex}}{C_1+C_2+C_{ex}}V_{ex} \;. \end{aligned} \tag{11}$$

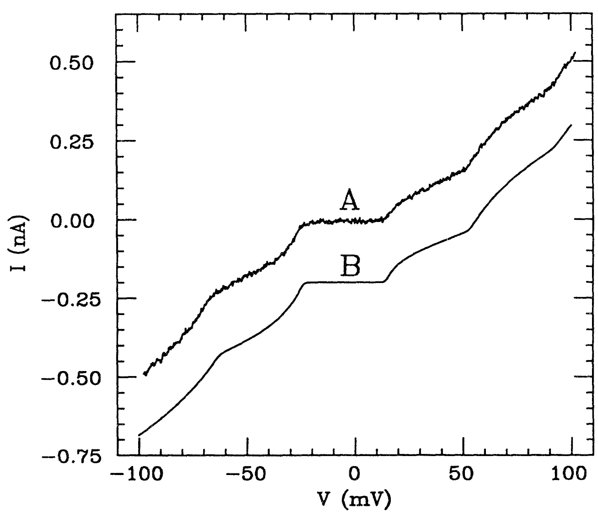


FIG. 2. Curve $A$: Experimental $I$-$V$ characteristic of a two-junction system obtained by probing a small indium droplet with a cryogenic scanning tunneling microscope. Curve $B$: Numerical fit of the experimental data of curve $A$, shifted by 0.2 nA for clarity. The parameters of the fitted curve are $C_1 = 4.14$ aF, $C_2 = 2$ aF, $R_1 = 132$ MΩ, $R_2 = 34.9$ MΩ, $V_p = 3.26$ mV, $T = 4.2$ K, and $\alpha = 24$ $V^{-2}$ (where $\alpha V^3/R$ is a nonlinear background term added to the tunneling rates).

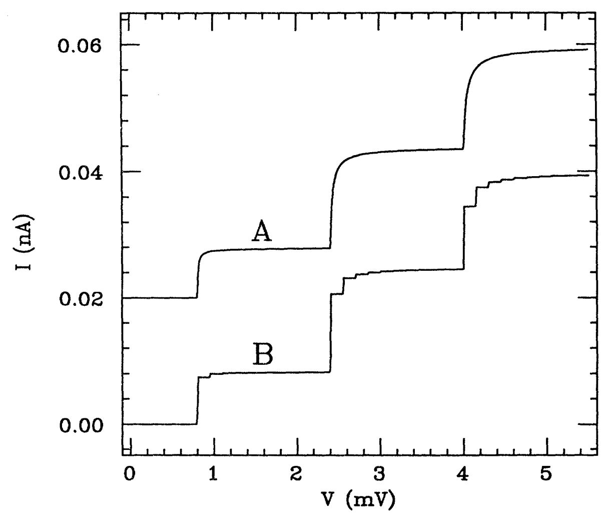


FIG. 3. Calculated $I$-$V$ characteristics for the two-junction system when the parameters are chosen such that clear charging steps are produced, $R_1 \gg R_2$ and $C_1 \gg C_2$. The parameters are $C_1 = 100$ aF, $C_2 = 1$ af, $R_1 = 100$ MΩ, $R_2 = 1$ MΩ, and $T = 0.01$ K. Curve $A$: $I$-$V$ characteristic calculated assuming a continuous middle electrode density of states. The curve is shifted vertically by 0.02 nA for clarity. Curve $B$: $I$-$V$ characteristic calculated assuming a discrete middle electrode density of states, with a level spacing of $\Delta E = 0.15$ meV.

The capacitive charging energy for this device is $E_c = e^2/2(C_1 + C_2 + C_{ex})$. Steady-state device characteristics for the system may then be generated using Eqs. (5), (6), and (10), and the above voltage equations.

With a simple modification in the tunneling rates one can also obtain a first approximation for the case when the discreteness of the middle electrode energy levels becomes important. For simplicity, consider the energy levels to be equally spaced and of zero width. A more realistic model would have states of a finite width dependent on the electronic relaxation time in the middle electrode.[14] The middle electrode density of states becomes

$$D_m(E - E_m) = D_{m0}\,\Delta E \sum_{n=0}^{+\infty} \delta(E - E_m - E_0 - n\,\Delta E) , \tag{12}$$

where $\Delta E$ is the level spacing and $E_0$ is the ground-state energy. Substituting this density of states into Eq. (7) gives the following for $r_1(N,V)$ (assuming $E_c \gg \Delta E$):

$$r_1(N,V) = \frac{\Delta E}{e^2 R_1} \sum_{n=0}^{+\infty} [(e^{[-eV_1(N,V) + E_c + E_0 + n\,\Delta E]/k_B T} + 1)(e^{-(E_0 + n\,\Delta E)/k_B T} + 1)]^{-1} . \tag{13}$$

Again, the other rates may be determined in a similar manner. Using Eqs. (5), (6), and the appropriate rate equations, we have calculated the $I$-$V$ characteristics for junction parameters that show well-developed charging steps. In Fig. 3, curve $A$, we show an $I$-$V$ characteristic for a continuous middle electrode density of states and exhibit the well-known "Coulomb staircase." When the middle electrode has a discrete density of states an additional structure appears in the $I$-$V$ characteristic, as shown in Fig. 3, curve $B$. Increasing the temperature and giving the discrete states finite width rounds the additional structure.

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