Numerical study of the totally asymmetric simple exclusion process that consists of only a single site for modeling the dynamics of Coulomb blockade in 2D quantum dot

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Numerical Study of the Totally Asymmetric Simple Exclusion Process that Consists of Only a Single Site for Modeling the Dynamics of Coulomb Blockade in 2D Quantum Dot

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Abstract. A theoretical study of the dynamical mechanism of Coulomb blockade using the totally asymmetric simple exclusion process (TASEP) consisting of only one site has been laid down in [1]. Coulomb blockade is the main idea behind the so-called quantum dot, which is a product in the advancement of nanotechnology. A quantum dot is a nano-scale system, which consists of only one electron. It offers exciting opportunities in the creation of semiconductor fabrication technology. In this study, a further examination is conducted into the relationship of the Coulomb blockade and the TASEP by obtaining numerical results of the density and current density of the electron trapped inside the dot as well as the tunneling of the electron through the dot. The results show that the density and current density agree with the electron being trapped inside the dot with high density and low current density, and the electron passing through the dot with a moderate value of the density and current density.

NANOTECHNOLOGY, COULOMB BLOCKADE, AND SINGLE ELECTRON TUNNELING

Nanoscale research and development have revolutionized today's technology becoming what is known today as nanotechnology. Nanoscience has evolved into a unique interdisciplinary subject which involves various specialized studies, such as physics[2], biology[3,4], chemistry[5], environment[6,7], medicine[8,9], and so forth. Products of nanoscience and nanotechnology are pouring into our daily life, e.g. toothbrush and toothpaste [10,11], food and packaging[12,13], kitchenware and household products[14], building constructions[15], computers and electronics[16,17], and so much more. Especially in the field of electronics, where nanotechnology finds one of its most fertile applications, a novel nanoscale structure has been created, i.e. quantum dot[18]. This system is obtained when an electron is being confined by an external potential in all three spatial coordinates. One of the interesting features of the quantum dot is the ability to mimic the behavior of an atom although it is ten or hundreds times bigger than an actual atom, e.g. discrete energy levels and the Zeeman effect[19]. Another interesting feature is that its physical properties depend on the voltage applied to the dot. Hence, the quantum dot is also designated as an artificial atom[1]. The quantum dot has been studied throughout many literatures and its various applications include optical and optoelectronic devices[20,21], quantum computing[22], DNA testing[23,24], and three-dimensional (3D) imaging[25]. Recently, Samsung has produced a television using quantum dots for its screen display [26].

An important machinery of how to control the number of electrons inside the dot is called Coulomb blockade[1,18]. It is the main object of this current study. Hence, an energy diagram given in Fig. 1 is provided to explain briefly the mechanism of the Coulomb blockade [Fig. 1(a)] as well as its counterpart, the single electron tunneling (SET) [Fig. 1(b)]. A quantum dot consists, primarily, of three parts, i.e. a source, an island, and a drain [see Fig. 1(a)]. The source is a reservoir of electrons which are going into the dot (island), the drain is a reservoir of

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electrons which come out from the dot, and the island is where the electron is supposed to be trapped (quantum dot). There are two kinds of applied voltages, which are involved here, i.e. the source-drain and gate voltages.

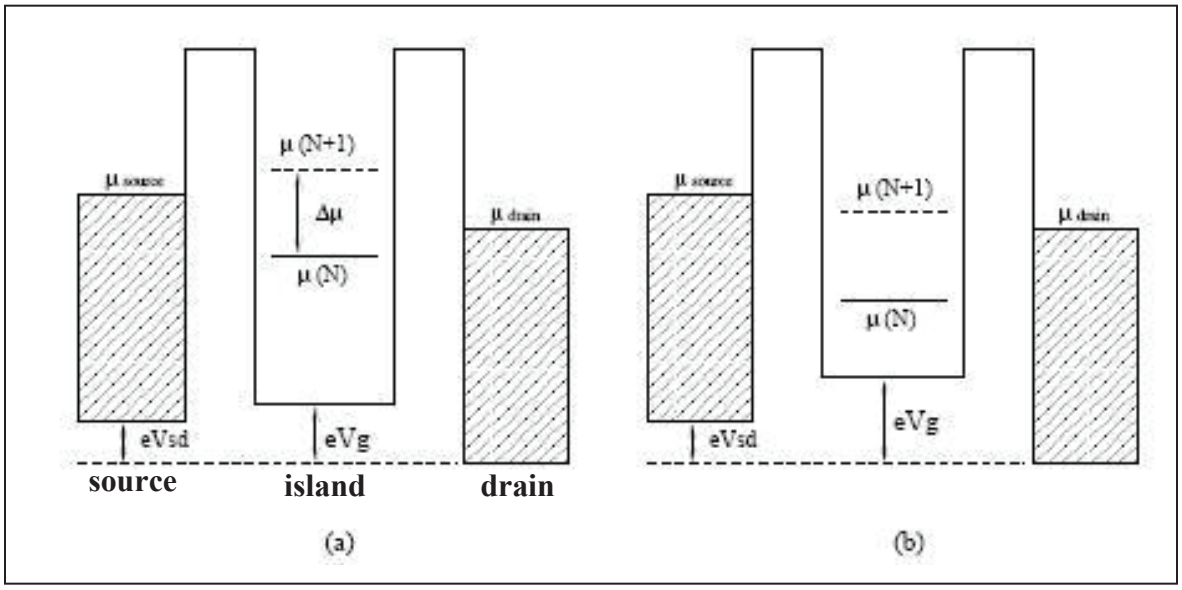

FIGURE 1. The energy diagram of the quantum dot. (a) is the Coulomb blockade and (b) is the single electron tunneling.

The Coulomb blockade may be described as follows. The source and drain are under the influence of their respective electrochemical potential, i.e.: μ_{source} and μ_{drain}, respectively. Both chemical potentials are connected through an applied source-drain voltage, V_{sd}, that is, $eV_{sd} = (\mu_{source} - \mu_{drain})$, where the latter is called the transport window and e is the electron charge unit. Now, the electrons inside the dot occupy the states up to the electrochemical potential of $\mu(N)$, where N is the total number of electrons. Therefore, the next state should be occupied by an electron which has a higher electrochemical potential, i.e. $\mu(N+1)$. However, since $\mu(N+1) > \mu_{source}$ at zero temperature, electrons may not enter the dot. Moreover, since $\mu(N) < \mu_{drain}$, the electrons cannot exit the dot [see Fig. 1(a)]. Hence, electrons are trapped inside the dot (island). This occurs for $k_BT << e^2/C$, where C is the total capacitance, k_B is the Boltzmann constant, and T is the temperature.

A second mechanism called the single electron tunneling is considered so that an electron may tunnel through the dot. This is based on Fig. 1(b). Here another voltage, which is the gate voltage, needs to be varied, such that $\mu(N+1) < \mu_{source}$. Therefore, an electron can move from the source to the dot and raise the next state higher than $\mu(N+1)$ preventing another electron from entering the dot. Moreover, since $\mu(N+1) > \mu_{drain}$, then the electron may exit the dot into the drain, decreasing the chemical potential back to $\mu(N)$.

THE DYNAMICAL MODEL: TOTALLY ASYMMETRIC SIMPLE EXCLUSION PROCESS IN ONE DIMENSION

The totally asymmetric simple exclusion process (TASEP) in one dimension (1D) is a simple mathematical model to explore the dynamics of hard-core classical-particles on discrete lattice sites, L. Each lattice site, i, may only be occupied by one and only one hard-core particle. The dynamics of the particles in the lattice sites are prescribed by the dynamical rule, i.e.: at any given time, a particle (particles) may jump to its (their) right nearest neighbor site(s) provided that the right nearest neighbor site(s) is (are) empty. The TASEP in 1D is a well-known particle hopping model [27] which is utilized to study many dynamical systems in various transport phenomena, e.g. DNA polymerization[28], the dynamics of motor protein in organism[29], the track of a group of ants[30], and road traffic jams[31].

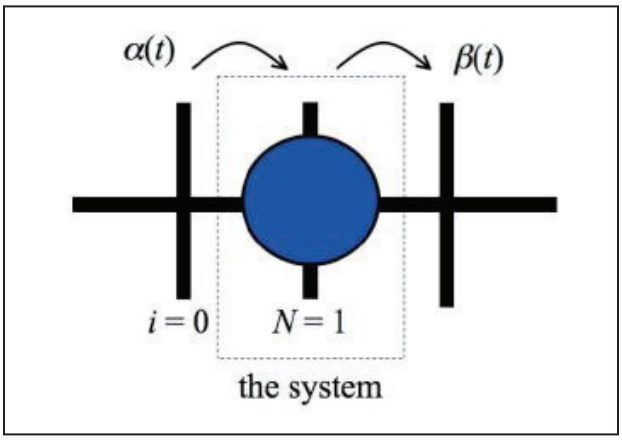

FIGURE 2. The TASEP that consists of only one site, i.e. $N = 1$. The dark vertical lines are lattice sites labeled by $i = 0, 1, 2$. Site $i = 0$ and 2 are reservoirs of particles where particles jump into and out of site $i = N = 1$ (the system), respectively. The dark (blue) circle is a hard-core particle occupying the system. A particle may enter site $i = 1$ with an input hopping rate of $\alpha(t)$ if there is no particle occupying site $i = 1$. A particle occupying site $i = 1$ may exit the site with an output hopping rate of $\beta(t)$.

Here, the TASEP is used to study the dynamics of electrons trap in the dot and their tunneling through the dot. With the aim of fulfilling the aforementioned objective, the TASEP with a single site is employed (see Fig. 2). This set-up is arguably the simplest arrangement of the model where we only consider one site, i.e.: $i = N = 1$, with N is the total number of sites. This single site represents the dot (island). Next, we make use of the open boundary condition where the single site is coupled to two reservoirs at each end of the site. The left reservoir, viz. $i = 0$, contains particles that may jump to the system (site $i = 1$) with input rate $\alpha(t)$ provided that there is no particle in the system. The right reservoir at $i = 2$ consists of particles that exit the system with output rate $\beta(t)$. With respect to the quantum dot above, the reservoirs of the single site TASEP at site $i = 0$ and $i = 2$ represent the source and drain, respectively.

The single particle occupation of the system in the TASEP is due to the hard-core inter-atomic potential between classical particles. This potential is a consequence of a purely infinite repulsive potential between two particles to a certain inter-atomic distance. Larger than this distance, the particles are non-interacting. Therefore, if there is a particle on site $i = 1$, then no other particle may sit on the site. However, the nature of the SET is completely different from that of the aforementioned potential. In the SET, an electron may 'jump' into and out of the dot because of the differences between electrochemical potentials. However, the two mechanisms look similar in the sense that there is only a single particle in the TASEP and SET. Hence the trapping or tunneling of a single electron in the dot is similar to a classical particle occupying or jumping on the lattice sites. That is why a relationship can be made between TASEP, Coulomb blockade, and SET.

THE CONNECTION BETWEEN THE TASEP, COULOMB BLOCKADE, AND SET

The conceptual relationship between the TASEP, Coulomb blockade, and SET is provided in [1]. First, as already mentioned above, the connection between the components of the TASEP and quantum dot is as follows: (i) site $i = 0$ of the TASEP represents the source, (ii) site $i = 1$ of the TASEP represents the dot (island), and (iii) site $i = 2$ of the TASEP represents the drain. Following the connection above is the density and current density of the electron tunneling or trapped inside the dot, that is,

$$\rho_1(t) = \rho_1(0) + e^{\frac{e}{k_B T}(V_g - V_{sd})} \int_0^t \{\rho_0(t')[1-\rho_1(t')] - \rho_1(t')[1-\rho_2(t')]\} dt'. \quad (1)$$

where $\rho_1(t)$ is the density of electrons in the dot ($i = 1$) at time t, $\rho_0(t)$ is the density of electrons in the source (site $i = 0$) at time t, $\rho_2(t)$ is the density of electrons in the drain ($i = 2$) at time t, and $\rho_1(0)$ is the initial density. Equation (1) is obtained using the continuity equation,

$$\frac{\partial \rho_1(t)}{\partial t} = J_{01}(t) - J_{12}(t), \tag{2}$$

such that the current density of electrons tunneling to the dot from the source is

$$J_{01}(t) = e^{\frac{e}{k_B T}(V_g - V_{sd})} \rho_0(t)[1 - \rho_1(t)], \tag{3}$$

and the current density of electrons exiting the dot is

$$J_{12}(t) = e^{\frac{e}{k_B T}(V_g - V_{sd})} \rho_1(t)[1 - \rho_2(t)]. \tag{4}$$

Equation (1) gives the average occupancy of electrons in the dot (i = 1), while equations (3) and (4) yield the average tunneling rate of electrons through the dot. It may be observed that both quantities depend on the gate and source-drain voltages. Using Eq. (1), by setting the initial density, $\rho_1(0)$, to some value and given the densities at site i = 0 and i = 2 at any given time, then the density at any given time, $\rho_1(t)$, can be obtained. Furthermore, the current density can be obtained using Eqs. (3) and (4).

MATERIAL AND METHODS

This is essentially a theoretical study which is a continuation of an earlier study conducted in[1]. The device utilized is Lenovo PC with Intel(R) Celeron(R) CPU 1000M @ 1.80 GHz processor and 2.00 GB memory. Here, the DEV C++ program language is used to obtain numerical solutions for the density and current density of the TASEP to study the dynamics of electrons in Coulomb blockade and SET. First, let $V_g > V_{sd}$ and $V_g - V_{sd} \rightarrow 0$. Then, let Eq. (2) evolves with time such that the stationary state is reached, i.e. the LHS of Eq. (2) equals to zero as the density does not depend on upon time. Hence, rearranging Eqns. (2), (3), and (4) yield:

$$\rho_1 = \frac{\rho_0}{1 - \rho_2 + \rho_0}. \tag{5}$$

The steady-state density of the single site TASEP is then calculated by varying the density of the reservoirs from 0 to 1.0. Moreover, the current density of the TASEP is obtained using Eq. (3) or (4).

RESULTS AND DISCUSSION

The results of this study show the density and current density of the TASEP with a single site in a steady state with a variation of the left and right reservoir densities. The results are then employed to examine the density of electrons in Coulomb blockade and SET.

The numerical one-body density profile of the TASEP with a single site is given in Fig. 3. It may be observed in Fig. 3 that there are various densities of the single site TASEP. For low densities of the left and right reservoirs, viz.: $\rho_0, \rho_2 < 0.5$, the density of the TASEP is quite low, thus this is the low-density regime. In this regime, the site is not occupied (empty) most of the time. This may be caused by (i) the low density of the left reservoir so that there is no particle going into the site, or (ii) the low density of the right reservoir such that the particle already exits the site. On the other hand, for high densities of the left and right reservoirs, that is $\rho_0, \rho_2 > 0.5$, the density of the site is quite high, therefore giving the high-density regime. Opposite to the former, in this regime, particles occupy the site most of the time. This is because of the high density of the left reservoir such that a particle has a high probability to fill the (empty) site, whereas the right reservoir is also in a high density preventing the particle to exit the site. Finally, for reservoir densities satisfying $\rho_0 + \rho_2 = 1.0$, except for $\rho_0 = 0.0$, $\rho_2 = 1.0$, the density is quite moderate, i.e. equal to 0.5, which means that particles have half a chance of occupying or exiting the site. In other words, particles are just 'tunneling' through the site. In this regime, we may interpret that the SET occurs.

From the density profile, the phase diagram may as well be obtained, which may be perceived in Fig. 4. The (red) dashed line on the main diagonal of the phase diagram is the region where the SET may occur, i.e.: very low and high densities of the left and right reservoirs, respectively. The Coulomb blockade occurs at the bottom of the phase diagram, that is, at $\rho_2 = 1.0$ (blue dot-dashed line).

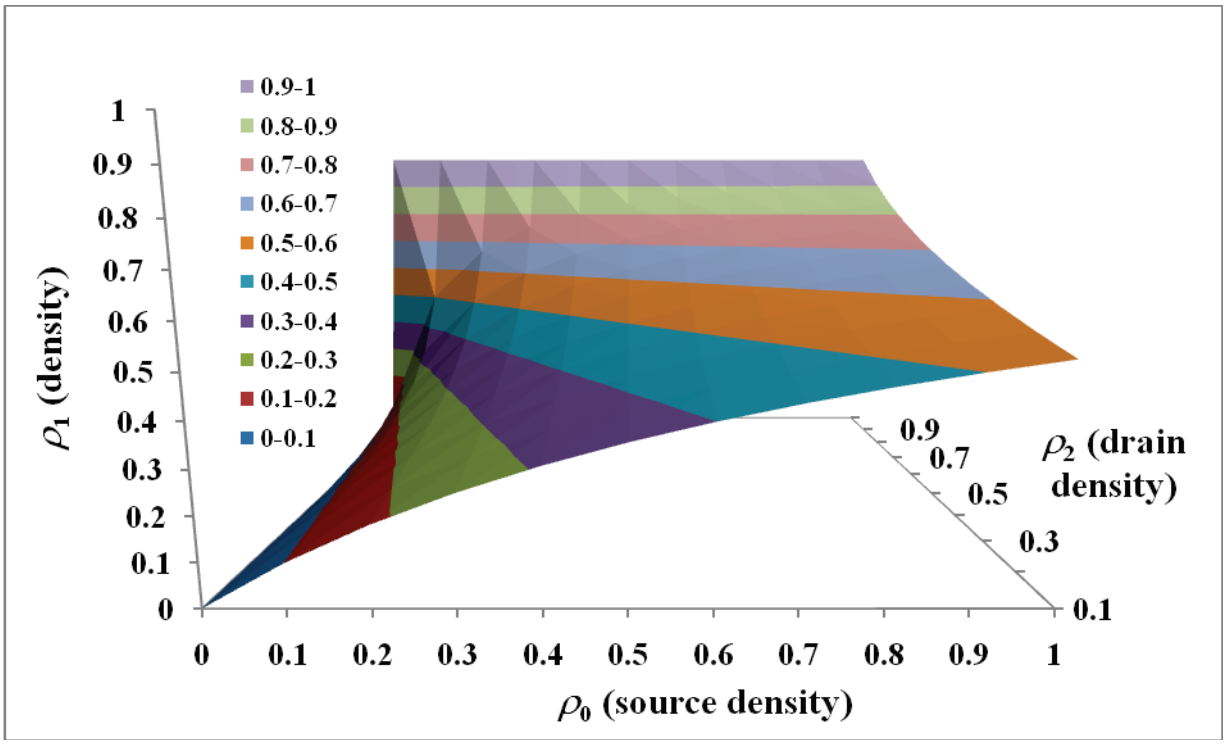

FIGURE 3. The density profile of the TASEP with a single site with a variation of the left (source) and right (drain) reservoirs densities.

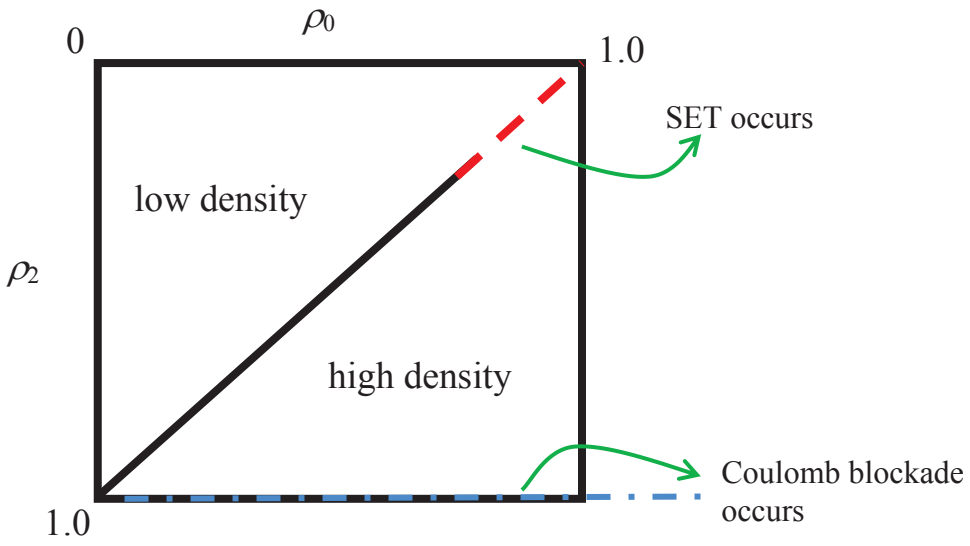

FIGURE 4. The phase diagram of the TASEP with a single site with a variation of the left and right reservoirs densities.

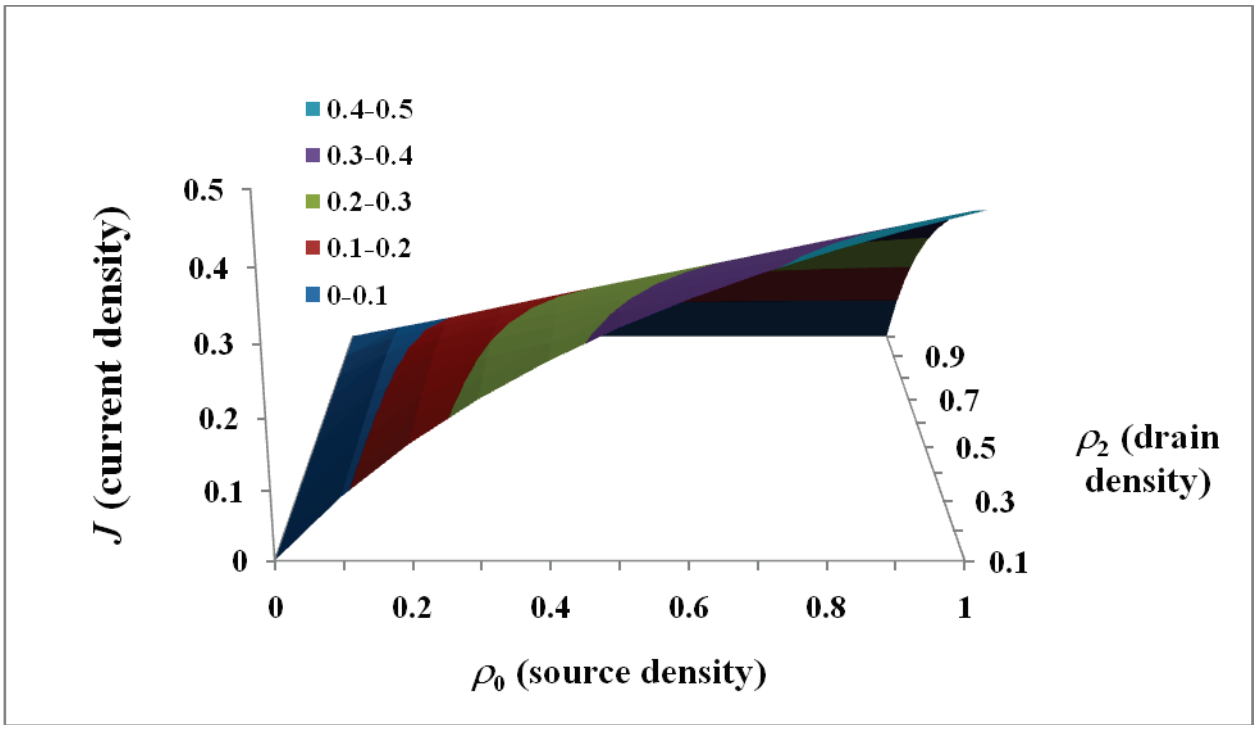

FIGURE 5. The current density profile of the TASEP with a single site with variation of the left (source) and right (drain) reservoirs densities.

Finally, the current density profile of the TASEP with a single site may be observed in Fig. 5. It may be examined that as the density of the right reservoir (drain) gets higher, the current density becomes smaller. Conversely, the higher the density of the left reservoir (source), the current density becomes higher. At high source density and very low drain density, the density current of particles is high, which indicates that occurrence of SET. For occupied drain or right reservoir, the current density is zero, which points out the Coulomb blockade.

CONCLUSION

The modeling of the Coulomb blockade and SET are investigated using the TASEP with only one site. The density and a current density of the TASEP in the site at steady state are obtained by varying the densities of the left and right reservoirs. The numerical solutions of the TASEP with a single site could indicate the occurrence of the Coulomb blockade and SET. The Coulomb blockade appears to be present for very high density of the right reservoir, while SET is obtained for very high source density and very low drain density.

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