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Towards the Dynamics of Coulomb Blockade in Quantum Dot via the Totally Asymmetric Simple Exclusion Process with a Single Site

Wipsar Sunu Brams Dwandaru

Soft Condensed Matter and Material Research Group
Physics Education Department, Faculty of Mathematics and Natural Science
Yogyakarta State University
Karangmalang Complex, Yogyakarta, 55281, Indonesia

Denny Darmawan

Soft Condensed Matter and Material Research Group
Physics Education Department, Faculty of Mathematics and Natural Science
Yogyakarta State University
Karangmalang Complex, Yogyakarta, 55281, Indonesia

Abstract

The advancement of nanotechnology opens exciting opportunities in the creation of semiconductor fabrication technology. It offers the production of small nano scale systems which consists of only one electron, i.e. quantum dot. The main idea behind a quantum dot is the Coulomb blockade. The dynamical mechanism of the Coulomb blockade can be studied by coupling the quantum dot to two reservoirs, viz. source and drain, at each end of the quantum dot. A potential difference of V_{sd} between the source and the drain is specified such that an electron asymmetrically tunnels from the source into the dot and out to the drain. The tunneling of the electron also depends on the gate potential, V_g, which is the potential applied to the dot. Based on the aforementioned description, a dynamical model is put forward to capture the qualitative and quantitative physical aspects of the quantum dot. The model is the totally asymmetric simple exclusion process or the TASEP.

Here, a connection between the quantum dot and the TASEP in one dimension with a single site is put forward. The hopping rate is connected to the gate potential and the source-drain potential. The dot is the single site lattice, whereas the source and the drain are the reservoirs. From this connection the density and current density of particles may be obtained.

Keywords: Coulomb blockade, gate potential, hopping rate, quantum dot, source-drain potential, TASEP

1 Introduction

Advancement in semiconductor material fabrication has given the science community the opportunity to explore and exploit a new world between the macroscopic world which obeys classical physics and the microscopic world which obeys quantum mechanics. This new world, which is called the mesoscopic world offers a large variety of interesting dynamical phenomena, one of which is the quantum dot. The aforementioned system is in the mesoscopic regime because its size ranges from nanometers to a few microns [1]. Hence, quantum dot is a part of the ongoing endeavor of nanoscience and nanotechnology.

A quantum dot is a physical system where electrons are confined by an external potential in all three spatial dimensions. An interesting feature of quantum dots is that they show similar physical properties which are seen in atomic physics, although the size of a quantum dot is hundreds of times bigger than a single atom. Similar atomic phenomena can be found in quantum dot, e.g. discrete energy levels and the Zeeman Effect. Another interesting feature of quantum dots is that instead of using different types of elements to see the dependencies of physical phenomena on the number of valence electrons inside an atom, the variation of the number valence electrons inside the quantum dot on a single device may be obtained just by varying the voltage on the dot. Therefore, this system is also known as an artificial atom [2 - 4].

The underlying mechanism where the number of electrons can be controlled inside a quantum dot is the so-called Coulomb blockade. This process may be explained using a diagrammatic representation given in Fig. 1. The states in the source are filled up to the electrochemical potential μ_{source} [Fig. 1(a)]. The electrochemical potential is defined as the sum of the Fermi energy, E_N, and the electrostatic potential. The states in the drain are also filled up to μ_{drain}. The source and the drain are connected by the applied source-drain voltage, i.e. $V_{\text{sd}} = (\mu_{\text{source}} - \mu_{\text{drain}})/e$. The difference between μ_{source} and μ_{drain} is known as the transport window. The electrons inside the dot fill the states up to the electrochemical potential of $\mu(N)$, so the next available state to be occupied by an electron has an electrochemical potential of $\mu(N+1)$. However, since $\mu_{\text{source}} < \mu(N+1)$ at zero temperature, electrons cannot tunnel into the dot, and since $\mu_{\text{drain}} > \mu(N)$, electrons cannot tunnel out of the dot. This is known as the Coulomb blockade which happens when $k_{\text{B}}T << e^2/C$, where C is defined as the total capacitance. In other

words, electrons are trapped inside the dot. In order to make a single electron tunnels through the dot, the gate voltage has to be varied. According to Fig. 1(b), since now $\mu_{\text{source}} > \mu(N+1)$, an electron may tunnel into the dot, hence making the next state higher than $\mu(N+1)$, such that the next electron may not enter the dot. The electrostatic potential inside the dot then increases by e^2/C (called by the charging energy). Furthermore, since $\mu_{\text{drain}} < \mu(N+1)$, an electron may tunnel out of the dot, hence dropping the electrochemical potential to $\mu(N)$ again. This discrete tunneling mechanism is called the single electron tunneling (SET).

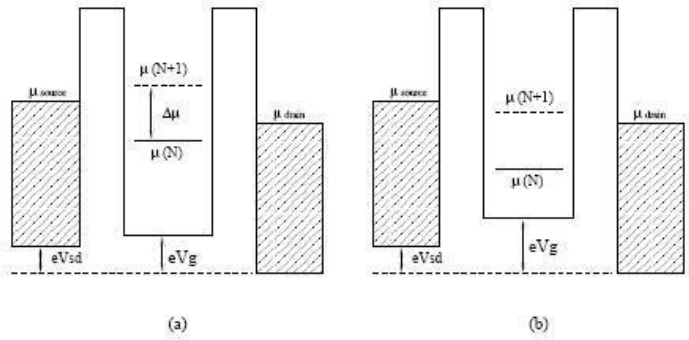

Fig. 1. Energy diagram in a quantum dot. (a) the Coulomb blockade, and (b) single electron tunneling

The theoretical background of the Coulomb blockade and SET has been established in some references, e.g. in [1, 5]. However, the discussion is largely based upon quantum mechanics and focuses on the electronic interaction behavior in the dot. Kouwenhoven et.al. [5] has provided a review on Coulomb oscillation inside the dot and the Coulomb staircase. Kouwenhoven and Marcus [1] describe the quantum dot based upon symmetry consideration. However, as the quantum dot is a mesoscopic system, it may also be discussed by considering the point of view of classical physics. Apparently, not so many enlightenments are available. Hence, in this article a simple mathematical model is put forward to study the dynamical aspects of quantum dot, i.e. Coulomb blockade and SET, which is based upon classical non-equilibrium statistical physics. The model is known as the totally asymmetric simple exclusion process or the TASEP.

In one dimension, TASEP is a well-known particle hopping model which has become a standard model for studying non-equilibrium driven systems [6 - 8]. The TASEP is a mathematical model whereby particles occupying one dimension lattice sites, $\mathcal{L}$, may jump to their (nearest) neighbor site so long as the neighbor site is not occupied by any other particle. The jump occurs towards one direction only, e.g. to the right, which produces one dimensional transport system. Variation to the TASEP has been conducted by Parmeggiani et.al. [9] by coupling it to Langmuir kinetics.

Further specifications are needed for the TASEP namely the dynamical rules and boundary conditions [10]. The dynamical rule illustrates the movement or hopping of

particles along the lattice sites as time evolves. This rule is specified systematically using an up-dating process on the microscopic level at each (discrete) time step. The dynamical rule used in this study is the sequential updating process. The up-dating process of this dynamical rule is that at each (discrete) time step, a site is chosen randomly with probability $1/(N+1)$, with N being the number of lattice sites. If there is a particle on the chosen site, then the particle on the chosen site may jump to its right nearest neighbor site with rate k given that there is no particle occupying the right nearest neighbor site [10]. Furthermore, the open boundary condition is applied. This boundary condition is realized by placing a reservoir at each end of $\mathcal{L}$. The left reservoir acts as a source of particles, where particles may enter $\mathcal{L}$. The rate at which particles enter the first site of $\mathcal{L}$ from the reservoir is called the input rate α. Meanwhile, the right reservoir serves as a sink for particles, where particles may exit from the last site of $\mathcal{L}$ to the reservoir. The rate at which particles exit the last site of $\mathcal{L}$ is called the output rate β.

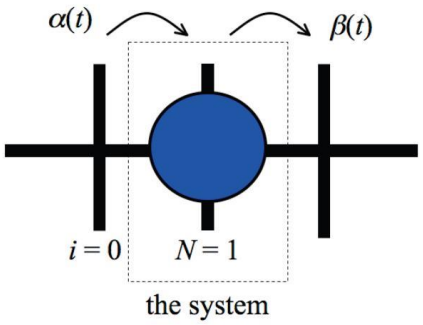

Fig. 2. The TASEP with a single site. The lattice system only consists of one site that is the site given in the dotted box. Site $i = 0$ is considered as the left reservoir and the site $N + 1$ acts as the right reservoir. The shaded (blue) circle is the particle occupying site $N = 1$

Here, the TASEP with only a single site ($N = 1$) with sequential updating and open boundary condition is employed. This is illustrated in Fig. 2. The single site is given in the dotted box, i.e. $N = 1$. The open boundary condition is provided by the sites between the system i.e. site $i = 0$ as the left reservoir and $i = N + 1$ as the right reservoir. A particle (given by the circle in Fig 2.) may hop from the left reservoir to the system with rate α and exit the system to the right reservoir with a rate β. The interaction of the particle follows one of the simplest potential, i.e. the hard core potential. It is a purely repulsive potential when two particles interact at some distance, σ, but for distances larger than σ the potential is zero. Hence, if there is a particle occupying site $N = 1$, then no other particle may occupy the site. On the other hand, if the site is empty, then a particle from the left reservoir may occupy the site.

An important notion which will be used is a relationship between the TASEP and the hard-core lattice gas model put forward by Dwandaru and Schmidt [11]. Originally, this connection is proposed to study a classical non-equilibrium system,

i.e. the TASEP, using an equilibrium system, viz. the hard-core lattice model via the classical density functional theory (DFT). The two systems share the same lattice system, $\mathcal{L}$, and share the same hard-core interaction of particles. The hard-core lattice gas model consists of a mixture of two species, i.e. monomers and dimers. A monomer is a particle that excludes its own site, whereas a dimer is a particle that excludes its own and its right nearest neighbor sites. The occupancies of the monomers and dimers are affected by the chemical potentials and the external potentials acting on each species.

The lattice fundamental measure theory (LMFT) is an extension of the DFT to discrete lattice systems [12, 13]. It is used to determine the exact excess (over ideal) free energy functional of the mixture. This functional is then linearized for small densities of the dimers. Minimization of the grand potential of the mixture yields the densities for the monomers and dimers. The relationship is given as follows: (i) the monomer density profile [$\rho_{\mathrm{m}}(i)$] is equivalent to the density profile of the TASEP [$\rho(t)$], ii) the dimer density profile [$\rho_{\mathrm{d}}(i)$] is equivalent to the current of the TASEP [$J_{i(i+1)}(t)$], and (iii) the ratio of fugacities of the mixture ($\exp\{\beta[\mu_{\mathrm{d}} - V_{\mathrm{d,ext}}]\}/\exp\{\beta[\mu_{\mathrm{m}} - V_{\mathrm{m,ext}}]\}$) is equivalent to the hopping rate of the TASEP, k. Thus, the connection between the monomer-dimer mixture and the TASEP may be given as a mapping as follows:

$$\rho_{\mathrm{d}}(i) \to J_{i(i+1)}(t), \tag{1}$$

$$\rho_{\mathrm{m}}(i) \to \rho_i(t), \tag{2}$$

and

$$\frac{\exp\{\beta[\mu_{\mathrm{d}} - V_{\mathrm{d,ext}}(i)]\}}{\exp\{\beta[\mu_{\mathrm{m}} - V_{\mathrm{m,ext}}(i)]\}} \to k, \tag{3}$$

where $\beta = 1/k_B T$, k_{B} is the Boltzmann constant, and T is the temperature. The combined density profiles of the monomers and dimers as obtained from solving the Euler-Lagrange equation [11] is

$$\rho_{\mathrm{d}}(i) = \frac{\exp\{\beta[\mu_{\mathrm{d}} - V_{\mathrm{d,ext}}(i)]\}}{\exp\{\beta[\mu_{\mathrm{m}} - V_{\mathrm{m,ext}}(i)]\}} \rho_{\mathrm{m}}(i)[1 - \rho_{\mathrm{m}}(i+1)]. \tag{4}$$

Inserting the mappings of (1), (2), and (3) into (4) yields the (mean-field) current density of the TASEP as

$$J_{i(i+1)}(t) = k\rho_i(t)[1 - \rho_{i+1}(t)]. \tag{5}$$

2 Method of Research

This work is essentially a theoretical study. Hence, the first step in conducting this study is literature study of the systems under consideration, which are the quantum dot, the TASEP, and the connection between the TASEP and the hard core lattice model. The next stage is to propose a connection between the quantum dot, i.e. the Coulomb blockade and the SET, to the TASEP, similar to that given in [11]. Finally, discussions are provided from the relationship obtained, especially concerning the dynamics of particles trapped inside the dot and particles tunneling through the dot.

Here, some results are explained concerning the dynamical study of the quantum dot using the TASEP with a single site.

3.1 The potentials of the quantum dot

A quantum dot is a system which consists of three components, that is the source, the dot, and the drain. A particle may be trapped inside the dot (Coulomb blockade) or tunnels from the source, to the dot, and out of the drain (SET). Both scenarios appear similar to the dynamics of the TASEP with a single site.

In this case, the quantum dot is considered as an equilibrium system. The movement of an electron through the dot is determined by the source-drain potential, V_{sd}. Also, whether or not the particle tunnels through the dot or going out from the dot depends upon the gate potential V_g. Firstly, a connection between the quantum dot and the hard-core lattice gas is given. This connection concerns the potentials of the quantum dot and the hard-core lattice gas. It is worth emphasizing that the nature of the interactions of the quantum dot is essentially different from the hard-core lattice gas. However, a similarity between the physical appearances of the two systems is exploited. First of all, the source-drain potential, V_{sd}, is associated to the chemical and external potentials of the monomers. This is because V_{sd} controls the *actual* particle moving through the dot, which is what (μ_m -$V_{m,ext}$) does towards the monomers. Secondly, the gate potential, V_g, is associated to the chemical and external potentials of the dimers. This is because V_g controls the actual jumping (movement) of particles from the source to the dot and to the drain, which is what (μ_d - $V_{d,ext}$) does towards the dimers. It may also be noticed that in the quantum dot there is no equivalent particle for the dimers. On the other hand, the electrons may be represented as monomers, although the interaction is different. The hard-core (repulsive) mechanism is not provided by the interaction between the electrons, but because of the intricate combination between V_{sd} and V_g. Hence, the relationship between the potentials of the quantum dot and the hard-core lattice gas may be given in a mapping as follows:

$$\left[\mu_{\mathrm{d}} - V_{\mathrm{d,ext}}(i)\right] \to V_g, \tag{6}$$

and

$$\left[\mu_{\mathrm{m}} - V_{\mathrm{m,ext}}(i)\right] \to V_{\mathrm{sd}}. \tag{7}$$

The mapping of (6) also indicates that the gate potential is connected to the current of electrons tunneling through the dot, and the mapping of (7) states that the source-drain potential is associated to the density of the electron. Hence, the left hand side of mapping (3) may be modified for the quantum dot according to (6) and (7) as

$$\frac{\exp\left\{\beta\left[\mu_{\mathrm{d}} - V_{\mathrm{d,ext}}(i)\right]\right\}}{\exp\left\{\beta\left[\mu_{\mathrm{m}} - V_{\mathrm{m,ext}}(i)\right]\right\}} \to \frac{\exp\left\{\beta V_{\mathrm{g}}\right\}}{\exp\left\{\beta V_{\mathrm{sd}}\right\}}. \tag{8}$$

The mapping (8) is used in the next section where the dynamics of the quantum dot is described for the Coulomb blockade and the SET.

3.2 The dynamics of the quantum dot

The dynamics of the quantum dot is elucidated using the TASEP with a single site. However, the TASEP is basically a classical model. Hence, a certain quantum depiction of the dot is left out for the moment, i.e. the discrete energy level. Here, it is assumed that the dot is a black box that may only be filled with one electron. The electron comes from the source and goes out to the drain. Thus, a connection may be made for the components of the quantum dot and the TASEP, that is (i) source → left reservoir, (ii) dot → the site, and (iii) drain → right reservoir. From the aforementioned relationship, the current density of the electron may be obtained via equation (5) by replacing (3) with (8), i.e.:

$$J_{i(i+1)}(t) = \frac{\exp\left\{\beta V_{\mathrm{g}}\right\}}{\exp\left\{\beta V_{\mathrm{sd}}\right\}} \rho_i(t)\left[1 - \rho_{i+1}(t)\right] = e^{\beta\left(V_{\mathrm{g}} - V_{\mathrm{sd}}\right)} \rho_i(t)\left[1 - \rho_{i+1}(t)\right], \tag{9}$$

where $\rho_i(t)$ is identified as the density of the electron at the dot (site i) at time t and $J_{i(i+1)}(t)$ is the current density of the electron moving from quantum dot i to the drain at time t. If the system is conserved then the continuity equation may be used,

$$\frac{\partial \rho_i(t)}{\partial t} = -\nabla J_{i(i+1)}(t), \tag{10}$$

where

$$\nabla J_{i(i+1)}(t) = J_{i(i+1)}(t) - J_{(i-1)i}(t). \tag{11}$$

Now, inserting equation (9) into equation (11) and then into equation (10), yields:

$$\frac{\partial \rho_i(t)}{\partial t} = e^{\beta(V_g - V_{sd})}\{\rho_{i-1}(t)[1-\rho_i(t)] - \rho_i(t)[1-\rho_{i+1}(t)]\}. \tag{12}$$

Equation (12) is a differential equation that consists of the density, $\rho_i(t)$, both on the right and left hand sides. This means that the equation is not closed and therefore may be solved self-consistently. The formal solution of the above differential equation is

$$\rho_i(t) = \rho_i(0) + e^{\beta(V_g - V_{sd})}\int_0^t \{\rho_{i-1}(t')[1-\rho_i(t')] - \rho_i(t')[1-\rho_{i+1}(t')]\}\mathrm{d}t', \tag{13}$$

where $\rho_i(0)$ is the density at $t = 0$ or the initial density. Equation (13) determines the density of the quantum dot as a function of time. It gives the average occupancy of electrons occupying the dot. Furthermore, if the system reaches steady state, then the density does not depend upon time, such that the left hand side of (12) is zero. For finite and non-zero values of $\exp\{\beta(V_g - V_{sd})\}$, equation (12) becomes

$$\rho_i = \frac{\rho_{i-1}}{1-\rho_{i+1}+\rho_{i-1}}. \tag{14}$$

Equation (14) may be solved recursively, i.e. determine ρ_i, then insert ρ_i into equation (14) to obtain ρ_{i+1}, and so forth. Equations (9), (12), (13), and (14) are the main equations obtained in this study. They are the macroscopic dynamical equations for systems yielded from the above relationship. The equations may be utilized for any finite number of quantum dots, $1 \le i \le N$.

However, in the quantum dot case, the system consists only of one site, viz. $i = N = 1$. Hence, inserting this into (14) and noting that $\rho_0 = 1.0$ (the source always contains an electron) and $\rho_2 = 0.0$ (the drain always empty), produces $\rho_1 = 0.5$. This is exactly what happens in the SET. The electron occupies the dot only half of the time in average, that is the electron occupies the dot from the source, and then (at the next time step) empties the dot by going out to the drain. Moreover, inserting the above information into equation (9) yields $J = 0.5\exp\{\beta(V_g - V_{sd})\}$. This indicates that the current density of the SET depends upon the potentials of the quantum dot. On the other hand, the trapping of an electron (a Coulomb blockade) may be realized by making V_{sd} constant and $V_g \to -\infty$. Now, inserting this into equation (13) yields $\rho_1 = \rho_1(0)$. This suggests that for the given specification of the potentials, the density of the electron in the dot at any time is constant, i.e. equals to its initial density. The density of the electron in the dot stays low or high at all time. Hence, the electron is trapped inside the dot or there is no electron in the dot. Inserting further the latter potentials into equation (9) produces $J = 0$, which means that there is no current throughout the system.

4 Conclusions

The relationship between the quantum dots with the TASEP has been proposed. The source is related to the left reservoir, the dot is connected to the site ($N = 1$), and the drain is related to the right reservoir. Dynamical equations for the current density and the density are obtained for the quantum dot using the continuity equation. The equation for the density is not a close equation thus may be solved self-consistently. The density of an electron in the SET is obtained for a value of 0.5, whereas for the Coulomb blockade the density follows its initial density. The current density for the electron of the SET depends upon the gate and the source-drain potentials, whereas the current density for the Coulomb blockade is zero.

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