

On the classical aspects of electrons tunnelling through a quantum dot via a driven lattice gas model in one dimension

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Abstract. A theoretical study of classical aspects, i.e.: density, current density, and average speed of electrons tunnelling through a quantum dot (QD) via a simple driven lattice gas model have been carried out. The study is conducted by considering a resemblance between the components of the QD with the components of the totally asymmetric simple exclusion process (TASEP) that consists of only a single site and open boundary conditions. The former consists of a source, an island, and a drain, which corresponds respectively to the left reservoir ($i = 0$), site $i = 1$, and the right reservoir ($i = 2$) of the latter. Explicit expressions of the density, current densities, and average speed for electrons tunnelling through the QD in the classical regime are obtained. At the steady state, the density of electrons tunnelling through the dot is 0.5 and the current density becomes $v/2$, where v is the speed of the electrons. Furthermore, the speed of the electrons may be obtained as functions of temperature and the difference between gate and source-drain potentials. For very low temperatures, the speed of electrons rapidly goes to zero pointing to the occurrence of Coulomb blockade.

1. Introduction

Nowadays, nanomaterial such as quantum dot (QD) have attracted much attention because of their superior electronic, optical, and magnetic properties due to confinement effects [1,2]. A confinement of an electron in all its three spatial coordinates is designated as a QD. A QD is a mesoscopic system which resembles an atom although it is tens or hundreds times bigger than an actual atom, e.g. the Zeeman Effect and discrete energy levels [3], hence entitling the QD as an artificial atom [4]. Another interesting feature is that its physical properties depend on the voltage applied to the dot, whereas an atom depends upon its valence electrons. The QD has been a subject of various applications including optical and optoelectronic devices [5,6], quantum computing [7], DNA testing [8,9], three dimensional (3D) imaging [10], and displays [11,12].

There are two mechanisms used in QD, namely Coulomb blockade (Figure 1A) and single electron tunnelling (SET) [Figure 1B] [13,14]. Coulomb blockade occurs when the electrons inside the dot create a strong Coulomb repulsion preventing other electrons to enter the dot. SET is a tunnelling mechanism where a single electron at a time may tunnel through the dot which occurs by varying the gate voltage, V_g . We may think of three components for the aforementioned mechanisms, i.e. a source, an island, and a drain (Figure 1). The source and drain are reservoirs of electrons which are going into and out of the dot (island), respectively. The island is where the electron is trapped inside the dot. The source and drain are associated to their respective electrochemical potentials, i.e.: μ_{source} and μ_{drain} . Both chemical

potentials are connected through the source-drain potential, V_{sd} , that is, $eV_{sd} = (\mu_{source} - \mu_{drain})$, where e is the electron unit of charge. The Coulomb blockade and SET are realized by differences in values between μ_{source} , μ_{drain} , and $\mu(N)$, where the latter is the chemical potential of N electrons inside the island.

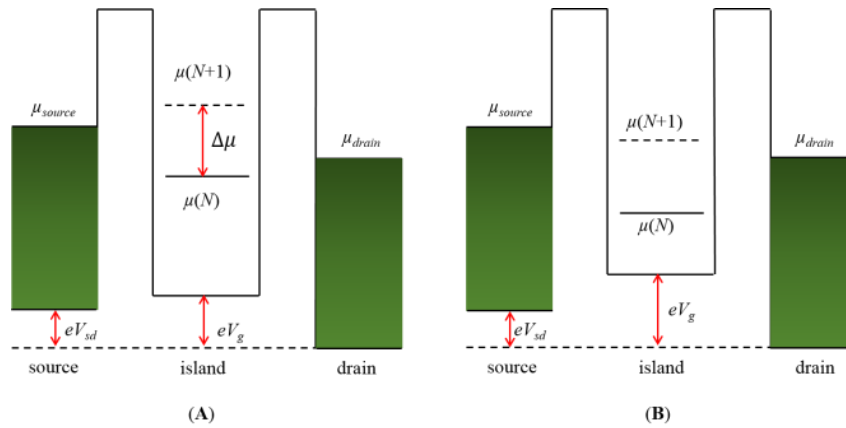


Figure 1. The energy diagram of a QD. (A) is the Coulomb blockade and (B) is the SET.

A standard mathematical model which can be utilized to study many physical properties of dynamical systems is the totally asymmetric simple exclusion process (TASEP) in one dimension (1D). This is a simple driven lattice gas model where hard-core particles occupying a discrete lattice sites, $i \in L$, may jump to their respective right-nearest neighbour sites, $(i + 1) \in L$, provided that the right-nearest neighbour sites are not occupied by any other (hard-core) particle. The jumping of particles is defined by hopping rules, which usually takes the sequential or parallel up-dating dynamics. The TASEP is also equipped with boundary conditions, which may be open or periodic. Furthermore, the model is a renowned particle hopping model [15] which is employed to investigate various transport phenomena, such as protein synthesis [16], motor protein in organism [17], the track of a group of insects [18], and road traffic congestions [19].

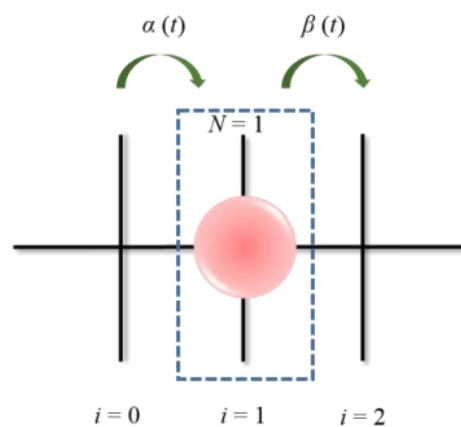


Figure 2. The TASEP that consists of only a single site, i.e.: $N = 1$.

The dark vertical lines are lattice sites labelled by $i = 0, 1, 2$. Site $i = 0$ and $i = 2$ are reservoirs of particles where a hard-core particle (pink coloured dot) jump into and out of the system, $i = N = 1$ (blue dashed rectangular lines), respectively. A hard-core particle may enter site $i = 1$ with an input rate of $\alpha(t)$ and exit the site with an output rate of $\beta(t)$ [green arrows].

Here, the TASEP which consists of only a single site (Figure 2) is utilized to study the dynamics of electrons tunnelling through the dot in the SET. This may be considered as the simplest arrangement of the model where only one site is used, i.e.: $i = N = 1$, with N is the total number of sites. The single site is attached to two reservoirs at each end of the site which indicates an open boundary condition. The left (right) reservoir, viz.: $i = 0$ ($i = 2$) allows particles to jump to (out of) the system (site $i = 1$) with input rate $\alpha(t)$ [output rate $\beta(t)$].

In this case, we present an application of TASEP consisting of only a few sites, e.g.: $1 \leq N \leq 3$ which is rarely investigated other than being used to confirm physical theories, let alone applied to model a physical system. It is necessary to emphasize here that this study offers an alternative approach in investigating classical aspects of the dynamics of a mesoscopic system, i.e. QD, through a simple classical dynamical model. However naive it may be, this study brings a new perspective in the relationship between dynamical models providing insights of one model (SET) through the other (TASEP with a single site), or vice versa. The results of explicit expressions for the average speed, density, and current densities of electrons tunnelling through the dot are worth scientific exploration and have not been reported before. This study enriches the many methods in describing the dynamics of electrons inside QD.

2. The Relationship

We may observe a physical resemblance of the TASEP with a single site and the two mechanisms in QD (Table 1). The system (site $i = 1$) of the TASEP represents the dot (island), the reservoirs of the TASEP at site $i = 0$ and $i = 2$ represent the source and drain, respectively.

Table 1. A connection between the components of the TASEP with a single site and QD.

No.	TASEP with a single site	connection	QD
1.	0	\longleftrightarrow	source
2.	1	\longleftrightarrow	island
3.	2	\longleftrightarrow	drain
4.	a particle occupies site $i = 1$	\longleftrightarrow	an electron inside the dot
5.	a particle jumps through site $i = 1$	\longleftrightarrow	an electron tunnelling the dot

The single particle occupation in site $i = 1$ of the TASEP is due to the hard-core inter-atomic potential between particles. This potential is obtained via a purely infinite repulsive potential between the centres of two particles until a certain inter-atomic distance. Beyond this distance, the particles are non-interacting. Hence, no other particle may occupy site $i = 1$ if the site is occupied by a particle. However, the nature of the Coulomb blockade and SET is completely different from that of the hard-core potential. In the QD, the movement or confinement of an electron is caused by chemical potential differences between the source, island, and drain, through the applied voltages. However, the two models look similar in the sense that there is only a single particle (electron) that may enter or exit the site (dot). Hence, the confinement (tunnelling) of a single electron in the dot is somewhat similar to a classical particle occupying (jumping out of) the lattice sites in the TASEP. Therefore, a connection can be constructed between TASEP, Coulomb blockade, and SET.

The intended relationship is realized in two stages. First, a relationship between the hard-core lattice gas model [20], the Coulomb blockade, and SET is constructed. Here, two species of hard-core particles are used, i.e. monomer and dimer. A monomer is a particle that excludes its own site, whereas a dimer is a particle that excludes its own and its right-nearest neighbour sites. Thus, the monomer corresponds to an electron that is confined in the dot, while the dimer corresponds to an electron that is tunnelling into and out of the dot. The results are static densities of the monomer and dimer in terms of the applied voltages of the QD. A physical understanding of these densities may be acquired by connecting them to

the TASEP with a single site in the second stage of the relationship. At this point, the monomer is associated to the particle occupying site $i = 1$ and the dimer is associated to the particle going into or out of site $i = 1$ of the TASEP. The densities of the monomer and dimer can then be associated to the density and current density of the TASEP, respectively [21]. Hence, giving the final results of the density of an electron confined in the dot and the current density of the electron tunnelling through the dot (Table 1).

3. Density, Current Density, and Average Speed of Electrons Tunnelling through a QD

The Following the above connection, we may obtain a continuity equation, i.e. [22]:

$$\frac{\partial \rho(t)}{\partial t} = J_{st}(t) - J_{dd}(t), \quad (1)$$

where $\rho(t)$ is the density of an electron in the dot at time t which gives the average occupancy of electrons in the dot,

$$J_{st}(t) = \exp \left[\frac{e}{k_B T} (V_g - V_{sd}) \right] \rho_s(t) (1 - \rho(t)), \quad (2)$$

is the current density of the electron entering the dot from the source, $\rho_s(t)$ is the density of electrons in the source at time t ,

$$J_{dd}(t) = \exp \left[\frac{e}{k_B T} (V_g - V_{sd}) \right] \rho(t) (1 - \rho_d(t)), \quad (3)$$

is the current density of the electron exiting the dot to the drain, and $\rho_d(t)$ is the density of electrons in the drain at time t . It may be observed that the current densities of the electron depend upon V_g and V_{sd} . Furthermore, by setting the input and output rates as

$$\alpha(t) = \exp \left[\frac{e}{k_B T} (V_g - V_{sd}) \right] \rho_s(t), \quad (4)$$

and

$$\beta(t) = \exp \left[\frac{e}{k_B T} (V_g - V_{sd}) \right] (1 - \rho_d(t)), \quad (5)$$

respectively, we may modify equations (2) and (3) to become

$$J_{st}(t) = \alpha(t) [1 - \rho(t)], \quad (6)$$

and

$$J_{dd}(t) = \beta(t) \rho(t), \quad (7)$$

respectively. Equations (6) and (7) give a simpler form of the current densities of electrons that depend explicitly only on the density of electrons in the dot and the input and output rates. Here, the dependency

of the current densities upon time, t , is through the density and the input and output rates. In order that the current density of electrons only depends upon the applied voltages, we may set $\rho_s(t) = 1.0$ and $\rho_d(t) = 0.0$. This indicates that at any time t , the source will always be filled with electrons and the drain will always be empty. Thus we may obtain the average speed of electrons tunnelling through the dot as

$$v = \exp\left[\frac{e}{k_B T} (V_g - V_{sd})\right], \quad (8)$$

which is time-independent and depends upon the temperature and the difference between the applied potentials. Hence, equations (6) and (7) becomes

$$J_{st}(t) = v[1 - \rho(t)], \quad (9)$$

and

$$J_{dd}(t) = v\rho(t), \quad (10)$$

where now the time dependency of the current densities only comes from the density of the electron in the dot. Equations (1), (9), and (10) determine the evolution of the density of electrons in the dot. This indicates that the density of electrons at any time may be obtained via the current densities by formally solving equation (1). This may be attained by inserting equations (9) and (10) into equation (1), giving:

$$\frac{\partial \rho}{\partial t} = v[1 - \rho] - v\rho = v[1 - 2\rho]$$

or

$$\int \frac{d\rho}{1 - 2\rho} = \int_{t_0}^t v dt.$$

Solving the LHS of the above integral via a substitution method produces an explicit expression for the density as a function of time, viz.:

$$\rho(t) = \frac{1}{2} [1 - e^{-2v(t-t_0)}]. \quad (11)$$

Furthermore, substituting equation (11) back into Equations (9) and (10), yields

$$J_{st}(t) = \frac{v}{2} [1 + e^{-2v(t-t_0)}], \quad (12)$$

and

$$J_{dd}(t) = \frac{v}{2} [1 - e^{-2v(t-t_0)}]. \quad (13)$$

Equations (11), (12), and (13) are a set of explicit equations that describe the dynamics of the electrons moving through the dot.

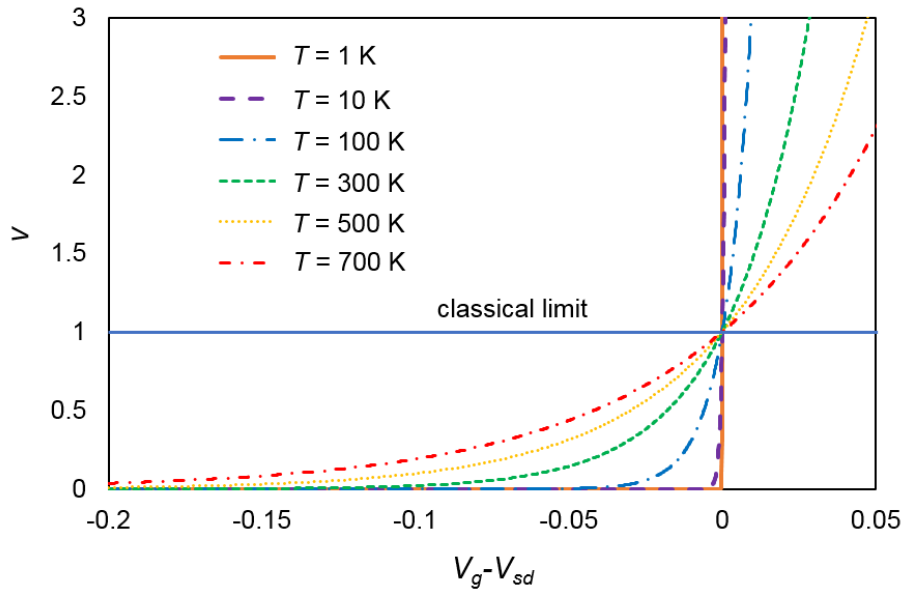


Figure 3. The average speed of electrons as functions of the applied potential differences, $V_g - V_{sd}$, at various temperatures, T .

First, we may plot the average speed of electrons in equation (8) against the difference of the applied potentials with temperature variations. This is given in Figure 3. The classical limit is obtained if the temperature is very high, i.e. $T \rightarrow \infty$, such that $v \rightarrow 1$, which is shown as a straight (blue) line. In this regime, the thermal fluctuations dominate over quantum events such that the speed of electrons is not affected by $V_g - V_{sd}$. As the temperature is decreased the speeds become an exponential form with respect to $V_g - V_{sd}$ consistent with Equation (8) and passing through a vertical line of $V_g = V_{sd}$ at $v = 1$. For the region of $V_g < V_{sd}$, as V_g becomes smaller (compared to a constant value of V_{sd}) v reduce to zero indicating the occurrence of Coulomb blockade. Accordingly, the density and current densities of electrons in Equations (11) - (13) become $\rho = J_{st} = J_{dd} = 0.0$. This means that an equilibrium condition is achieved where an electron may not enter the island (dot). Moreover reducing the temperature increases the region of $V_g - V_{sd}$ where the Coulomb blockade may occur, hence shifting the ‘switch’ between Coulomb blockade and electrons tunnelling or vice versa to smaller values of $|V_g - V_{sd}|$. For very low temperature, the ‘switch’ is located at $V_g = V_{sd}$, i.e. for $V_g < V_{sd}$, $v = 0$ (Coulomb blockade), and $V_g > V_{sd}$, $v \rightarrow \infty$ (electrons tunnelling). For the region of $V_g > V_{sd}$ only electron tunnelling takes place as $v \neq 0$. Lowering the temperature in this region increases the speed of the electrons and at very low temperatures $v \rightarrow \infty$. However, as $v \rightarrow \infty$, the current densities tend to infinite as well ($J_{st}, J_{dd} \rightarrow \infty$), but the density remains finite ($\rho = 0.5$).

For some long evolution time, i.e. $t \rightarrow \infty$, Equations (11) – (13) may achieve a steady state condition where the density does not depend again upon time, i.e.: $\rho = 0.5$, and $J_{st} = J_{dd} = v/2$ does not vanish, as shown in Figure 4. This implies that at steady state the dot (island) has half a chance in average of being

occupied by an electron or being empty. This is of course in accordance with the SET where electrons may alternately enter and exit the dot through the source and drain, respectively. Hence, the SET may be thought of being in a non-equilibrium steady state (NESS) condition with a non-vanishing current of $v/2$. It may also be observed in Figure 4(a) that increasing the speed of the electrons tunnelling through the dot causes the system to reach NESS faster.

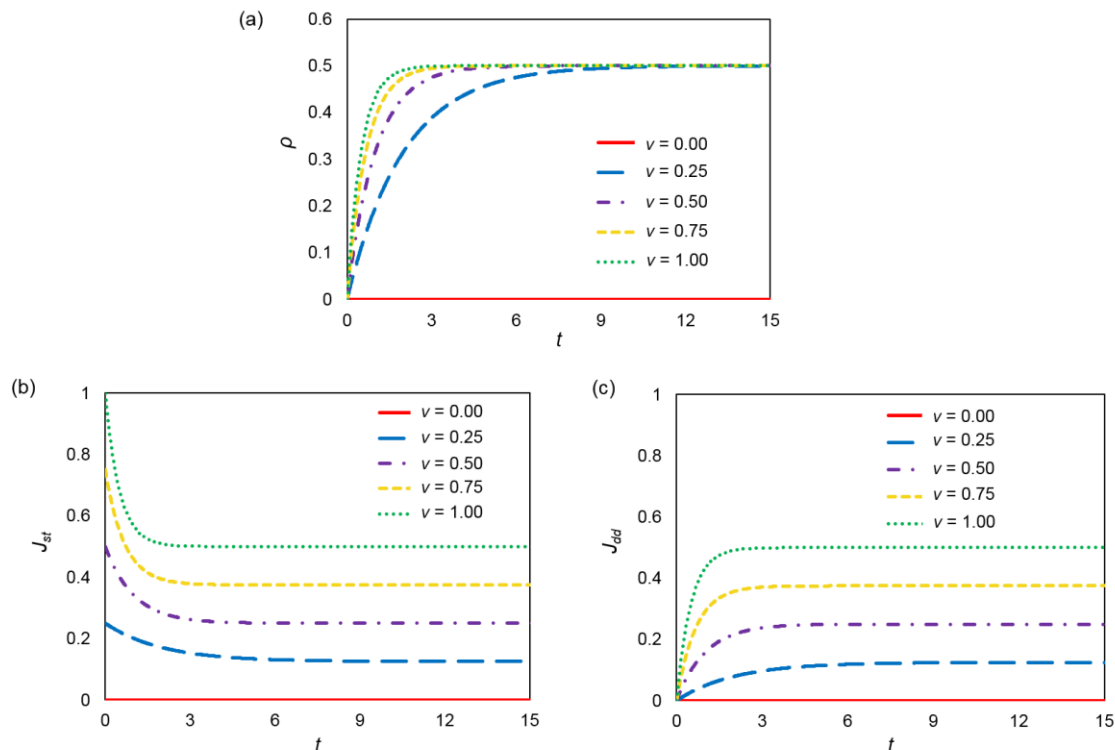


Figure 4. (a) The density of electron in the dot, ρ , (b) the current density of the electron entering the dot from the source, J_{st} , and (c) the current density of the electron exiting the dot to the drain, J_{dd} , as functions of time for various speeds, v .

4. Conclusion

Explicit classical expressions of the density, current densities, and the average speed of electrons tunnelling through a QD are obtained. This may be realized using a relationship between the TASEP with a single site and the QD through the hard-core lattice gas model. The density and current densities of electrons are obtained via the density and current density of the hard-core particles of the TASEP with a single site. In steady state, the Coulomb blockade is obtained when the average speed of the electrons is zero, i.e. for low temperatures, such that $\rho = J_{st} = J_{dd} = 0$. SET is an NESS which is attained for $\rho = 0.5$ and $J_{st} = J_{dd} = v/2$, respectively.

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