Thermoelectric Current and Coulomb-Blockade Plateaus in a Quantum Dot

Kristinn Torfason\textsuperscript{a,b}, Andrei Manolescu\textsuperscript{a}, Sigurdur I. Erlingsson\textsuperscript{a}, Vidar Gudmundsson\textsuperscript{b}

\textsuperscript{a}School of Science and Engineering, Reykjavik University, Menntavegi 1, IS-101 Reykjavik, Iceland
\textsuperscript{b}Science Institute, University of Iceland, Dunhaga 3, IS-107 Reykjavik, Iceland

Abstract

A Generalized Master Equation (GME) is used to study the thermoelectric currents through a quantum dot in both the transient and steady-state regime. The two semi-infinite leads are kept at the same chemical potential but at different temperatures to produce a thermoelectric current which has a varying sign depending on the chemical potential. The Coulomb interaction between the electrons in the sample is included via the exact diagonalization method. We observe a saw-tooth like profile of the current alternating with plateaus of almost zero current. Our calculations go beyond the linear response with respect to the temperature gradient, but are compatible with known results for the thermopower in the linear response regime.

1. Introduction

The electrical conduction of open nanoelectronic devices driven by electric potentials or fields generated in various ways is a major topic in mesoscopic physics. Outside this area complementary research on thermoelectric currents, thermopower, and related thermal properties in the quantum regime for systems like quantum dots has been more difficult, but on a growing trend in the last two decades. Temperature control down to the milli Kelvin range and temperature gradients at nanoscale are attainable in the laboratories and generate new scientific opportunities [1].

The thermopower of quantum dots was initially studied theoretically by Beenakker and Staring [2]. They calculated the Seebeck coefficient

$$S = -\lim_{\Delta T \to 0} \frac{V}{\Delta T},$$

(1)

where $V$ is the voltage generated across the quantum dot weakly connected to electron reservoirs at a temperature bias $\Delta T$, under the condition that the current between the two reservoirs is zero. They obtained oscillations of $S$ around $S = 0$ as function of the Fermi energy in the reservoirs, with symmetric positive and negative values. The Coulomb electron-electron interaction in the quantum dot was included in the charging (“orthodox”) model, and the result of it was a saw-tooth profile of the thermopower, with oscillations having the positive slope smaller than the negative slope. The predicted results were confirmed in subsequent experimental work by the same team [3] and also by Dzurak et al. [4]. Few years later Dzurak et al. published a new series of measurements which show that at temperatures below 100 mK the saw-tooth oscillations of the thermopower vs. the Fermi energy alternate with plateaus of zero thermopower [5]. A qualitative graph of the thermopower is shown in Fig. 1.

While the saw-teeth were attributed to sequential tunneling and high temperatures [2], the zero plateaus were initially attributed to many-body effects. Later on Turek and Matveev derived a theory of the thermopower of quantum dots in which the zero plateau at low temperature is a result of cotunneling [6]. A more complex cotunneling theory, beyond the limit of weak tunnel coupling, and including quantum fluctuations, was proposed by Kubala and König [7], and later by Billings et al. who also included exchange effects [8]. Further experimental results were interpreted in terms of sequential-tunneling dominated thermopower at high temperatures, leading to a saw-tooth profile, and cotunneling onset at low temperatures, leading to zero plateaus [9]. In a recent experimental paper by Svensson et al. [10] the thermopower of quantum dots is systematically investigated and the lineshape is carefully analyzed in various conditions. Periodic sequences of a negative peak followed by positive peak followed by a zero plateau of the thermopower of the quantum dot as function of chemical potential in the leads are clearly seen over large intervals of chemical potentials. The interpretation of these results is done using a Landauer formula with an empirical transmission function.

In the constant interaction model the effects of the Coulomb interaction are taken into account using only a charging energy, with no other effects on the energy spectrum [11, 12]. The transport is described by a series of resonances, and in between the resonance peaks there are zero current plateaus. This is the standard Coulomb blockade picture [12]. In the Landauer-Buttiker approach this phenomena is described using a transmission function $T(E)$ representing the resonances in the transport, usually a Lorentzian of width $\Gamma$ centered on some resonance ener-
where $G$ is the conductance of the system. The conductance in case (i) is determined by peaks of width $\sim kT$, with exponential suppression between adjacent resonances (assuming $kT \ll \Delta E$). The ratio of $I$ and $G$ will thus lead to a saw-tooth like pattern without plateaus in $V_{Th}$, even though there are plateaus in $I$. In case (ii) the conductance is proportional to the Lorentzian peak, which tends to zero like $1/E^2$ outside the resonances. In this case the thermal voltage is saw-tooth like but with plateaus between resonances.

In the present paper we use the generalized master equation (GME) as a tool to understand the electric currents generated in an open quantum dot due to a temperature bias. The dot is connected to external leads seen as electron reservoirs and kept at the same chemical potential. We obtain the currents in the leads produced by a finite temperature bias. We calculate the time dependent currents when the leads are gradually coupled to the sample and we find numerically the asymptotic currents in the leads in the steady state. To our knowledge the master equation has not been commonly used for the thermoelectric response of open systems. One approach was performed by Koch et al. who used in fact rate equations, neglecting the off-diagonal elements of the reduced density operator, but including cotunneling [14]. Our method is not restricted to the linear response to a small temperature gradient. We obtain a line shape of the currents vs. the chemical potential as illustrated in Fig. 1 for low temperatures, where zero plateaus are also expected for the thermopower [5, 9, 10], as illustrated in Fig. 1. Our method however does not include cotunneling effects, but only sequential tunneling. Instead, the Coulomb interaction in the dot is completely incorporated using the method of exact diagonalization. We also discuss time dependent and transient currents in the system and the effect of a third terminal attached to the quantum dot. The third terminal was proposed in order to create a phase-breaking mechanism inside the dot [15].

The paper is organized as follows: The model and the methodology are described in Section 2, analytical calculations in Section 3, the numerical results are presented in Section 4, and the conclusions in Section 5.

2. The Model

The physical system consists of a sample connected to two leads acting as particle reservoirs. We shall adopt a tight-binding description of the system: the sample is a short quantum wire and the leads are 1D and semi-infinite. The sample can also be seen as an elongated quantum dot. In this work we consider a sample of 3 sites. This number optimizes the computational time and the physical phenomenology which we intend to describe. A sketch is given in Fig. 2. The left lead (or the source, marked as $L$) is contacted at one end of the sample and the right lead (or the drain, marked as $R$) is contacted at the other end.
The function \( \langle \psi_{qt} \rangle \) describes the time-dependent coupling between the single-particle basis states of the isolated sample and the states \( \{ \psi_{qt} \} \) of the leads:

\[
H_T(t) = \sum_n \sum_{\ell} \int dq \chi_{\ell}(t) (T_{q\ell}^d c_{q\ell}^d d_n + \text{h.c.}) .
\] (7)

The function \( \chi_{\ell}(t) \) describes the time-dependent switching of the sample-lead contacts, while \( d_n^{\dagger} \) and \( c_{q\ell} \) create/annihilate electrons in the corresponding single-particle states of the sample or leads, respectively. The coupling coefficient

\[
T_{q\ell} = V_t \psi_{q\ell}(0) \phi_n(i_{\ell}) ,
\] (8)

involves the two eigenfunctions evaluated at the contact sites \((0, i_\ell)\), \(0\) being the site of the lead \(\ell\), and \(i_\ell\) the site in the sample. The wave functions in the leads are \(\psi_{q\ell}(0) = \sqrt{\sin q/2\pi} \) with \(\tau\) the hopping energy in the leads (the same for all leads), the energy spectrum of the leads being \(\epsilon_q = 2\tau \cos q\) [16]. The hopping energy in the sample, denoted as \(t_s\), will be considered different than in the leads, and will be used as the energy unit. In Fig. 2 the lead left is connected to the site \(i_L = 1\) and the right lead on the site \(i_R = 3\). The parameter \(V_t\) plays the role of a coupling constant between the sample and the leads.

We will ignore the Coulomb effects in the leads, where we assume a high concentration of electrons and thus strong screening and fast particle rearrangements. The GME is formulated in the Fock space and therefore it is natural to include the Coulomb electron-electron interaction in the dot in a complete many-body manner and to calculate the exact many-body states using a straight forward diagonalization in the basis of occupation numbers. This method is known as exact diagonalization in the community of mesoscopic physics, but often called configuration interaction by quantum chemists. The many-electron states (MES) are calculated in the Fock space built on non-interacting single-particle states [17]. Since the sample is open the number of electrons is not fixed, but the Coulomb interaction conserves the number of electrons, which means the interacting eigenvectors are linear combinations of the non-interacting eigenvectors with a fixed number of particles.

The equation of motion for our system is the quantum Liouville equation,

\[
ih\dot{W}(t) = [H(t), W(t)] ,
\] (9)

where \(W(t)\) is the statistical operator of the total system made by the sample plus leads, which are connected at time \(t=0\). Before the connection, at \(t<0\), the sample and the leads are independent and in equilibrium, meaning that \(W(t<0) = \rho_{\ell R}\), i.e. simply the product of the density operator of the sample, \(\rho_{\ell}\), the left lead and the right lead \(\rho_R\).

Following the Nakajima-Zwanzig technique [18] we define the reduced density operator (RDO), \(\rho(t)\), by tracing out the degrees of freedom of the environment, the leads in our case, over the statistical operator of the entire system, \(W(t)\)

\[
\rho(t) = T_{\ell L} T_{R} W(t) .
\] (10)

For a sufficiently weak coupling strength \((V_t)\) one obtains the non-Markovian integro-differential master equation for the RDO

\[
\dot{\rho}(t) = -i\hbar^{-1} [H_S, \rho(t)] - \frac{1}{\hbar^2} \sum_{\ell} \int dq \chi_{\ell}(t) \left[ T_{q\ell}, \Omega_{q\ell}(t) \right] + \text{h.c.} ,
\] (11a)

where the operators \(\Omega_{q\ell}\) and \(\Pi_{q\ell}\) are defined as

\[
\Omega_{q\ell}(t) = e^{-itH_S} \int_0^t ds \chi_{\ell}(s) \Pi_{q\ell}(s) e^{i(s-t)\epsilon_q} e^{itH_S} ,
\]

\[
\Pi_{q\ell}(s) = e^{isH_S} \left( T_{q\ell} \rho(s)(1-f_s) - \rho(s) T_{q\ell} f_s \right) e^{-isH_S} ,
\] (11b)

and \(f_s\) is the Fermi function of the lead \(\ell\) describing the state of the lead before being coupled to the sample. The operators \(T_{q\ell}\) and \(T_{q\ell}^d\) describe the "transitions" between two many-electron states (MES) when one electron enters the sample or leaves it.

The GME is solved numerically by calculating the matrix elements of the RDO in the basis of the interacting MES, in small time steps, following a Crank-Nicolson algorithm. More details of the derivation of the GME can be found in Ref. [16]. The calculation of the interacting MES is described in Ref. [17]. The switching functions \(\chi_{\ell}(t)\) must be defined. For example any function starting at zero and gradually increasing to one can be used to obtain the steady state in the asymptotic limit. In principle any other
time dependence can be used, like steps or periodic functions.

Mean values of observables can be obtained by taking the trace of product of the corresponding operator and the RDO. The total time dependent charge in the sample is found by using the number operator $N = \sum_m d_m^\dagger d_m$:

$$\langle Q(t) \rangle = e \langle \text{Tr} \{ \rho N \} \rangle = e \sum N \sum_{\alpha N} \langle \alpha_N | \rho(t) | \alpha_N \rangle,$$  \hspace{1cm} (12)

where $\alpha_N$ denotes the (Coulomb interacting) MESs with fixed number of electrons $N$. Remark that one can also calculate the partial charge accumulated on $N$-particle MESs.

The currents in the leads are then found by taking the derivative of Eq. (12) with respect to time. The time derivative of Eq. (3) can be substituted by the right-hand side of the GME [Eq. (11a)] and so it is possible identify the currents in each lead,

$$\langle J_{e_i}(t) \rangle = -\frac{1}{\hbar^2} \sum N \sum_{\alpha N} \int dq \chi_i(t) \langle \alpha_N | \{ \mathcal{T}_{q_{\ell}} \mathcal{Q}_{q_{\ell}}(t) \} | \alpha_N \rangle$$

$$+ \text{h.c.} \hspace{1cm} (13)$$

3. GME With One Energy Level

To better understand the thermal effects in the GME we solve the GME for a sample with one single site (a single level quantum dot). To simplify Eq. (11a) we start by inserting

$$\rho(s) = U_s^\dagger(t-s) \rho(t) U_s(t-s)$$

$$= e^{iH_s(t-s)\hbar} \rho(t) e^{-iH_s(t-s)\hbar},$$  \hspace{1cm} (14)

i.e. we propagate the density matrix backwards in time and take it outside the time integral in Eq. (11b). In fact this is the Markov approximation.

The Fock space contains now only two states, the vacuum state with energy 0 and a single particle states with energy $E > 0$. We use here $E = 2$ units of $E_s$. Of course, for a one-site model the hopping energy $E_s$ has no meaning, the result being only the diagonal term in the lattice Hamiltonian. We want to find the occupation of these states, i.e. the diagonal elements of the RDO, for this two-level model. In this case Eqs. (11) are greatly simplified because only one of the transfer matrix elements, $\langle T_{q_{\ell}} \rangle$, is non-zero:

$$\langle 1 | \mathcal{T}_{q_{\ell}} | 0 \rangle = \sum_n T_{\ell n_q}^\dagger \langle 1 | d^\dagger_{n_q} | 0 \rangle = T^\dagger_{q_{\ell}}.$$  \hspace{1cm} (15)

This simplifies the commutator Eq. (11a) and gives

$$\frac{\partial}{\partial t} \langle 0 | \rho | 0 \rangle = -\frac{2}{\hbar^2} \sum_{\ell} \int dq \text{Re} \left\{ \langle 0 | \mathcal{Q}_{q_{\ell}}(1) | 1 | \mathcal{T}_{q_{\ell}} | 0 \rangle \right\}.$$  \hspace{1cm} (16)

The trace of the RDO is 1, therefore the other diagonal element is given by $\langle 1 | \rho | 1 \rangle = 1 - \langle 0 | \rho | 0 \rangle$. Only one matrix element for $\Omega$ is needed to find the diagonal elements of the RDO

$$\langle 0 | \Omega_{q_{\ell}} | 1 \rangle = \frac{\langle 0 | \mathcal{T}_{q_{\ell}}^\dagger | 1 \rangle}{\epsilon_{q_{\ell}}(q) - E} \left\{ e^{-i\epsilon_{q_{\ell}}(q)t} - 1 \right\}$$

$$\times \left\{ (1 | \rho | 1) (1 - f_L(\epsilon_{q_{\ell}})) - (0 | \rho | 0) f_L(\epsilon_{q_{\ell}}) \right\}.$$  \hspace{1cm} (17)

The $q$-integral can be evaluated in the steady-state limit if we admit that for $t \rightarrow \infty$ the real part of $\langle 0 | \Omega_{q_{\ell}} | 1 \rangle$ contains a delta function $\delta(\epsilon_{q_{\ell}}(q) - E)$. With this approximation we actually neglect the level broadening due to the lead-dot coupling [19]. That broadening will be discussed in the next section. In the steady-state limit the diagonal values of $\rho$ approach a constant value and thus the right hand side of Eq. (16) must be zero. Using Eq. (8) and the delta function one obtains

$$\sum_{\ell} V^2_{\ell} \left\{ (1 | \rho | 1) (1 - f_L(E)) - (0 | \rho | 0) f_L(E) \right\} = 0.$$  \hspace{1cm} (18)

Therefore the occupations in the steady-state are

$$\langle 0 | \rho | 0 \rangle = 1 - \frac{\sum_{\ell} V^2_{\ell} f_L(E)}{\sum_{\ell} V^2_{\ell}}, \hspace{1cm} (19)$$

and the current is

$$J_{e_i} = \frac{V^2_{\ell}}{\tau} \left\{ (1 | \rho | 1) (1 - f_L(E)) - (0 | \rho | 0) (1 - f_L(E)) \right\}.$$  \hspace{1cm} (20)

The equation for the occupation and the currents in the leads was derived using the fact that in the steady-state $\rho$ is constant and thus its time derivative is zero. This implies that in the steady state the currents in the left and right leads are equal: what goes into the sample must also go out. Therefore using Eq. (19) we can eliminate $\rho$ from Eq. (20) and we obtain:

$$J_L = \frac{1}{\tau^2} \frac{V^2_L V^2_R}{V^2_L + V^2_R} \left( f_L(E) - f_R(E) \right),$$

$$J_R = \frac{1}{\tau^2} \frac{V^2_L V^2_R}{V^2_L + V^2_R} \left( f_R(E) - f_L(E) \right).$$  \hspace{1cm} (21)

Which makes it clear that in the steady-state the currents are equal, but with opposite signs $J_L = -J_R$, with positive “in” from the left led, and negative “out” into the right lead.

The results of the analytical calculations can be seen in Fig. 3. In Fig. 3(a) we show the results for a thermal bias, i.e. for different temperatures in the leads, $T_L > T_R$ and $\mu_L = \mu_R$, and also for an electrochemical bias, i.e. $T_L = T_R$ and $\mu_L > \mu_R$. Fig. 3(b) shows the charge in the system calculated using Eq. (19). The current generated thermically can be positive or negative, the transition occurring when the Fermi level is equal to the energy of the single level $\mu_{L,R} = E$. At this point the state is half filled and the current in the leads is zero. The probability of a transition to/from the energy level to/from the left and
right lead is equal. When the state is less than half filled, a transition from the energy level to the right lead has a higher probability than to the left lead. This gives a positive current flowing from the left to the right. Once the state is more than half filled a transition from it to the left lead is more probable. Giving a negative current flow from the right to the left. This difference in transition probability is due to different temperatures at the left and right lead.

According to Eq. (21) the current is essentially the difference of two Fermi functions. For the thermolectric current they are centered at the same chemical potential, but they have different widths. For the pure electric current they are centered at two different chemical potentials, but they have the same width. Therefore the width of the current peaks in Fig. 3 are only due to the temperatures or chemical potentials. For example the width of the current created by the chemical potential bias, at half height, should be \( \Delta \mu + 2k_B T = 0.15 + 2 \times 0.1 = 0.35 \), which is consistent with Fig. 3. (The level width \( \Gamma \) has been neglected.)

We can conclude this section with the idea that the thermolectric currents can be understood as being related to the difference between two Fermi functions with the same center but different widths. Therefore, as pointed out recently by Tagani and Soleimani [20], there are two reasons for the current to become zero: (1) half filling, where the two Fermi functions are equal to 0.5, and (2) integer filling, where both are 0 or 1. This idea will help us to understand more complex results incorporating many-body effects. For comparison the currents generated by an electrochemical potential bias are given by the difference between two Fermi functions of the same width but with different centers, and thus have a constant sign and a maximum at half filling.

4. Results for a Many-Body System

The MESs of the sample are characterized by the electrochemical potentials \( \mu_N^{(i)} := \mathcal{E}_N^{(i)} - \mathcal{E}_{N-1}^{(i)} \), where \( \mathcal{E}_N^{(i)} \) is an energy of the sample spectrum containing \( N \) particles, \( i = 0 \) indicating the ground state and \( i > 0 \) the excited states. In Fig. 4 we see the electrochemical potential diagram for a system with three lattice points and Coulomb interaction strength \( u_c = 2.0 \) (units of \( t_s \)).

The system has three single particle states with energies \( E_1^0 = 2 - \sqrt{2} \approx 0.59 \), \( E_1^1 = 2 \), \( E_1^2 = 2 + \sqrt{2} \approx 3.41 \), three two-particle states with energies \( E_2^0 = 4 \), \( E_2^1 = 6 \), \( E_2^2 = 7 \) and one three-particle state with energy \( E_3^0 = 11 \). For the single-particle states \( (N = 1) \) the chemical potentials are in fact the single-particle energies. The effects of the Coulomb interaction on the two \( (N = 2) \) and three-particle states \( (N = 3) \) is to shift them upwards. Fig. 5 shows the current in the left lead in the steady state for both \( u_c = 0.0 \) and \( u_c = 2.0 \). The green vertical lines represent the chemical potentials in Fig. 4. The blue line (---) shows the current for a system with no Coulomb interaction. The current is zero at the points \( \mu \approx 0.5, \mu = 2 \) and \( \mu \approx 3.5 \). These points correspond to half filling of states. In between such points the current is again zero when integer filling occurs (e. g. for \( \mu \approx 1.2 \)). The filling can be seen in Fig. 6(a), were the charging of the single, two- and three-particle states is shown for the non-interacting case. At the point \( \mu \approx 0.5 \) the single particle states are half charged, and at \( \mu = 2 \) the two-particle states
are half charged and the single particle half discharged. The last point \( \mu \approx 3.5 \) is the point where the two-particle states are half discharged and the three-particle state half filled. The red line (---) shows the current for the same system with Coulomb interaction \((u_c = 2.0)\). The effects of the Coulomb is to create plateaus of zero current at \( \mu = 2 \) and \( \mu \approx 5.5 \). These points correspond to integer filling of states.

![Figure 5: Comparison of the current in the left lead with and without Coulomb interaction. Red solid line (---) has the Coulomb strength \( u_c = 2.0 \) while the blue dashed line (---) has \( u_c = 0.0 \). The temperature is \( k_B T_L = 0.25 \) in the left lead and \( k_B T_R = 0.10 \) in the right lead. The lead-dot coupling parameters are \( V_L = V_R = 0.75 \) and the hopping energy in the leads is \( \tau = 4 \) (units of \( t_s \)).](image)

Fig. 6(b) shows the charging for the system with Coulomb interaction \((u_c = 2.0)\). The blue line (---) shows the total charge and has integer fillings at \( \mu = 2 \) and \( \mu = 5 \). At \( \mu = 2 \) the single particle states (---) are completely filled and at \( \mu = 5 \) the two-particle states (---) are filled. While the points \( \mu \approx 0.5 \), \( \mu \approx 3.5 \) and \( \mu = 7 \) correspond to half filling.

In Fig. 7 we show the current for two different temperatures. The red dashed line (---) has the temperatures \( k_B T_L = 0.25 \) and \( k_B T_L = 0.10 \) in the left and right leads respectively. The blue solid line (---) has the same temperature difference between the leads \( \Delta k_B T = 0.15 \) but the temperature has been increased by 0.35 in both leads. The temperature in the left lead is then \( k_B T_L = 0.55 \) and \( k_B T_R = 0.40 \) in the right lead. One effect of increasing the temperature in both leads is that the current increases in magnitude. The zeroes in the current due to half filling are not affected but the plateaus due to integer filling are raised or lowered and reduced. This behavior can be also explained using the charging diagram. Comparing Fig. 6(c) with Fig. 6(b) one can see that around chemical potential \( \mu = 2 \), due to the increased temperature, the population of single particle states decreases considerably from one, but the population of the two-particle states increases considerably from zero. Therefore the single particle states create a negative current whereas the two-particle states create a positive one (as illustrated in Fig. 3). The sum of these two contributions create the total current, in this case positive. For chemical potentials around 5.5 the total current is a combination of two-particle and three-particle components. The population of the two-particle states is less than one, but larger than one half, hence with a negative contribution to the current, whereas the three-particle population is between zero and half, hence with a positive contribution. In this case the total current is negative.

![Figure 6: Charge as a function of the chemical potential. Brown solid line (---) shows charging for the single particle states, black dotted lines (---) for two-particle states, violet dashed lines (---) for the three-particle state, and blue dashed lines (---) show the total charge. (a) Without Coulomb interaction, \( k_B T_L = 0.25 \) and \( k_B T_L = 0.10 \). (b) With Coulomb interaction \((u_c = 2.0)\), \( k_B T_L = 0.25 \) and \( k_B T_L = 0.10 \). (c) With Coulomb interaction \((u_c = 2.0)\), \( k_B T_L = 0.55 \) and \( k_B T_L = 0.40 \).](image)

![Figure 7: A comparison of the current in the left lead for two different temperatures. The red dashed line (---) has \( k_B T_L,R = (0.25, 0.10) \). While the blue solid line (---) has \( k_B T_L,R = (0.55, 0.40) \). The temperature difference between the leads is the same in both cases \( \Delta k_B T = 0.15 \).](image)

It is interesting to compare the current created by a temperature bias with that due to an electrochemical bias in the many-body case. This is what we show in Fig. 8. The current driven by the thermal bias is the same as in Fig. 7. The temperature and chemical potential differences.
between the left and right leads are identical on the energy scale. Obviously in the later case the current is positive, with peaks indicating the half filling of the ground state with \( N \) electrons, and with zero values in between these peaks, indicating the Coulomb blocking of the transport. We also obtain a small peak at \( \mu = 2 \) which corresponds to a small current going through the first excited single-particle state. The magnitude of the Coulomb interaction is incorporated in the energetic separation between the main peaks and may be estimated from the energetic length of the zero plateau of the thermoelectric current.

Now we can estimate the level broadening due to the coupling between the leads and the dot, \( \Gamma \). For example, the first peak of the current produced by the chemical potential bias around \( \mu = 0.6 \) has a width at half height of 0.58 (units of \( \tau_s \)). As shown in the previous section the broadening corresponding to the bias window is \( \Delta \mu = 2k_B T = 0.35 \). The difference can be attributed to the coupling, i.e. \( \Gamma = 0.58 - 0.35 = 0.23 \). This result is consistent with calculations at lower bias windows and temperatures (not shown). In principle the broadening due to coupling is proportional to the coupling coefficients, Eq. 8, which are not simple parameters, but a matrix elements and functions of energy which are hidden in the numerical solution of the GME. Nevertheless, in general, from previous studies \([16, 17, 21]\), we expect \( \Gamma \) a fraction of \( V_L \) like 25-50% or so. Comparing the estimated \( \Gamma = 0.23 \) with the thermal energies used \( 0.10 < k_B T < 0.55 \) we can conclude that our results correspond to an intermediate parameter regime, in between the situations presented in Fig. 1.

Another comparison we want to make is between the complete Coulomb effects, which we describe via the exact diagonalization of the sample Hamiltonian, and the charging model which is usually invoked in problems related to the Coulomb blockade. The latter is known as the “orthodox” model and it assumes that the energy of a two-particle state is the sum of the energy of the first two single particle states plus some charging energy estimated as the electron charge divided by the capacitance of the quantum dot \([12]\). This is essentially a mean field assumption. In order to compare the two approaches we calculate the current generated by the temperature bias by using the non-interacting eigenvectors in the many-body sample Hamiltonian (i.e. the basis in the Fock space), and the ground state energy of the sample for 2 electrons as given by the exact treatment. With this ansatz we describe uncorrelated particles with the energies of the exact states. The results are shown in Fig. 9. In the “orthodox” model the plateau of the thermoelectric current, at least for a number of electrons between one and two, softens or vanishes, possibly depending on strength of the Coulomb interaction. Our interpretation of this result is that the zero plateaus of the thermoelectric currents are at least partially and effect of electron-electron correlations, not captured by the “orthodox” model of the Coulomb blockade.

Next we show results for a sample attached to three leads, i.e. with a third lead connected to site number 2. Such a setup was proposed recently \([15]\) in a different context, where the third terminal was used as a phase breaking mechanism of the ballistic electron propagation between the other two terminals. In our case the third lead has a different effect: it softens the Coulomb blocking of the currents by allowing the electrons entering the sample to diffuse into the third terminal. In Fig. 10 one can see how the zero plateaus of the thermoelectric current vanish in the presence of the third terminal, indicating the additional degree of freedom offered to the electrons injected into the sample.

Finally we also show time dependent currents generated by a temperature bias. Until now we discussed only the currents in the steady state obtained by time integration, i.e. in the asymptotic time limit. But the important advantage of the GME is that one can examine the transient regime in the system or another kind of time evolution. Fig. 11 shows time dependent currents of a turnstile model.
with a thermal bias. The temperature of the left lead is \(k_B T_L = 0.25\) and of the right lead \(k_B T_R = 0.10\). The switching functions \(\chi(t)\) start at zero and continue with sinusoidal pulses, as shown in the lower panels of Fig. 11. A phase shift of half a cycle between the left and right lead is included. The current is in both leads are shown for two cases, \(\mu_L = \mu_R = 3.25\) and \(\mu_L = \mu_R = 3.75\). Earlier, in Eq. (21), we used the sign rule such currents which enter into the sample or exit from it have opposite signs. In this example we prefer to consider positive the currents from left to right and negative those from right to left. The currents follow the shape of the pulses applied to the contacts. Initially the pulses are large because the system starts out empty. The initial charging of the system is from both leads, with a positive current from \(L\) into the sample and a negative current from \(R\) also into the sample. After the transient phase the pulses stabilizes and the system enters in a periodic (steady) state. In Fig. 11(a) the current pumped in each cycle is positive whereas in Fig. 11(b) the current pumped over each cycle is negative. This is qualitatively different from an analog pumping in the presence of chemical potential bias with the same temperature in the leads. In that case only positive net current can be transported over the sample in one complete cycle [21].

5. Concluding remarks

In this work we performed an exploratory study of the current driven through an open quantum dot in a thermopower setup using the generalized master equation (GME). The quantum dot has been connected to two leads having different temperatures and the same chemical potential. The quantum dot has been defined with a finite number of discrete states. The GME method allows us to describe time dependent, transient, and also steady states, by numerical integration in time. We also included the electron-electron interaction in the sample using the exact diagonalization procedure. We obtained currents generated by a temperature bias between two leads in qualitative agreement with the experimental results for the thermopower of quantum dots at low temperatures [10], with saw teeth alternating with zero plateaus. The plateaus of the thermopower have been explained by other authors with the cotunneling processes across the leads through the dot [6]. Our formulation of the GME does not include cotunneling, but only the sequential tunneling. Therefore in our model the zero plateaus of the current can be explained using the level spacing, the Coulomb blocking, and electron-electron correlations. Cotunneling effects may indeed contribute to the plateaus of the current and including them into the GME for a multilevel system is a computational challenge and the goal of a future work.

Our study may also be compared with a recent work on the thermoelectric properties of serially coupled quantum dots [20]. Those authors used rate equations and a short-range Hubbard model for the electron-electron interaction and obtained the saw teeth of the thermopower. Our sample is designed as a series of sites, and therefore each site can also be interpreted as a single quantum dot with a single bound state. Therefore our model can be naturally used for serially coupled dots.

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7. References

References

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