Turnstile pumping through an open quantum wire

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\textbf{Abstract.} We use a non-Markovian generalized master equation (GME) to describe the time-dependent charge transfer through a parabolically confined quantum wire of a finite length coupled to semi-infinite quasi-two-dimensional (2D) leads. The quantum wire and the leads are in a perpendicular external magnetic field. The contacts to the left and right leads depend on time and are kept out of phase to model a quantum turnstile of finite size. The effects of the driving period of the turnstile, the external magnetic field, the character of the contacts and the chemical potential bias on the effectiveness of the charge transfer of the turnstile are examined, in both the absence and the presence of the magnetic field. The interplay between the strength of the coupling and the strength of the magnetic field is also discussed. We observe how the edge states created in the presence of the magnetic field contribute to the pumped charge.

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The time-dependent properties of semiconductor nanostructures and their response to electric pulses are currently being studied through transient current measurements and in a pump-and-probe configuration [1]–[3]. Along with these experimental developments, theoretical schemes for the description of time-dependent transport have emerged. The methods include the non-equilibrium Keldysh–Green function formalism [4, 5], scattering theory [6] and more recently the generalized master equation (GME) adapted for electronic transport [7]–[9].

These methods were used mostly for studying the transient currents generated by a time-dependent potential applied on the sample or by a time-dependent coupling between the leads and the sample. An example of the first category is the time-dependent pumping of electrons through a small open system [4]. In the second category, we mention the transient currents and the geometrical effects imposed by the lateral confinement of the sample [8, 10]. In recent work, we investigated the modulation of the drain current when a sequence of square pulses is applied to the source probe connected to a quantum dot and a short quantum wire described within the lattice model [11]. That study was motivated by the experiments of Naser et al [3].

In this work, we further exploit the GME method and study the transport properties of a quantum wire operating in a turnstile regime. The turnstile pump is a single-electron device where the sample is periodically connected and disconnected with the left and right leads, respectively, but with a relative phase shift. It was experimentally created by Kouwenhoven et al [12] by modulating in time the two tunneling barriers between a quantum dot and two leads. The electrons were driven by a finite bias between the leads. This setup is different from a quantum pump where a current is generated by asymmetric external oscillations, but without a bias. In the experiment of Kouwenhoven et al, the barrier heights oscillate out of phase in the following sense. In the first half-cycle, electrons enter from the source probe in the system but there is no current in the drain probe because the corresponding tunneling barrier is high enough to prevent this. In the second half-cycle the source is disconnected, the drain contact opens, and a discharge of the dot follows. It was found that an integer number of electrons are transmitted through the structure in each pumping cycle.

More recently, due to the general interest in applications of nanoelectronic devices, more complex turnstile pumps have been studied by numerical simulations, such as one-dimensional (1D) arrays of junctions [13] or 2D multidot systems [14]. In this paper, we predict that the turnstile operation can also be performed in a quantum wire sample and in an external magnetic
field as well. Our results are obtained using a parabolic lateral confinement model both for the quantum wire and for the leads. We put special effort on describing the lead–sample contacts. In a previous work, we studied the turnstile transport through a sample described by a lattice (tight-binding) model. The sample was a 1D system with two or three sites and the transport calculations were performed using nonequilibrium Keldysh–Green functions [15]. The quantum wire considered in this present work is much more complex. We start from the single-particle Hamiltonian of a 2D wire of length $L_x$ parabolically confined along the $y$-direction and with hard-wall conditions at $\pm L_x/2$. The eigenfunctions of the Hamiltonian were described in detail in [10] and will not be repeated here.

The material is organized as follows. In section 2, we briefly review the main equations of the model and of the GME method; section 3 is devoted to the numerical results for zero magnetic field (3.1), in the presence of a magnetic field (3.2) and to the edge states (3.3). The conclusions are given in section 4.

2. Model

We consider an isolated finite quantum wire of length $L_x = 300$ nm, extended in the $x$-direction. The width of the wire is defined by a parabolic confinement potential in the $y$-direction with the characteristic energy $\hbar \Omega_0 = 1.0$ meV. The quantum wire is terminated at $\pm L_x/2$ with hard wall potentials. In addition, we have two semi-infinite leads, one extended from $-L_x/2$ to $-\infty$ and the other one from $+L_x/2$ to $+\infty$. Both have a parabolic confinement in the $y$-direction with an energy of 0.8 meV and are also terminated at $\pm L_x/2$ with hard walls. The leads and the finite quantum wire, or the system, are all subjected to an external constant magnetic field $\mathbf{B} = B \hat{z}$. The length of the wire, $L_x$, and the magnetic length modified by the parabolic confinement $a_w = \sqrt{\hbar/(m^* \Omega_w)}$, with $\Omega_w^2 = \Omega_0^2 + \omega_c^2$ and the cyclotron frequency $\omega_c = eB/(m^*c)$, are convenient length scales in the calculations. We assume the GaAs effective mass, $m^* = 0.067 m_e$. The many-electron Hamiltonian of the system composed of the semi-infinite leads and the finite quantum wire, but isolated from each other, is

$$H(t) = \sum_a E_a c_a^\dagger c_a + \sum_{q,l=L,R} \epsilon_l(q) c_{ql}^\dagger c_{ql},$$

where an electron in the system is created (annihilated) by the operators $d_a^\dagger (d_a)$, and in the leads by $c_{ql}^\dagger (c_{ql})$. $E_a$ are the energies of the SES labeled as $a = 1, 2, 3, \ldots$ in increasing order, $\epsilon_l(q)$ is the energy spectrum of the left and right leads, labeled as $l = L$ and $l = R$, respectively, and $q$ represents a discrete label of subbands and a continuous quantum number labeling states within each subband. At $t = 0$, the system is coupled to the leads with the Hamiltonian

$$H_T(t) = \sum_l \chi_l(t) \sum_{q,a} \left[ T_{qa}^l c_{ql}^\dagger d_a + (T_{qa}^l)^* d_a^\dagger c_{ql} \right],$$

with $\chi_l(t)$ describing the time dependence of the coupling, such that $\chi_l(t < 0) = 0$, and $T_{qa}^l$ describing the coupling strength of state $a$ and $q$ in the system and the leads, respectively.

The coupling is defined by a nonlocal overlap integral of the the wave functions in the system and in the leads, in the region of contact around $\pm L_x/2$. The coupling coefficients are defined phenomenologically with the tensor [10]

$$T_{aq}^l = \int d\mathbf{r} d\mathbf{r}' \left( \Psi_{aq}^l(\mathbf{r}) \right)^* \Psi_{a}^l(\mathbf{r}) g_{aq}^l(\mathbf{r}, \mathbf{r}'),$$

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where the overlap kernel is modeled by

\[ g_{aq}(r, r') = g_0^l \exp \left[ -\delta_1^l (x - x')^2 - \delta_2^l (y - y')^2 \right] \exp \left( -\frac{|E_a - \epsilon^l(q)|}{\Delta^l_E} \right). \]  

(4)

It is natural to assume that the coupling coefficients depend on the states in the sample and in the leads, since these are the ‘in’ and ‘out’ states for tunneling. In our model, the wave functions are derived for the isolated systems with hard walls in the \( x \)-direction, and thus they vanish at the sample–lead interface and do not overlap. Therefore, the intuitive ansatz, equations (3) and (4), is a convenient way of describing the coupling. The character of a wave function in the sample, whether it is a bulk or an edge state (as may be in a magnetic field), does matter for the contact with the states in the leads. The effective coupling of states with higher energy is also enhanced in our model due to the higher penetration into the contact area. The strength of the coupling between the leads and the sample is defined by the parameter \( g_0^l \), which captures the tunneling rate at the contact between each lead and the sample, and also by the parameters \( \delta_1^l \), \( \delta_2^l \) and \( \Delta^l_E \), which adjust the spatial overlap of lead and sample wave functions in the contact region. In our calculations, these coupling parameters will be the same for both leads and hence the label \( l \) will be omitted.

The system can be subjected to a bias \( \Delta \mu = \mu_L - \mu_R \), and in order to reduce the number of many-electron states (MES) to a reasonable number, in the following calculations we limit the number of single-electron states (SES) for the particular calculation by selecting a window of relevant states around the bias window (BW), i.e. \([\mu_R - \Delta, \mu_L + \Delta] \), such that the transport properties are not changed significantly by extending the window. We consider these states relevant for the transport, or ‘active’, while all the other states are ‘frozen’, being either permanently occupied or permanently empty. In addition to the electrons frozen in the states below the active window (which are not included in the transport calculation), we also assume the lowest active state occupied at the moment \( t = 0 \), i.e. when the contacts begin to operate. In this way, the transient phase is shorter than if we would assume an empty active window, and we can spend less computing time until the system reaches the periodic state.

The periodic phase of the evolution can be described by the Floquet method in the Fourier domain and we are able to include in the time evolution the transient phase between the initial coupling and the periodic states.

The time evolution of the total system—finite wire and leads—after the coupling at \( t = 0 \) can be described by the Liouville–von Neumann equation for the statistical operator \( W(t) \). The evolution of the finite wire itself can be captured by the reduced density operator \( \rho(t) = \text{Tr}_L \text{Tr}_K W(t) \) (RDO), i.e. by averaging over the the lead variables. In the resulting integro-differential equation, we retain only the lowest order (quadratic) terms in \( H_T \) in the kernel and obtain [8, 10]

\[ \dot{\rho}(t) = -\frac{i}{\hbar}[H_S, \rho(t)] - \frac{1}{\hbar^2} \sum_{l=L,R} \int dq \chi_l(t)([T_l, \Omega_{ql}(t)]) + \text{h.c.}, \] 

(5)

where we have introduced two operators to compactify the notation

\[ \Omega_{ql}(t) = U_S^\dagger(t) \int_{t_0}^t \text{d}s \chi_l(s) \Pi_{ql}(s)e^{i\hbar(s-t)/h\epsilon_l(q)} U_S(s), \]

\[ \Pi_{ql}(s) = U_S(s)(T_l^\dagger \rho(s)(1 - f_l) - \rho(s)T_l^\dagger f_l)U_S^\dagger(s), \]
with $U_S(t) = e^{i(t/\hbar)H_S}$, and a scattering operator $\mathcal{T}$ acting in the many-electron Fock space of the system

$$\mathcal{T}_l(q) = \sum_{\alpha,\beta} \mathcal{T}_{\alpha\beta}^l(q)|\alpha\rangle\langle\beta|,$$

$$\mathcal{T}_{\alpha\beta}^l(q) = \sum_{a} \mathcal{T}_{a\alpha}^l(\alpha|d^+_a|\beta).$$

Equation (5) is applicable when the coupling between the leads and the sample is relatively weak (tunneling regime), i.e. weaker than the kinetic energy inside the leads or inside the sample. In other words, the contacts and the sample create an effective potential barrier between the left and right leads. Implicitly, this means that the time evolution of the sample is slow. The solution of equation (5), i.e. $\rho(t)$, can actually be seen as a power series in $H_T^2$, like the solution of a Dyson equation. Hence, the correction to the density matrix of the isolated sample is more than second order in $H_T$. Therefore, in practice it is difficult to say rigorously where the border between weak and strong coupling is. It is, however, known that if the coupling is too strong, the occupation numbers may become negative and thus unphysical. (The occupation numbers, or ‘populations’, are the diagonal elements of the RDO.) Although we always check in our calculations, strictly speaking this condition does not guarantee the validity of the RDO. So, in practice, we cannot avoid choosing our contact parameters in a semi-empirical manner.

With the RDO, it is possible to calculate the statistical average of the charge operator $Q_S = e\sum_a d^+_a d_a$ for the coupled system,

$$\langle Q_S(t) \rangle = \text{Tr}[W(t)Q_S] = \text{Tr}_S[[\text{Tr}_R\text{Tr}_L W(t)]Q_S]$$

$$= \text{Tr}_S\{\rho(t)Q_S\} = e \sum_{a,\mu} i^\mu_\alpha \langle \mu|\rho(t)|\mu \rangle,$$

with the traces assumed over the Fock space. The average time-dependent spatial distribution of the charge can also be obtained,

$$\langle Q_S(r, t) \rangle = e \sum_{ab} \sum_{\mu\nu} \Psi^\mu_a(\mathbf{r})\Psi^\nu_b(\mathbf{r}) \rho_{\mu\nu}(t) \langle v|d^+_a d_b|\mu\rangle.$$  

The net current flowing into the sample is

$$\langle J(t) \rangle = \langle J_L(t) \rangle - \langle J_R(t) \rangle$$

$$= \frac{d\langle Q_S(t) \rangle}{dt} = e \sum_{a} \sum_{\mu} i^\mu_\alpha \langle \mu|\dot{\rho}(t)|\mu \rangle.$$  

The total current in equation (9) is given by the left-hand side of the GME, equation (5), and the partial currents associated with each SES and each lead corresponds to the terms of the sum on the right-hand side (the trace of the commutator of $\rho$ and $H_S$ is zero). The functions that modulate the coupling between the leads and the quantum wire are built in the following way: for $0 \leq t < T_l$, we use the Fermi-like function $f(t) = (e^{\gamma t} + 1)^{-1}$, with $\gamma = 1.0 \text{ ps}^{-1}$, and we define $\chi_l(t) = 1 - 2f(t)$, where $l = L, R$ is the lead index. Then, for $t \geq T_l$, $\chi_l(t)$ becomes step-like functions alternating between 0 and 1, both with the same period $T$, but with a delay of $T/2$. In this way, we mimic the on/off contact switching done in the turnstile experiments. We choose $T_L < T_R = T_L + T/2$, which means that we first switch off the left contact while the right one is still on. Then the left is turned on again while the right is turned off that and so on.
Figure 1. The energy spectrum of the leads versus the scaled wave vector $q a_w$. The subband index is $n = 0, 1, 2, 3$. Dots indicate the energy spectrum of the isolated sample, horizontal wide dashed lines the chemical potentials $\mu_L = 1.48$ meV and $\mu_R = 0.78$ (BW1) and horizontal narrow dashed lines $\mu_L = 2.48$ meV and $\mu_R = 1.78$ meV (BW2).

The solution of the GME, equation (5), is obtained numerically using the Crank–Nicolson algorithm [8, 18]. The time derivative of the RDO is evaluated as the mean value of the forward and backward derivatives over a finite time step $\tau$, chosen small enough to capture correctly the dynamical details of the sample. On the right-hand side of the GME, we initially approximate $\rho(t) \approx \rho(t - \tau)$ and then we perform iterations (typically 10–20) until $\rho(t)$ is convergent.

3. Numerical calculations, results and discussion

3.1. No magnetic field

The energy spectrum of the leads and of the sample are shown in figure 1. The leads have parabolic subbands while the sample has discrete levels. The maximum energy for each subband shown in the graph indicates the corresponding maximum wave vector in the $q a_w$-integration of the GME. The chemical potentials in the leads defining the BW are shown with the dashed horizontal lines. We consider two BWs: BW1 with chemical potentials $\mu_L = 1.48$ meV and $\mu_R = 0.78$ meV and BW2 with $\mu_L = 2.48$ meV and $\mu_R = 1.78$ meV, respectively. In both cases, the applied bias is $eV_{\text{bias}} = \mu_L - \mu_R = 0.70$ meV. In the numerical calculations of the reduced statistical operator, we also include the sample states with energy outside the BW, between the limits $\mu_R - \Delta$ and $\mu_L + \Delta$ with $\Delta = 0.1$ meV. The first active window contains four SESs and the second one contains five SESs.

In figure 2, we show the time-dependent total occupation $n_t$ of the relevant (active) SES for BW1 and BW2. The electrons occupying the states situated below and above the active windows are not included, but only those on the relevant states (or within the active windows). In this example, the parameters characterizing the coupling of the sample to the leads are $g_0 a_w^{3/2} = 926$ meV (with $a_w$ measured in nm), $\delta_1 a_w^2 = 1.0$, and $\delta_2 a_w^2 = 2.0$. The large value for $g_0 a_w^{3/2}$ is consistent with the small overlap of the wave functions from the lead and from the sample mandated by the large values for $\delta_1 a_w^2$ and $\delta_2 a_w^2$. The largest contribution to the overlap
Figure 2. The time-dependent total occupation of the relevant SES for a system occupied initially with one electron for the first (solid) and second (dotted) BWs. The time coupling functions $\chi_l(t)$, with $l = L, R$, are shown for reference. Other parameters: $g_0a_0^{3/2} = 926$ meV, $\delta_1a_0^2 = 1.0$, $\delta_2a_0^2 = 2.0$ and $T = 60$ ps. In each case, there is one electron on the lowest relevant state at the initial moment.

The efficiency of the turnstile operation depends on the pulse length $T$. The previous results have been obtained with $T = 60$ ps. In those setups, the system transfers at least two electrons per cycle. Since the present GME method is valid for weak lead–sample coupling, the tunneling of the electrons from the leads to the sample and back is relatively slow. Therefore by increasing
or decreasing the pulse duration, the transferred charge increases or decreases, respectively. Denoting by $T_t$ the characteristic tunneling time, if $T \leq T_t$ the turnstile operation is not expected to work, the allowed time for the charging and discharging of the system being too short. This is the case for $T = 10$ ps, as shown in figure 4, when clearly very little charge can enter and leave the system in a pumping cycle. Actually, the time $T_t$ depends on the pairwise coupling (or overlap) of each state of the leads to each state of the sample with energies within the BW. But in order to obtain significant pumping effects, the pulse duration has to include the time of flight (or propagation time) of electrons along the wire. This extra time depends on the energy of the electrons injected from the left lead all the way into the right lead.

Therefore, for a longer pulse, $T = 40$ ps, the turnstile pumping process is able to transfer charge through the sample. The occupation number has a triangular shape in time and it becomes periodic after 2–3 cycles. During the initial cycle, which includes the initial charging phase, the system accumulates more than two electrons and the steady state is already reached at about 30 ps when the charge in the system is saturated. This is possible because the right
contact is still off. This charging time gives us a rough estimation of the coupling energy, $T_{qa} \approx \hbar / t \approx 0.02$ meV. Graphs of the coefficients $T_{qa}$ will be shown later in the presence of a magnetic field (figure 9).

The right contact opens for the first time at 45 ps allowing more than one electron charge to pass into the right lead. For a longer period, such as $T = 60$ ps, the occupation number develops toward a saw tooth profile typical for the charging/relaxation processes. The asymmetry of the charge peaks is determined by the direction of the bias: the electrons leave the sample faster than they entered. The system drives almost two electrons from one lead into the other, which is remarkable given the length of our sample (300 nm).

Another important aspect in our model is the strength of the lead–sample coupling, i.e. the parameters $g_0$, $\delta_1$ and $\delta_2$ in equation (6). Our GME implementation is restricted to the lowest order in $H_T$ (quadratic), supplying the integro-differential equation (5), and thus the parameters have to be appropriately selected.

To have an idea of the relation between the pumping amplitude and the coupling strength, we show in figure 5 three calculations performed with three strengths of the coupling, which we consider in relative terms as weak, intermediate and strong. In order to compare with the results obtained in the presence of a magnetic field shown in the next examples, the scaled parameters $g_0 a_w^{3/2}$ and $\delta_1 a_w^2$ are chosen such that the physical values $g_0$ and $\delta_1$ are the same as for $B = 0.9$ T (to be shown in the next subsection). The time-dependent occupation of the states in the active window is shown for longer times than in the previous figures to indicate better the final periodic regime.

It is not surprising to see that the pumping amplitude increases with the coupling strength, since tunneling of electrons becomes more likely. The same can be said about the current, which is essentially the time derivative of the charge, and it is visible in figure 5 that the slope of the charging increases with the coupling strength. This can also be seen in the net (average) slope of the sawtooth evolution for the weak coupling. The increase in the transient current with the coupling strength has also been shown recently by Sasaoka et al [19], although in a quantum dot pumping device.

Figure 5. The time-dependent total occupation for $B = 0$ T and three values of the coupling strength. Weak: $g_0 a_w^{3/2} = 1408$ meV, $\delta_1 a_w^2 = 1.85$, $\delta_2 a_w^2 = 3.7$. Intermediate: $g_0 a_w^{3/2} = 1408$ meV, $\delta_1 a_w^2 = 1.39$, $\delta_2 a_w^2 = 2.77$. Strong: $g_0 a_w^{3/2} = 1824$ meV, $\delta_1 a_w^2 = 1.39$, $\delta_2 a_w^2 = 2.77$. The pulse period is $T = 60$ ps.
3.2. Magnetic field present

Following our ansatz used to describe the system–leads coupling, equations (3) and (4), we can visualize systems where the physical parameters $g_0$, $\delta_1$ and $\delta_2$ should be assumed constant and others where the scaled values $g_0 a_w^{3/2}$, $\delta_1 a_w^2$ and $\delta_2 a_w^2$ should be kept constant with changing values of the magnetic field rather. In the following, we explore both possibilities. Our choice of $\Delta E = 0.25 \hbar \Omega_w$ depends also on the value of the magnetic field, but we have checked that variations in this parameter between a scaled version and a fixed physical one will only lead to vanishing quantitative changes in calculations where we consider a range in the $q$ integration of the GME (5) that includes four subbands of the leads. This choice of $\Delta E$ guarantees always the same number of subbands in the calculation.

In the presence of a magnetic field, in a first approximation one might expect the amplitude of the charge oscillations to decrease, the reason being that the electronic trajectories bend due to the Lorentz force and the electrons might return to the source lead rather than traveling directly to the drain lead. At the same time, we know that a magnetic field generally reduces backscattering. In figure 6, where we show the time-dependent total charge for different values of the magnetic field, we see a reduction of the charge oscillations with increasing magnetic field. For comparison, we include the $B = 0$ case, also shown in figures 2 and 4. To compare the results with and without magnetic field, we initially keep the same coupling parameters as measured with respect to the modified magnetic length, $a_w$, i.e. $g_0 a_w^{3/2} = 926$ meV, $\delta_1 a_w^2 = 1.0$ and $\delta_2 a_w^2 = 2.0$. The modified magnetic length $a_w$ decreases with increasing magnetic field.

We select the BWs like BW2, with three states included in the window and two marginal states in the extended regions. The energy levels and the wave functions depend on the strength of the magnetic field, both in the sample and in the leads. In order to make the comparison shown in figure 6 meaningful for each value of the magnetic field, we shift the chemical potentials in the leads such that the same energy levels of the quantum wire sample are contained in the BW with a fixed width.

Again the charging time is inversely proportional to the coupling strength, as already mentioned at the end of subsection 3.1 for $B = 0$, and so the slope of each tooth is large or small.
depending on whether the coupling is large or small. The same can be said about the net slope of the mean number of electrons. In figure 6, the magnetic field is changed while the coupling is constant in normalized units. The magnetic field is included in the length $a_w$, which decreases with increasing $B$. Therefore, the spatial width of the Gaussian kernel $g_{0a}(r, r')$ decreases at constant $\delta a_w^2$. Large $B$ implies large $\delta$’s, or a narrow Gaussian, and thus weak coupling and small slope.

The efficiency of the turnstile pump tends to decrease with increasing magnetic field. For $B = 0$ an amount of charge $Q_p \approx 1.8$ electrons can be transmitted along the wire sample in one cycle, and for $B = 0.2 \ T$, $Q_p \approx 1.2$. For stronger magnetic fields, $Q_p$ drops to 0.8 for $B = 0.4 \ T$, and $Q_p < 0.5$ at $B > 0.6 \ T$. It is also clear that, at least for the present coupling parameters, the charging time increases in the presence of the magnetic field. During the initial cycle, i.e. for $t < 60 \ ps$, there is less charge accumulated in the system in the normal switching regime than for $B = 0$, and also the charging process continues even after the pumping begins. The periodic regime is reached after a number of cycles, which increases with $B$.

Although the presence of the magnetic field reduces the electron transfer, the pumped charge still increases with increasing coupling between the leads and the sample. To show that we solve the GME for a fixed magnetic field $B = 0.9 \ T$ for three sets of coupling parameters, which we again call (in relative terms) weak, intermediate and strong coupling, respectively, see figure 7(a). The parameters for the weak coupling are the same as in figure 6. For the intermediate coupling we use $g_{0a}^{\frac{3}{2}} = 926 \ meV$, $\delta_1 a_w^2 = 0.75$ and $\delta_2 a_w^2 = 1.5$. For the strong coupling $g_{0a}^{\frac{3}{2}} = 1200 \ meV$, $\delta_1 a_w^2 = 0.75$ and $\delta_2 a_w^2 = 1.5$. These parameters correspond to the same physical parameters that were used in figure 5. So, if we now compare the results at $B = 0.9 \ T$ with the results at $B = 0$, we see quite similar charge amplitudes, but somewhat more sensitive to the coupling strength at $B = 0.9 \ T$. For example, at $B = 0.9 \ T$, we obtain $Q_p \approx 0.4$ electron at low coupling, $Q_p \approx 1.2$ at intermediate coupling and $Q_p \approx 2.4$ at strong coupling. For $B = 0$, these numbers are $Q_p \approx 0.3$, 1.2 and 1.8, as can be read from figure 5.
Figure 8. (a) The time-dependent total occupation of the relevant SESs for \( B = 0.9 \text{–} 1.2 \text{ T} \). (b) The total current entering the system from the left lead and the total current exiting the system into the right lead for \( B = 1.0 \text{ T} \). Parameters: \( g_0 a_w^{3/2} = 1200 \text{ meV}, \delta_1 a_w^2 = 0.75 \) and \( \delta_2 a_w^2 = 1.5 \). The pulse period \( T = 60 \text{ ps} \).

We believe that the increased sensitivity of the pumping to the contact strength in the presence of the magnetic field is a result of the edge states created in the sample. The edge states are indeed more and more pronounced with increasing magnetic field, and so is the pumped charge if the edge states are in good overlap with the coupling region. This is shown in figure 7(b) for the example with \( g_0 \) and \( \delta_{1,2} \) corresponding to constant and (relatively) strong physical coupling between the sample and leads. After an initial decrease, \( Q_p \) reaches a minimum and then it increases due to the contribution of the edge states. In this case, the onset of the effects due to the edge states is at \( B \approx 0.6 \text{ T} \).

Next, in figure 8(a), we show the results for higher magnetic fields, but this time with fixed normalized coupling. The apparent reduction in amplitude with increasing magnetic field is now an effect of the indirect reduction of physical strength of the contacts. Nonetheless, for a magnetic field of 1 T, we obtain \( Q_p \) of about two electrons, which is still more than that at zero magnetic field. The curve for \( B = 0.9 \text{ T} \) in figure 8(a) is identical to that of figure 7 and is included for comparison. The time-dependent total currents in the left and right leads are shown in figure 8(b) for \( B = 1 \text{ T} \). The currents suddenly vanish at each contact when the contact is closed. The currents have a trapezoidal shape for the pulse duration \( t = 60 \text{ ps} \), but they become triangular for shorter pulses such as \( T = 10 \text{ ps} \) (not shown).

3.3. Analysis of edge states

Clearly, states in the sample with higher probability at the contact edges contribute more to the pumping. In figure 9, we show the coupling strength of each of the five states of the finite wire involved in the transport for each magnetic field of figure 8, only for the lowest subband of the leads. The general trend of the coupling coefficients is to decrease with increasing magnetic field. So the decrease in the pumping as the magnetic field increases can be explained by the decrease in the coupling strength. The contribution of each state to the transport is given by an integration over all of the lead states \( q \) in the GME.

To show the contribution of each state to the transport, we show in figure 10 the time-dependent occupation of all five states included in the calculation for \( B = 1.2 \text{ T} \), which are the
Figure 9. The coupling energies between the states $a = 6–10$ and the states of the lowest subband in the left (or the right) lead for $B = 0.9–1.2\,\text{T}$. $g_0a_w^{3/2} = 1200\,\text{meV}$, $\delta_1a_w^2 = 0.75$ and $\delta_2a_w^2 = 1.5$.

Figure 10. The time-dependent total occupation of the relevant SESs for $B = 1.2\,\text{T}$. $g_0a_w^{3/2} = 1200\,\text{meV}$, $\delta_1a_w^2 = 0.75$ and $\delta_2a_w^2 = 1.5$, $T = 60\,\text{ps}$.

states numbered 6–10 in the single-electron energy spectrum of the finite wire. It is clear that the three middle states $a = 7, 8, 9$ contribute unequally to the pumping. These states are well inside the BW, but the coupling energies are slightly different, as seen in figure 9 for $B = 1.2\,\text{T}$. For the other values of the magnetic field shown in figure 9, the states within the BW have nearly equal coupling to the leads and consequently nearly equal contributions to transport. So in general the coupling strength may depend on the state and so does the corresponding partial current. States 6 and 10 included in figure 10 are slightly outside the BW and obviously their contribution to transport is smaller.
Figure 11. The probability density of the single-electron eigenstates of the sample, numbers 6–10, for $B = 1$ T. The coupling parameters are the same as in figure 8.

In figure 11, we show the probability density associated with the five active SES (numbers 6–10) of the finite quantum wire. The figures indicate that all five states have the characteristics of an edge state. The coupling parameters are the same as for figure 8. In vanishing magnetic field, the probability density of the active states is on average smeared over the finite wire. As the magnetic field increases, the Lorentz force squeezes the probability of some states close to the edge of the finite wire. This also happens at the hard-wall ends of the wire, the contact area. This fact explains why increasing the coupling through increasing $g_0$ should be more effective at high magnetic field. From figure 11, it is evident that the edge states will have different coupling strengths to the leads due to the difference in their finer structure in the contact area. This finer structure in the contact area of the wire induces differential coupling to the states in the different subbands of the leads.

The time-dependent charge in the quantum wire is shown in figure 12 for the parameters used in figure 8(b). The charge distribution reflects the geometry of the quantum wire and of the five SESs involved, and indicates the propagation of the electrons in the system. The selected time moments cover the initial charging cycle plus a part of the next cycle. It is interesting to observe how the electrons are injected at the left contact into the sample traveling along the quantum wire on the upper edge channel and how they are reflected back at the right contact traveling along the lower channel.

We show first the charge density soon after the coupling of the system to the leads, at $t = 1.52$ ps when the distribution is the same at both contact regions. At $t = 14.43$ ps, more charge is accumulated in the sample and the distribution is more pronounced on the left part of the central region. This is consistent with the currents shown in figure 8(b), where we see that at this moment the current from the left lead is higher than the current in the right lead. In the next three snapshots the distribution of the charge is not changing in time because the steady state is
Figure 12. The average spatial charge distribution in the quantum wire for $B = 1$ T at different moments of time. The coupling parameters are the same as in figure 8.

reached, as visible in figure 8(a) for $B = 1$ T. Then, in the next snapshots, one can see how the charge concentrates to the left or to the right of the sample when the current in the left lead or in the right leads increases, respectively.

4. Summary

The turnstile conduction of a 2D parabolic wire, seen as ‘the sample’, attached to semi-infinite leads of a similar parabolic shape has been studied using a non-Markovian GME method. This system is far more complex than the simple two- or three-level system with 1D leads considered in an earlier publication based on the Keldysh–Green functions approach [15]. The eigenstates of the leads and of the finite wire have been calculated in an external perpendicular magnetic field using a combination of analytical and numerical methods for large functional basis sets. We have taken into account the subband structure of the leads to which it is attached. We have also described phenomenologically the coupling between the states in the leads and the states in the finite wire as a nonlocal overlap of the wave functions from both sides of the contact.

We have analyzed the effects of the BW, pulse length and magnetic field on the evolution in time of the number of electrons in the sample. We have found that longer pulses are more favorable for the turnstile pumping as the electrons need time to propagate along the sample wire. One or two electrons could be transferred through the 300 nm wire using pulses of 40 or 60 ps.

Comparison of the results obtained with and without a magnetic field is a difficult issue. If a magnetic field is present, all energies shift, all wave functions change (both in the sample and...
in the leads) and also all elements of the coupling tensor $T_{qa}$ between lead and sample states change. Of course, these changes depend on the strength of the field. Therefore, it is difficult to create similar conditions for two different field values, i.e. the same number of states in the BW and the same coupling energies, in order to compare only the amplitude of the pumped charge. To do that, we have selected the parameters describing the phenomenological coupling of the leads to the finite wire in two different ways, both scaled and not scaled with the effective width of the sample, which implicitly depends on the magnetic field. This is an issue that can only be better resolved with a more involved microscopic model of the coupling and comparison to experiments where the coupling strength could be varied, for example by using finger-strip gates.

The charge distribution inside the system, figure 12, emphasizes the dynamics induced by the charging/discharging sequences. The charge propagation along edge states in a strong magnetic field indicates that the optimal turnstile period depends on the external magnetic field. Experimental studies of turnstile pumping in quantum wires have to clarify the relationship between the magnetic field, pumping amplitude and contact strength.

We have already included the Coulomb interaction in our GME formalism using an implementation built on an exact numerical diagonalization of a truncated Fock space [20, 21]. We observed Coulomb blocking on the one hand in the regime of weakly coupled leads and sample [20], or delocalization of states enhancing the total current through the sample on the other hand for systems with more detailed potential landscape [21]. Here, we have neglected the Coulomb interaction to concentrate our attention on other components and variables influencing turnstile pumping through a finite quantum wire. It was not clear initially whether a GME formalism for a weakly coupled system and leads would be adequate to describe a turnstile action in the system. Our experience with the Coulomb interaction indicates that qualitatively the turnstile pumping will also take place with the Coulomb interaction present; of course, the results will be quantitatively affected, depending on the parameters of the operation. However, since in this work we were interested mostly in the conductive states and not in the Coulomb blocking effects, we believe the Coulomb interaction will not change dramatically the present results, but we see the inclusion of the Coulomb interaction in the present model as a challenging future task.

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