Quantised charge pumping through multiple quantum dots

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We study electron pumping through a system of barriers, whose heights are deformed adiabatically. We derive a simple formula for the pumped charge \( Q \) in terms of the total reflection and transmission amplitudes and phases. The pumped charge increases with the number of barriers \( (n_b) \) and shows an interesting step-like behaviour, with the steps appearing at integer values of \( Q \). The pumped charge also tends towards quantisation with the increase of the amplitude of the time-varying potential. The value of the quantised pumped charge is shown to be correlated to the discontinuity of the reflection phase.

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A parametric electron pump is a device which generates a dc current at zero bias by cyclic deformations of the system parameters [1,2]. The parameters of the Hamiltonian are slowly varied as a periodic function of time such that the Hamiltonian returns to itself at the end of one cycle, but charge has been pumped through the system. In the last few years, electron pumps consisting of small semi-conductor dots have received a great deal of experimental [3,4] and theoretical attention [5–9].

Of more recent interest are the quantum pumps in open dot systems, where quantum interference of the electronic wave-function rather than Coulomb blockade (CB) is expected to play the major role. Such a pump has been fabricated by Switkes et al [10]. A scattering approach to such a parametric electron pump was pioneered by Brower [6] where the pumped current was related to parametric derivatives of the scattering matrix. Using this, several theoretical papers [11–13] have investigated the connection between resonant transmission and the pumped charge. In general, the pumped charge is not quantised; however, it has been shown that when the pumping contour encloses almost all of a resonance line, the charge pumped is almost quantised [12]. It has also been shown that inclusion of inter-electron interactions using the Luttinger liquid formalism [14] leads to charge quantisation even with just a double barrier system, due to the insulating nature of the Luttinger wire in the presence of any barrier.

Although for the case of a rigidly sliding potential \( U(x-\nu t) \), where the periodicity in time \( T \) is related to the periodicity in space \( L \) by \( T = nL/\nu \), \( n \) =integer, it can be proved using topological arguments that the charge is quantised [1], it is not so obvious that those arguments hold for more general cases where the Galilean principle does not hold. Several explicit examples were considered by Niu [2] but quantisation has been shown only for potentials which are spatially periodic.

In this letter, we derive a simple formula for the pumped charge in terms of the reflection and transmission amplitudes of the system -

\[
Q = \frac{e}{2\pi} \int_0^\tau dt \ 1 - \frac{e}{2\pi} \int_0^\tau dt \ t^2 (\theta + \phi), \tag{1}
\]

where \( \tau \) is the time period of the perturbation in the potential which causes the charge to be pumped and \( r, \theta \) and \( \gamma, \phi \) are the reflection and transmission amplitudes and phases respectively. We show that quantisation occurs whenever the contribution from the second term vanishes.

We also explicitly demonstrate the quantisation of the pumped charge, due to interference effects, when we increase the number of tunnel barriers \( (n_b) \) or equivalently increase the number of dots \( (n_d = n_b - 1) \) through which the current is measured. We work with open quantum dots with large transmissions and explicitly show how the charge pumped through the device changes with the number of dots. It is expected [1,2] that for a fully spatially periodic system, \( (n_b \ or \ n_d \rightarrow \infty) \), the charge pumped will be quantised. However, here we see that for reasonable values of the barrier strengths and pumping strengths, (almost) quantisation occurs even with 4-6 dots. We also see that the pumped charge, as a function of the number of dots, shows an interesting step-like behaviour. The pumped charge increases with the number of barriers and then saturates near an integer. Beyond that, it rises again with the number of barriers, till it saturates at the next integer. This tendency towards quantisation is also seen as a function of the amplitude of the pumping potential. This clearly indicates the special stability that occurs when an integer number of electrons are pumped through the system. Note that this stability is purely quantum mechanical in origin and is not due to interactions or CB physics, which allows electrons to be added only one by one to the dot. Here, we are completely ignoring interaction effects and there is no CB since the dots are well-coupled to the leads.

Although we use \( \delta \)-function barriers for the explicit calculation, we expect the results to be robust to changing the form of the barriers. Following the work of Ref. [15],
we also expect these results to be robust to weak disorder and to weak interactions.

We start with a system of coupled quantum dots as shown in Fig. 1. The barriers forming the dot are periodically modulated as

\[ V_i = V_0 + V_p \cos(\omega t), \quad i \leq n_b/2 \text{ for } n_b = \text{even}, \]
\[ i \leq n_b/2 + 1 \text{ for } n_b = \text{odd}, \]
\[ V_i = V_2 = V_0 + V_p \cos(\omega t + \delta), \] for the remaining. \hspace{1cm} (2)

Here \( \omega \) is related to the time period as \( \omega = \pi/2\pi \) and \( \delta \) is the phase difference between the two time-varying potentials. Such a potential breaks the parity symmetry and allows the shape of all the dots to be varied. If the dots are coupled to the leads by a single channel quantum point contact, then it is sufficient to treat the dot within a one-dimensional effective Hamiltonian. The width of the dots (effectively the width of the quantum well that we use) is given by \( a \). We are mainly interested in the region where \( V_0 \leq E_F \) since we are in the resonant tunneling regime and not in the CB regime.

The effective single channel \( S \)-matrix for this system of \( n_b \) barriers can be written as

\[ S = \begin{pmatrix} r e^{i\theta} & t e^{i\phi} \\ t e^{i\phi} & r e^{i\theta} \end{pmatrix} \]
\hspace{1cm} (3)

where the parameters \( r, t, r', \theta, \theta' \) and \( \phi \) are functions of the Fermi energy \( E_F \) and the amplitudes of the time-varying potentials \( V_i(t) \). Their explicit forms can be found, in terms of the parameters of a single well, (in the adiabatic limit), by solving the time-independent Schrodinger equation for the potential \( V_i(t) \) given in Eq. 2, for each value of \( t \). The reflection amplitudes are not the same because the time-varying potentials explicitly violate parity. The potential also violates time-reversal invariance. But since in the adiabatic approximation, we are only interested in snapshots, at each value of the time, the Hamiltonian is time-reversal invariant and hence, the transmission amplitudes are the same for the 12 and 21 elements in the \( S \)-matrix.

By the Brouwer formula \([6]\), the charge pumped can directly be computed from the parametric derivatives of the \( S \)-matrix. For a single channel, it is given by

\[ Q = \frac{e}{2\pi} \int_0^\tau dt \text{Im} \left( \frac{\partial S_{11}}{\partial V_1} S_{12}^* V_1 + \frac{\partial S_{12}}{\partial V_1} S_{11}^* V_1 \right) \]
\[ + \frac{\partial S_{11}}{\partial V_2} S_{12}^* V_2 + \frac{\partial S_{12}}{\partial V_2} S_{11}^* V_2 \] \hspace{1cm} (4)

where \( S_{ij} \) denote the matrix elements of the \( S \)-matrix and \( V_1 \) and \( V_2 \) are the time derivatives of the \( V_1, V_2 \) given in Eq. 2. For the form of the \( S \)-matrix given in Eq. 3, this is just

\[ Q = \frac{e}{2\pi} \int_0^\tau dt (r^2 \dot{\theta} + t^2 \dot{\phi}) . \] \hspace{1cm} (5)

Thus, the pumped charge is directly related to the amplitudes and phases that appear in the scattering matrix. Note that \( Q \) can also be written in the form of Eq. 1 where the first term is clearly quantised since \( e^{i\theta} \) has to return to itself at the end of the period. So the only possible change in \( \theta \) can be in integral multiples of \( 2\pi \). The second term is the ‘dissipative’ term which prevents the perfect quantisation. It is easy to see the analogy of Eq. 1 with Eq. 19 of Ref. [7].

The form in Eq. 5 also indicates that \( Q \) is quantised whenever either \( r \) or \( t \) is zero throughout the period. When the Fermi energy lies in a gap, \( (t = 0, r = 1) \) the charge is quantised. This is what happens for spatially periodic potentials as discussed in Ref [1,2]. The charge is also quantised when there is total transmission \( (t = 1, r = 0) \) through almost the whole period. This is essentially the case studied in Ref [12], where they find quantised charges whenever the pumping contour encloses almost all of the resonance line.

In the rest of the letter, we compute the transmission and reflection coefficients, the phases and the quantised charges for various cases, and see that the pumped charge is almost quantised even when the number of barriers is quite small. We study the variation of \( Q \) as a function of the number of barriers, as a function of \( E_F \) and as a function of the pumping amplitudes. We also study \( Q \) as a function of the separation \( a \) between the barriers and as a function of the phase difference \( \delta \).

Strictly speaking, to remain within adiabatic approximation under which the Brouwer formula is derived, the energy level spacing in the dots \( \Delta \) has to be larger than the energy scale defined by the frequency of the time-varying parameter \( E_\omega = \hbar \omega \). It is only under this approximation that the snapshot picture of studying the static \( S \)-matrix for different time points within the period is valid. A better approach to go beyond the adiabatic approximation [16,17] is to use the Floquet states. However, here we use the adiabatic approximation even in the continuum limit \( (E_F \geq V_0) \), where the energy levels are almost continuous and \( \Delta \to 0 \), and a few energy levels cross the Fermi level within a period. For sufficiently small \( \omega \), we expect this approximation to still yield qualitatively correct results.

- Single dot case or \( n_b = 2 \) : Here, we compute the scattering matrix for two \( \delta \)-function barriers at a distance \( a \)
Pumped Charge - First Peak

The transmission does not fall to zero after reaching a maximum, does not become small (for a double-barrier system, the Fermi level in one period. Also, since the transmission peak in the small pumped current, occurs at the Fermi level versus $E$ in Fig. 3 for the first and second peaks. Clearly, $Q$ increases with the number of barriers. The first peak reaches quantisation with just $n_b = 6$ whereas the second peak requires $n_b = 9$. The most significant feature here is the step-like structure or plateau structure near integer quantisation. (The quantisation for the first peak can be clearly seen, at 1 for $n_b = 6$, at 2 for $n_b = 10$ and at 3 for $n_b = 14$. For the second peak, we have only gone up to the value of one for $Q$, since it is progressively more cumbersome to go to larger number of barriers. But we have checked that the trend is the same.) For $n_b \rightarrow \infty$, the system would be spatially periodic and perfect quantisation would have been expected. However, what is interesting and unexpected is the formation of plateaux for small values of $n_b$.

![FIG. 2](image)

**FIG. 2.** $Q$ and the average transmission amplitude per period versus $E_F$ for $n_b = 6$ barriers. We have set $V_0 = 1$, $V_p = 0.4$, $\omega = 1$, $a = 4$ and $\delta = \pi/2$.

- **Multiple dot case or $n_b > 2$**: Here, we have computed the $S$-matrix, and obtained the transmission and reflection coefficients, their phases and the pumped charge for $n_b$ ranging from 3 to 14 (2 to 13 quantum dots). For each value of $n_b$, the pumped charge and the average transmission amplitude (obtained by integrating the transmission amplitude over one period and dividing by the period), is plotted as a function of the Fermi energy $E_F$, between $E_F < V_0$ to $E > V_0$. This is shown in Fig. 2 for a typical case ($n_b = 6$). The pumped charge is a maximum just when the transmission rises from zero. Since $E_F \ll V_0$ is the CB limit, which is not the limit we are studying, our main focus is on the charge pumped when $E \sim V_0$ (the second peak in Fig. 2). Peaks at higher values of $E_F$ become progressively smaller. However, we often work with the first peak also for illustrative purposes, since we have not included CB in our formalism.

The magnitude of the (position of maximum as a function of $E_F$) pumped charge as a function of $n_b$ is plotted in Fig. 3 for the first and second peaks. Clearly, $Q$ increases with the number of barriers. The first peak reaches quantisation with just $n_b = 6$ whereas the second peak requires $n_b = 9$. The most significant feature apart. Following Ref. [11], to obtain numerical results, we set $a = 4$ and $\omega = 1$. We find, however, that our results are independent of $\omega$ and hence $\omega$ can be made as small as we wish. Our energy units are set by $\hbar = 2m = k_B = 1$, where $k_B$ is the Boltzmann constant. So for $a = 100A^c$, which is a typical value of the mean free path in GaAs, the energy unit in our system of units is $E = 5.6meV$, which corresponds to a temperature of $T = 65^oK$. With these units, we set $V_0 = 1$ and $V_p = 0.4$. We have also set the phase difference $\delta = \pi/2$ to obtain the maximum pumped charge. Here, we essentially reproduce the results of Wei et al [11]. We have also checked that the peak in the small pumped current, occurs at the Fermi level, when one transmission maxima passes through the Fermi level in one period. Also, since the transmission does not become small (for a double-barrier system, the transmission does not fall to zero after reaching a maximum), there is a large dissipative term in the pumped charge, which explains why the charge pumped is small.

![FIG. 3](image)

**FIG. 3.** $Q$ (in units of $e$) as a function of the number of barriers $n_b$. The top line is for the first peak and the line below is for the second peak. The parameter specifications are the same as for Fig. 2.

![FIG. 4](image)

**FIG. 4.** Transmission and reflection amplitudes ($t$ and $r$) and phases ($\phi$ and $\theta$) and the pumped charge $Q$ as a function of time (for a single period $\tau = 2\pi$) for $n_b = 10$ barriers (left panel) and $n_b = 4$ barriers (right panel). $Q$ is measured in units of $e$ and $\phi$ and $\theta$ in radians.

The correlation of the pumped charge with the values of the phases and amplitudes of the reflection and transmission coefficients is shown in Fig. 4 for a couple of typical cases. In the top left panel, $Q$ is plotted along with the $\theta$ and $\phi$ as a function of time for one full period, for the system with $n_b = 10$. For this system, we know from Fig. 3, that the total pumped charge is (al-
most) quantised at $Q = 2$. From the figure, we see that $\phi$ comes back to itself at the end of one period, but $\theta$ has a discontinuity. It changes by $2 \times 2\pi$ in one period. Thus, the first term in Eq. 1 gives a factor of 2. The criterion for quantisation is that the second term should vanish. The correlation of the quantisation with the (approximate) vanishing of the second term can also be seen by looking at the figure. In the left panel, we note that where the transmission amplitude $t$ is large, both $\theta$ and $\phi$ change very little and almost symmetrically. On the other hand, where $\theta$ and $\phi$ change very rapidly, the amplitude $t$ is very small. In the right panel, for contrast, we have studied $n_b = 4$ where $Q$ is not quantised. We see that the change in $\theta$ is $2\pi$ so that the first term in Eq. 1 gives 1. But here, there are rapid and non-symmetric changes in $\theta$ and $\phi$ when $t$ is large. Hence, here, the second term is non-zero and there is no quantisation of $Q$ near unity. Features similar to the left and right panels are consistently seen whenever there is quantisation and whenever there is no quantisation respectively.

The qualitative features described above do not change when we change the ratio of $V_p$ to $V_0$. In fact, as $V_p/V_0$ increases, we find that the value of $Q$ and the tendency towards quantisation increases. This is seen in Fig. 5. We have also checked that $Q$ is periodic in the separation $a$ (shown as inset in Fig. 6.). In the weak pumping limit, as the amplitude $V_p$ is sufficiently small, we expect the charge pumped to be proportional to $\sin \delta$ [6], but as $V_p$ increases, the sinusoidal shape is expected to be distorted. This feature is seen in Fig. 6. For $V_p \sim 0.05$, the dependence on $\delta$ is sinusoidal, but here $Q$ is quite small. As $V_p$ increases, $Q$ increases, but there is also an increasing distortion of the sinusoidal shape.

To summarise, in this letter, we have shown that the pumped charge shows an interesting step-like behaviour as we increase the number of dots through which the charge is pumped and also as we increase the pumping amplitude. We have derived and demonstrated the relation between $Q$ and the transmission and reflection coefficients of the effective $S$-matrix. $Q$ is quantised whenever the contribution from the transmission amplitude vanishes - i.e., whenever there is no dissipation. The main point of this letter is to emphasize that this can occur due to quantum interference, even for transmission through a few (4-6) dots and not only for an infinite spatially periodic system. The experimentally testable prediction here is that the pumped charge increases as the number of barriers through which is transmitted increases, and reaches quantisation with a few barriers.

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\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig5.png}
\caption{FIG. 5. $Q$ as a function of the amplitude $V_p$ of the time-varying potential for different $n_b$.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig6.png}
\caption{FIG. 6. Pumped charge as a function of the phase difference $\delta$ for $n_b = 6$ barriers. The inset shows it as a function of the separation $a$ between barriers.}
\end{figure}

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