Non-adiabatic charge pump: an exact solution

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We derived a general and exact expression of current for quantum parametric charge pumps in the non-adiabatic regime at finite pumping frequency and finite driving amplitude. The non-perturbative theory predicts a remarkable plateau structure in the pumped current due to multi-photon assisted processes in a double-barrier quantum well pump involving only a single pumping potential. It also predicts a current reversal as the resonant level of the pump crosses the Fermi energy of the leads.

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Parametric charge pump is a device that drives the flow of a DC electric current by a time dependent variation of two or more device parameters. The quantum parametric pump has received considerable attention both experimentally and theoretically. A very useful and clear transport theory on quantum parametric pump was provided by Brouwer\textsuperscript{2,3} for the adiabatic regime, \textit{i.e.} in the $\omega \to 0$ limit, where $\omega$ is the frequency of driving force of the pump. Since then there have been several attempts devoted towards the understanding of parametric pumping at finite frequency, \textit{i.e.} for the more general non-adiabatic regime. These theories were all based perturbative schemes either in terms of pumping frequency or in pumping amplitude. Recently, a Floquet scattering matrix theory was developed\textsuperscript{12} and an exact solution obtained for an oscillating double-barrier pump structure. Despite the progress, so far a general and non-perturbative theory for quantum parametric pump has not been reported. Such a theory will be very important to establish a general and unambiguous physical picture of quantum charge pumps for the non-adiabatic regime, and provide new features not accessible by perturbative theories. It is the purpose of this Letter to present the exact solution for the current delivered by a quantum parametric pump at \textit{both} finite driving frequency and amplitude.

Our theory is based on Keldysh non-equilibrium Green’s functions (NEGF)\textsuperscript{13} and is non-perturbative. It reproduces not only all previous theories in their perspective limits, but also reveals qualitative new and interesting transport properties of quantum parametric pump. Our theory is also applicable to the case where the driving potential is in the interior of the pump. Because of the generality of our theory, it is now possible to investigate situations beyond the established physics of adiabatic pump. As an example, we investigate a peculiar case of a quantum-well charge pump driven by only a single parameter: such a pump is only possible in the non-adiabatic regime. In particular, if the pumping potential is located at the barriers of the quantum well, the pumped current exhibits remarkable plateaus due to a multi-photon assisted pumping process. The width of the plateaus is determined by $\hbar \omega$ while their height vary depending on the pumping amplitude and the coupling strength between the pump and the leads. By tuning a gate voltage, the resonant level of the quantum well crosses Fermi energy of the leads and a pumped current reversal is observed. On the other hand, if the pumping potential is at the center point of the quantum well, due to the spatial symmetry the pumped current vanishes exactly. Moving away from this symmetric point, the pumped current increases rapidly by several orders of magnitude and similar plateaus in pumped current are observed.

Now we derive the pumped current in the non-adiabatic regime. Assuming that the time-dependent driving potential has the following form $H(t) = (V/2) \exp(i\omega t_1) + (V^* /2) \exp(-i\omega t_1)$ where $V$ is the effective pumping potential profile. Neglecting interaction between electrons in the ideal leads labeled by $L$ and $R$, we start from the expression of time averaged current in standard NEGF theory,

$$I_{\alpha} = -\frac{q}{\tau} \int_0^\tau dt \int dt_1 \text{Tr}[G^\alpha(t, t_1) \Sigma_{\alpha}^{<}(t_1, t) + G^\alpha(t, t_1) \Sigma_{\alpha}^{>}(t_1, t) + c.c.]$$

(1)

where $\tau = 2\pi / \omega$ is the period of pumping cycle. Using the following double time Fourier transform

$$G^\alpha(t_1, t_2) = \int \frac{dE_1}{2\pi} \int \frac{dE_2}{2\pi} e^{-iE_1t_1+iE_2t_2} G^\alpha(E_1, E_2)$$

(2)

with $\gamma = r, a, <$, Eq.(1) becomes,

$$I_{\alpha} = -\frac{q}{2N\tau} \int \frac{dE_1}{2\pi} \int \frac{dE_2}{2\pi} \text{Tr}[(G^\alpha(E_1, E_2) - G^a(E_1, E_2)) \Sigma_{\alpha}^{<}(E_2, E_1) + G^{<}(E_2, E_1) \Sigma^{>}_{\alpha}(E_2, E_1) - \Sigma^{<}_{\alpha}(E_2, E_1) \Sigma^{>}_{\alpha}(E_2, E_1)]$$

(3)

where we have extended the integration range for $dt$ in Eq.(1) to $[-N\tau, N\tau]$ with $N > \infty$. Note that in Eq.(3), the matrix $G^{\alpha}$ has element $G^{\alpha}(E_1, E_2)$. It is also easy to show that $G^\alpha - G^a = -iG^\alpha T G^\alpha$. Using the fact that $G^{<} = G^2 \Sigma^< G^a$ and $\Sigma^{<}(E_2, E_1) = 2\pi \delta(E_1 - E_2) \Sigma^<(E_1)$ (no external bias), we obtain
\[ I_\alpha = \frac{q}{2N\tau} \int \frac{dE_1 dE_2}{2\pi} \text{Tr} [\Gamma_\alpha(E_1)G^r(E_1, E_2) \Gamma(E_2)G^a(E_2, E_1)] (f(E_2) - f(E_1)) \]
\[ \Gamma_n(E)G^a(E + n\omega) = \Gamma_n(E)G^a(E + n\omega, E) (f_n(E) - f(E)) \]

Using the identity
\[ \sum_{n = -\infty}^{+\infty} = 2N\tau \int dE/(2\pi) \]
we finally arrive at
\[ I_\alpha = \frac{q}{(2N\tau)^2} \int \frac{dE}{2\pi} \sum_{n = -\infty}^{+\infty} \text{Tr} [\Gamma_\alpha(E)G^r(E, E + n\omega) \Gamma_n(E)G^a(E + n\omega, E)] (f_n(E) - f(E)) \]

where \( \Gamma_n(E) = \Gamma(E + n\omega) \) and \( f_n(E) = f(E + n\omega) \).

From the Dyson equation, we have
\[ G^r(t, t') = G^{\alpha r}(t, t') + \int G^r(t, t_1)H'(t_1)G^{\alpha r}(t_1, t')dt_1 \]

where \( G^{\alpha r} \) is the equilibrium Green’s function. Taking a double-time Fourier transform of Eq.\((7)\), we find
\[ G^r(E_1, E_2) = 2\pi G^{\alpha r}(E_1)\delta(E_1 - E_2) + \int \frac{dE}{2\pi} G^r(E_1, E_2 + E)H'(E)G^{\alpha r}(E_2) \]

Since \( H'(E) = \pi[V\delta(E + \omega) + V^*\delta(E - \omega)] \), we obtain
\[ G^r(E_1, E_2) = 2\pi G^{\alpha r}(E_1)\delta(E_1 - E_2) + [G^r(E_1, E_2 - \omega)V + G^r(E_1, E_2 + \omega)V^*]G^{\alpha r}(E_2)/2 \]

Using this equation, the general expression of \( G^r(E, E + n\omega) \) can be obtained. To simplify notation, we use the following abbreviations \( G_n^r(E) \equiv G^r(E, E + n\omega) \) and \( G_n^{\alpha r}(E) \equiv G^{\alpha r}(E + n\omega) \). We then have
\[ G_0^r = 2\pi G_0^{\alpha r}\delta(0) + (G_1^rV^* + G_{-1}^rV)G_0^{\alpha r}/2 \]
\[ G_1^r = (G_2^rV^* + G_0^rV)G_2^{\alpha r}/2 \]
\[ G_{-1}^r = (G_0^rV^* + G_{-2}^rV)G_{-1}^{\alpha r}/2 \]

If we restrict ourselves for single photon process only, we can neglect \( G_2^r \) in Eq.\((10)\) and obtain
\[ G_0^r(E) = \frac{2\pi\delta(0)}{[G_0^{\alpha r}(E)]^{-1} - \Sigma_1(E)} \]

where \( 2\pi\delta(0) = \int dE = 2N\tau \). Here the self-energy \( \Sigma_1(E) = \pi(VG_0^{\alpha r}V^* + V^*G_0^{\alpha r}V)/4 \).

The exact solution of \( G_n^r \) by including all photon processes can be obtained by iterating the following equation obtained from Eq.\((10)\),
\[ G_n^r = (G_{n+1}^rV^* + G_{n-1}^rV)G_n^{0\alpha r}/2 \]
we obtain
\[ G_n^r = G_{n, -1}V G_n^{0\alpha r} \frac{1}{2\alpha_n} \]
where \( \alpha_n^r = [(a_n, \bar{a}_n), (a_{n+1}, \bar{a}_{n+1}),...] \) with \( a_n = iV G_{n+1}^{0\alpha r}/2 \) and \( \bar{a}_n = iV^* G_{n-1}^{0\alpha r}/2 \). The continued fraction \([(a_1, \bar{a}_1), (a_2, \bar{a}_2),...] \) is defined as
\[ [(a_1, \bar{a}_1), (a_2, \bar{a}_2),...] = 1 + a_1 + \frac{1}{\bar{a}_1 + \frac{1}{a_2 + \frac{1}{\bar{a}_2 + \ldots}}} \]

From Eq.\((13)\), we obtain \( G_1^r = G_0^r V G_1^{0\alpha r}/(2\alpha_1^r) \) and \( G_{-1}^r = G_0^r V G_{-1}^{0\alpha r}/(2\beta_{-1}^r) \). Here \( \beta_{-1}^r = [(b_{-n}, \bar{b}_{-n}), (b_{n-1}, \bar{b}_{n-1}),...] \) with \( b_{-n} = iV G_{n-1}^{0\alpha r}/2 \) and \( \bar{b}_{-n} = iV G_{n-1}^{0\alpha r}/2 \).

Substituting the expressions of \( G_{\pm 1}^r \) into Eq.\((10)\), we have
\[ G_0^r(E) = \frac{2\pi\delta(0)}{[G_0^{\alpha r}(E)]^{-1} - \Sigma(E)} \]
with
\[ \Sigma(E) = VG_0^{0\alpha r}V^* + V^*G_{-1}^{0\alpha r} \frac{1}{2\beta_{-1}^r} \]

Once \( G_1^r \) is obtained, \( G_n^r \) can be calculated recursively from Eq.\((13)\). Eqs.\((11)\), \((12)\), \((13)\) and \((14)\) form the central result of this paper. Note that \( G_n^{0\alpha r} \) is the Green’s function for the process of absorbing (emitting) n-photons whereas \( G_n^r \) is the renormalized n-photon Green’s function containing the contribution of multi-photon process. From Eq.\((13)\), we see that \( G_n^r \) is at least of the order of \( V^n \). For this reason, as we will see below that in the resonant tunneling regime, the summation in Eq.\((10)\) converges rapidly even in the strong pumping regime. Using the fact that \( G^* \Gamma G = G^* \Gamma G \), it is easy to show \( \sum_\alpha I_\alpha = 0 \), i.e., current conservation for parametric pumping.

Eq.\((10)\) reproduces all previously known results of parametric pumping. We give two examples here. First, in Ref.\((1)\) the pumped current is obtained using perturbation theory for finite pumping frequency up to the second order in pumping amplitude\((13)\). This result is recovered by only keeping the terms \( n = \pm 1 \) in Eq.\((10)\) to obtain \( G_1^r = G_0^r V G_1^{0\alpha r}/2 \). Hence Eq.\((10)\) becomes,
\[ I_\alpha = q \int \frac{dE}{8\pi} \sum_{n = \pm 1} \text{Tr} [\Gamma_\alpha G_0^{0\alpha r} V G_{n+1}^{0\alpha r} G_{n}^{0\alpha r} G_{n}^{0\alpha r} V^* G_{n}^{0\alpha r} f_n - f) \]

which is exactly the same as that of Ref.\((1), (3)\). Second, we consider the well-studied adiabatic regime \( \omega \to 0 \) where the instantaneous approximation for the Green’s function is appropriate. We transform Eq.\((10)\) to the Wigner representation using
\[ G^\gamma(t_1, t_2) = \int \frac{dE}{2\pi} e^{-iE(t_1 - t_2)} G^\gamma(E, T) \]
where \( T = (t_1 + t_2)/2 \) and \( G^\dagger \) is the NEGF in the Wigner representation. We then have
\[
G^a_n = \int dT G^r(E, T) e^{-i\omega T}
\] (19)
Substituting Eq. (19) into Eq. (8) and keep only the \( O(\omega) \) term, we obtain
\[
I_a = \frac{q}{(2\pi)^2} \int \frac{dE}{2\pi} \int_{-\infty}^{+\infty} dT dT' \sum_{n=0}^{+\infty} n\omega \text{Tr} [\Gamma_\alpha(E)] G^r(E, T') \exp(-i\omega(T - T')) \partial_E f(E)
\] (20)
Note that
\[
\int dT \sum_{n=0}^{+\infty} n\omega G^r(E, T) \exp(-i\omega(T - T')) = -2iN\tau \partial_T G^r(E, T')
\] (21)
where we have used Eq. (8). Eq. (20) now becomes,
\[
I_a = \frac{-iq}{\tau} \int_0^{\infty} dT \int \frac{dE}{2\pi} \text{Tr} [\Gamma_\alpha \partial_T G^r(T) \Gamma G^a(T)] \partial_E f(E)
\] (22)
this is exactly the Brouwer's formula \([2] \) for adiabatic pumping.

In the following we calculate pumped current using Eq. (8) for a symmetric double \( \delta \)-barrier structure given by \( U(x) = V_0 \delta(x + a) + V_0 \delta(x - a) \). For this system, the Green's function \( G(x, x') \) can be calculated exactly \( [3] \). In the adiabatic theory, two pumping potentials are needed in order to give a nonzero pumping current. At finite frequency, a single pumping potential was reported to be enough to pump a current \([3] \), which is peculiar, and our exact non-perturbative theory derived above allows us to investigate this situation clearly and unambiguously.

We chose the single pumping potential to be sinusoidal \( V(x, t) = V_p \cos(\omega t) \delta(x - x_0) \), and we calculate pumped current from the left lead at zero temperature and set \( V_0 = 200 \) unless specified otherwise. A gate voltage \( v_g \) is applied to the double barrier structure so that the resonant single particle energy level is controlled by it. We fix the Fermi level of leads in line with the resonant level at \( v_g = 0 \). Finally, the unit is set by \( h = 2m = q = 2a = 1 \).

For GaAs material with well width \( a = 1000 \text{ Å} \), the energy unit is \( E = 0.056 \text{ meV} \) which corresponds to \( \omega = 13.2 \text{ GHz} \). The unit for pumped current is \( 5 \times 10^{-10} \text{ A} \).

Fig.1 shows the pumped current versus the gate voltage in the strong pumping regime for \( x_0 = -a \), \( V_p = 160 \), and \( \omega = 1 \). Following observations are in order. (1) The pumped current displays a series of remarkable plateaus. The width of a plateau is equal to \( \hbar \omega \) whereas the height of the plateau depends on \( V_p \) and \( V_0 \) in a nonlinear fashion. (2) The pumped current reverses its direction when the resonant level across the Fermi level of the lead, i.e., when \( v_g \) changes sign. As a result, we see from Fig.1 that the pumped current is quenched near \( v_g = 0 \). (3) The height of the current plateaus for negative \( v_g \) is considerably larger than those of positive \( v_g \). To understand these results, we rewrite Eq. (12) as
\[
I_L = q \int \frac{dE}{2\pi} \sum_{n=1}^{+\infty} F_n(E)(f_n(E) - f(E))
\] (23)
with
\[
F_n(E) = \frac{q}{(2\pi)^2} \text{Tr} [\Gamma_L(E)G^r(E, E + n\omega) \Gamma_n(E)]
\]
\[
G^a(E + n\omega, E) - \Gamma_n(E)G^r(E + n\omega, E)
\]
\[
\Gamma(E)G^a(E, E + n\omega)
\] (24)
We notice that kernel \( F_n \) consists of two terms: one due to photon absorption process [1] and the other to photon emission process. These two contributions differ by a sign indicating the competition between the photon absorption and emission processes similar to that discussed in Ref. [1]. In Fig.2 we plot the integrand of Eq. (23), \( F_n(E) \), for \( n = 1, 2, 3 \) (solid line, dotted line, dashed line, respectively). The sidebands due to photon absorption (when \( v_g < 0 \) and photon emission are clearly seen (for an \( n \)-photon emission process, the energy has been shifted by \( n\omega \) due to the transformation from Eq. (8) to Eq. (23)). To obtain pumped current, one integrates these sidebands over energy. For the \( n \)-th sideband (\( n > 0 \)), the integral range is \([v_g - n\omega, v_g]\) it is therefore clear that the plateau structure is a direct result of multi-photon assisted processes. The positive current is due to photon absorption processes and the current reverses its sign if photon emission process dominates. The behavior of current reversal has been observed before for pumping in Carbon nanotube [3] charge quantization, [4] and heat current generated during the pumping [5], although from completely different origins. Due to the energy dependence of coupling between the pump and the leads, the sideband is asymmetric with a larger peak for photon absorption process. As a result, the height of the current plateau is larger for photon absorption process. Our numerical plots show that this plateau structure persists for different frequencies and pumping amplitudes. Our analysis show that there are two effects which affect the current plateau structure. The first is barrier heights of the quantum well: current plateaus can only be observed in the strong tunneling regime and they disappear for low barrier height. The second is temperature: the plateau structure is rounded off at finite temperature and destroyed when temperature reaches \( \sim 200 \text{ mK} \) for \( \omega = 10 \text{ GHz} \).

When the pumping potential is inside of the double-barrier structure, we found a similar plateau structure due to the same photon assisted processes. In Fig.3, the pumped current as a function of pumping position \( x_0 \) is plotted at a fixed \( v_g = -0.67 \) for a much smaller pumping amplitude \( v_p = 6 \). We observe that the pumped current \( I_p \) is antisymmetric about the center of the pump. As expected for a symmetric structure, \( I_p \) vanishes identically.
at $x_0 = 0$. At $x_0 = -0.5$, we found $I_p = 2 \times 10^{-6}$. Fig. 3 shows that $I_p$ can increase by three orders of magnitude by varying the position of the pumping potential away from the barriers.

In summary, we have derived a non-perturbative and exact current expression for parametric pumping at finite frequency and finite pumping amplitude. This theory can also account for the case of pumping potential located in the interior of the scattering region. Our theory reproduces all previously known results in both adiabatic regime and in perturbative theory. For a double-barrier quantum well pump, we predicted current plateaus to appear due to multi-photon assisted processes with the plateau width given by the pumping frequency. As the gate voltage is varied and the resonance level sweeps through the Fermi energy of leads, the pumped current is found to reverse its direction.

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