Theory of one-dimensional double-barrier quantum pump in two-frequency signal regime

M. M. Mahmodian(a) and M. V. Entin(b)

Institute of Semiconductor Physics, Siberian Division, Russian Academy of Sciences - Novosibirsk, 630090 Russia

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Abstract – A one-dimensional quantum pump with oscillating double δ-like barriers/wells is studied. We assume that the oscillations contain two frequencies ω and 2ω. The alternating signal leads to the direct current across the structure even in a symmetric system. The properties of this quantum pump are studied in a wide range of the system parameters.

Introduction. – The quantum pump is a microscopic device with two or more contacts in which periodically changing inner potential produces a stationary current. Quantum pumps were the subject of many recent papers (for example, [1–7]). The macroscopic analogue of quantum pumps is the photogalvanic (photovoltaic) effect studied in detail in the last decades [8–12]. A considerable number of papers on quantum pumps were dedicated to analytically solvable, adiabatic approach [3,4]. Just this approach results in the quantization of charge transport [5].

The directed flow of particles is a general property of systems with no inversion symmetry subjected to external force with zero mean. This effect was multiply studied in the last decade both in classical and quantum systems, see, for example, [13–16].

In the recent papers [6,7] we have carried out an extensive study of the simplest model of the one-dimensional quantum pump, containing two delta-like harmonically oscillating barriers/wells. This model demonstrates a rich behavior which is ruled by a variety of system parameters.

The present paper deals with a similar system, namely a quantum wire with two narrow gates, to which alternating bi-chromatic voltages are applied. The stationary bias between the source and the drain is supposedly absent. The considered model is described by a one-dimensional time-dependent potential:

\[ U(x, t) = (u_{11} \sin \omega t + u_{12} \sin 2\omega t) \delta(x + d) + (u_{21} \sin \omega t + u_{22} \sin 2\omega t) \delta(x - d). \] (1)

In particular, this model appears in the problem of optical heterodyning when it is necessary to stabilize a 2ω optical source by means of an ω standard source.

To produce a stationary current both spatial and time irreversibility of the system are needed. This asymmetry is provided by the presence of two frequencies and two barriers. In fact, the time dependence of the barrier height distinguishes the direction t and −t and the difference of the barriers marks the specific spatial direction.

The system under consideration has an even richer variety of regimes of the pump operation, depending on the system parameters, e.g. frequency and amplitudes, than the single-frequency case. The effect is sensitive to the phase coherence of alternating signals and can exist even in the symmetric systems. The stationary current is possible also in the case of different amplitudes of alternating fields.

If \( u_{12} = u_{22} = 0 \) or \( u_{11} = u_{21} = 0 \), the problem reduces to harmonic voltages studied before. If \( u_{12} = u_{21} = 0 \) or \( u_{11} = u_{22} = 0 \) the current is determined by the asymmetry of the external signal rather than the asymmetry of the static system. To some extent this limit is an analogue of the coherent photovoltaic effect [17], namely the appearance of a stationary current in a homogeneous medium under illumination by two intercoherent light sources with frequencies ω and 2ω. (A similar effect, caused by a random or deterministic external field with non-zero odd means was studied in [16].)

The adiabatic pump corresponds to the low-frequency (\( \omega \to 0 \)) limit. In the adiabatic regime the charge transfer per cycle is proportional to some integral over the area covered by two parameters in the phase space [3]. In our case the parameters are coefficients of delta-functions.
\{u_1(t), u_2(t)\}. We shall concentrate on the case when \(u_1(t) \propto u_2(t)\), so that they cover in the phase plane \(\{u_1(t), u_2(t)\}\) a close loop, namely, a cut, with zero area. Hence, the current vanishes and the considered case lies beyond the limits of the adiabatic approach.

We study the system both analytically, basing on the perturbational consideration, and numerically, if the alternating voltage is strong.

**Basic equations.** The solution to the Schrödinger equation with the potential (1) is searched in the form

\[
\psi = \sum_n e^{-i(E + n\omega)t} \left\{ \begin{array}{ll}
\delta_n e^{-\frac{i p_n x}{\hbar}} + r_n e^{-\frac{i p_n x}{\hbar}}, & x < -d, \\
\delta_n e^{\frac{i p_n x}{\hbar}} + b_n e^{\frac{i p_n x}{\hbar}} - i u_1 e^{-\frac{i p_n x}{\hbar}}, & x < d, \\
\gamma_n e^{\frac{i p_n x}{\hbar}}, & x > d.
\end{array} \right.
\]

Here \(2d\) is the distance between \(\delta\)-barriers (wells), \(p_n = \sqrt{p^2 + n^2}\omega^2\) and \(p = \sqrt{E}\), quantities \(u_{ij}\) are measured in units of \(\hbar/m d\) (\(m\) is the electron mass), \(p, E, \) and \(\omega\) are the energy, energy, and frequency measured in units of \(\hbar/d, h^2/2m d^2,\) and \(h/2m d^2\), respectively. The wave function eq. (2) corresponds to the wave incident on the barrier from the left. (In the final formulas, we mark the directions of the incident waves by indices “\(+\)” and “\(-\)”.) The form of solution eq. (2) corresponds to absorption (for \(n > 0\)) or emission (\(n < 0\)) of \(n\) field quanta by an electron after interaction with the vibrating barriers; \(n = 0\) relates to the elastic process. Quantities \(t_n\) and \(r_n\) give the corresponding amplitudes of transmission (reflection). If the value of \(p_n\) becomes imaginary, the waves moving away from the barriers should be treated as damped waves, so that \(\text{Im} p_n > 0\).

The transmission amplitudes obey the equations:

\[
t_n = e^{-i(p + p_n)} T_n, \quad u_{12} u_{22} g_{n-2} T_{n-2} - (u_{12} u_{21} g_{n-2} + i u_{11} u_{22} g_{n-2}) T_{n-3} - i u_{12} e^{-2ip_n} - u_{11} u_{21} g_{n-1} + i u_{22} e^{-2ip_n} + u_{11} u_{22} g_{n+1}) T_{n-1} - (u_{11} u_{21} (g_{n-1} + g_{n+1}) + u_{12} u_{22} (g_{n-2} + g_{n+2}) - 2ip_n e^{-2ip_n} T_n - (u_{12} u_{21} g_{n+2} - i u_{11} e^{-2ip_n} - i u_{21} e^{-2ip_n} + (i u_{12} e^{-2ip_n} + u_{11} u_{22} g_{n-1} + u_{12} u_{22} g_{n+2}) T_{n+1} + (u_{12} u_{21} g_{n+2} + u_{11} u_{22} g_{n+1}) T_{n+3} + u_{12} u_{22} g_{n+2} T_{n+4} - 2ip\delta_{n,0}. (3)
\]

Here, \(g_n = \sin 2p_n/p_n\). The equations for transmission amplitudes \(T_n\) are obtained from eqs. (3) by replacing \(u_{11} \leftrightarrow u_{21}\) and \(u_{12} \leftrightarrow u_{22}\).

Provided that electrons from the right and left of the pump are in equilibrium, and that they have identical chemical potentials \(\mu\), the stationary current is

\[
J = \frac{e}{\pi \hbar} \int dE \sum_n (|T_n|^2 - |T_n|^2) f(E)\theta(E + n\omega), \quad (4)
\]

where \(f(E)\) is the Fermi distribution function, and \(\theta(x)\) is the Heaviside step function. The current is determined by the transmission coefficients with real \(p_n\) only.

At a low temperature, it is convenient to differentiate the current with respect to the chemical potential:

\[
G = \frac{\partial}{\partial \mu} J = G_0 \sum_n \theta(\mu + n\omega)(|T_n|^2 - |T_n|^2)_{p = p_F}. \quad (5)
\]

Here \(G_0 = e^2/\pi \hbar\) is the conductance quantum and \(p_F\) is the Fermi momentum. The resultant quantity \(G\) can be treated as a two-terminal photoconductance (the conductance for simultaneous change of the chemical potentials of source and drain).

**Theory of perturbations.** In the low-amplitude limit the stationary current (its derivative \(G\)) is proportional to \(G \propto A_1 u_1 u_2 + A_2 u_2 u_2\). This behavior corresponds to the coherent photovoltaic effect [17].

Let us consider the case of a symmetric system with \(u_{11} = -u_{21} = u_w, u_{12} = -u_{22} = u_{2w}\). The system symmetry leads to the dependence \(G \propto u_2^2 u_{2w}\). This follows from the replacement \(u_w \rightarrow -u_w\) and \(u_{2w} \rightarrow -u_{2w}\) that exchanges the expressions for the transmission amplitudes \(T_n^+\) and \(T_n^-\). The contributions to \(T_n\) which do not change by such replacement subtract each other in the stationary current. The main contribution to the current arises from the terms in \(T_n\) that change sign by this replacement and hence is proportional to \(u_2^2 u_{2w}\), namely from the corresponding terms in the transmission coefficients \(T_0, T_{\pm 1}, T_{\pm 2}^+\):

\[
T_0 \propto 1 + A_0 u_2^2 u_{2w}, \quad T_{\pm 1} \propto A_{\pm 1} u_w + B_{\pm 1} u_w u_{2w}, \quad T_{\pm 2} \propto A_{\pm 2} u_w^2 + B_{\pm 2} u_{2w}, \quad (6)
\]

where \(A_0, A_{\pm 1}, B_{\pm 1}, A_{\pm 2}, B_{\pm 2}\) are some coefficients, depending on \(\omega\) and \(p\). Taking into account eqs. (6), we obtain

\[
G = 4G_0 u_2^2 u_{2w} \text{Re} [A_0 + A_{\pm 1} B_{\pm 1}^* + A_{\pm 2} B_{\pm 2}^*]. \quad (7)
\]

Substituting the quantities \(A_0, A_{\pm 1}, B_{\pm 1}, A_{\pm 2}, B_{\pm 2}\), we have

\(\text{see eq. (8)}\).

The expression eq. (8) tends to infinity at \(p_{-1} = 0\) and \(p_{-2} = 0\) (the threshold of emission of one and two photons) like \(1/p_{-1}, 1/p_{-2}\). This divergence is conditioned by the density of states characteristic for the one-dimensional system. However, applicability of the perturbations theory is violated near the threshold points \(p_{-1} = 0\) and \(p_{-2} = 0\).

The divergent behavior is limited by accounting for the finite amplitude of the alternating signal. In particular, the threshold singularity of \(G\) at \(p_{-1} = 0\) arises from \(T_{-1}\) and \(T_0\). To find the correct dependence near \(p_{-1} = 0\), we took the most singular equations (3) for \(n = 0\) and \(n = -1, 67002-p2\).
\[ G = G_0 u_2^2 u_{2\omega} \left\{ \frac{1}{\mathcal{P}^2 \mathcal{P}_2^2} \left( (p - 2p_2) p_1 \sin 2p_1 - (p - 2p_1) p_2 \sin 2p_2 \right) \sin 2p - \mu (p_1 - p_2) \sin 2p_1 \sin 2p_2 \right\} + \theta(\omega - \mu) \left( p - 2p_1 \right) \left( e^{-2|p_1| - \cos 2p_1} \sin 2p - \mu (p_1 - p_2) \sin 2p_1 \sin 2p_2 \right) \]
\[ \times \left( p - 2p_1 \right) \left( e^{-2|p_1| - \cos 2p_1} \sin 2p - \mu (p_1 - p_2) \sin 2p_1 \sin 2p_2 \right) \]
\[ + \frac{\theta(\mu - \omega)}{|p - 2p_1|^2} \left( p - 2p_1 \right) \left( e^{-2|p_1| - \cos 2p_1} \sin 2p - \mu (p_1 - p_2) \sin 2p_1 \sin 2p_2 \right) \]
\[ + \frac{\theta(\mu - \omega)}{|p - 2p_1|^2} \left( (p - 2p_1) p_1 \sin 2p_1 - (p - 2p_1) p_2 \sin 2p_2 \right) \sin 2p + \mu (p_1 - p_2) \sin 2p_1 \sin 2p_2 \]
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Fig. 2: The dependence of $G$ on frequency for antipodal voltages $u_{11} = u_{12} = 1$, $u_{21} = u_{22} = -1$, $p_F = \sqrt{0.5}$.

Fig. 3: The value of $G$ vs. the Fermi momentum. Here $\omega = 2$, $u_{21} = u_{22} = -1$, $u_{11} = u_{12} = 1$ (solid curve) and $2$ (dashed curve). The delta-functions oscillate from well to barrier values in antiphase. The curves differ from each other by the asymmetry of oscillations. The minimum of the solid curve $G = -10.5$ goes out of the boundaries.

Fig. 4: $G$ vs. the Fermi momentum for large frequency $\omega = 50$ and different $u_{11} = u_{12}$. Here $u_{21} = u_{22} = -1$. The singularity corresponds to the single-photon threshold $p_F = \sqrt{\omega}$.

Fig. 5: The dependence of $G$ on the amplitudes $u_{11} = u_{12} = -u_{21} = -u_{22}$ for $p_F = \sqrt{0.5}$ and different small frequencies. Insert: the threshold resonance case $\omega = 0.5 = p_F^2$. For $u_{ij} \to 0$, $G \propto 1/u_{11}$.

Harmonic signals only (if $u_{11} = -u_{21} \neq 0$, $u_{12} = u_{22} = 0$ or $u_{11} = u_{21} = 0$, $u_{12} = -u_{22} \neq 0$) [6].

Figure 1 illustrates the perturbative regime. The main figure, calculated with use of eqs. (8), contains peaks caused by the threshold singularities in the points $\omega = p_F^2$ and $\omega = p_F^2/2$. The exact dependence of $G$ on $\omega$ (found according to eqs. (3)) contains the threshold singularities in all points $\omega = p_F^2/n$. They are shown for the domain of lower frequencies in the left insert to the figure. The singularities exponentially decay for large numbers $n$ (small $\omega$) that corresponds to their multi-photon nature.

The region of low frequency corresponds to the adiabatic approximation, which is commonly used for consideration of quantum pumps. In accord with what said above, fig. 1 shows the decay of the current with the decrease of frequency. At the same time, the finite value of the current results from the absence of exact adiabaticity.

The right insert to fig. 1 depicts the neighborhood of the singularity $\omega = p_F^2$ and its smoothing by a finite value of the alternating voltage according to exact eqs. (3) or approximate eqs. (9) (see also insert to fig. 5).

The frequency dependence of $G$ for larger voltages is depicted in fig. 2. The oscillations of $G$ are condensed near zero frequency $\omega$ in accordance with the formula $\omega = p_F^2/n$. The complicated structure of $G$ in the low-frequency region is explained by overlapped multi-photon resonances which reduce with $n$.

Figure 3 shows the dependence of $G$ on the Fermi momentum $p_F$. The current oscillates with the Fermi momentum due to the interference of the electron waves in the structure. Besides, the current possesses singularities caused by the resonances with the zero-energy state and their photon repetitions. The value of $G$ vanishes at zero momentum. The singularities at $p_F = \sqrt{\omega}$ grow with the amplitude. The dashed curve in fig. 3 differs from the solid...
The density of states and are conditioned by the high-order processes when an electron occurs at the bottom of the permitted band after emission of one or many photons of alternating field. They are partly smoothed by the finite value of the alternating voltage. This process can be described as a two-level mixing by alternating field where one is the initial electron state and the other is the state of the electron at the bottom. Together with the real processes of emission, the virtual processes play a role in the appearance of weak singularities below the thresholds.

The case of in-phase alternating field gives zero current in the strict adiabatic approximation. The found current in the low-frequency limit lies beyond the adiabatic case.

The current has oscillatory behavior as a function not only of the Fermi momentum and voltage frequency, but also as a function of voltage values. The latter corresponds to the similar behavior of transition amplitudes for the simpler problem of a single vibrating delta-functional potential.

Let us discuss the role of dissipation. The system under consideration is open, so the dissipation in contacts is immanently present in the system. This differentiates the present problem from a problem about a particle driven by a periodic homogeneous force in a periodic lattice, considered in the theory of the photogalvanic effect [8–11], where the stationary flow results from momentum non-conservation in scattering processes. (A similar process in a spatially periodic system [15] is conditioned by the frictional character of velocity noise; the same system driven by a homogeneous periodic external field obviously exhibits no stationary flow.) Yet the dissipation is not essential in the transition probability through a small device (and hence transport coefficients do not depend on relaxation constants). In most cases it is so while the transit time stays less than the relaxation time, even if the frequency is comparable with the electron energy. Nevertheless, the dissipation can smooth away tiny peculiarities of dependencies.

\[ G \propto u_{11} \]

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![Fig. 6: The dependence of $\mathcal{G}$ on the amplitudes $u_{11} = u_{12} = -u_{21} = -u_{22}$ (antipodal voltages like in fig. 3 (solid curve)) for $p_F = \sqrt{\omega}$ and different signal frequencies. For $u_{ij} \to 0$, $\mathcal{G} \propto u_{11}$.](image)
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