Quantum pumping with adiabatically modulated barriers in graphene

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Abstract

We study the adiabatic quantum pumping characteristics in the graphene modulated by two oscillating gate potentials out of phase. The angular and energy dependence of the pumped current is presented. The direction of the pumped current can be reversed when a high barrier demonstrates stronger transparency than a low one, which results from the Klein paradox. The underlying physics of the pumping process is illuminated.

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Generally speaking, the transport of matter from low potential to high potential excited by absorbing energy from the environment can be described as a pump process. Its counterpart in quantum mechanics involves coherent tunneling and quantum interference. Since the experimental realization of the quantum pump, research on quantum charge and spin pumping has attracted increasing interest. The current and noise properties in various quantum pump structures and devices were investigated such as the magnetic-barrier-modulated two dimensional electron gas, mesoscopic one-dimensional wire, quantum-dot structures, mesoscopic rings with Aharonov-Casher and Aharonov-Bohm effect, magnetic tunnel junctions. Correspondingly, theoretical techniques have been put forward for the treatment of the quantum pumps [Refs.(2, 3, 18) and references therein]. One of the most prominent is the scattering matrix approach for ac transport, as detailed by Moskalets et al. who derived general expressions for the pump current, heat flow, and the shot noise for an adiabatically driven quantum pumps in the weak pumping limit. The pump current was found to vary in a sinusoidal manner as a function of the phase difference between the two oscillating potentials. It increases linearly with the frequency in line with experimental finding. Recently, Park et al. obtained an expression for the admittance and the current noise for a driven nanocapacitor in terms of the Floquet scattering matrix and derived a nonequilibrium fluctuation-dissipation relation. The effect of weak electron-electron interaction on the noise was investigated by Devillard et al. using the scattering matrix renormalized by interactions. Applying the Greens function approach, Wang et al. presented a nonperturbative theory for the parametric quantum pump at arbitrary frequencies and pumping strengths. Independently, Arrachea presented a general treatment based on nonequilibrium Green functions to study transport phenomena in quantum pumps.

Work on graphene (discovered by Geim and his colleagues almost 5 years ago) heated up quickly as researchers realized that the materials two-dimensionality caused it to show unusual quantum behaviors. Graphene transistors, chemical sensors, electrodes, scales and frequency generators are some proposed potential applications. Even though graphene is a low-energy system consisting of a two dimensional honeycomb lattice of carbon atoms, its quasiparticle excitations can be fully described by the (2+1)-dimensional relativistic Dirac equation. The fundamental property of the Dirac equation is often referred to as the charge-conjugation symmetry. Klein paradox and chiral
tunneling are two major effects of it in graphene. A sufficiently strong potential, being repulsive for electrons, is attractive for positrons and results in positron states inside the barrier. Matching between electron and positron wave functions across the barrier leads to the high-probability tunneling described by the Klein paradox. The chirality of quasiparticles requires conservation of pseudospin (which is linked to different components of the same spinor wave function and is parallel/antiparallel to the direction of motion of electrons/holes) during tunneling and induces angular anisotropy in transmission in single- and multi-barrier structures in graphene. Due to its unusual structure, many extraordinary behaviors of devices based on graphene have been observed, such as the conductance minimum\textsuperscript{21,27}, resonant tunneling\textsuperscript{28}, the shot noise with the Fano factor close to 1/3\textsuperscript{27,29,30,31,32}, the unconventional Quantum Hall effect\textsuperscript{33} and the edge-state-related quantum spin Hall effect\textsuperscript{34,35}, and the electronic cooling effect\textsuperscript{36}. However, a graphene-based quantum pump has not yet been considered in literature.

In this work, we focus on an adiabatic quantum pump device based on a graphene monolayer modulated by two oscillating gate potentials. The Klein paradox featured pump current is obtained and illuminated.

The crystal structure of undoped graphene layers is that of a honeycomb lattice of covalent-bond carbon atoms. One valence electron corresponds to one carbon atom and the structure is composed of two sublattices, labeled by A and B. In the vicinity of the K point and in the presence of a potential U, the low-energy excitations of the gated graphene monolayer are described by the two-dimensional (2D) Dirac equation

\[ v_F (\sigma \cdot \hat{p}) \Psi = (E - U) \Psi, \] (1)

where the pseudospin matrix \( \sigma \) has components given by Pauli’s matrices and \( \hat{p} = (p_x, p_y) \) is the momentum operator. The “speed of light” of the system is \( v_F \), i.e., the Fermi velocity \( (v_F \approx 10^6 \text{ m/s}) \). The eigenstates of Eq. (1) are two-component spinors \( \Psi = [\psi_A, \psi_B]^T \), where \( \psi_A \) and \( \psi_B \) are the envelope functions associated with the probability amplitudes at the respective sublattice sites of the graphene sheet.

In the presence of a one-dimensional confining potential \( U = U(x) \), we attempt solutions of Eq. (1) in the form \( \psi_A(x, y) = \phi_A(x)e^{ik_y y} \) and \( \psi_B(x, y) = i\phi_B(x)e^{ik_y y} \) due to the translational invariance along the \( y \) direction. The resulting coupled, first-order differential
The equations read as

\[ \frac{d\phi_B}{d\xi} + \beta \phi_B = (\varepsilon - u)\phi_A, \]

\[ \frac{d\phi_A}{d\xi} - \beta \phi_A = -\varepsilon \phi_B. \]

Here \( \xi = x/L \), \( \beta = k_y L \), \( u = U L/\hbar v_F \), and \( \varepsilon = E L/\hbar v_F \) (\( L \) is the width of the structure).

For a double-barrier structure with two square potentials of height \( U_1 \) and \( U_2 \) respectively, Eqs. (2) and (3) admit solutions which describe electron states confined across the well and propagating along it. The transmission and reflection amplitude \( t \) and \( s \) is determined by matching \( \phi_A \) and \( \phi_B \) at region interfaces.

Following the standard scattering approach\(^2\)\(^3\)\(^37\), we introduce the fermionic creation and annihilation operators for the carrier scattering states. The operator \( \hat{a}^\dagger_L(E, \theta) \) or \( \hat{a}_L(E, \theta) \) creates or annihilates particles with total energy \( E \) and incident angle \( \theta \) in the left lead, which are incident upon the sample. Analogously, we define the creation \( \hat{b}^\dagger_L(E, \theta) \) and annihilation \( \hat{b}_L(E, \theta) \) operators for the outgoing single-particle states. Considering a particular incident energy \( E \) and incident angle \( \theta \), the scattering matrix \( s \) follows from the relation

\[
\begin{pmatrix}
    b_L \\
    b_R
\end{pmatrix} = \begin{pmatrix}
    r & t' \\
    t & r'
\end{pmatrix} \begin{pmatrix}
    a_L \\
    a_R
\end{pmatrix},
\]

where, \( t \) and \( r \) are the scattering elements of incidence from the left reservoir and \( t' \) and \( r' \) are those from the right reservoir.

The frequency of the potential modulation is small compared to the characteristic times for traversal and reflection of electrons and the pump is thus adiabatic. In this case one can employ an instant scattering matrix approach, i.e. \( s(t) \) depends only parametrically on the time \( t \). To realize a quantum pump one varies simultaneously two system parameters, e.g.\(^2\)\(^3\)

\[
X_1(t) = X_{10} + X_{\omega,1} e^{i(\omega t - \varphi_1)} + X_{\omega,1} e^{-i(\omega t - \varphi_1)},
\]

\[
X_2(t) = X_{20} + X_{\omega,2} e^{i(\omega t - \varphi_2)} + X_{\omega,2} e^{-i(\omega t - \varphi_2)}.
\]

Here, \( X_1 \) and \( X_2 \) are measures for the two barrier heights \( U_1 \) and \( U_2 \), which can be modulated by applying two low-frequency (\( \omega \)) alternating gate voltages. \( X_{\omega,1} \) and \( X_{\omega,2} \) are the corresponding oscillating amplitudes with phases \( \varphi_{1/2} \); \( X_{10} \) and \( X_{20} \) are the static (equilibrium) components.

As in the work of Moskalets and Büttiker\(^3\), in the weak pumping limit (\( X_{\omega,j} \ll X_{j0} \)) and at zero temperature, the pump current could be expressed in terms of the scattering matrix.
as follows.

\[ I_\alpha = \frac{e\omega}{2\pi} \sum_{j_1,j_2} X_{\omega,j_1} X_{\omega,j_2} \frac{\partial s_{\alpha\beta}}{\partial X_{j_1}} \frac{\partial s^*_{\alpha\beta}}{\partial X_{j_2}} 2i \sin (\varphi_{j_1} - \varphi_{j_2}). \] 

(6)

The mechanisms of an adiabatic quantum pump can be demonstrated in a mesoscopic system modulated by two oscillating barriers (see Fig. 1). We here consider a quantum pump without the effect of the Klein paradox and look into the latter afterwards. To prominently picture the charge flow driven process within a cyclic period, the two potential barriers are modulated with a phase difference of \( \pi/2 \) in the manner of \( U_1 = U_0 + U_{1\omega} \sin t \) and \( U_2 = U_0 + U_{2\omega} \sin(t + \pi/2) \). Our discussion is within the framework of the single electron approximation and coherent tunneling. The Pauli principle is taken into account throughout the pumping process. The Fermi energy of the two reservoirs and the inner single-particle state energy are equalized to eliminate the external bias and secure energy-conserved tunneling. As shown in Fig. 1, the transmission strengths between one of the reservoirs and the inner single-particle state are denoted by \( t_1-t_4 \). When \( t \in [0, \pi/2] \), \( \sin t \) changes from 0 to 1 and \( \sin(t + \pi/2) \) changes from 1 to 0. Considering the time-averaged effect, the chance of \( U_1 > U_2 \) and \( U_1 > U_2 \) is equal. Therefore, the probability of \( t_1 \) and \( t_3 \) balance out. The tunneling quantified by \( t_2 \) and \( t_4 \) do not occur since the inner particle state is not occupied. When \( t \in [\pi/2, \pi] \), \( \sin t \) changes from 1 to 0 and \( \sin(t + \pi/2) \) changes from 0 to -1. \( U_1 > U_2 \) invariably holds in this time regime. The probability of \( t_3 \) prevails and a net particle flow is driven from the right reservoir to the middle state. When \( t \in [\pi, 3\pi/2] \), \( \sin t \) changes from 0 to -1 and \( \sin(t + \pi/2) \) changes from -1 to 0. The probability of \( t_2 \) and \( t_4 \) balance out and the tunneling quantified by \( t_1 \) and \( t_3 \) are excluded from the Pauli principle. No net time-averaged tunneling occur. When \( t \in [3\pi/2, 2\pi] \), \( \sin t \) changes from -1 to 0 and \( \sin(t + \pi/2) \) changes from 0 to 1. \( U_1 \) maintains a lower height than \( U_2 \), which drives the particle in the inner state to the left reservoir. Through one whole pumping cycle, electrons (and positrons in graphene) are pumped from the right reservoir to the left by absorbing energy from the two oscillating sources. The tunneling is governed by quantum coherence. In each period, the pumping process repeats and the particles are driven continuously in the same direction as time accumulates. Direction-reversed current can be obtained with reversed phase difference of the two oscillating gates. The direction of the pumped current is from the phase-leading gate to the phase-lagged one without exception when we assume that higher barriers admit smaller transmission probability. It can find resemblance in its
classical turnstile counterpart\textsuperscript{38} with the fore-opened gate admits transmission ahead of the later-opened one driving currents in corresponding manner.

We now consider the pumped current in the graphene-based conductor. In the numerical calculations, the parameters $U_{10} = U_{20} = 100$ meV, $L = 200$ nm, $U_{\omega,1} = U_{\omega,2} = 0.1$ meV. The phase difference of the two oscillating gate potentials $\Delta \phi = \phi_1 - \phi_2$ is set at a constant value of 0.5 (in radian). The unimpeded penetration of quasiparticles (quasielectrons and quasiholes) through high and wide potential barriers described by Klein paradox is an exotic property of graphene resulting from its particular double degenerate light-cone-like band structure. Considering a graphene-based double-barrier structure, it is possible to pump current from one reservoir to the other at zero external bias by oscillating the potential barrier heights. To demonstrate the Klein paradox induced pumping properties, we present in Figs. 2 and 3 the angular and energy dependence of the pumped current respectively with constant phase difference of the two gate voltages. The positive pumped current is defined to be from the left reservoir to the right. From Fig. 2, we observe zero net electron/positron flow at normal incidence for all incident energies. It is an effect of Klein tunneling. In terms of the conservation of pseudospin, the barrier always remains perfectly transparent for angles close to the normal incidence $\theta = 0$. Therefore, the adiabatic oscillation of the two gate potentials out of phase would allow equal transmission rightward and leftward for normal incidence throughout the period of their cyclic changes, which generates no net current flow. Finite current flow is pumped at the angles where pseudospin matching produces prominent transmission. For $E = 25$ meV, the pumped current is positive. For $E = 78$ meV, the pumped current is negative. For $E = 92$ meV, the pumped current curve flips back to the positive half plane of the figure. For $E = 98$ meV, the pumped current is positive for some incident angles and negative for others. It is shown here the pumped current can shift direction when the incident angle or energy change for fixed $\Delta \phi$. The accumulated contribution of electrons tunneling from different angles to the pumped current is shown in Fig. 3. It can be seen that the flow direction of the angle-averaged pumped current can change from rightward to leftward and reversely as the energy changes. This is remarkable since in quantum pumps based on usual mesoscopic nanoscale conductors considered in literature the direction of the pumped current is determined by the phase difference of the two oscillating parameters and remains constant when the latter is fixed (see the preceding introduction).
The results can be interpreted by the mechanism of the pumping process. Different from conventional tunnel barriers, the transmission probability in graphene through a high barrier can exceed that of a low barrier characterized by the Klein paradox. A numerical comparison is given in Fig. 4. In a pumping cycle, the phase-lagged gate can admit transmission in advance of the phase-leading when a high barrier is more transparent than a low one. Therefore the direction of the current flow can be reversed in such conditions. Accordingly, the angle-averaged pumped current can be in either direction even with the phase of the pump source fixed.

In summary, a quantum pump device involving the graphene-based ballistic tunneling structure is investigated. For two independent adiabatically modulated parameters of this device a finite net charge current is transported. The physical mechanism of quantum pumping is presented within the framework of single-particle approximation and coherent tunneling. It is observed that the direction of the pumped current can be reversed when a high barrier demonstrates stronger transparency than a low one, which is a result of the Klein paradox.
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FIG. 1: The tunneling scenario of an adiabatic quantum pump. The two shadowed blocks represent the left and right electron reservoirs respectively. The two barriers oscillate adiabatically in time. The middle bar indicates the single-particle state between the two barriers. The Fermi levels of the two reservoirs are the same and are leveled to the single-particle state within the conductor. $t_1-t_4$ indicate the transmission amplitudes between one of the two reservoirs and the middle single-particle state.

FIG. 2: Angular dependence of the pumped current for different quasiparticle energy.

FIG. 3: Energy dependence of the angle-averaged pumped current.

FIG. 4: Angular dependence of the static transmission probability of tunneling from the left reservoir to the right without gate potential oscillation for different heights of the right barrier. The height of the left barrier is fixed to be 100 meV. The Fermi energy of the reservoir is 72 meV.
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