AC field induced quantum rectification effect in tunnel junctions

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We study the appearance of directed current in tunnel junctions (quantum ratchet effect), in the presence of an external ac field $f(t)$. The current is established in a one-dimensional discrete inhomogeneous "tight-binding model". By making use of a symmetry analysis we predict the right choice of $f(t)$ and obtain the directed current as a difference between electron transmission coefficients in opposite directions, $\Delta T = T^{LR} - T^{RL}$. Numerical simulations confirm the predictions of the symmetry analysis and moreover, show that the directed current can be drastically increased by a proper choice of frequency and amplitudes of the ac field $f(t)$.

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A great attention has been devoted to theoretical and experimental studies of a transport rectification in various physical, chemical and biological systems \cite{1,2}. In particular this peculiar effect appears in the form of a directed current as a system is exposed to a time-dependent ac force with zero mean. Such a directed motion (current) has been observed in molecular motors \cite{1,3}, in Josephson junction coupled systems \cite{4,5}, and in systems of cold Rb atoms in laser fields \cite{6}, just to name a few.

In most studies the appearance of directed current has been analyzed by making use of the model of a particle moving in the presence of both space and time periodic potentials \cite{2,7,8,9}. The effects of dissipation and interaction with a heat bath have been taken into account, and in many cases the decrease of dissipation as a system approaches the Hamiltonian limit, leads to a substantial increase of the directed current \cite{9}. By making use of a symmetry analysis of the dynamic equations of motion, it has been shown that the directed current occurs as a space-periodic potential is asymmetric (ratchet potential) and/or all important symmetries of an ac force, i.e. time-reversal and shift symmetry, are broken \cite{9,10}. Notice here, that the latter case can be easier realized in experiments. It has been established that more complex systems described by generic Boltzman transport equation \cite{10}, Fokker-Planck equation \cite{7,8,11}, etc. also display a directed current. Moreover, the directed energy transport has been obtained in the case of interacting many particle systems described by nonlinear partial differential equations \cite{12,13}.

Most previous studies analyzing both the dissipative and Hamiltonian limits, were heavily based on a classical nonlinear regime of particle motion. A next step is to obtain the directed transport in systems displaying quantum-mechanical behavior. The quantum regime of directed transport for a few particular systems has been studied in Refs. \cite{2,3,14,15,16}. It was shown that a dissipationless quantum system in a single energy band tight-binding approximation does not support directed current \cite{14}, and although a quantum Brownian particle can display a directed motion and even numerous current reversal in the presence of an asymmetric ratchet potential, one still needs to take into account the dissipative effects \cite{15}. Notice that a quantum ratchet effect has been observed in Josephson junction arrays \cite{5} as the directed motion of a Josephson vortex in a ratchet potential with two interacting energy bands.

On the other hand there is a class of intrinsically quantum phenomena involving a particle tunneling through a potential barrier where effects connected with the dissipation in tunnel region can be diminished. The particular examples of systems displaying these phenomena are the ballistic regime in mesoscopic devices, various tunnel junctions, tunneling through quantum (molecular) wires, etc. Recently the directed current has been obtained for electrons that tunnel through the barrier containing the asymmetrically distributed energy levels in the presence of harmonic ac drive \cite{10,16}. However, in this case the dissipation caused by the coupling to the leads is crucial in order to obtain a nonzero directed current. Thus, it is interesting to obtain general conditions for the appearance of directed transport in tunnel (dissipationless in the tunnel region) systems that are subject to an externally applied ac drive.

In this Letter we consider electron tunneling through a one-dimensional potential barrier $U(x)$ in the presence of an externally applied ac force $f(t)$. Moreover, we will restrict ourselves to the elastic scattering case, i.e. the energy of incoming electron coincides with the energy of transmitted electrons. By making use of symmetry arguments we obtain the conditions for the directed current in such a system and verify these arguments by direct numerical simulations. We show how the directed cur-
current can be resonantly enhanced by a proper choice of the frequency and amplitudes of ac drive. Notice here, that the obtained current can be considered as a particular example of the widely discussed quantum pump effect [13, 14, 20].

In the absence of dissipation the propagation of electrons through the potential barrier \( U(x) \) (\( U(x)_{x \to \pm \infty} \to 0 \)) is described by the one-dimensional Schrödinger equation. The externally applied ac force \( f(t) \) induces a time-dependent potential that is odd in space, i.e. \(-x f(t)\).

The crucial characteristics of electron propagation is the transmission coefficient \( T(E) \) which in the elastic case depends on the energy of electron \( E \). Moreover, we will distinguish the electron transmission coefficients in the opposite directions: \( T^{LR}(E) \) as the electron moves from left to right and \( T^{RL}(E) \) as the electron moves from right to left. Thus, the directed current in such a system appears if a symmetry is broken and the difference \( \Delta T(E) = T^{LR}(E) - T^{RL}(E) \) is not zero. The symmetry properties of the transmission coefficient \( T(E) \) can be analyzed by making use of the Green function method [21] and especially its representation in the form of path integral [22]. Indeed, the transmission coefficient \( T(E) \) is written in the form:

\[
T(E) \propto \int_{-\infty}^{\infty} d\tau e^{-iE\tau} G(x_1, x_2; t),
\]

where the coordinates \( x_1 \) and \( x_2 \) are located on the different sides of the barrier. Thus the symmetry of transmission coefficients \( T^{LR(RL)}(E) \) and correspondingly the absence of directed current is determined by a symmetry of the Green function \( G(x_1, x_2; t) \) with respect to the permutation of \( x_1 \) and \( x_2 \). In order to obtain the condition allowing a nonzero directed current we represent the Green function in the form of the path integral [22]:

\[
G(x_1, x_2; t) = \int D[u(t)] e^{-\int_{-\infty}^{\infty} dt \frac{m}{\hbar} \left( \frac{d}{dt} u(t) \right)^2 - U(u(t)) + u(t)f(t)}. \tag{2}
\]

Here, \( m \) is the electronic effective mass, and all paths \( u(\tau) \) start from the coordinate \( x_1 \) at \( \tau = -\infty \) and pass the point with the coordinate \( x_2 \) at \( \tau = t \). A most important symmetry transformation is time reversal. We notice that time reversal \( \tau \to -\tau \) changes (permutes) the coordinates \( x_1 \) and \( x_2 \), and the Green function \( G(x_1, x_2; t) \) is invariant with respect to this permutation and correspondingly the directed current is absent, provided \( f(t) \) is symmetric [23]:

\[
f(t) = f(-t). \tag{3}
\]

A simple consequence of such a time-reversal symmetry is that the directed current vanishes for an arbitrary potential \( U(x) \) in the absence of an ac force.

Next, we consider another symmetry operation: reflection in space. In this case the symmetry operation \( x \to -x \), and correspondingly \( u \to -u \) in the integral of Eq. (2), changes the coordinates \( x_1 \) and \( x_2 \) but leaves the Green function \( G(x_1, x_2; t) \) invariant, provided the potential \( U(x) \) is symmetric and the ac force is shift symmetric:

\[
U(x) = U(-x); \quad f(t) = -f(t + \frac{\pi}{\omega}), \tag{4}
\]

where \( \omega \) is the period of ac force.

It is interesting to mention that the conditions [3] and [4] of the absence of directed transport obtained for the quantum-mechanical system, coincide with ones obtained for classical dynamical systems in Hamiltonian limit [10, 11]. Thus, a simplest choice to obtain the directed current is to use the symmetric potential \( U(x) \) and the ac force \( f(t) \) allowing to break the shift symmetry and time-reversal symmetry

\[
f(t) = f_1 \sin \omega t + f_2 \sin(2\omega t + \varphi). \tag{5}
\]

Note that only for the phase shift \( \varphi = \pm \pi/2 \) the ac force \( f(t) \) possesses the time-reversal symmetry, and the directed current has to vanish.

To verify the above presented analysis and also to study the dependence of the directed current on the frequency and amplitudes of the ac drive, we consider a particular example of a tunnel junction, namely a large and wide barrier between two narrow-band electrodes (Fig. 1). The ac force of the type [5] is applied to the barrier region. In a simplest case this system can be described by a standard tight-binding model in the presence of a time-dependent scattering potential:

\[
i\hbar \dot{\psi}_n^f = \epsilon_0^2 (2\psi_n - \psi_{n+1} - \psi_{n-1}) + U_n \psi_n - f_n(t) \psi_n. \tag{6}
\]

The potential \( U_n \) and \( f_n(t) \) have the form:

\[
U_n = \begin{cases} 
U_0, & -2 \leq n \leq 2 \\
0, & n < -2, \quad n > 2.
\end{cases} \tag{7}
\]

\[
f_n(t) = \begin{cases} 
n f(t), & -2 \leq n \leq 2 \\
0, & n < -2, \quad n > 2.
\end{cases} \tag{8}
\]

For simplicity the hopping between the sites determined by \( c_0 \), is assumed to be the same in the electrodes and in the barrier region. Note here, that this model can be directly used also for the analysis of electron propagation through the periodic chain of impurities with symmetrical (see, Fig. 1) or asymmetrical distribution of energy levels [13, 17].

We use \( c_0 = 0.1 \) to ensure that the case of elastic scattering (one channel scattering) was realized. The height of the barrier was fixed \( U_0 = 1 \) and thus, in the absence of ac drive the transmission coefficient was negligibly small ( \( \approx 10^{-12} \)). In order to resonantly enhance the
transmission coefficient and the directed current the frequency \( \omega = 0.5 \) was used. For this particular value of \( \omega \) both harmonics in (5) give a contribution to the resonant enhancement. Such an enhancement of the transmission coefficient is due to a well known photon assisted tunneling. As the ac drive is applied, the electron can absorb one or two photons, then propagate through the barrier region with the enhanced energy \( \tilde{E} = E + 2\hbar \omega \geq U_0 \) and emit the phonons at the end of this region. The transmission coefficient \( T(E) \) for such a process can be large and moreover, can be different for electrons propagating in different directions.

To calculate the transmission coefficient we turn to a numerical investigation. We developed a scheme that generalizes the one given in [24], and allows to compute the transmission coefficient for any time-periodic scattering potential. The details of this method can be found in [24], and this scheme has been used in order to calculate the phonon scattering by time-periodic and localized in space breathers [25].

The dependence of the computed transmission coefficient \( T^{LR}(q) \) on the wave vector \( q \) of electron propagating from left to right is shown in Fig. 2. Notice here that in our model the wave vector \( q \) is determined by a standard relationship: \( E = 4c_0^2 \sin^2(q/2) \). As expected the transmission coefficient drastically increases and moreover, displays the effect of resonant tunneling for particular values of the energy \( E \) of a propagating electron. For these values of energy the transmission coefficient is close to one. Notice that the resonant transmission obtained for the electron wavevector \( q = \pi/2 \) has a simple physical origin. Indeed, for this particular energy the resonant condition \( qL = 2\pi \), where \( L \) is the length of the barrier region, is satisfied and the transmission has a maximum. As the amplitudes of ac force \( f_{1,2} \) or the phase shift \( \varphi \) vary additional resonances appear in the dependence \( T^{LR}(q) \) (see Fig. 2). These resonances in

\[
T^{LR}(q) \sim 0.043 \quad \text{(around 7.5\% from the value of } T(E) \text{)}
\]

has been found for particular values of \( f_{1,2} \).
Notice, here that an increase of the spatial extension of the ac drive “spot” can lead to a substantial decrease of both transmission coefficient and directed current. It is due to a specific of our model where a small value of coupling $c_0$ has been chosen.

The physical origin of the considered rectification effect is the quantum-mechanical interference between various paths of an electron with different absorption (emission) of photons. For this particular case of ac induced resonant propagation in tunnel junctions, this interference is especially transparent. As an electron propagates from left to right it absorbs one or two photons on the left side of a junction, and after the propagation, emits the photons on the right side of the junction. The amplitude of this process is $A(-f_1^2 + if_2 e^{i\varphi})(-f_1^2 + if_2 e^{-i\varphi})$, where $A$ is the amplitude of electron transmission with an enhanced energy. Similarly, for the electron propagating from right to left we obtain the amplitude $A(-f_1^2 - if_2 e^{i\varphi})(-f_1^2 - if_2 e^{-i\varphi})$, and correspondingly, the difference in the transmission coefficients occurs, which is proportional to $\cos(\varphi)$.

In order to observe this resonant rectification effect the ac drive of the frequency that is a half of the barrier height has to be used. Moreover, the second harmonic around 0 can lead to the directed current [20]. The importance of time-reversal ac forces can lead to the directed current [20]. The time-reversal symmetry for a quantum pump effect has been first stressed in Ref. [20]. The importance of time-reversal symmetry for a quantum pump effect has been first stressed in Ref. [20].

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