Fano resonance in the nonadiabatic pumped shot noise of a
time-dependent potential well

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Abstract

We use the Floquet scattering theory to study the correlation properties of the nonadiabatic pumped dc current and heat flow through a time-dependent potential well. Oscillator induced quasibound states of electrons can transit to the Floquet states leading to resonant tunneling effect. Virtual electron scattering processes can produce pumped heat flow, pumped shot noise and pumped heat flow noise, with presence of time and spatial reversal symmetry. When one of the Floquet levels matches the quasibound level there strikes a “Fano” resonance.

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I. INTRODUCTION

Quantum pumping is a transport phenomenon, which was originally proposed by Thouless. It can give directed current in a quantum phase coherent nanoscale conductor by time-dependent modulation of external and internal parameters. Theoretical and experimental research of quantum pumping has become a very important and active direction in mesoscopic physics. It is also significant in the field of quantum dynamic theory. Quantum pumped current and noise has been investigated in various mesoscopic systems, such as nanowire, mesoscopic rings, quantum-dot structures, spin-orbit coupled conductors, magnetic tunnel junction, graphene, and superconductor junction with Majorana fermions, etc. Quantum pumping has been experimentally observed in 1999. The pumped shot noise, which is produced by the quantum coherence of charge carriers, can give rich physical information in mesoscopic transport systems, which is more significant in nanoscale quantum devices than in the traditional non-quantum devices.

The Floquet scattering matrix approach was developed for nonadiabatic transport and noise properties as detailed by Moskalets et al. General expressions for the pumped current, heat flow, and shot noise are derived for adiabatically and non-adiabatically driven quantum pumps. This approach stresses the existence of sidebands of electrons passing the time-dependent scatterer and these sidebands are connected to the currents and noise directly. The adiabatic scattering theory for quantum pumping leads naturally to a geometrical description. Recently, Park and Ahn derived an expression for the admittance and the current noise for a driven nanocapacitor in terms of the Floquet scattering matrix and obtained a non-equilibrium fluctuation dissipation relation. The scattering matrix renormalized by interaction has been used by Devillard et al. to study the effect of weak electron-electron interaction on the noise. A non-perturbative theory for the parametric quantum pump at arbitrary frequencies and pumping strengths was presented by Wang et al, using the Green’s function approach. Based on non-equilibrium Green’s functions, Arrachea presented a general treatment to investigate transport phenomena in quantum pumps. Under the geometric framework, there have been beautiful mathematical descriptions from the current to the noise.

In this work we focus on the non-adiabatic quantum pump driven by a single oscillating potential well. Incoming and outgoing waves with the Floquet energy spacing of a photon
characterized by the driving frequency $\omega$ between two adjacent channels arises. The Floquet scattering matrix $S$ can be constructed to treat the quantum mechanical pumped current as well as the noise. Due to the time-reversal symmetry the system under consideration does not exhibit a directed current. However, energy and information is transfused into the pump from exterior by instantaneous transport within a driving cycle. Fano resonance was found in the transmission spectrum of a non-adiabatically oscillating quantum well, which could not be directly observed due to vanishing pumped current. Supposing the resonance feature can be characterized in the correlation, we investigated its noise and heat flow properties in this work.

II. MODEL AND NUMERICAL CALCULATIONS

We use the Floquet scattering theory to investigate the quantum pumping properties of a one-dimensional width-$L$ time-dependent potential-well sketched in Fig. 1. The time-dependent potential, which oscillates with frequency $\omega$ and is located between $x = -L/2$ and $x = L/2$ has the form

$$U(x, t) = \begin{cases} 
0, & \text{others,} \\
U_0 + U_1 \cos(\omega t), & -L/2 < x < L/2. 
\end{cases}$$

The time-dependent Hamiltonian of the electrons can be expressed as

$$H(t) = -\frac{\hbar^2}{2m^*} \frac{\partial^2}{\partial x^2} + U(x, t).$$

$m^* = 0.067m_e$ is the effective mass of electrons and our discussion is based on single electron approximation and coherent tunneling. Using the Floquet approach, wave functions in the three scattering regimes can be written as

$$\Psi_L(x, t) = \sum_{n=-\infty}^{\infty} \left( a_n^l e^{ik_n x} e^{-iE_n t/\hbar} + b_n^l e^{-ik_n x} e^{-iE_n t/\hbar} \right), x \leq -L/2,$n

$$\Psi_M(x, t) = e^{-iE_F t/\hbar} \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} (a_m e^{i\kappa_m x} + b_m e^{-i\kappa_m x}) J_{n-m} \left( \frac{\hbar}{\omega} \right) e^{-i\omega t}, -L/2 \leq x \leq L/2,$n

$$\Psi_R(x, t) = \sum_{n=-\infty}^{\infty} \left( a_n^r e^{-ik_n x} e^{-iE_n t/\hbar} + b_n^r e^{ik_n x} e^{-iE_n t/\hbar} \right), x \geq L/2.$$n

In the left and right free regions, the incident and outgoing electron waves consists of infinite number of sidebands, as shown in Fig. 1. $E_n = E_F + n\hbar\omega$ is the eigenenergy of
the $n$-th order Floquet state with the Fermi energy $E_F$ and $k_n = \sqrt{2m^*E_n/\hbar^2}$ is the corresponding wave vector. $n$ are integers varying from $-\infty$ to $+\infty$ in an ideal exactness. While $E_n < 0$, $k_n$ is imaginary meaning an evanescent mode, the current for this channel vanishes. $a^{l/r}_n$ and $b^{l/r}_n$ are the probability amplitudes corresponding to those flowing out of and flowing into the left/right leads, respectively. The Floquet scattering matrix can be constructed by their relations. For example, if we set $a^l_0 = 1$, $b^l_n$ corresponds to the reflection amplitude from the left lead to the left lead in the $n$-order Floquet channel, and so on.

\[
\kappa_m = 2m^*\sqrt{(E_F + m\hbar\omega - U)/\hbar}
\]

is wave vector in the middle oscillating quantum well region. $J_n$ is the first kind of Bessel function deriving from $\exp(-ix\sin\beta) = \sum_{n=-\infty}^{\infty} J_n(x)e^{in\beta}$, which only exists in the oscillating region. $a_m$ and $b_m$ are the wave function amplitudes in the oscillating region and present only in the continuity equation solving processes.

By solving equations of the boundary conditions at interfaces

\[
\Psi_L(0,t) = \Psi_M(0,t), \quad \Psi_M(a,t) = \Psi_R(a,t),
\]

and

\[
\frac{\partial \Psi_L(0,t)}{\partial x} = \frac{\partial \Psi_M(0,t)}{\partial x}, \quad \frac{\partial \Psi_M(a,t)}{\partial x} = \frac{\partial \Psi_R(a,t)}{\partial x},
\]

which must hold for all time, the Floquet scattering matrix can be obtained by some matrix algebra. The Floquet scattering matrix connects different Floquet modes as

\[
\begin{pmatrix}
  b^l \\
  b^r
\end{pmatrix} = \underbrace{\begin{pmatrix}
  R & T' \\
  T & R'
\end{pmatrix}}_{S} \begin{pmatrix}
  a^l \\
  a^r
\end{pmatrix},
\]

with $a^{l/r}$ and $b^{l/r}$ column vectors made up of $a^{l/r}_n$ and $b^{l/r}_n$ of all $n$'s. $T/T'$ and $R/R'$ are matrices with their elements the transmission and reflection amplitudes between Floquet bands. From the scattering matrix we can obtain the transmission probability.

\[
T = \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} \frac{\text{Re}(k_n)}{\text{Re}(k_m)} |t_{nm}|^2,
\]

where $t_{nm}$ measures the transmission amplitude incoming from the $m$-th Floquet channel and going into the $n$-th Floquet channel. Transmission of evanescent modes would vanish as only the real part of the outgoing wave vectors is considered.

We are interested in the element $s_{\alpha\beta}(E_n,E)$ of the Floquet scattering matrix $S$ given in Eq.(6). It measures the scattering amplitude of the electron incident through lead $\beta$ with
energy $E$ and leaving through lead $\alpha$ with energy $E_n$. By interacting with the oscillating potential the electron absorb or lose energy quanta of $n\hbar\omega$, with its final energy $E_n = E \pm n\hbar\omega$.

For the non-adiabatic quantum pump, the Floquet scattering matrix is sensitive to the spatial symmetry of the potential. If the system is present of perturbations broken the spatial symmetry or time-reversal symmetry it can pump a dc current. With only one oscillating potential, both the spatial symmetry and time-reversal symmetry is present in the device, thus no pumped current exists.

$$I = 0$$ (8)

The heat flow is carried by the non-equilibrium particles, which occurs in the process of scattering and the direction of heat flow is defined as from the oscillating potential to the reservoirs

$$I_{\alpha}^H = \frac{1}{\hbar} \int_0^\infty dE \sum_{\gamma} \sum_{n} (E_n - \mu) |s_{\gamma\alpha} (E_n, E)|^2 [f_0 (E) - f_0 (E_n)]$$ (9)

Here $f_0 (E)$ is equilibrium Fermi distribution function.

The problem of current noise is closely connected with the matrix elements of $s_{\alpha\beta} (E_n, E)$. For a phase-coherent conductor the noise is sensitive to the quantum-mechanical interference effects. We can describe the correlation function $S_{\alpha\beta} (t_1, t_2)$ of the current as

$$S_{\alpha\beta} (t_1, t_2) = \frac{1}{2} \langle \hat{I}_\alpha (t_1) \hat{I}_\beta (t_2) + \hat{I}_\beta (t_2) \hat{I}_\alpha (t_1) \rangle ,$$ (10)

where $\Delta \hat{I} = \hat{I} - \langle \hat{I} \rangle$, and $\hat{I}_\alpha (t)$ is the quantum-mechanical current operator in the lead $\alpha$, which can be expressed as

$$\hat{I}_\alpha (t) = \frac{e}{\hbar} \int dE dE' \left[ \hat{b}_\alpha^\dagger (E) \hat{b}_\alpha (E') - \hat{a}_\alpha^\dagger (E) \hat{a}_\alpha (E') \right] e^{i(E-E')t/\hbar}$$ (11)

with $\hat{a}_\alpha (E)$ and $\hat{b}_\alpha (E)$ annihilation operators of the incident and outgoing electrons to the driven potential and

$$\hat{b}_\alpha (E) = \sum_{\beta} \sum_{n} s_{\alpha\beta} (E, E_n) \hat{a}_\beta (E_n).$$ (12)

Using Eqs. (1.10) and (1.11) we find the pumped shot noise $S_{\alpha\beta}^h$ and pumped heat flow noise $S_{\alpha\beta}^h$ expressed in terms of the Floquet scattering matrix as follows

$$S_{\alpha\beta} = \frac{e^2}{\hbar} \int_0^\infty \sum_{\gamma, \delta} \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} \sum_{p=-\infty}^{\infty} M_{\alpha\beta\gamma\delta} [f_0 (E_n) - f_0 (E_m)]^2,$$ (13)
\[ S_{\alpha\delta}^{H} = \frac{1}{\hbar} \int_{0}^{\infty} dE \sum_{\gamma, \delta} \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} \sum_{p=-\infty}^{\infty} M_{\alpha\beta\gamma\delta} (E - \mu) (E_p - \mu) \left| f_0 (E_n) - f_0 (E_m) \right|^2 , \]  

(14)

with

\[ M_{\alpha\beta\gamma\delta} = s_{n\gamma}^* (E, E_n) s_{\alpha\delta} (E, E_m) s_{p\delta}^* (E_p, E_m) s_{\beta\gamma} (E_p, E_n) \]  

(15)

describing the quantum-mechanical exchange during scattering of electrons with energy \( E_n, E_m \) incident from leads \( \gamma, \delta \) and outgoing to the leads \( \alpha, \beta \) with energy \( E, E_p \), respectively.

Current flux conservation secures that \( S_{LL} = S_{RR} = -S_{LR} = -S_{RL} \) and \( I_{L}^{H} = I_{R}^{H} \). We consider one of the four and label \( S_{LL} \) as \( S_{I}^{H} \), \( S_{H}^{LL} \) as \( S_{H} \), and \( I_{L}^{H} = H \). To magnify the resonance spectrum, we also considered the derivatives of the noise and heat flow over the Fermi energy with

\[ S_{I/H}^{d} = \frac{dS_{I/H}}{dE_F} , \quad H^{d} = \frac{dH}{dE_F} . \]  

(16)

III. NUMERICAL RESULTS AND DISCUSSION

In this paper we have adopted the Floquet scattering matrix approach to investigate the pumped effect of phase coherent mesoscopic systems of noninteracting electrons. The Floquet scattering matrix describes existence of sidebands of electrons entering and exiting the pump. The nonequilibrium electrons generated by the pump carry heat from the oscillating potential to the reservoirs and transfer charge between the two reservoirs. Only the first sidebands \( (n = \pm 1) \) are excited if the oscillating amplitude is small.

The total transmission probability \( T = \sum_{n=0}^{5} |t_{0n}|^2 \) as a function of the incident energy is shown in Fig. 2. We take into account different Floquet sidebands both above and below the incident energy, with \( n = 0, \pm 1, \ldots, \pm N \). \( N = 5 \) cutoff is used, with its precision satisfactory for the small driving amplitude. In the quantum well there exists a quasibound state, when the first order Floquet sideband overlaps with the quasibound level, a “Fano” resonance occurs (also confer Fig. 1), which was discovered in Ref. 36. Due to time and spatial reversal symmetry, no charge current is generated by a single oscillating quantum well. It is known that when pumped charge current is zero, the pumped shot noise can be considerably large due to virtual transmission processes.\(^5,29\) We suppose that the nonequilibrium transmission properties can be recorded in the shot noise spectrum and the “Fano” resonance can thus be observed.
We calculated the pumped current noise, heat noise and heat flow driven by the nonadiabatic oscillating quantum well using the Floquet scattering scheme with Eqs. (9), (13), and (14). Their variation as a function of the Fermi energy was depicted in Fig. 3. The pumped current noise, heat noise and heat flow increases with the Fermi energy when more energy channels contribute to the transport for larger Fermi energies. For a small driving amplitude in our case, most of the transmission comes from the original incident level and the two first order Floquet sidebands \( n = 0, \pm 1 \). When these bands completely go out of the quantum well with \( E_F \approx \hbar \omega \), a decrease occurs in the noise spectrum. Noise is an effect of correlation, concrete or virtual. When all the active Floquet bands are out of the quantum well, the transmitting electron “sees” no structure in the conductor therefore ballistic transport governs giving rise to the shot noise decrease. An inflection could be found at the Fermi energy \( E_F \approx 0.826 \) meV corresponding to the “Fano” resonance in the total transmission. The magnification of the inflection point is shown in the insets. Since the transport properties are an accumulating effect of all energy channels, contribution of a single energy channel of the resonance is limited. To magnify and experimentally observe the “Fano” resonance of the nonadiabatic quantum pump, we calculated the differentials of the pumped charge and heat noise to the fermi energy and dramatic resonance pattern could be found.

Differentials of the pumped current noise, heat noise, and heat flow as a function of the Fermi energy are shown in Fig. 4. These curves have a sharp dip followed by a peak at \( E_F \approx 0.826 \) meV, demonstrating an asymmetric “Fano” resonance, which ensures that there exists a quasibound state (the energy of the quasibound state is \( E_B \approx -0.176 \) meV) in the deep quantum well. Electrons in the propagating states can emit photons and drop into the quasibound state and bounce back before exiting the well, thus contributing to the transport (see Fig. 1). The heat flow also shows a sharp peak at the resonance Fermi energy. The pumped noise properties can be interpreted as follows. At the resonant Fermi energy, transport process and the electron-electron correlation achieve maximal strength. The nonequilibrium electrons created by the oscillating scatterer move in different directions carried the heat flow into the electron reservoirs of the two sides. The differential shot noise demonstrates peaks corresponding to the “Fano” resonance, as a result of the virtual motion of nonequilibrium electrons.
IV. CONCLUSIONS

We considered the noise properties of a nonadiabatic quantum pump driven by an oscillating potential well. Due to time and space reversal symmetry no dc charge current can be produced. Due to virtual transmission of the electrons, heat current is not zero with its direction from the conductor into the leads at both reservoirs. To experimentally observe the “Fano” resonance found in the transmission\textsuperscript{36}, we investigated the heat current and shot noise of the charge and heat current. Sharp “Fano”-shape resonance was found. The differential current noise, heat noise, and heat flow demonstrate peak structure from the interaction of electrons with the oscillating potential when one of the Floquet sideband matches the quasibound state. Electrons in incident channel can drop into the quasibound state by emit photons. Similarly, electron in the bound state can also absorb photons and bounce back into the Floquet channels. Thus a “Fano” resonance occurred. The resonance position of the Fermi energy is then governed by the energy of the static quasibound state.

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FIG. 1: Profile of the quantum pump formed by an oscillating quantum well. Two adjacent Floquet states have energy spacing of $\hbar \omega$. There is a quasibound state in the potential well with the binding energy $E_b$. Energy is infused into the system by ac modulation of the potential well. Fano resonance occurs when one of the Floquet sideband overlaps with the quasibound state. Equilibrium well depth is $U_0$ and its variation in time has the form of $U_1 \cos(\omega t)$. 
FIG. 2: Total transmission probability $T = \sum_{n=0}^{5} |t_{0n}|^2$ as a function of the incident energy.\textsuperscript{36} Driving amplitude $U_1 = 5$ meV, static well depth $U_0 = 20$ meV, well width $L = 10$ Å, and energy quanta of the driving frequency $\hbar \omega = 1$ meV. A resonance occurs at $E_F \approx 0.826$ meV.
FIG. 3: (a) Current shot noise $S_I$, (b) heat flow shot noise $S_H$, and (c) heat flow $H$, as functions of the Fermi energy. An inflection occurs at $E_F \approx 0.826$ meV corresponding to the resonance in transmission. Insets are the zoom-in of the inflection point.
FIG. 4: Energy differentials of the current noise $S_i^d$, heat flow noise $S_H^d$, and the heat flow $H^d$, as functions of the Fermi energy. Sharp resonance could be seen at the inflection in Fig. 3 with $E_F \approx 0.826$ meV.