We investigate the Pauli blocking factor in quantum pumps using Floquet formalism. Even though the time dependent potentials in quantum pumping can not only cause inelastic scatterings but also break the micro-reversibility, i.e. $T^+(E',E) \neq T^-(E,E')$, the Pauli blocking factor is unnecessary when the scattering process through the scatterer is coherent. The well defined scattering states extending from one reservoir to the others form a complete non-orthogonal set. Regardless of the non-orthogonality one can obtain the pumped currents using the field operator formalism. The current expression finally obtained do not contain Pauli blocking factor.

Quantum transport through artificially fabricated nano/mesostructures has been extensively studied both experimentally and theoretically during the past years. Conductances between two reservoirs through the nano/mesostructures can be calculated by using Landauer-Büttiker formalism [1] when no dephasing process occurs in the scatterer region. The current through the scatterer can then be obtained from

$$I = \frac{e}{h} \int dE dE' \left[ T^+(E',E) f_L(E) - T^-(E,E') f_R(E') \right],$$

(1)

where $T^+(E',E)$ represents the transmission probability for scattering states incident from the left at energy $E$ and emerging to the right at $E'$, and $T^-(E,E')$ is defined in a similar manner for the reverse direction. $f_L$ ($f_R$) is the Fermi-Dirac distribution in the left (right) reservoir. There has been some debate and confusion for using this formula [1-8] since Eq. (1) close not contain the so-called Pauli blocking factors. The fermionic nature of the electrons is taken care of in an ad hoc way by factors $1 - f$ to suppress scattering into occupied states, so that the current is given by

$$I = \frac{e}{h} \int dE dE' \left[ T^+(E',E) f_L(E) [1 - f_R(E')] - T^-(E,E') f_R(E') [1 - f_L(E)] \right].$$

(2)

Usually these two expressions Eqs. (1) and (2) give the same results since the difference between them, $[T^+(E',E) - T^-(E,E')] f_L(E) f_R(E')$, vanishes when $T^+(E',E) = T^-(E,E')$, i.e., the micro-reversibility holds. The question can arise, however, if the system lack of this micro-reversal symmetry is considered. One of the relevant example is a quantum pump.

The quantum pump is a device that generates a dc current at zero bias potential through cyclic change of system parameters [9,10]. Recently, adiabatic charge pumping in open quantum dots has attracted considerable attention [11–20], and was experimentally realized by Svitkes et al. [21]. After a cycle of the adiabatic shape change we return to the initial configuration, but the wavefunction may have its phase changed from the initial wavefunction. This is the geometric or Berry’s phase [22]. The additional phase is equivalent to some charges that pass through the quantum dot, namely, pumped charge [9]. In another point of view, the quantum pump is a time dependent system driven by (at least) two different time periodic perturbations with the same angular frequency and a phase difference. One can deal with this problem using not only adiabatic approximation but also Floquet approach [23–25]. Recently, it has been shown that in the adiabatic limit with small strength of the oscillation potentials the Floquet and the adiabatic approach give exactly equivalent results [24].

More than two periodically oscillating perturbations with a phase difference ($\neq n\pi$, $n$ is an integer) break the time reversal symmetry [8], and consequently $T^+(E',E) \neq T^-(E,E')$. Therefore, the currents obtained from Eq. (1) and (2) are different from each other in quantum pumps [5,8]. The question immediately arises: which one is correct in quantum pumps? It is noted that this problem still exists even in the adiabatic limit, which will be shown below. We would like to make a conclusion first. Even though the time dependent scatterer like the case of quantum pumping can not only cause inelastic scatterings but also break the micro-reversibility, the Pauli blocking factor is unnecessary when the scattering process through the scatterer is coherent.

The existence of the Pauli blocking factors is intimately related to the “scattering states” [1]. If we fill up the energy eigenstates with the electrons in both reservoirs independently and then transfer the electrons from one to the other reservoir, the Pauli blocking factors cannot be avoided. If the transport is coherent across the scatterer, however, one can define a single wavefunction extending from one reservoir to the other (more precisely reflected and transmitted waves in every connected reser-
voirs) and then fill up these scattering states. In this con-
ideration the concept of transferring the electron from
one to the other reservoir is automatically eliminated, so
is the Pauli blocking. The scattering states of the
problem with static scatterer was proven to be orthogonal and
complete [26].

Consider the Schrödinger equation $i\hbar \partial / \partial t)\psi = H(t)\psi$
for an electron with mass $\mu$ and $H(t) = -\nabla^2 / 2\mu + U(x,t)$, where $U(x,t + T) = U(x,t)$ and $U(x,t) = 0$ at $x \rightarrow \pm \infty$.
For an energy $E = \hbar^2 k^2 / 2\mu$ ($k > 0$) of the incoming par-
ticle the scattering states as a solution of the Schrödinger
equation can be defined as

$$
\chi_E^\pm(x,t) = \left\{ \begin{array}{ll}
E \rightarrow \hbar k \rightarrow \pm \infty, \\
E \rightarrow \hbar k \rightarrow +\infty,
\end{array} \right.
$$

where $E_n = E + n\hbar\omega$, $k_n = \sqrt{2\mu E_n} / \hbar$, and the normal-
ization is ignored. Here we have reflection and transmis-
sion coefficients $r_{E_n,E}^+$ and $t_{E_n,E}^+$, which can be obtained
from unitary Floquet scattering matrices $S$ [24,27,28].

The matrix $S$ has the following form

$$
S(\epsilon) = \left( \begin{array}{ccccccc}
r_{00} & r_{01} & \cdots & t'_{00} & t'_{01} & \cdots \\
r_{10} & r_{11} & \cdots & t_{10} & t'_{11} & \cdots \\
\vdots & \vdots & \ddots & \vdots & \vdots & \ddots \\
t_{00} & t_{01} & \cdots & r'_{00} & r'_{01} & \cdots \\
t_{10} & t_{11} & \cdots & r_{10} & r'_{11} & \cdots
\end{array} \right),
$$

where $r_{\alpha\beta}$ and $t_{\alpha\beta}$ are the reflection and the transmission amplitudes respectively, for modes incident from the left
with an Floquet energy $\epsilon$ which take continuous values in the
interval $[0,\hbar\omega]$; $r'_{\alpha\beta}$ and $t'_{\alpha\beta}$ are similar quantities for
modes incident from the right. The above transmis-
ion and reflection coefficients are related to the matrix
elements of $S$ in terms of $t_{E_n,E}^+$ and $r_{E_n,E}^+$, etc. with
$E = \epsilon + \beta\hbar\omega$ and $\alpha = n + \beta$.

For $E' - E \neq m\hbar\omega$ ($m$ is an integer) the orthogonality
of these scattering states can be immediately proven by
using the orthogonality of the functions $e^{\pm ik}$. When $E' - E = m\hbar\omega$, however, we obtain at any fixed time

$$
\langle \chi_E^+ | \chi_{E'}^+ \rangle \propto \sum_{E_n > 0} \left( r_{E_n,E}^+ E_n,E + m\hbar\omega + t_{E_n,E}^+ E_n,E + m\hbar\omega \right)
$$

and

$$
\langle \chi_E^+ | \chi_{E'}^- \rangle \propto \sum_{E_n > 0} \left( r_{E_n,E}^+ E_n,E + m\hbar\omega + t_{E_n,E}^+ E_n,E + m\hbar\omega \right)
$$

One can find the same result for $\langle \chi_E^- | \chi_{E'}^\pm \rangle$ using the similar procedure used in Eq. (7). The unitarity of
the Floquet scattering matrix does not guarantee the orthogon-
ality of the scattering states. In the multichannel scatter-
ing problem with a static scatterer the orthogonality is drawn from the orthogonality of the channel eigen-
functions.

We consider the completeness of the scattering states.
A solution of the time periodic Hamiltonian can be
formally written as

$$
\Psi(x,t) = e^{-i\epsilon t} \sum_{n=-\infty}^{\infty} \psi_n(x)e^{-i\alpha t}.
$$

Since the potential is zero at $x \rightarrow \pm \infty$, $\psi_n(x)$ is given by the following form

$$
\psi_n(x) = \left\{ \begin{array}{ll}
A_n e^{i k_n x} + B_n e^{-i k_n x}, & x \rightarrow -\infty \\
C_n e^{i k_n x} + D_n e^{-i k_n x}, & x \rightarrow +\infty,
\end{array} \right.
$$

where $k_n = \sqrt{2\mu (\epsilon + n\hbar\omega) / \hbar}$. One can immediately
know that the linear combination of $A_n \chi_E^+ + D_n \chi_E^-$
completely cover all Floquet type solutions. The scattering
states form a complete set for describing the solution of a
scattering problem with time periodic potential. We have
shown the scattering states $\chi_E^\pm$ form a complete
non-orthogonal set.

We derive the current using these scattering states.
The time dependent electron field operator can be obtained
in the following form [29,30]

$$
\Psi(x,t) = \sum_{\sigma} \int dE \chi_E^\sigma(x,t) \frac{a_{\sigma E}}{\sqrt{hv(E)}}
$$

where $a_{\sigma E}$ and $v(E)$ is an annihilation operator for elec-
trons in the scattering states $\chi_E^\sigma(x,t)$ and the velocity,
respectively. Even though the scattering states do not
form orthogonal bases we need only the completeness to be
sure that the expansion of Eq. (10) is valid. Using
this field operator the current operator is also expressed as

$$
J(x,t) = (ie / 2m) \Psi^+ (x,t) \nabla \Psi (x,t) + H.c.
$$

$$
= \frac{e}{m} \sum_{\sigma, \sigma'} \int dE dE' \text{Im} \left( \langle \chi_{E'}^{\sigma'} | \nabla \chi_E^\sigma \rangle \frac{a_{\sigma' E}}{\sqrt{hv(E)} v(E') \sqrt{hv(E)}} \right).
$$
and Re["ad\(1\)(E)] with \(\lambda = 22.5\) meV·nm, \(\phi = \pi/2\), \(\mu = 0.067m_e\), \(d = 50\) nm, and \(T = 9.09\) ps.

The quantum mechanical (or thermal) average of the current operator becomes

\[
\langle J(x,t) \rangle = \frac{e}{m} \sum_\sigma \int dE \text{Im}(\chi_E^\sigma \nabla \chi_E^\sigma) \frac{\langle a_\sigma^+E a_\sigma E \rangle}{hv(E)}
\]

\[
+ \frac{e}{m} \sum_\sigma \sum_{E_n > 0, n \neq 0} \int dE \text{Im}(\chi_E^\prime \nabla \chi_E^\prime) \frac{\langle a_\sigma^+E a_\sigma E \rangle}{h\sqrt{v(E)v(E_n)}}
\]  

(12)

We evaluate Eq. (12) taking \(x \to \infty\) and averaging over space and time. One can then obtain the pumped current as following

\[
I = \frac{e}{h} \sum_{E_n > 0} \int dE \left[ T_{E_n,E}^+ f_L(E) - T_{E_n,E}^- f_R(E) \right],
\]

(13)

where we exploit the unitarity of the scattering matrix [31]. Here, \(T_{E_n,E}\) denotes \((k_n/k)|t_{E_n,E}^\pm|^2\). The final result, Eq. (13), exactly corresponds to Eq. (1), i.e. the current without Pauli blocking factor.

Now we consider the adiabatic limit. The adiabatic condition in the quantum pump implies that any time scale of the problem considered must be much smaller than the period of the oscillation of an external pumping [12]. We can then define the instantaneous scattering matrix with time dependent parameters, namely \(X_n(t)\),

\[
S_{ad}(E,t) = S_{ad}(E,X_1(t),X_2(t),\cdots).
\]

(14)

Due to the time periodicity of \(X_n\)’s, using Fourier transform one can obtain the amplitudes of side bands for

\[
S_{ad,n}(E) = \frac{1}{T} \int_0^T dt \ e^{i\omega t} S_{ad}(E,X_1(t),X_2(t),\cdots).
\]

(15)

The micro-reversibility condition in this expression is given by \(t_{ad,n}(E) = t_{ad,-n}(E + \hbar \omega)\), where \(t_{ad}\) and \(t_{ad}'\) represent the adiabatic transmission amplitude for the forward and the backward direction, respectively.

We show, in Fig. 1, that \(t_{ad,1}(E) = t_{ad,-1}(E + \hbar \omega)\) for a simple model system, a 1D two harmonically oscillating \(\delta\)-function barriers with the strengths \(X_1 = \lambda \cos(\omega t + \phi)\) and \(X_2 = \lambda \cos(\omega t + \phi + \delta\) respectively, separated by a distance \(d\) [14], are clearly deviated from each other, which implies the micro-reversibility of adiabatic quantum pumps is also broken. Note that in this model system \(t_{ad}(E) = t_{ad}'(E)\). The Pauli blocking factor was ignored in Brouwer’s approach since Brouwer’s theory is based upon a formula due to Büttiker, Thomas, and Prêtre [32], where they obtained the current operator from the difference between the incoming and the outgoing distributions of the electrons without Pauli blocking factors. This current can also be acquired by using the scattering states, consequently without Pauli blocking factor [29].

Figure 2 shows the pumped currents obtained from Floquet approach with and without Pauli blocking factor,
and Brouwer’s formula in the same model used above under the adiabatic regime (the Wigner delay time is much smaller than $T$ [24]) and with small amplitudes of the oscillating strength. It is clearly seen that the current with Pauli blocking factor deviates from that of Brouwer’s approach which nearly coincide with the current without Pauli blocking factor [24]. It is worth noting that quantitative behavior of the pumped currents with and without Pauli blocking looks quite similar: the pumped current $I \propto \lambda^2 \sin \phi$ as shown in the insets of Fig. 2. In Ref. [8], however, the temperature dependence of the pumped currents was expected to be distinct.

Finally, it is noted that if any kind of dephasing such as electron-electron interaction and electron-phonon interaction is involved in the scattering processes it is still an open problem whether the Pauli blocking factor is required.

In conclusion, we have shown that the Pauli blocking factor is unnecessary in quantum pumps when the scattering process through the quantum pump is coherent. The well defined scattering states form a complete non-orthogonal set. One can obtain the pumped currents without the Pauli blocking factor using the field operator formalism with these scattering states. Even in the adiabatic limit the problem of Pauli blocking factor still exists. The Pauli blocking factor was ignored in Brouwer’s adiabatic formalism, so that in the adiabatic limit with small strength of the pumping potential the pumped currents obtained from the Floquet theory without Pauli blocking factor show good agreement with those drawn from Brouwer’s formula.

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