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Symmetry and environment effects on rectification mechanisms in quantum pumps

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We consider a paradigmatic model of quantum pumps and discuss its rectification properties in the framework of a symmetry analysis proposed for ratchet systems. We discuss the role of the environment in breaking time-reversal symmetry and the possibility of a finite directed current in the Hamiltonian limit of annular systems.

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Recently there has been a good amount of experimental and theoretical activity devoted to studying quantum pumps[1–5] and quantum ratchets.[6] The basic underlying idea is the generation of a net current as a response to a time-dependent external field without a net static bias. The potential applications of this effect capture increasing interest within the communities of condensed matter physics and chemistry.

The paradigm of a ratchet system is a device with broken spatial symmetry affected by a zero-mean time-dependent force. An additional ingredient is the coupling to an environment, which is usually represented by reservoirs or some external noise. An important point in the investigation of the ratchet effect has been the understanding of the role played by the symmetries in the rectification properties of the related devices. In particular, a very simple criterion has been proposed in order to decide whether a system driven by a time-dependent field is able to support a dc current.[7] It could be stated as follows: current rectification is not possible in systems where the symmetry operations leading to a change in the sign of the relevant current, $J(t) \to -J(t)$, leave the ensuing equations for its time evolution invariant. This criterion is completely general and applies to both adiabatic and nonadiabatic regimes. Its validity has been mainly explored in the framework of classical systems.

Recent advances of material science have enabled the experimental realization of the ratchet effect in quantum pumps.[1,2] Charge and spin currents have been generated as a response to two harmonic potentials with a phase lag, which induce out-of-phase oscillations at the walls of a quantum dot. Experiments have been performed in linear arrays where the quantum dot is in contact with leads. Under these operational conditions these devices are actually open quantum systems and time-inversion symmetry breaking is introduced in the problem not only because of the phase lag between the potentials but also through the coupling to the environment. An interesting alternative setup is obtained by bending the structure to form a ring to generate a dc current along its circumference. An important example of this class is a ring threaded by a time-dependent magnetic flux. In the case of a flux with a linear dependence on time, Bloch oscillations take place due to the induced constant electric field and the coupling to reservoirs is essential to rectify this current.[8,9]

In this work we consider the setup of Fig. 1, which corresponds to a double-barrier structure embedded into a ring. The ring is connected to two reservoirs with the same chemical potential μ and two harmonic potentials with a phase lag are applied at the barriers. Our aim is to perform a careful analysis of the relevant symmetries of the system on the basis of the scheme of Ref. 7 proposed for ratchet systems. We investigate the possibility of a directed current in the limit where the coupling to the reservoirs tends to zero as well as the role of the environment in the rectification properties of quantum pumps.

We consider a tight-binding chain of N sites with constant hopping w and two barriers of height E_b. The ends of the chain are connected to reservoirs. The chain is closed with a hopping w' along the bond $\langle 1N \rangle$. The Hamiltonian for the full system reads

$$H = H_1 + H_2 + H_C(t) - w_0 \sum_{k_1} (c_1^\dagger c_{k_1} + \mathrm{H.c.}) - w_0 \sum_{k_2} (c_N^\dagger c_{k_2} + \mathrm{H.c.}), \quad (1)$$

where H_1 and H_2 are free-electron Hamiltonians with degrees of freedom labeled by k_1, k_2, respectively, which represent the reservoirs. The latter are coupled to the ring

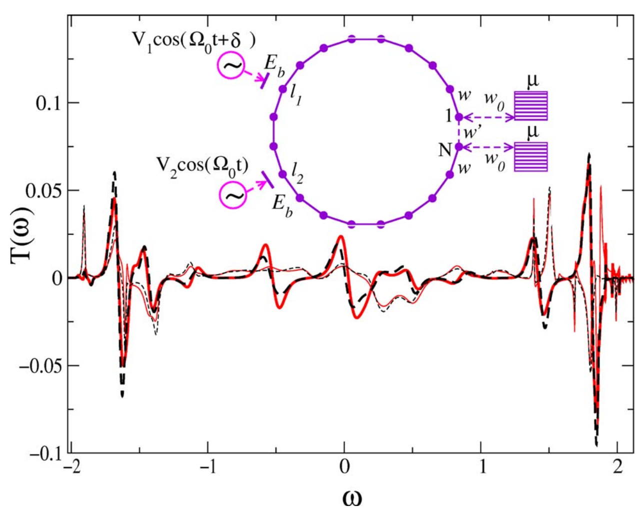

FIG. 1. (Color online) Transmission function for a ring with $N=20$ sites, $l_1=9$, $l_2=12$ barriers of height $E_b=1$, $V_1=V_2=0.5$, $w_0=1$, and $\delta=\pi/2$. Solid red (dark gray) and dashed black lines correspond, respectively, to $w'=0.1, 0$. Thick and thin lines correspond to $\Omega_0=0.05$ and 0.3, respectively. A scheme of the setup is also included.

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through a hopping w_0. The Hamiltonian of the ring containing the two oscillating barriers reads

$$H_C(t) = -w\sum_{l=1}^{N-1}(c_l^\dagger c_{l+1} + \text{H.c.}) - w'(c_1^\dagger c_N + \text{H.c.}) + [E_b + V_1\cos(\Omega_0 t + \delta)]c_{l_1}^\dagger c_{l_1} + [E_b + V_2\cos(\Omega_0 t)]c_{l_2}^\dagger c_{l_2}. \tag{2}$$

This model has two interesting limits: for $w'=0$, $w_0\neq 0$ it corresponds to the linear array studied in Ref. 10, while for $w_0=0$, $w'\neq 0$ it corresponds to the ring isolated from the reservoirs. In the latter case, the spatial coordinates satisfy periodic boundary conditions $l+N\equiv l$. We assume that reservoirs and barriers are symmetrically placed defining a mirror line along a diameter (see the scheme of Fig. 1). Their positions satisfy $l_1=-l_2+1$. The relevant symmetry operations to analyze are

$$\begin{aligned}&\mathcal{S}_1: \quad l \to -l+1, \quad t \to t-\delta/\Omega_0,\\ &\mathcal{S}_2: \quad t \to -t,\end{aligned} \tag{3}$$

which cause a spatial inversion combined with a shift in the time coordinate, and a time inversion, respectively.

The ring isolated from the reservoirs ($w_0=0$) defines a Hamiltonian, or closed, system. We now show that if $H_C(t)$ is invariant under $\mathcal{S}_1$ or $\mathcal{S}_2$, the directed current along the ring vanishes.

The evolution of a single-particle wave function $\Psi(t)=\Sigma_l \psi_l(t)$ is determined by (we work in units where $\hbar=1$)

$$-i\frac{\partial}{\partial t}\psi_l(t) - \sum_{m=1}^{N}\varepsilon_{l,m}(t)\psi_m(t) = 0, \tag{4}$$

where $\varepsilon_{l,m}(t)=-w_l\delta_{m,l+1}-w_{l-1}\delta_{m,l-1}+\delta_{l,m}[\delta_{l,l_1}v_1(t)+\delta_{l,l_2}v_2(t)]$, $w_l=w$, $l=1,\ldots,N-1$, $w_N=w'$, and $v_1(t)=E_b+V_1\cos(\Omega_0 t+\delta)$, $v_2(t)=E_b+V_2\cos(\Omega_0 t)$. The ensuing time-dependent current is

$$J_l^{isol}(t) = ew_l\,\text{Im}[\psi_l^*(t)\psi_{l+1}(t)]. \tag{5}$$

Since the applied fields are harmonic with frequency Ω_0, it is verified that $J_l^{isol}(t+\tau_0)=J_l^{isol}(t)$, with $\tau_0=2\pi/\Omega_0$. The dc component of this current is independent of l, due to the continuity condition. It is defined as

$$J^{isol} = \frac{1}{\tau_0}\int_0^{\tau_0} J_l^{isol}(t) = \frac{1}{N\tau_0}\sum_{l=1}^{N}\int_0^{\tau_0} J_l^{isol}(t). \tag{6}$$

For $V_1=V_2$ and $\delta=0,\pi$, the matrix elements of the Hamiltonian $\varepsilon_{l,m}(t)$ are invariant under $\mathcal{S}_1$ and $\mathcal{S}_2$. Hence, applying $\mathcal{S}_1$ to Eq. (4), it is found that $\psi_l(t)=\psi_{-l+1}(t-\delta/\Omega_0)$, while applying $\mathcal{S}_2$, it is found that $\psi_l(t)=\psi_l^*(-t)$. In the first case, we obtain $J_l^{isol}(t)\to -J_{-l}^{isol}(t-\delta/\Omega_0)$, while in the second one, $J_l^{isol}(t)\to -J_l^{isol}(-t)$. In the two cases, the final consequence is $J^{isol}=0$.

In summary, it becomes clear that, in order to have $J^{isol}\neq 0$ we need geometrical arrangements with broken $\mathcal{S}_1$ and $\mathcal{S}_2$ symmetries. In the case of a symmetric static setup like the one we are considering, $\mathcal{S}_1$ can be dynamically broken by applying time-dependent potentials with (i) $V_1\neq V_2$ and/or (ii) $\delta\neq 0,\pi$. Instead, condition (ii) must be satisfied in order to break $\mathcal{S}_2$. Altogether, we conclude that in the Hamiltonian limit, $\delta\neq 0,\pi$ is a necessary condition that the pumped two-barrier system must satisfy in order to support a finite net current.

We now refer to the setup of Fig. 1 with $w_0\neq 0$. As mentioned before, the linear arrangement is contained in the limiting case $w'=0$. In the latter limit the dc current vanishes as $w_0\to 0$.[10] Instead, the above symmetry analysis suggests that this may not be the case in the ring geometry ($w'\neq 0$) when $\delta\neq 0,\pi$. A convenient theoretical framework to study transport phenomena in driven open quantum systems is provided by the nonequilibrium Green's function formalism.[9,10] For reservoirs with the same chemical potential μ, the dc component of the current flowing along the ring reads

$$J_l = e\int_{-\infty}^{\infty} d\omega\, f(\omega)T_l(\omega), \tag{7}$$

where we assume zero temperature; hence, $f(\omega)=\Theta(\mu-\omega)$. The transmission function is[10]

$$T_l(\omega) = \frac{1}{\pi\tau_0}w_l|w_0|^2\int_0^{\tau_0} dt\,\rho_0(\omega)\text{Im}[G_{l,1}^R(t,\omega)G_{1,l+1}^A(\omega,t) + G_{l,N}^R(t,\omega)G_{N,l+1}^A(\omega,t)], \tag{8}$$

where $G_{l,m}^R(t,\omega)$ is the Fourier transform of the retarded Green's function, with respect to the difference of time $t-t'$, at the time of observation t. The advanced Green's function is $G_{l,m}^A(\omega,t)=[G_{m,l}^R(t,\omega)]^*$ and $\rho_0(\omega)$ is the density of states of the reservoirs. In this geometrical arrangement, there is in general a net charge flow between ring and reservoirs. Hence, $T_l(\omega)=T(\omega)$, $J_l=J$ for $l=1,\ldots,N-1$, and $T_N(\omega)=T'(\omega)$, $J_N=J'$, with $J'\neq J$, which of course verify the Kirchhoff rules. The exact retarded Green's function is the solution of the following linear set:[10]

$$G_{m,n}^R(t,\omega) = G_{m,n}^0(\omega) + \sum_{j=1}^{2}\frac{V_j}{2}e^{i(\delta_j+\Omega_0 t)}G_{m,l_j}^R(t,\omega-\Omega_0)G_{l_j,n}^0(\omega) + \sum_{j=1}^{2}\frac{V_j}{2}e^{-i(\delta_j+\Omega_0 t)}G_{m,l_j}^R(t,\omega+\Omega_0)G_{l_j,n}^0(\omega), \tag{9}$$

where $\delta_1=\delta$, $\delta_2=0$, while $G_{m,n}^0(\omega)$ is the retarded Green's function of the equilibrium ring with barriers connected to reservoirs without time-dependent voltages.

We now show results for different pumping conditions and strengths of coupling to the reservoirs. We consider two infinite tight-binding chains of bandwidth W for the reservoirs, described by the density of states $\rho_0(\omega)=4\sqrt{1-\omega^2/W^2}\Theta(W-\omega)$. All energies are expressed in units of w.

First, we would like to point out that the coupling to the reservoirs introduces inelastic scattering events and the propagation of the wave packet along the ring loses its coherence. Hence, for strong coupling to the reservoirs, the system evolves smoothly from the annular to the linear geometry as $w'\to 0$ and we expect that the transport properties of the ring do not significantly differ from those of the linear array. This feature is illustrated in Fig. 1, where we show that

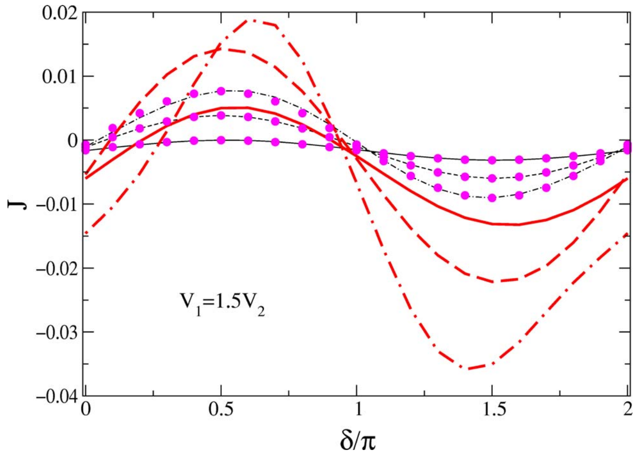

FIG. 2. (Color online) dc current J as a function of the phase lag for $V_2=1.5V_2$ and $w_0^2=0.5$. Thin black and thick red (dark gray) lines correspond to $V_1=0.2$ and 0.5, respectively. Solid, dashed, and dot-dashed lines correspond to $\Omega_0=0.05$, 0.1, and 0.6. Circles correspond to fits with the function $J=A_0+A_1\sin(\delta)$. The chemical potential is $\mu=0.1$ and $w'=1$. Other parameters are as in Fig. 1.

for $w_0=1$ and small w' we can almost exactly reproduce the transmission function $T(\omega)$ of the linear array.

In what follows, we consider $w'=w$ and a symmetric static arrangement with barrier positions l_1 and l_2 equidistant to the reservoirs ($l_1=-l_2+1$). We turn to show that a finite net current J may be obtained for $\delta=0,\pi$ if the pumping amplitudes are different ($V_1\neq V_2$). For small V_1,V_2, Eq. (9) can be solved perturbatively and when this solution is replaced in Eq. (8) for $l=N/2$, we obtain

$$\begin{aligned}T(\omega) \sim w|w_0|^2\rho_0(\omega)\Bigg\{\Bigg[\left(\frac{V_1}{2}\right)^2-\left(\frac{V_2}{2}\right)^2\Bigg]\gamma_1(\omega)\\ \times \mathrm{Im}[G^0_{N/2,1}(\omega+\Omega_0)G^{0^*}{}_{N/2+1,1}(\omega+\Omega_0)\\ +G^0_{N/2,1}(\omega-\Omega_0)G^{0^*}{}_{N/2+1,1}(\omega-\Omega_0)]\\ +\frac{V_1V_2}{2}\sin(\delta)\gamma_2(\omega)[|G^0_{N/2,1}(\omega+\Omega_0)|^2\\ -|G^0_{N/2,N}(\omega+\Omega_0)|^2-|G^0_{N/2,1}(\omega-\Omega_0)|^2\\ +|G^0_{N/2,N}(\omega-\Omega_0)|^2]\Bigg\},\end{aligned} \tag{10}$$

where $\gamma_1(\omega)=|G^0_{l_1,1}(\omega)|^2+|G^0_{l_1,N}(\omega)|^2$ and $\gamma_2(\omega)=\mathrm{Re}\{G^0_{l_1,1}(\omega)[G^0_{l_1,N}(\omega)]^*\}$. Therefore, it is found that the net current behaves as $J\sim B_0[(V_1/2)^2-(V_2/2)^2]+B_1V_1V_2\sin(\delta)$, B_0 and B_1 being real coefficients. The exact solution of J as a function of δ is shown in Fig. 2. For the smallest V_1, there is agreement with the functional behavior suggested by Eq. (10). For higher V_1, departures from this behavior are observed. In any case, the feature we want to emphasize is that for $\delta=0,\pi$, symmetry $\mathcal{S}_1$ is dynamically broken for $V_1\neq V_2$, but $\mathcal{S}_2$ is still an exact symmetry of the Hamiltonian $H_C(t)$ for the isolated system. A nonvanishing J at these points is a consequence of the fact that the latter symmetry is broken due to the coupling to the reservoirs. Another issue worth mentioning is that the functional behavior of J we are finding is just the one observed in the experimental work.[1]

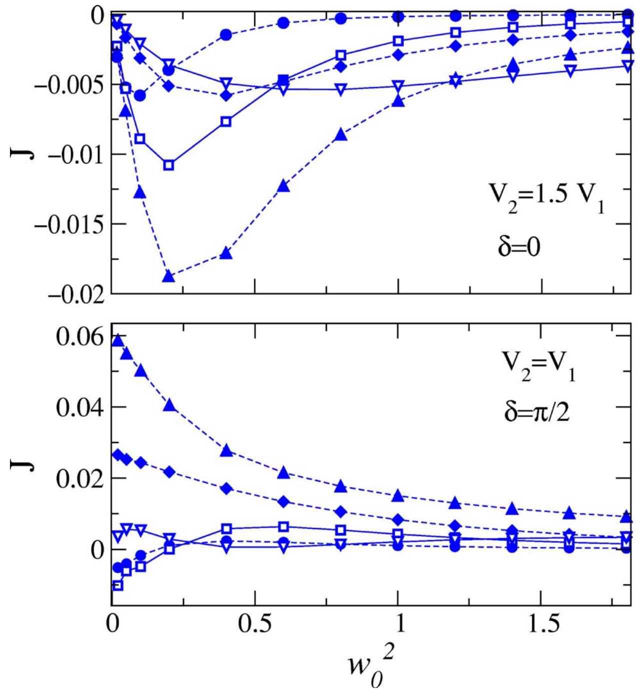

FIG. 3. (Color online) dc current J as a function of the coupling to the reservoirs. Upper panel corresponds to $V_1=1.5V_2$ and $\delta=0$ and lower panel corresponds to $V_1=V_2$, with $V_1=0.5$ and $\delta=\pi/2$. Circles, squares, diamonds, and up and down triangles correspond to $\Omega_0=0.01$, 0.05, 0.45, 0.6, and 0.75, respectively. Other parameters are as in Fig. 2.

The role of the environment in breaking time-reversal symmetry is highlighted in Fig. 3. For finite w_0, $\mathcal{S}_2$ is broken due to the coupling to the reservoirs. The figure illustrates the behavior for $\mathcal{S}_1$ dynamically broken in two different ways: The upper panel corresponds to $\delta=0$ and $V_1\neq V_2$, while the lower one to $V_1=V_2$ and $\delta=\pi/2$. In the first case symmetry $\mathcal{S}_2$ is restored as $w_0\to 0$. Thus, $J\to 0$ as the system evolves toward the Hamiltonian limit. Instead in the second case, $\mathcal{S}_2$ remains broken at $w_0=0$ and J may achieve a finite value.

Finally, let us comment on the behavior of J as a function of the pumping frequency Ω_0. For low V_1,V_2, an expansion of Eq. (10) in powers of Ω_0 leads to $J\propto\Omega_0$. For completeness, we also show in Fig. 4 the exact behavior of J for arbitrary Ω_0, V_1, and V_2. A large $|J|$ is obtained when Ω_0 is resonant (i.e., when it coincides with the energy difference between two levels of the isolated system). The inset shows that J changes linearly in Ω_0 for small enough pumping frequencies, which is typical of adiabatic driving.[3,4] Such a linear behavior is, however, not expected when the coupling to the environment vanishes. This is because in that limit $G^0_{m,n}(\omega)$ corresponds to a sequence of poles at the energy levels of the free ring and it is not possible to perform a power expansion of Eq. (10). Furthermore, for small pumping amplitudes, the structure of Eq. (9) suggests that J is only sizable for resonant Ω_0, in agreement with Ref. 5.

Previous discussions in the literature on the role of symmetries in quantum pumps suggest different behavior in adia-

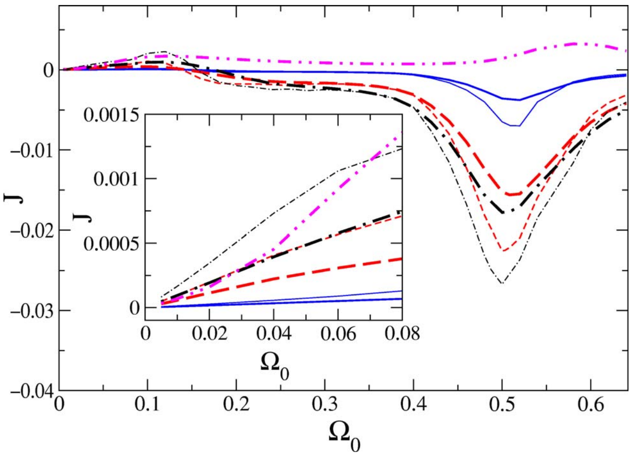

FIG. 4. (Color online) dc current J as a function of the pumping frequency Ω_0 for $\delta=\pi/2$. Thin and thick lines correspond to couplings to the reservoirs $w_0^2=0.5$ and 1, respectively. Blue (black) solid and red (dark gray) dashed lines correspond to $\mu=-1.14$ and $V_1=V_2=0.2$ and 0.5, respectively. Black dash-dotted lines correspond to $\mu=-1.14$ and $V_2=1.5V_1$ with $V_1=0.5$. Magenta (gray) two-dot-dashed line corresponds to $V_1=V_2=0.2$ and $\mu=0.1$. Other parameters are as in Fig. 2. The inset shows a zoom for small Ω_0.

batic and nonadiabatic regimes. The idea of adiabatic driving is associated with small pumping amplitudes and low frequency Ω_0 compared to the inverse of the typical time for the particle propagation through the device. While in practice this definition implies $J\propto\Omega_0$, this concept is usually formulated in terms of some approximation for the scattering matrix[3,4] and it has been pointed out that this definition strictly applies only to isolated systems.[5]

The symmetry analysis carried out in this work leads us to conclude that in open quantum systems the fundamental condition to be satisfied, in order to obtain a dc current, is spatial inversion symmetry breaking in the Hamiltonian $H_C(t)$. Since we have not introduced any assumption regarding the pumping amplitudes and frequencies, we conclude that this condition should apply to both adiabatic and nonadiabatic regimes. Let us support with examples the fact that this conclusion applies, in particular, to the adiabatic regime. We can mention, at least, three models with time-inversion invariance in the Hamiltonian limit but broken spatial inversion symmetry where J behaves linearly in the pumping frequency. (i) The system considered in the present work with $\delta=0,\pi$, $V_1\neq V_2$, finite w_0 and arbitrary (even zero) w' (see Fig. 4). (ii) Only one pumping potential applied away from a symmetric point under spatial inversion. In Ref. 10 this problem has been solved in a linear array and identical procedure and conclusions apply for the annular geometry with contacts to reservoirs. (iii) A ring threaded by a linear time-dependent flux coupled to reservoirs. This basic problem generated interesting discussions some time ago on the nature of resistive behavior.[8] More recently it has been exactly solved.[9] For low enough driving, the dc current is linear in the induced emf, which is the effective pumping frequency of this problem. In all these systems, the key point is that time-inversion symmetry breaking is introduced by their coupling to the environment. Another important conclusion is that time-inversion symmetry breaking in the Hamiltonian $H_C(t)$ is, instead necessary to obtain a dc current in the isolated ring. In order to achieve this, a minimum of two time-dependent voltages with a phase lag noncommensurate with π are needed.

To finalize, we mention that the setup of Fig. 1 with vanishing w' and finite w_0 can be viewed as a schematic model to capture the role of symmetries in the transport properties of the system studied in Ref. 1. Our results are consistent with the behavior $J=A+B\sin(\delta)$ observed in that experiment and suggest that the small finite J at $\delta=0,\pi$ can be naturally explained as a consequence of a slight difference in the amplitudes of the pumping voltages.

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