Quantum pumping in deformable quantum dots

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The charge current pumped adiabatically through an elastically deformable quantum dot suspended between electrodes is studied within the Green's function approach. Differently from the nondeformable case, the current shows an undefined parity with respect to the pumping phase φ . The unconventional current-phase relation, analyzed in the weak pumping regime, is due to a dynamical phase shift ϕ_D caused by the elastic deformations of the central region (classical phonons). The role of the quality factor Q of the oscillator, the effects induced by a mechanical resonance and the implications for current experiments on molecular systems are also discussed.

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I. INTRODUCTION

The idea of adiabatic pumping, i.e., of producing a dc current at zero bias voltage by time periodic modulation of two system parameters, dates back to the work of Thouless.¹ The pumping is *adiabatic* when the parameters change slowly as compared to all internal time scales of the system and the average charge pumped per period does not depend on the specific time dependence² of the parameters. Using the concept of emissivity proposed by Büttiker *et al.*, [3](#page-5-2) Brouwer⁴ related the charge pumped in a period to the derivatives of the instantaneous scattering matrix of the conductor with respect to the time-varying parameters. Since then, a general framework to compute the pumped charge through a conductor has been developed for noninteracting and interacting electrons[.5,](#page-5-4)[6](#page-5-5) Then the interest in the pumping phenomenon has shifted to the experimental^{τ} investigations of confined nanostructures, as quantum dots, where the realization of the periodic time-dependent potential can be achieved by modulating gate voltages applied to the structure.⁷

On the other hand, the modern miniaturization techniques have allowed the realization of artificial structures of the same length scale of molecular objects so that the charge distribution and shape of the system may well change during their operation. The process of hybridization obtained by joining artificial manmade structures with macromolecules makes possible to get systems whose electrical response is strongly affected by electromechanical tunable interaction. This happens because at molecular scale the elastic forces controlling the structure of the system are of the same order of magnitude with respect to the electrostatic forces related to the charge distributions. The interplay between electrostatic and structural degrees of freedom can be experimentally studied by means of the carbon-based technology allowing a full integration between manmade nanostructures and molecular conductors (as in particular the fullerene C_{60}). In such systems, whose theory has been formulated by Gorelik *et al.*,^{[8](#page-5-7)} the interplay between mechanical and electromagnetic degrees of freedom is responsible for a mechanical instability that causes a self-oscillating behavior due to a selfconsistent bistable potential. The current induced by this socalled *charge shuttle phenomenon*[9](#page-5-8) is proportional to the frequency of the oscillating part of the system, while the electric charge transported per cycle is an integer multiple of the elementary charge −*e*. The coupling between charge transport and vibrational properties of these molecular systems has been observed by H. Park *et al.*[10](#page-5-9) in an experiment on a single-molecule C_{60} -based transistor. Similar effects have also been observed in experiments on the transport properties of suspended carbon nanotubes where the activation of the breathing modes (i.e., radial deformations of the nanotube) has been obtained using scanning tunneling microscope (STM) tip. 11 These systems are nowadays known as nanoelectromechanical systems (NEMS) and are very important in clarifying the role of the electron-phonon interactions in molecular conductors and manmade artificial systems.

Within the previous scenarios, an interesting question is what type of effect would induce the mechanical degrees of freedom (oscillations) on quantum pumping properties. In particular, one can imagine to realize an adiabatic quantum pump with a deformable quantum dot capable of changing its configuration under the combined effect of electrostatic and elastic forces. This proposal can be realized, for instance, by coupling a suspended nanotube¹² to external leads through two tunable tunnel barriers. Suspended nanotubes of \sim 0.5 μ m of length present a mechanical resonance frequency of \sim 200 MHz, i.e., of the same order of the adiabatic pumping frequency and a quality factor $Q \sim 100-150$ (see, for instance, Fig. 3 of Ref. 12). Thus the mentioned molecular systems are good candidates to explore the adiabatic quantum pumping through a deformable system.

In this work, by employing a Green's function approach, we derive an expression of the adiabatic pumping current through a deformable quantum dot subject to a static electric field E_{ϱ} generated by a back gate and coupled to two external leads kept at the same chemical potential. The pumped current in this system is generated by the adiabatic variation of the tunneling rates between the noninteracting leads and the deformable quantum dot. During the pumping cycle the deformable dot is charged with a finite density and reacting to the presence of the electric field E_g by deforming itself and changing its energy. The dynamical effects related to the mechanical deformation of the system are considered as adiabatic and are described by using a classical formalism. The small deformation limit is considered to avoid interesting but very complicated nonlinear effects.¹³

An important point is that the parametric pump we have in mind is very different from a shuttle device. Indeed, the shuttle consists of a self-oscillating system able to selfsustain a mechanical oscillation of a small grain when a dc bias is applied to the external leads. In this setup, the charge is transported on the shuttle and is released to the closest lead, the charge on the grain being almost constant during the shuttling time. Thus a crucial ingredient is the possibility to reach closely a given lead to enhance the tunneling rate which then depends strongly on the position of the shuttle in the direction of charge transport (longitudinal direction). Alternatively, we are proposing here a parametric pumping, the only difference from the original work of Thouless¹ being the inclusion of a classical variable associated to the transverse oscillations of the central region subjected to a back gate. In our pumping setup, the tunneling rates are unsensitive to the position of the central region in the longitudinal direction and only depends on the transverse motion of the center of mass of the central region. The self-oscillating phenomena present in the shuttle dynamics (see e.g.¹⁴) are then absent in our proposal.

The plan of the paper is the following. In Sec. [II,](#page-1-0) we introduce the model Hamiltonian and the relevant parameters. In Sec. [II A,](#page-2-0) the classical dynamics of the variable *x* describing the motion of the center of mass of the central region is studied within the small deformation limit (i.e., in linear response). In Sec. II B, we derive the weak pumping formula for the current which includes the effects of the additional phase shift ϕ_D due to the dynamics of the *x*-variable. In Sec. [III,](#page-3-1) we present the results of the pumped current at zero temperature by discussing the role of the mechanical oscillations including the effects of the dissipation and conclusions are drawn in Sec. [IV.](#page-5-14)

II. MODEL

The system under study is shown in Fig. [1.](#page-1-1) It consists of a deformable quantum dot (QD) coupled to two external leads, namely the right lead (RL) and the left lead (LL), kept at the same chemical potential μ . The middle region is biased by a back gate, which generates a time-independent electric field E_{ϱ} that exerts an electrostatic force $eE_{\varrho}n$, when the electron charge on the QD region is −*en* being −*e* the electron charge, while $n = \langle d^{\dagger} d \rangle$). The QD region, which can be made of a nanotube or a C_{60} molecule, is thus deformed under the effect of E_g and reaches its equilibrium configuration when the elastic force is balanced. The electron transport in the QD is generated by the adiabatic parametric pumping consisting in the out-of-phase modulation of the two tunnel barrier strength $V_{l,r}(t)$ at the interface with the external leads.

In order to study the transport through the quantum dot, we consider as classical the variables associated to the mechanical deformation of the QD region, namely the position *x* and the momentum *P* of the center of mass, while the electron transport is treated within the quantum theory. Such

FIG. 1. (Color online) The deformable quantum dot-based device consisting of a molecular conductor connected to the external leads via two tunnel barrier whose strength can be tuned periodically in time by using suitable top gates. In the middle region an electric field *Eg* affects the center of mass dynamics of the QD. Such dynamics takes place in the direction perpendicular to the electrons transport. The periodic out-of-phase raising/lowering of the barriers strength enables the charge/discharge of the central region which reacts to the electric field E_g due to the electrostatic force.

approximation is justified when the center of mass dynamics is much slower compared to the electron dynamics (i.e., $\Omega \ll \Gamma/\hbar$, being Ω the mechanical frequency of the dot and Γ the tunneling rate controlling the dot-leads dynamics). In the following, we consider a mechanical frequency Ω of the central region comparable to the frequency ω of the pump and thus of the order of 100–300 MHz or less. The Hamiltonian describing the system is the following[:15](#page-5-15)

$$
H = \sum_{k\alpha=L,R} \epsilon_k c_{k\alpha}^\dagger c_{k\alpha} + (\epsilon_0 - eE_g x) d^\dagger d + \sum_{k\alpha} \left[V_\alpha(t) d^\dagger c_{k\alpha} + \text{H.c.} \right] + \frac{P^2}{2M} + \frac{M\Omega^2 x^2}{2},
$$
\n(1)

where the first term describes the Hamiltonian of the free electrons in the LL and RL written in term of the creation (annihilation) operators $c_{k\alpha}^{\dagger}(c_{k\alpha})$, the second term describes the QD energy in terms of the displacement *x*, the third term represents the tunneling between the leads and the QD, while the last two terms describe the classical degrees of freedom related to the center of mass motion of the QD region having mass *M* and bare resonance frequency Ω . The model Hamil-tonian Eq. ([1](#page-1-2)) represents an effective minimal model for the description of the dynamics of molecular objects coupled to soft vibrational degrees of freedom and was first proposed in Refs. [16.](#page-5-16)

The energy on the QD thus depends on the classical state of the oscillator while the oscillator is affected by the charge state of the QD. Differently from the charge shuttle case, where the tunneling strength V_α depends on the longitudinal position of the shuttle, in the present analysis such dependence is not important and will be neglected in the following analysis.

From the classical Hamilton equations, $\dot{P} = -\partial_x \langle H \rangle$, \dot{x} $= \partial_p \langle H \rangle$ the following equation for the center of mass motion 17 is obtained,

$$
M\ddot{x} + \beta \dot{x} + M\Omega^2 x = eE_g \langle d^\dagger d \rangle. \tag{2}
$$

where βx represents a phenomenological dissipative term in-cluded in Eq. ([2](#page-2-1)) independently from the Hamiltonian equations. On the r.h.s. the term $eE_g\langle d^{\dagger}d \rangle$ is the electrostatic force acting on the deformable dot when the charge density *–e* $\langle d^{\dagger}d \rangle$ is present on it. Under the adiabatic hypothesis, the variable *x* and the ac pumping terms $V_a(t)$ can be considered as slow varying parameters, and thus, we can compute the retarded Green's function of the quantum dot within the average-time approximation[:18](#page-5-18)

$$
G^{r}(E,t) = \frac{1}{E - \epsilon(x) + i\frac{\Gamma(t)}{2}}
$$

$$
\epsilon(x) = \epsilon_0 - eE_g x,
$$
 (3)

where the wide band limit for the self-energy has been considered, while $\Gamma(t) = \sum_{\alpha} 2\pi \rho V_{\alpha}^*(t) V_{\alpha}(t)$, ρ being the density of states of the external leads $(\rho_l = \rho_r = \rho)$. The modulation of the tunnel strengths $V_\alpha(t)$ is responsible for an adiabatic modulation of the linewidth $\Gamma(t) = \sum_{\alpha} \Gamma_{\alpha}(t)$, where $\Gamma_{\alpha}(t) = \Gamma_{0}^{\alpha}$ $+\Gamma^{\omega}_{\alpha} \sin(\omega t + \varphi_{\alpha})$. In addition, under no bias voltage applied to the external leads and within the zero temperature limit (T=0), the charge density $-e\langle d^{\dagger}d \rangle$ on the quantum dot region can be determined by the relation $\langle d^{\dagger} d \rangle$ $=\pi^{-1}\int_{-\infty}^{\mu} \text{Im}\lbrace G^r(E,t)\rbrace dE$ whose explicit expression is given by:

$$
\langle d^{\dagger} d \rangle = \frac{1}{2} + \frac{1}{\pi} \arctan\left[\frac{\mu - \epsilon(x)}{\Gamma(t)/2}\right],\tag{4}
$$

 μ being the chemical potential of the external leads. As shown in Eq. (4) (4) (4) , the charge density on the dot follows instantaneously the *x* dynamics, and thus, the equation for the mechanical degree of freedom can be solved at each time. Once the solution for $x \equiv x(t)$ has been obtained, the retarded Green's function of the dot can be calculated.

The instantaneous current pumped in the lead α can be computed within the Green's function technique by considering the variation of the charge $q = -e \langle d^\dagger d \rangle$ with respect to the small and slow harmonic variations of the parameters $X_i(t)$: $\delta q(t) = \sum_i \partial_{X_i} q \delta X_i(t)$. By setting $X_1 = \epsilon(x(t))$ and X_2 $=\Gamma(t)$ and by making use of Eq. ([4](#page-2-2)), the time derivative of $q(t)$ is given by

$$
\frac{dq}{dt} = -\frac{e}{2\pi} |G'(E = \mu, t)|^2 \{\Gamma(t)\partial_t \epsilon(x) + [\mu - \epsilon(x)]\partial_t \Gamma(t)\}.
$$
\n(5)

Noticing that $\Gamma(t) = \sum_{\alpha} \Gamma_{\alpha}(t)$, the r.h.s. of Eq. ([5](#page-2-3)), can be written as $\Sigma_{\alpha}I^{\alpha}(\mu,t)$ and thus the expression for the current pumped in the lead α within the zero temperature limit is recovered[.18](#page-5-18) Under time averaging over one pumping period, the first term in Eq. ([5](#page-2-3)) vanishes and the relation $\overline{I}^l = -\overline{I}^r$ is verified. The dc current pumped per cycle is given by:

$$
\bar{I}^{\alpha} = \frac{\omega}{2\pi} \int_0^{2\pi/\omega} I^{\alpha}(\mu, t) dt,
$$
\n(6)

 ω being the pumping frequency. In the following, we focus on the weak pumping limit and confine our analysis to the case of small deformation of the central region. Within this approximation the equation of motion of the *x* variable can be linearized and the related solution can be expressed in a simple form.

A. Dynamics of the mechanical degrees of freedom

In this subsection, we treat the dynamics of the *x*-variable within the linear approximation and consider the weak pumping limit, $\Gamma_{\alpha}^{\omega} \ll \Gamma_0$. Let us first note that $\langle d^{\dagger} d \rangle$ depends on the instantaneous position x of the deformable quantum dot and such dependence induces a non linear term in the dynamics as shown by Eqs. (2) (2) (2) and (4) (4) (4) . To linearize Eq. (2) , we expand $x(t)$ around the equilibrium position \bar{x} and write $x(t) = \overline{x} + \xi(t)$. Substituting $x(t) = \overline{x} + \xi(t)$ in Eq. ([4](#page-2-2)) we get the following weak pumping and small deformation expansion:

$$
\langle d^{\dagger} d \rangle \simeq n_0 - \frac{\lambda \xi(t)}{\pi} \text{Im} \{ G_0^r(E = \mu) \} - \sum_{\alpha} \frac{\Gamma_{\alpha}^{\omega}(t)}{2\pi} \text{Re} \{ G_0^r(E = \mu) \},\tag{7}
$$

where n_0 is defined from Eq. ([4](#page-2-2)) by setting $\xi(t)=0$ and $\int_{\alpha}^{\omega}(t) = 0$, while $G_0^r(E=\mu) = [\mu - \tilde{\epsilon}_0 + i \Sigma_{\alpha} \Gamma_0^{\alpha/2}]^{-1}$, $\tilde{\epsilon}_0 = \epsilon_0 - \lambda \bar{x}$, and $\Gamma_{\alpha}^{\omega}(t) = \Gamma_{\alpha}^{\omega} \sin(\omega t + \varphi_{\alpha})$. Substituting Eq. ([7](#page-2-4)) in Eq. ([2](#page-2-1)) and by introducing the adimensional displacement $\eta(\tau)$ $=\xi/x_0$ and time $\tau=\Omega t$ we get the following linear equation:

$$
\ddot{\eta} + Q^{-1} \dot{\eta} + \alpha^2 \eta = -\frac{\overline{\lambda}}{2\pi} \sum_{\alpha} \Gamma_{\alpha}^{\omega}(\tau) \text{Re}\{G_0^r(E=\mu)\}, \quad (8)
$$

where Q represents the quality factor of the oscillator (notice that $\beta = M\Omega/Q$, $\bar{\lambda} = \lambda/(M\Omega^2 x_0)$, while $\alpha^2 = \bar{\Omega}^2/\Omega^2$, $\bar{\Omega}$ being the renormalized oscillation frequency,

$$
\widetilde{\Omega} = \sqrt{\Omega^2 + \text{Im}\{G_0^r(E = \mu)\}\lambda^2 / (\pi M)}.
$$
\n(9)

The solution of Eq. (8) (8) (8) can be obtained by the classical response function $\chi(\tau)$ which is solution of the equation $\hat{D}\chi(\tau) = \delta(\tau)$ where $\hat{D} = \left[\frac{d^2}{d\tau^2} + Q^{-1}\frac{d}{d\tau} + \alpha^2\right]$ is a linear differential operator. Under the effect of the forcing term $F(\tau)$, the r.h.s. of the Eq. ([8](#page-2-5)), the displacement $\eta(\tau)$ of the deformable quantum dot can, thus, be obtained as $\eta(\tau) = \int_{-\infty}^{\infty} d\tau' \chi(\tau - \tau') F(\tau')$. Therefore, the explicit solution for the *x* variable is

$$
x(t) = \bar{x} - \frac{|\chi|\bar{\lambda}x_0}{2\pi} \text{Re}\{G_0^r(E=\mu)\}\sum_{\alpha} \Gamma_{\alpha}^{\omega} \sin(\omega t - \phi_D + \varphi_{\alpha}),
$$
\n(10)

where the quantities $|\chi|$ and ϕ_D come from the exponential representation $|\chi| \exp(i\phi_D)$ of the Fourier transform of the response function $\chi(s) = (\alpha^2 - s^2 - isQ^{-1})^{-1}$,

$$
|\chi(s)| = \frac{1}{\sqrt{(\alpha^2 - s^2)^2 + s^2 Q^{-2}}}
$$

and

$$
\phi_D(s) = \arctan\left(\frac{Q^{-1}s}{\alpha^2 - s^2}\right).
$$

From Eq. ([10](#page-2-6)) is evident that the dynamical phase ϕ_D of the classical response function χ plays an important role in the quantum pumping. The knowledge of the dynamics of the deformable quantum dot allows us to derive the retarded Green's function Eq. (3) (3) (3) and thus the pumped current.

B. Pumped currents within the weak pumping case

In this subsection, we derive the expression of the charge current adiabatically pumped under the influence of the center of mass dynamics of the central region. By introducing the retarded Green's function in Eq. (6) (6) (6) and performing an expansion of the integrand up to second order terms in Γ^{ω}_{α} , the current pumped in the left lead i_l in units of $-\frac{e\omega}{2\pi}$ can be written as 19

$$
i_{l} = i_{eq}^{l} - \frac{E_{p}|\chi|}{2\pi} |G_{0}^{r}(E = \mu)|^{2} \text{Re}\{G_{0}^{r}(E = \mu)\}\
$$

$$
\times \text{Im}\{G_{0}^{r}(E = \mu)\}\Gamma_{l}^{\omega}\Gamma_{r}^{\omega}\left[\sin(\phi_{D})\cos(\varphi)(\Gamma_{0}^{r} - \Gamma_{0}^{l}) + \sin(\phi_{D})\left(\frac{\Gamma_{l}^{\omega}}{\Gamma_{r}^{\omega}}\Gamma_{0}^{r} - \frac{\Gamma_{r}^{\omega}}{\Gamma_{l}^{\omega}}\Gamma_{0}^{l}\right) - \cos(\phi_{D})\sin(\varphi)(\Gamma_{0}^{l} + \Gamma_{0}^{r})\right], \tag{11}
$$

where the *polaronic energy* $E_p = \bar{\lambda} \lambda x_0 / 2 = \lambda^2 / (2M\Omega^2)$ has been introduced. The current i_{eq}^{l} is the current pumped when the quantum dot is in its equilibrium position \bar{x} and whose expression is

$$
i_{eq}^{l} = \frac{\Gamma_{r}^{\omega} \Gamma_{l}^{\omega}}{2} \sin(\varphi) \text{Im}\{G_{0}^{r}(E=\mu)\} \text{Re}\{G_{0}^{r}(E=\mu)\}. \quad (12)
$$

Equation (11) (11) (11) , which is the main result of this work, clearly shows that the classical phase ϕ_D , coming from the *x* dynamics, may strongly affect the current-phase relation compared to the static situation where an odd behavior of the current with respect to the pumping phase φ is expected. When λ goes to zero, e.g., by switching off the central gate $(E_g=0)$, the standard weak pumping current is recovered. Furthermore, from detailed analysis of Eq. (11) (11) (11) one sees that when the pumping frequency ω becomes very close to the renormalized resonance frequency Ω the pumped current is significantly modified by the additional terms related to the oscillation of the quantum dot. Even within the small displacement approximation, the amplitude of the second term on the r.h.s. of the Eq. (11) (11) (11) proportional to E_pQ can become comparable to the term proportional to $\Gamma_l^{\omega} \Gamma_r^{\omega}$ for suitable values of E_g and thus the system may present interesting oscillation-induced effects on the pumped current. The oscillation-related terms of the current consist of three dis-

FIG. 2. (Color online) Behavior of $sin(\phi_D)$ (dashed line) and $cos(\phi_D)$ (dashed-dotted line) as a function of the normalized pumping frequency ω . The remaining parameters have been fixed as follows: $\epsilon_0 = 0$, $E_p = 0.015$, and $\Gamma_0^l = \Gamma_0^r = 1$, $Q = 20$.

tinct contributions. Two of them are related to the pumping phase φ and are proportional to sin ϕ_D and cos ϕ_D , while the remaining one is independent from the pumping phase and can be interpreted as a rectification term. Concerning the terms containing the pumping phase, the current-phase relation is no more an odd function of φ due to the presence of terms of the form $\sin(\phi_D)\cos(\varphi)$ and $\cos(\phi_D)\sin(\varphi)$ that can be recognized as interference terms. If the oscillator has a very high Q (low dissipation), the terms proportional to $\sin(\phi_D)$ become relevant only very close to the resonance frequency (see Fig. [2](#page-3-3)), while the term proportional to $sin(\varphi)$ is the dominant one. Thus for weak dissipation, the odd symmetry of the current-phase relation is preserved almost everywhere in the parameters space. On the other hand, when the quality factor of the oscillator is decreased, i.e., for increasing values of the dissipation, the additional terms with phase dependence different from the odd ones start to become relevant. Our analysis, thus, relates the dissipation of the center of mass motion to the presence of the anomalous terms in the current-phase relation.

Let us note that the mechanism related to the presence of a dynamical phase shift is more general than the context we are describing here and can in principle be present every time a quantum system is coupled to a subsystem with a classical dynamics (as, for instance, a classical RLC circuit).

Finally, we also stress that the $cos(\varphi)$ term of the pumped current we derived in the present analysis has also been obtained in different contexts. For example, in Ref. [20](#page-5-20) where the effect of the inelastic scattering within a two terminal parametric pump was treated by means of the *fictitious leads method*. In that work a third fictitious lead with a time dependent chemical potential was introduced. In our case, even in the absence of inelastic phenomena, the deformable quantum dot behaves similarly to the fictitious lead of Ref. [20](#page-5-20) and thus a $cos(\varphi)$ term appears. Interferencelike terms in the current-phase relation were also obtained in Ref. [21](#page-5-21) where an adiabatic quantum pump in the presence of external ac voltages was considered.

III. RESULTS

In the following, we fix the zero of the energy at the Fermi level $(\mu=0)$ and consider the zero temperature limit to

FIG. 3. (Color online) Pumped current normalized to $-e\omega/(2\pi)$ computed as a function of the pumping frequency ω . The dasheddotted line corresponds to the current pumped in the absence of *polaronic* coupling (i.e., $E_p = 0$), while the dashed curves in both the panel represent the current pumped through the system in the presence of mechanical oscillations, $E_p \neq 0$. The upper panel is obtained for $\varphi = \pi/2$, while the lower panel for $\varphi = 0$. The remaining parameters have been fixed as follows: $\epsilon_0 = 0.7$, $E_p = 0.015$, $\Gamma_0^l = 1.2$, Γ_0^r $=1, \Gamma_l^{\omega} = 0.3, \Gamma_r^{\omega} = 0.5, \text{ and } Q = 150.$

study the pumped current $[Eq. (11)]$ $[Eq. (11)]$ $[Eq. (11)]$ as a function of the relevant system parameters. All the energies are expressed in units of Λ =10 μ eV which is of the same order of magnitude of the static linewidth Γ_0^{α} and the *polaronic energy* E_p is assumed as a small quantity compared to Λ . Since the *polaronic energy* can be tuned by means of the electric field *Eg*, in the following we assume that the displacement of the central region is a fraction of 10^{-12} m and thus $E_p < 10$ μ eV. In starting our analysis we notice that the behavior of the pumped current depends strongly on the value of the pumping frequency since both the response function χ and the dynamical phase are functions of ω . This is clearly seen in Fig. [2](#page-3-3) where $sin(\phi_D)$ and $cos(\phi_D)$ are shown as a function of the pumping frequency ω (normalized to the mechanical frequency Ω) while the quality factor is fixed at a relatively low value $Q=20$ (high dissipation).

When the mechanical dissipation is high, the $sin(\phi_D)$ becomes a broad peak close to the renormalized mechanical resonance, while $cos(\phi_D)$ presents a steplike behavior as a function of ω close to Ω . Thus, the presence of some dissipation mechanism allows for the presence of an even function of the pumping phase φ in the current-phase relation.

In Figs. [3](#page-4-0) we analyze the pumped current as a function of the pumping frequency ω and by fixing the remaining parameters as follows: $\epsilon_0 = 0.7$, $E_p = 0.015$, $\Gamma_0^l = 1.2$, $\Gamma_0^r = 1$, Γ_l^{ω} =0.3, Γ_r^{ω} =0.5, and *Q*=150, where we set $\varphi = \pi/2$ in the upper panel and $\varphi=0$ in the lower panel. The dashed-dotted curves in both the panels represent the current computed at $E_p=0$, i.e., in the absence of deformations of the central region, while the dashed line represents the current pumped through the system when the system is coupled to the clas-

FIG. 4. (Color online) Pumped current normalized to $-e\omega/(2\pi)$ computed as a function of the pumping frequency ω and by fixing $Q = 150$ (dashed curve) and $Q = 75$ (dashed-dotted curve). The remaining parameters have been fixed as follows: $\varphi = \pi/2$, $\epsilon_0 = 0.7$, $E_p = 0.015$, $\Gamma_0^l = 1.2$, $\Gamma_0^r = 1$, $\Gamma_l^{\omega} = 0.3$, and $\Gamma_r^{\omega} = 0.5$.

sical phonons. Again we observe that when the system is driven on resonance by the external ac parameters of the pump, the oscillations of the dot are responsible for the enhancement of the current close to the mechanical frequency Ω , while for pumping frequencies different from the resonance one the system shows a current intensity similar to the static case. Furthermore, the specific value of the pumping phase φ can strongly affect the symmetry of the pumped currents as a function of the pumping frequency. Indeed, as is shown in the lower panel of Figs. [3](#page-4-0) for pumping frequencies around the resonance frequency Ω , the sign of the current is reversed. The behavior of the pumped current as a function of the pumping frequency ω is qualitatively consistent with the one measured in Ref. [22](#page-5-22) (see Fig. 2a of the cited work) where a suspended carbon nanotube with $Q=80$ and $\overline{\Omega}$ =55 MHz has been considered to analyze the electricalinduced *guitar-string-like* oscillation modes. In Fig. [4](#page-4-1) the pumped current is shown as a function of the pumping frequency for two different values of the quality factor, namely $Q=75$ (dashed-dotted line) and $Q=150$ (dashed line), while the remaining parameters have been fixed as $\varphi = \pi/2$, ϵ_0 =0.7, E_p =0.015, Γ_0^l =1.2, Γ_0^r =1, Γ_l^{ω} =0.3, and Γ_r^{ω} =0.5. As shown, higher values of Q (lower dissipation) permit to enhance the pumped current close to the mechanical frequency. The influence of the oscillation-related terms on the currentphase relation is shown in Fig. [5](#page-4-2) where the pumped current is reported in the presence and not of the deformations. As

FIG. 5. (Color online) Pumped current normalized to $-e\omega/(2\pi)$ computed as a function of the pumping phase φ . The remaining parameters have been fixed as follows: $Q=150$, $\omega/\Omega=1$, $\epsilon_0=0.7$, E_p =0.015 (dashed line) or E_p =0 (dashed-dotted line), Γ_0^l =1.2, Γ_0^r $=1, \Gamma_l^{\omega} = 0.15, \text{ and } \Gamma_r^{\omega} = 0.5.$

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we see when $E_p \neq 0$ a nonzero pumped current appears even for $\varphi = 0, 2\pi$, i.e., a rectification term is present.

IV. CONCLUSIONS

We studied the adiabatic quantum pumping through a deformable quantum dot coupled to two external leads in the presence of time varying barriers strength and analyzed the oscillations induced effects on the pumped current. The outof-phase adiabatic modulation of the coupling to the leads is responsible for the charging/discharging of the central deformable region, which is subject to an electrostatic field *Eg*. The dynamics of the center of mass displacement *x* of the central region introduces an additional phase shift ϕ_D which affects the pumped current. In particular the deformation induced terms modify the current-phase relation by introducing even contributions in the pumping phase φ . Such terms depend strongly on the quality factor *Q* and are suppressed when the mechanical dissipation is low. Furthermore, the current pumped is enhanced when the pumping frequency ω is very close to the mechanical resonance frequency Ω , the enhancement factor being determined by the *Q* factor. Finally, we demonstrated that the pumping mechanism can in principle be used to characterize the mechanical properties of a molecular resonator allowing to study the response function $\chi(t)$. Thus, our proposal can be seen as a complementary tool in the investigation of the mechanical response of a nanoresonator. On the other hand, the deformations of the central region permit to enhance the pumped current for values of the pumping frequency close the to mechanical one, thus rendering measurable the pumping current, which otherwise remains difficult to detect. Experimentally our proposal can be realized by modifying the experimental set up proposed in Ref. [22,](#page-5-22) which is particularly suitable due to the relatively low value of the resonance frequency i.e., 55 MHz) fulfilling the adiabatic requirement considered in our work.

- 1 D. J. Thouless, Phys. Rev. B 27, 6083 (1983).
- ²B. Altshuler and L. Glazman, Science **283**, 1864 (1999).
- 3M. Büttiker, H. Thomas, and A. Prêtre, Z. Phys. B **94**, 133 $(1994).$
- ⁴ P. W. Brouwer, Phys. Rev. B **58**, R10135 (1998).
- 5B. Spivak, F. Zhou, and M. T. Beal Monod, Phys. Rev. B **51**, 13226 (1995); F. Zhou, B. Spivak, and B. Altshuler, Phys. Rev. Lett. 82, 608 (1999); Yu. Makhlin and A. D. Mirlin, *ibid.* 87, 276803 (2001); O. Entin-Wohlman, A. Aharony, and Y. Levinson, Phys. Rev. B 65, 195411 (2002); M. Moskalets and M. Büttiker, *ibid.* 66, 035306 (2002); Phys. Rev. B 66, 205320 $(2002).$
- 6 H. Pothier, P. Lafarge, C. Urbina, D. Esteve, and M. H. Devoret, Europhys. Lett. 17, 249 (1992); I. L. Aleiner and A. V. Andreev, Phys. Rev. Lett. 81, 1286 (1998); M. Blaauboer and E. J. Heller, Phys. Rev. B 64, 241301(R) (2001); B. L. Hazelzet, M. R. Wegewijs, T. H. Stoof, and Yu. V. Nazarov, *ibid.* **63**, 165313 (2001); R. Citro, N. Andrei, and Q. Niu, *ibid.* 68, 165312 (2003); P. W. Brouwer, A. Lamacraft, and K. Flensberg, *ibid.* 72, 075316 (2005); L. Arrachea, A. Levy Yeyati, and A. Martin-Rodero, *ibid.* 77, 165326 (2008); Fabio Cavaliere, Michele Governale, and Jürgen König, Phys. Rev. Lett. **103**, 136801 $(2009).$
- 7Kazuhito Tsukagoshi and Kazuo Nakazato, Appl. Phys. Lett. **71**, 3138 (1997); K. Tsukagoshi, K. Nakazato, H. Ahmed, and K. Gamo, Phys. Rev. B 56, 3972 (1997); M. Switkes, C. M. Marcus, K. Campman, and A. C. Gossard, Science **283**, 1905 (1999); S. K. Watson, R. M. Potok, C. M. Marcus, and V. Umansky, Phys. Rev. Lett. 91, 258301 (2003); J. J. Vartiainen, M. Mottonen, J. P. Pekola, and A. Kemppinen, Appl. Phys. Lett. 90, 082102 (2007).
- 8L. Y. Gorelik, A. Isacsson, M. V. Voinova, B. Kasemo, R. I. Shekhter, and M. Jonson, Phys. Rev. Lett. **80**, 4526 (1998).
- 9^9 For a detailed description of the shuttle devices see A. Donarini, Ph.D. thesis, Technical University of Denmark, 2004.
- 10H. Park, J. Park, A. Lim, E. Anderson, A. Alivisatos, and P. McEuen, Nature (London) 407, 57 (2000).
- ¹¹B. J. LeRoy, S. G. Lemay, J. Kong, and C. Dekker, Nature (London) 432, 371 (2004).
- ¹²K. Jensen, C. Girit, W. Mickelson, and A. Zettl, Phys. Rev. Lett. 96, 215503 (2006).
- ¹³ A. N. Cleland, *Foundations of Nanomechanics* (Springer-Verlag, Berlin, 2003).
- 14F. Pistolesi and Rosario Fazio, Phys. Rev. Lett. **94**, 036806 $(2005).$
- 15A similar Hamiltonian has been studied in F. Pistolesi, Ya. M. Blanter, and Ivar Martin, Phys. Rev. B 78, 085127 (2008) to describe the dynamics of a molecular object coupled to a soft vibrational degree of freedom.
- 16M. Galperin, M. A. Ratner, and A. Nitzan, Nano Lett. **5**, 125 (2005); D. Mozyrsky, M. B. Hastings, and I. Martin, Phys. Rev. B 73, 035104 (2006).
- 17 The semiclassical treatment of the dynamics of the *x*-variable is essentially the same as the one considered for a shuttle devices by A. Donarini and A.-P. Jauho, Physica E (Amsterdam) 22, [7](#page-2-4)21 (2004). The difference in the dynamics described by Eq. (7) of that work and our Eq. (2) (2) (2) is the presence of the vertical displacement of the middle region cosidered in this work.
- ¹⁸ J. Splettstoesser, M. Governale, J. König, and R. Fazio, Phys. Rev. Lett. 95, 246803 (2005).
-
- ¹⁹The property $i_l = -i_r$ of the current is verified. 20 M. Moskalets and M. Büttiker, Phys. Rev. B **64**, 201305(R) $(2001).$
- 21 M. Moskalets and M. Büttiker, Phys. Rev. B 69 , 205316 (2004).
- 22V. Sazonova, Y. Yaish, H. Üstünel, D. Roundy, T. A. Arias, and P. L. McEuen, Nature (London) 431, 284 (2004).