

Nonadiabatic charge pumping by oscillating potentials in one dimension: results for infinite system and finite ring

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(Dated: September 21, 2010)

We study charge pumping when a combination of static potentials and potentials oscillating with a time period T is applied in a one-dimensional system of non-interacting electrons. We consider both an infinite system using the Dirac equation in the continuum approximation, and a periodic ring with a finite number of sites using the tight-binding model. The infinite system is taken to be coupled to reservoirs on the two sides which are at the same chemical potential and temperature. We consider a model in which oscillating potentials help the electrons to access a transmission resonance produced by the static potentials, and show that non-adiabatic pumping violates the simple $\sin \phi$ rule which is obeyed by adiabatic two-site pumping. For the ring, we do not introduce any reservoirs, and we present a method for calculating the current averaged over an infinite time using the time evolution operator $U(T)$ assuming a purely Hamiltonian evolution. We analytically show that the averaged current is zero if the Hamiltonian is real and time reversal invariant. Numerical studies indicate another interesting result, namely, that the integrated current is zero for *any* time-dependence of the potential if it is applied to only one site. Finally we study the effects of pumping at two sites on a ring at resonant and non-resonant frequencies, and show that the pumped current has different dependences on the pumping amplitude in the two cases.

PACS numbers: 73.23.-b, 73.63.Nm, 72.10.Bg

I. INTRODUCTION

The idea that oscillating potentials applied to certain points in a one-dimensional system can pump a net charge between two reservoirs at the same chemical potential has been studied extensively for many years, both theoretically [1-42] and experimentally [43-49]. For the case of non-interacting electrons, theoretical studies of this phenomenon have used adiabatic scattering theory [9-17], Floquet scattering theory [21-23], the non-equilibrium Green function formalism [24-27], and the equation of motion approach [36, 37]. The case of interacting electrons has been studied using a renormalization group method for weak interactions [50], and the method of bosonization for arbitrary interactions [51-61]. Other interesting studies of pumping include adiabatic quantum pumping in graphene where the electrons obey the Dirac equation [62], and classical pumping on a finite ring by oscillating hopping rates at two sites [63].

With the exception of a few papers [22, 24-27, 49], the earlier studies of charge pumping have generally considered systems in which oscillating potentials are applied to two or more sites. In such cases, it is known that if the oscillation frequency ω is small, the dc part of the pumped current is proportional to ω ; the charge pumped per cycle (with time period $2\pi/\omega$) therefore has a finite value in the adiabatic limit $\omega \rightarrow 0$. However, it has been noted in Refs. 22 and 24-27 that an oscillating potential applied to a single site can also pump charge provided that the system has no left-right symmetry; this can happen if, for instance, appropriate static potentials are present. Most studies of charge pumping have also been limited to infinite systems in which the left and right sides of the system (called the leads or reservoirs) are associated with certain

chemical potentials and temperatures. Charge pumping on a finite ring has been studied in a few papers for adiabatic [13-16] and nonadiabatic situations [23, 25, 26].

In this paper, we will study charge pumping in both an infinite system as well as on a finite ring for non-interacting electrons. We will study the effects of oscillating potentials applied to either one site or more than one site. We will not assume the oscillation frequency to be small (i.e., the adiabatic limit), but will assume the oscillation amplitudes to be small. For the infinite system, we will assume the existence of reservoirs, but for the finite ring, we will assume that the system is not coupled to any reservoirs and that the time evolution is purely Hamiltonian. We will see that results obtained in the two cases differ in some interesting ways. We will restrict our analysis to zero temperature and spinless electrons, since spin does not play an essential role in the absence of interactions between the electrons.

The plan of the paper is as follows. In Sec. II, we will examine charge pumping in the infinite system. For convenience, this will be studied in the continuum limit using a linearized form of the energy-momentum relation; namely, we will use the massless Dirac equation with both right and left moving modes. We will assume the system to be coupled to reservoirs on the two sides, and the chemical potentials and temperature of these will be introduced using the formalism of Refs. 22 and 23. This implicitly assumes that an electron, after passing through the region with the static and oscillating potentials, equilibrates with whichever lead it enters; the precise mechanism for energy or momentum relaxation in the reservoirs will not be specified in our calculation. As a specific example, we will consider a model in which the static potentials have transmission resonances at certain energies,

and potentials oscillating at exactly the right frequency can then lead to enhanced charge pumping [38, 39]; in this model, we show how a competition between different processes can lead to either maxima or minima in the pumped current. We find that the pumped charge is of second order in the strengths of the oscillating potentials and can be much larger for two-site pumping compared to one-site pumping. We also find that the ‘sin ϕ ’ rule, which has been discussed earlier in the adiabatic limit $\omega \rightarrow 0$ for pumping by two oscillating potentials with a phase difference of ϕ [4, 43], breaks down if ω is larger than the resonance width.

In Sec. III, we will study charge pumping on a finite ring using a tight-binding Hamiltonian to describe the electrons; no reservoirs will be introduced. We will present a formalism for calculating the long-time averaged current if there are potentials oscillating with a time period T ; this is done by considering the eigenstates of the unitary time evolution operator $U(T)$. Next, we will assume that the system begins in a specific initial state corresponding to a particular filling at zero temperature. We will then evolve the system using only the Hamiltonian, without introducing any mechanisms for momentum relaxation and phase decoherence; this means that the system will never reach a steady state and that its properties depend on the initial state. We will show analytically that if the Hamiltonian is real and time reversal invariant, then charge pumping cannot occur even if the system has no left-right symmetry. Numerically, we also find that if the Hamiltonian is real and if an oscillating potential is applied to only one site, then charge pumping does not occur even if the oscillating potential is not time reversal invariant and the system has no left-right symmetry. It is therefore necessary to apply oscillating potentials to at least two sites in order to pump charge. We will also study what happens at both non-resonant and resonant frequencies; the latter means that the oscillation frequency is equal to the energy difference between a filled state and an empty state of the time-independent part of the Hamiltonian. (We would like to mention here that charge pumping on a ring at resonant and non-resonant frequencies has also been studied earlier in Ref. 23). In the Appendix, we will present details of the calculation of the eigenstates of $U(T)$ to first order in the oscillating potentials, both for the non-resonant and resonant cases. We will show there that the pumped charge can receive contributions at either zero-th or first order in the oscillating potential in the resonant case but only at second order in the non-resonant case. In Sec. IV, we will summarize our results and emphasize the different assumptions that we have made in the models defined on the infinite line and on a ring. Finally, we will discuss possibilities for experimentally testing our results in two kinds of systems, namely, mesoscopic rings and aromatic molecules.

II. CHARGE PUMPING ON AN INFINITE LINE

In this section, we will study charge pumping on an infinite line. Our model consists of a gapless system of non-interacting spinless electrons subject to some static and oscillating potentials. We will assume that the regions lying far to the left and far to the right of all the potentials have the same chemical potential given by the Fermi energy E_F (we will work at zero temperature). Assuming that the oscillating frequency is small compared to the bandwidth, we will linearize the energy-momentum dispersion around E_F . Let us denote the Fermi velocity and Fermi wave number by $v_F = (dE/dp)_{E=E_F}$ and k_F respectively. [The relation between k_F and E_F is governed by the underlying microscopic model. For instance, in a tight-binding lattice model with the dispersion $E = -2\gamma \cos k$, where γ is the nearest-neighbor hopping amplitude, we have $E_F = -2\gamma \cos k_F$ where $0 < k_F < \pi$]. We can then define the electron field operator

$$\psi(x) = \psi_R(x) e^{ik_F x} + \psi_L(x) e^{-ik_F x}, \quad (1)$$

where ψ_L and ψ_R are the fermionic field operators for the left and right moving electrons. In terms of these fields, the Hamiltonian in the presence of several point-like potentials is given by $H = H_0 + V$, where

$$\begin{aligned} H_0 &= \int dx \, i v_F \left(-\psi_R^\dagger \frac{\partial \psi_R}{\partial x} + \psi_L^\dagger \frac{\partial \psi_L}{\partial x} \right), \\ V &= \int dx \sum_p \delta(x - x_p) U_p(t) \psi^\dagger(x) \psi(x). \end{aligned} \quad (2)$$

In the absence of the potential V , the eigenstates of H are given by $\exp[i(\pm kx - Et)]$, where $E = v_F k$, and $\pm k$ refer to right and left moving modes respectively; note that we are measuring the energy E and the wave number k with respect to E_F and k_F respectively, and we have set $\hbar = 1$. Using Eq. (1), we find that the equations of motion for ψ_R and ψ_L are given by [61]

$$\begin{aligned} & i \frac{\partial \psi_R}{\partial t} + i v_F \frac{\partial \psi_R}{\partial x} \\ &= \sum_p \delta(x - x_p) U_p(t) (\psi_R + \psi_L e^{-i2k_F x_p}), \\ & i \frac{\partial \psi_L}{\partial t} - i v_F \frac{\partial \psi_L}{\partial x} \\ &= \sum_p \delta(x - x_p) U_p(t) (\psi_L + \psi_R e^{i2k_F x_p}). \end{aligned} \quad (3)$$

We can solve these equations by integrating over small regions from $x_p - \epsilon$ to $x_p + \epsilon$ to find the discontinuities in the fields at $x = x_p$.

Let us now consider two types of point-like potentials: $a_m \delta(x - x_m)$ which are time independent, and $w_n(t) \delta(x - x_n)$ which oscillate in time as $w_n(t) = b_n \cos(\omega t + \phi_n)$. We will assume that the oscillation amplitudes b_n are

small compared to v_F and will generally calculate the pumped charge to the lowest non-zero order in the b_n 's. Let us first assume that $b_n = 0$ for all n , and that we can completely solve the problem with the static potentials. This can be described in terms of a scattering matrix S as follows. If \mathcal{R} denotes the region within which all the static potentials are present, then an electron incoming from a region far to the left of \mathcal{R} (which we denote as $x \ll \mathcal{R}$) with unit amplitude and energy and wave number given by E and $k = E/v_F$ respectively will have a wave function $\psi(x)e^{-iEt}$ given by

$$\begin{aligned} \psi(x) &= e^{ikx} + r_L(E) e^{-ikx} \text{ for } x \ll \mathcal{R}, \\ &= t_R(E) e^{ikx} \text{ for } x \gg \mathcal{R}, \end{aligned} \quad (4)$$

where r_L and t_R denote the reflection and transmission amplitudes. Similarly, an electron incoming from a region far to the right of \mathcal{R} with unit amplitude and energy and wave number given by E and $-k = -E/v_F$ respectively has the wave function $\psi(x)e^{-iEt}$, where

$$\begin{aligned} \psi(x) &= e^{-ikx} + r_R(E) e^{ikx} \text{ for } x \gg \mathcal{R}, \\ &= t_L(E) e^{-ikx} \text{ for } x \ll \mathcal{R}. \end{aligned} \quad (5)$$

Assuming that all these reflection and transmission amplitudes are known, let us now turn on the oscillating potentials, all of which we take to lie to the left of \mathcal{R} , and proceed as follows.

An electron incoming from the left of \mathcal{R} with unit amplitude and energy (wave number) E_0 ($k_0 = E_0/v_F$) will now have a wave function $\psi(x, t)$ of the form

$$\begin{aligned} \psi &= e^{i(k_0x - E_0t)} + \sum_j r_{L,j} e^{i(-k_jx - E_jt)} \text{ for } x \ll \mathcal{R}, \\ &= \sum_j t_{R,j} e^{i(k_jx - E_jt)} \text{ for } x \gg \mathcal{R}, \end{aligned} \quad (6)$$

where $E_j = E_0 + j\omega$, $k_j = E_j/v_F$, and $r_{L,j}$ and $t_{R,j}$ will now generally be functions of both E_0 and E_j . Similarly, an electron incoming from the right of \mathcal{R} with unit amplitude and energy (wave number) E_0 ($k_0 = E_0/v_F$) will have a wave function $\psi(x, t)$ of the form

$$\begin{aligned} \psi &= e^{i(-k_0x - E_0t)} + \sum_j r_{R,j} e^{i(k_jx - E_jt)} \text{ for } x \gg \mathcal{R}, \\ &= \sum_j t_{L,j} e^{i(-k_jx - E_jt)} \text{ for } x \ll \mathcal{R}, \end{aligned} \quad (7)$$

where $E_j = E_0 + j\omega$, $k_j = E_j/v_F$, and $r_{R,j}$ and $t_{L,j}$ will be functions of both E_0 and E_j .

The sums over the side band index j in Eqs. (6-7) will go from $-\infty$ to ∞ for a Dirac electron. But, in practice, j gets cut off for two reasons. First, if the energy E_j goes above or below the bandwidth of the system, the corresponding wave function decays exponentially as $|x| \rightarrow \infty$; such a state does not carry any current. Secondly, if all the pumping amplitudes b_n are small, one can show, using Eqs. (3) recursively, that the leading order terms in

$r_{R/L,j}$ and $t_{R/L,j}$ are given by $|b_n|^{|j|}$ if $j \neq 0$; this goes to zero exponentially as $|j| \rightarrow \infty$. Hence, if ω is much smaller than the bandwidth and E_0 is not too close to the edges of the band, the contributions of the higher side bands become very small long before the energy E_j reaches the band edges.

We will now calculate the different reflection and transmission amplitudes using Eqs. (3). To first order in b_n , only the first side bands with $j = \pm 1$ survive. If the oscillating potentials are given by

$$\sum_n \delta(x - x_n) b_n \cos(\omega t + \phi_n), \quad (8)$$

we find that

$$\begin{aligned} t_{R,\pm 1} &= -\frac{i}{2v_F} t_R(E_{\pm 1}) \sum_n b_n e^{\mp i\phi_n} \\ &\quad \times [e^{\mp i\omega x_n/v_F} + r_L(E_0) e^{-i(k_{\pm 1} + k_0 + 2k_F)x_n}], \\ r_{R,\pm 1} &= -\frac{i}{2v_F} t_R(E_{\pm 1}) t_L(E_0) \\ &\quad \times \sum_n b_n e^{\mp i\phi_n} e^{-i(k_{\pm 1} + k_0 + 2k_F)x_n}. \end{aligned} \quad (9)$$

Similar expressions can be derived for $t_{L,\pm 1}$ and $r_{L,\pm 1}$, but these will not be required below. The expressions in Eqs. (9) can be understood as arising from a sum over paths as explained in Ref. [37].

Given all the transmission and reflection amplitudes $t_{R/L,j}$ and $r_{R/L,j}$, the dc part of the current in, say, the right lead is given by [22, 23]

$$\begin{aligned} I_{R,dc} &= q \int_{-\infty}^{\infty} \frac{dE_0}{2\pi} \sum_j [|r_{R,j}|^2 \{f_R(E_0) - f_R(E_j)\} \\ &\quad + |t_{R,j}|^2 \{f_L(E_0) - f_R(E_j)\}], \end{aligned} \quad (10)$$

where q is the charge of the electron, and $f_\alpha(E) = 1/[e^{\beta(E - \mu_\alpha)} + 1]$ is the Fermi function in the lead α . At zero temperature, $f_\alpha(E) = 1$ if $E < \mu_\alpha$ and 0 if $E > \mu_\alpha$. If we assume zero bias, $\mu_R = \mu_L = 0$ (we are defining energy with respect to E_F), and restrict ourselves to terms of second order in the b_n 's, we obtain the expression

$$\begin{aligned} I_{R,dc} &= q \int_{-\omega}^0 \frac{dE_0}{2\pi} [|r_{R,1}|^2 + |t_{R,1}|^2] \\ &\quad - q \int_0^\omega \frac{dE_0}{2\pi} [|r_{R,-1}|^2 + |t_{R,-1}|^2]. \end{aligned} \quad (11)$$

In the adiabatic limit $\omega \rightarrow 0$, we can show from this that, up to order ω , the current will involve only cross-terms of the form $\sum_{m < n} b_m b_n \sin(\phi_m - \phi_n)$ multiplied by terms involving x_m and x_n . Let us call this the 'sin ϕ ' rule; it implies that two potentials cannot pump current if their phase difference is 0 or π . We also see that if there is an oscillating potential at only site, there is no current at order ω . These features arise because of the

near cancellation in Eq. (11) between $|r_{R,1}|^2$ and $|r_{R,-1}|^2$ and between $|t_{R,1}|^2$ and $|t_{R,-1}|^2$ at order ω . However, the $\sin \phi$ rule does not hold, and an oscillating potential at even one site can pump current, if ω is larger than the resonance width; in that case $E_0 + \omega$ and $E_0 - \omega$ will be sufficiently different from each other so that $|r_{R,1}|^2$ and $|r_{R,-1}|^2$ or $|t_{R,1}|^2$ and $|t_{R,-1}|^2$ are no longer almost equal to each other. The violation of the $\sin \phi$ rule will be explicitly demonstrated below for the case of pumping at two sites.

We will now illustrate the above results for the case in which there are two static δ -function potentials given by

$$a_1 \delta(x - x_1) + a_2 \delta(x - x_2). \quad (12)$$

Defining $u_i = a_i/v_F$, we find the following expressions for the reflection and transmission amplitudes as functions of the wave number k ,

$$\begin{aligned} t_R &= t_L = \frac{1}{1 + i(u_1 + u_2) - u_1 u_2 (1 - e^{i2(k+k_F)(x_2-x_1)})}, \\ r_L &= t_R [-iu_1 e^{i2(k+k_F)x_1} - iu_2 e^{i2(k+k_F)x_2} \\ &\quad + u_1 u_2 (e^{i2(k+k_F)x_1} - e^{i2(k+k_F)x_2})], \\ r_R &= t_R [-iu_1 e^{-i2(k+k_F)x_1} - iu_2 e^{-i2(k+k_F)x_2} \\ &\quad - u_1 u_2 (e^{-i2(k+k_F)x_1} - e^{-i2(k+k_F)x_2})]. \end{aligned} \quad (13)$$

These expressions simplify considerably if $u_1 = u_2 = u$, i.e., if we have a symmetric double barrier. Defining $\theta = (k + k_F)(x_2 - x_1)$, we obtain

$$|t_R|^2 = |t_L|^2 = \frac{1}{1 + 4u^2 (\cos \theta + u \sin \theta)^2}. \quad (14)$$

We then see that $|t_R| = |t_L| = 1$, i.e., there is a resonance, whenever $\tan \theta = -1/u$. This occurs at $\theta = (n + 1/2)\pi$ for $u \rightarrow 0$ and at $n\pi$ for $u \rightarrow \infty$. For $|u| \gg 1$, the resonances are very sharp, with $|t_R|^2$ dropping to $1/2$ when one deviates from one of the resonant values of θ by $1/(2u^2)$, namely, when k_F deviates from one of the resonant values by $1/(2u^2|x_2 - x_1|)$.

Similar to other models considered in the earlier literature, we can now study what happens when an electron is incident on the symmetric double barrier with an energy E_0 which is *not* at resonance, but the pumping frequency is such that $E_0 + \omega$ or $E_0 - \omega$ is equal to one of the resonant energies called E_r . Then the oscillating potentials can change the energy of the electron to E_r which can then transmit through the double barrier. Thus the pumping can help the electrons to access a resonance. We will compare below the cases of pumping at one site versus two sites, and also study the dependence of the pumped current on the phase difference ϕ in the case of two-site pumping.

In Fig. 1, we show the pumped dc current $I_{R,dc}$ versus the Fermi energy E_F when there is a static and symmetric double barrier and an oscillating potential is applied at one site lying on the left of the double barrier. As E_F increases, we observe first a maximum at $E_F = 0.883$,

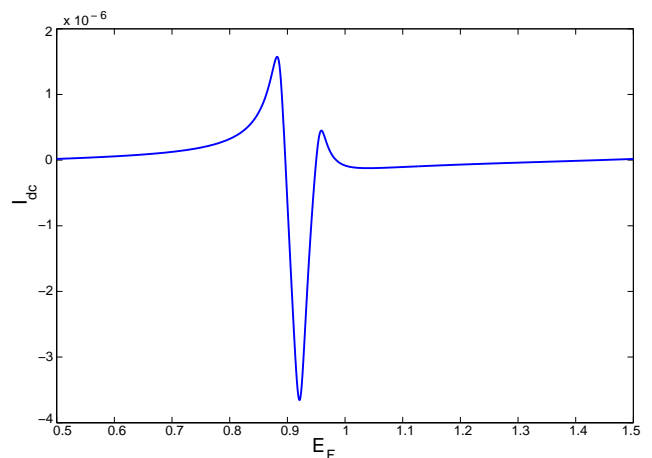


FIG. 1: (Color online) Current pumped through a symmetric double barrier by an oscillating potential applied at one site as a function of E_F . The barrier strengths u_i are both equal to 4, and their positions are at 0 and π . The resonant energy is $E_r = 0.917$, and no bias is applied. The oscillating potential is applied at the position $-\pi$ with an amplitude 0.2 and frequency 0.035. We set $v_F = 1$. The locations of the two maxima and the minimum in the middle are discussed in the text.

then a minimum at 0.921, and then a small maximum at 0.960. These features arise for the following reasons. The first maximum at 0.883 coincides with $E_r - \omega$ within a spread given by the resonance width $1/(2\pi u^2) \simeq 0.010$ (note that this is significantly less than the pumping frequency $\omega = 0.035$). This occurs because an electron approaching from the left reservoir with an energy equal to $E_F = E_r - \omega$ can get boosted up to the energy E_r due to the oscillating potential; it can then transmit through the double barrier. The minimum at 0.921 coincides with E_r ; note that this corresponds to a negative current, namely, the current is flowing to the left. This occurs due to a combination of two effects. An electron approaching from the right reservoir with an energy equal to $E_F = E_r$ transmits through the double barrier; it can then get boosted to the energies $E_r \pm \omega$ by the oscillating potential, which means that it cannot transmit back to the right through the double barrier. Similarly, an electron approaching from the left reservoir with the an energy equal to $E_F = E_r$ can get boosted to the energies $E_r \pm \omega$ by the oscillating potential, which means that it cannot transmit to the right through the double barrier. Hence, in both cases, the electron finds it easier to go to the left than to the right, leading to a net current to the left. Finally, the small maximum at 0.960 coincides with $E_r + \omega$. This maximum is not very robust; its height can change easily depending on the values of the various parameters because it is a result of several competing processes. An electron approaching from the right reservoir with an energy equal to E_r (which is less than E_F) transmits through the double barrier; it can

then get boosted to the energies $E_r \pm \omega$ by the oscillating potential and then escape to the left reservoir. On the other hand, an electron approaching from the left reservoir with an energy equal to $E_r \pm \omega$ can get boosted to the energy E_r by the oscillating potential, which means that it can then transmit to the right through the double barrier. Depending on which of these is larger, the net current can be positive or negative.

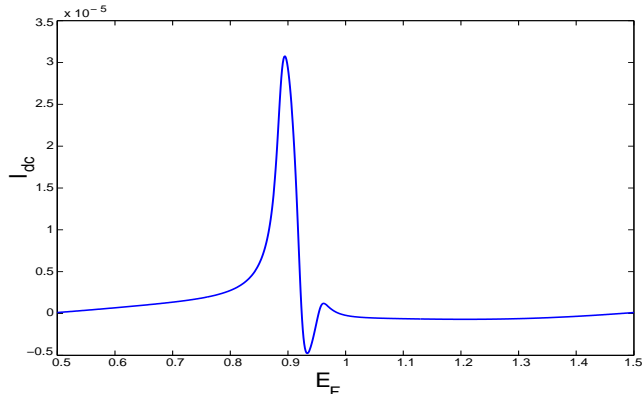


FIG. 2: (Color online) Current pumped through a symmetric double barrier by oscillating potentials applied at two sites. The barrier strengths are both equal to 4, and their positions are at 0 and π . The resonant energy is $E_r = 0.917$, and no bias is applied. The oscillating potentials are applied at the positions $-\pi$ and -2π with the same amplitude 0.2 and frequency 0.035, but with a phase difference of $\pi/2$. We set $v_F = 1$. The locations of the maxima and the minimum are discussed in the text.

In Fig. 2, we show the pumped dc current versus the Fermi energy E_F when there is a symmetric double barrier and oscillating potentials are applied at two sites (lying on the left of the double barrier) with a phase difference of $\pi/2$ between the two potentials. Just as in Fig. 1, as E_F increases, we observe first a maximum at $E_F = 0.895$, then a minimum at 0.932, and then a small maximum at 0.963. The reasons for all these features are the same as the ones discussed above for Fig. 1. We observe that the maximum value of the pumped current in Fig. 2 is about 10 times the corresponding value in Fig. 1, showing that pumping by two oscillating potentials can be much more effective than by one oscillating potential. This can be qualitatively understood as follows. If oscillating potentials are applied to K sites, and their effects add up constructively, the reflection and transmission amplitudes in the first side band would be of the order of K times what one would get if there was pumping at only one site; this is evident from Eqs. (9). The pumped current would therefore be magnified by a factor of K^2 .

In Fig. 3, we show the pumped dc current as a function of the phase difference between oscillating potentials applied at two sites, for four different values of the Fermi energy E_F . These values have been chosen to lie between

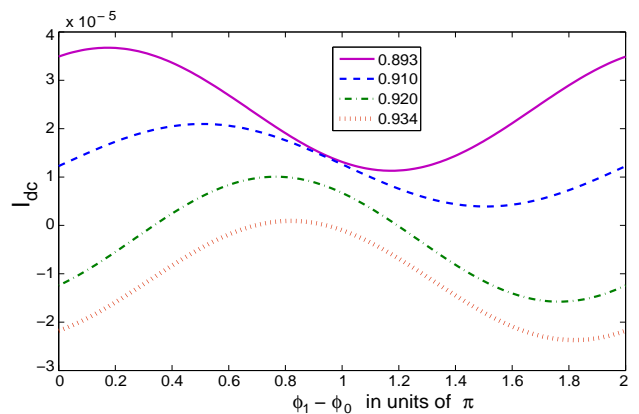


FIG. 3: (Color online) Current pumped through a symmetric double barrier by oscillating potentials applied at two sites as a function of the phase difference $\phi_2 - \phi_1$, for four different Fermi energies given by 0.893 (magenta solid line), 0.910 (blue dashed line), 0.920 (green dotted-dashed line) and 0.934 (red dotted line). The barrier strengths are both equal to 4, and their positions are at 0 and π . The resonant energy is $E_r = 0.917$, and no bias is applied. The oscillating potentials are applied at the positions $-\pi$ and -2π with the same amplitude 0.2 and frequency 0.035. We set $v_F = 1$.

the first maximum and the minimum observed in Fig. 2. We observe that all the four curves are approximately of the form $d_1 + d_2 \sin(\phi_2 - \phi_1 + d_3)$, where the values of d_1 , d_2 and d_3 are different for the different curves. All of these differ from a simple $\sin \phi$ rule which would correspond to the parameters d_1 and d_3 being equal to 0. This violation of the $\sin \phi$ rule occurs here because we have chosen ω to be larger than the resonance width. The demonstration of this violation is one of the main results of this section.

The results in this section can be generalized to finite temperatures by using the appropriate Fermi functions in Eq. (10). One of the effects of a finite temperature T is to introduce a finite phase decoherence length given by $l_\phi = \hbar v_F / (k_B T)$ [64]. We expect this to destroy the resonance produced by the static double barrier when l_ϕ becomes smaller than the distance between the barriers; hence the peaks in the pumped current will become broad and eventually disappear.

III. CHARGE PUMPING ON A FINITE RING

In this section, we will study what happens when oscillating potentials are applied to a finite-sized ring which is *not* coupled to any reservoirs. This study may possibly be of interest in the context of transport in mesoscopic rings or even molecular rings [10] which are either not coupled to any reservoirs or are so weakly coupled to reservoirs that the momentum relaxation and phase decoherence times are much longer than the time period of

the oscillating potentials. (A discussion of the possible experimental applications of our work will be presented in Sec. IV). Once again, we will consider non-interacting spinless electrons. The Hamiltonian will be taken to be of the tight-binding form with nearest-neighbor hopping amplitudes and on-site potentials which are either static or oscillating with a time period T . Namely, we have $H = H_0 + V(t)$, where

$$H_0 = - \sum_{n=1}^N \gamma (c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_n) + \sum_{n=1}^N a_n c_n^\dagger c_n, \\ V(t) = \sum_{n=1}^N w_n(t) c_n^\dagger c_n, \quad (15)$$

where $w_n(t) = w_n(t+T)$ with T denoting the time period. (We will set the hopping amplitude $\gamma = 1$ in all our numerical calculations). Note that we have included all the static potentials in H_0 . We will impose the condition that

$$\int_0^T dt w_n(t) = 0 \quad (16)$$

for all n ; if necessary, this can be ensured by adding a constant to $w_n(t)$ and subtracting the same constant from a_n in H_0 . We are therefore assuming that V satisfies

$$\int_0^T dt V(t) = 0. \quad (17)$$

We will impose periodic boundary conditions, so that $N+1 \equiv 1$ in Eq. (15). It will be convenient below to rewrite the operators in Eq. (15) as $N \times N$ matrices in the one-particle basis. Namely,

$$(H_0)_{jk} = -\gamma (\delta_{j,k+1} + \delta_{j,k-1}) + \sum_n a_n \delta_{j,k} \delta_{j,n}, \\ (V(t))_{jk} = \sum_n w_n(t) \delta_{j,k} \delta_{j,n}. \quad (18)$$

We will now study various features of this model; in particular, we will calculate the current averaged over one time period for different choices of the oscillating potential $V(t)$. We will assume that the system is not connected to any external reservoirs and has no mechanism for momentum relaxation or phase decoherence. We will begin with a given initial state in which the lowest p energy levels of the Hamiltonian H_0 in Eq. (15) are filled (so that the filling fraction is p/N), and then evolve the system in time using only the total Hamiltonian H given by Eq. (15). Consider the current operator for the bond $(n, n+1)$,

$$\hat{J}_n = -i (c_n^\dagger c_{n+1} - c_{n+1}^\dagger c_n), \quad (19)$$

or, in matrix form,

$$(\hat{J}_n)_{jk} = -i (\delta_{j,n} \delta_{k,n+1} - \delta_{j,n+1} \delta_{k,n}). \quad (20)$$

(Note that this matrix is Hermitian, imaginary and antisymmetric). We can then obtain the average value of the current at that bond by calculating the expectation value of \hat{J}_n over many time periods as described below; let us denote this average value by I_{dc} . Note that in the absence of reservoirs, the system will not reach a steady state. The quantity I_{dc} should therefore not be thought of a steady state current; it is merely the current averaged over many time periods. We will see that apart from the average part called I_{dc} , the current continues to oscillate in an aperiodic manner even if we wait for a period of time which is much longer than T .

The time evolution of the system is governed by the unitary time evolution operator

$$U(t) = \lim_{M \rightarrow \infty} \mathcal{T} \prod_{j=1}^M e^{-iH(t_j)dt}, \quad (21)$$

where \mathcal{T} stands for time ordering (namely, $\mathcal{T}\mathcal{O}(t_1)\mathcal{O}(t_2) = \mathcal{O}(t_1)\mathcal{O}(t_2)$ if $t_1 > t_2$), and we have divided the time t into M equal steps, i.e., $dt = t/M$ and $t_j = (j-1/2)dt$; eventually, we have to take the limit $M \rightarrow \infty$. We now consider $U(T)$ where T is the time period. Let v_j and $e^{i\theta_j}$ denote the eigenstates and corresponding eigenvalues of $U(T)$, with $j = 1, 2, \dots, N$. Due to the periodicity of H in time, we see that $U(sT)v_j = e^{is\theta_j}v_j$ for any positive integer s . Let us assume for simplicity that there is no degeneracy, so that $e^{i\theta_j} \neq e^{i\theta_k}$ if $j \neq k$; we can take the v_j 's to form an orthonormal basis.

We observe that if the periodic potentials in Eq. (15) are all shifted in time by the same amount, i.e., $w_n(t) \rightarrow w_n(t+\tau)$, where τ lies in the range $[0, T]$, this generally changes the unitary operator $U(T)$. However, if we redefine the vectors $v_j \rightarrow v'_j = U(\tau)v_j$, we can use the periodicity of $w_n(t)$ to show that the v'_j will be eigenstates of the new operator $U'(T)$ with the *same* eigenvalues $e^{i\theta_j}$. This can be proved as follows. Let us introduce a two-parameter notation for the time evolution operator

$$U_2(t', t) = \lim_{M \rightarrow \infty} \mathcal{T} \prod_{j=1}^M e^{-iH(t_j)dt}, \quad (22)$$

where $t_j = t + (j-1/2)dt$, and $dt = (t' - t)/M$. According to this notation, what we called $U(t)$ earlier is actually $U_2(t, 0)$ and the time shifted operator $U'(T)$ is $U_2(T + \tau, \tau)$. The periodicity of $w_n(t)$ then implies that $U_2(T + \tau, \tau)U_2(\tau, 0) = U_2(\tau, 0)U_2(T, 0)$, namely, that $U'(T)U(\tau) = U(\tau)U(T)$. Hence $U(T)v_j = e^{i\theta_j}v_j$ implies that $v'_j = U(\tau)v_j$ satisfies $U'(T)v'_j = e^{i\theta_j}v'_j$. Next, let us define the matrix for the current averaged over one time period,

$$(\hat{J}_n)_{jk} = \frac{1}{T} \int_0^T dt v'_j{}^\dagger U^\dagger(t) \hat{J}_n U(t) v_k. \quad (23)$$

Then we can use the identity $U(t)U^\dagger(\tau) = U(t-\tau)$, for $t \geq \tau$, to show that

$$v'_j{}^\dagger U^\dagger(t) \hat{J}_n U(t) v_k = (v'_j)^\dagger U^\dagger(t-\tau) \hat{J}_n U(t-\tau) v'_k. \quad (24)$$

Integrating both sides of Eq. (24) over one time period T , we see that the quantities $(\hat{J}_n)_{jk}$ defined in Eq. (23) are invariant under a shift in time by an arbitrary amount τ .

We now begin with an initial one-particle state ψ_a at time $t = 0$. This can be written as a linear superposition, $\psi_a = \sum_j c_{aj} v_j$, where $c_{aj} = v_j^\dagger \psi_a$. If we evolve this initial state using the Hamiltonian H , the current averaged over an infinitely long time will be given by

$$\begin{aligned} J_n(\psi_a) &= \lim_{s \rightarrow \infty} \frac{1}{sT} \int_0^{sT} dt \psi_a^\dagger U^\dagger(t) \hat{J}_n U(t) \psi_a \\ &= \lim_{s \rightarrow \infty} \frac{1}{s} \sum_{m=0}^{s-1} \sum_{j,k} e^{im(\theta_k - \theta_j)} c_{aj}^* c_{ak} (\hat{J}_n)_{jk}. \end{aligned} \quad (25)$$

Since we have assumed that there is no degeneracy, i.e., $e^{i(\theta_k - \theta_j)} \neq 1$ if $j \neq k$, we see that

$$\lim_{s \rightarrow \infty} \frac{1}{s} \sum_{m=0}^{s-1} e^{im(\theta_k - \theta_j)} = \delta_{j,k}. \quad (26)$$

Hence Eq. (25) simplifies to

$$J_n(\psi_a) = \sum_{j=1}^N |c_{aj}|^2 (\hat{J}_n)_{jj}. \quad (27)$$

We thus have a simple expression for the current averaged over an infinite amount of time, even though the current will oscillate in an aperiodic manner at all times due to the factor of $e^{im(\theta_k - \theta_j)}$ in Eq. (25). Finally, if we start at $t = 0$ with p electrons occupying the orthonormal states ψ_a , where $a = 1, 2, \dots, p$, the current averaged over an infinite time will be given by

$$I_{dc} = \sum_{a=1}^p \sum_{j=1}^N |c_{aj}|^2 (\hat{J}_n)_{jj}. \quad (28)$$

We have numerically computed the diagonal part of the averaged current $(\hat{J}_n)_{jj}$ for several different situations. For the case in which H is real, we have made the following observations, all of which will be seen to be quite different from the situation on the infinite line.

(i) If the periodic potentials $w_n(t)$ are shifted in time by an amount τ as described above, the value of $(\hat{J}_n)_{jj}$ changes in general. This is because the overlaps $|c_{aj}|^2$ of the new eigenstates v'_j with the initial states ψ_a is given by

$$|c_{aj}|^2 = |v_j^\dagger U^\dagger(\tau) \psi_a|^2 \quad (29)$$

which will generally depend on τ , except in the trivial limit in which all the oscillating potentials $w_n(t)$ are set equal to zero. Hence the averaged current given in Eq. (28) will vary with τ , even though $(\hat{J}_n)_{jj}$ is independent of τ as discussed earlier. All this is quite different from the situation on the infinite line where the time averaged

current does not change if all the periodic potentials are shifted in time by the same amount.

We note, however, that the dependence of I_{dc} on the shift τ (or, equivalently, the overall phase of all the oscillating potentials) is weak if the amplitudes of all the oscillating potentials are small compared to the hopping amplitude γ . This statement will be made more precise below.

(ii) If the periodic potential is time reversal invariant, i.e., if $w_n(t) = w_n(-t)$ which is also equal to $w_n(T - t)$ due to the periodicity in time, then $(\hat{J}_n)_{jj} = 0$ for each value of j . We will present an analytical proof of this below. From this it follows that $(\hat{J}_n)_{jj} = 0$ even if the periodic potential is time reversal invariant only up to a shift, i.e., if $w_n(t) = w_n(\tau - t)$ for some value of τ . This too differs from the situation on the infinite line where the averaged current is non-zero even if the periodic potential is time reversal invariant, as long as the static potentials break the left-right symmetry.

(iii) If the periodic potential is applied to only one site, then $(\hat{J}_n)_{jj} = 0$ even if the potential has no particular symmetry in time. We have found this numerically for a wide variety of potentials $w_n(t)$; $(\hat{J}_n)_{jj}$ always turns out to be zero to very high precision. We have no analytical understanding of this remarkable result. This is also different from the situation on the infinite line where we have already seen that an oscillating potential applied to only one site can pump current if the static potentials break left-right symmetry.

We will now prove analytically that $(\hat{J}_n)_{jj} = 0$ if H is real and $w_n(t) = w_n(T - t)$ for all n . Following the notation of Eq. (21), this property of $w_n(t)$ implies that

$$(e^{-iH(t)dt})^* = (e^{-iH(T-t)dt})^{-1}, \quad (30)$$

and therefore that $U^*(T) = U^{-1}(T)$. Hence $U(T)v_j = e^{i\theta_j} v_j$ implies that $U(T)v_j^* = e^{i\theta_j} v_j^*$. The non-degeneracy of the eigenvalues of $U(T)$ then implies that v_j^* must be proportional to v_j . Hence we can multiply the v_j 's by appropriate phases to ensure that $v_j^* = v_j$ for each value of j . Next, we can use Eq. (30) to show that

$$U(T-t) = U^*(t)U(T) \quad (31)$$

for any value of t lying in the range $[0, T]$. We can now combine Eq. (31) with the reality of v_j to show that $v_j^\dagger U^\dagger(T-t) \hat{J}_n U(T-t) v_j$, which must be real since \hat{J}_n is Hermitian, is equal to $v_j^\dagger U^\dagger(t) \hat{J}_n^* U(t) v_j = -v_j^\dagger U^\dagger(t) \hat{J}_n U(t) v_j$ since $\hat{J}_n^* = -\hat{J}_n$. We thus see that

$$(\hat{J}_n)_{jj} = \frac{1}{T} \int_0^T dt v_j^\dagger U^\dagger(t) \hat{J}_n U(t) v_j = 0 \quad (32)$$

due to an exact cancellation of the integrand at the times t and $T - t$.

In Fig. 4, we show that the current integrated over one time period is zero if an oscillating potential is applied to only one site; as a specific example, we have considered

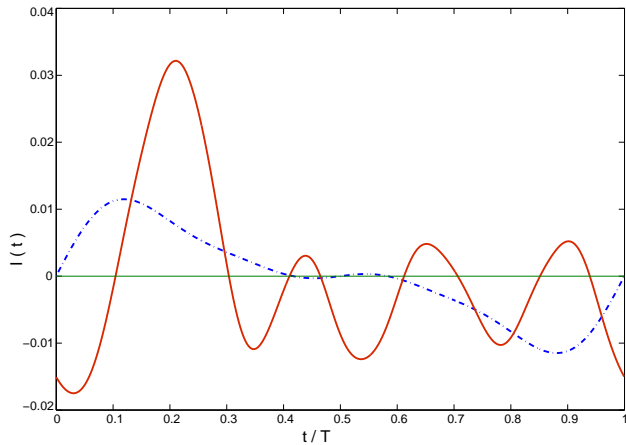


FIG. 4: (Color online) Instantaneous current at various times over one time period $T = 10\pi$ (corresponding to $\omega = 0.2$) for an oscillating potential applied at one site, for the third eigenstate of $U(T)$ for a six-site system. Two cases are considered: the oscillating potential is (i) time-reversal invariant (blue dashed line), and (ii) not time-reversal invariant (red solid line). A static potential of strength 1 is applied at site 2, while the oscillating potential is applied at site 3. For case (i) with an oscillating potential $\cos(\omega t) + 0.2 \cos(2\omega t)$, we see an exact cancellation between the values at times t and $T - t$, while case (ii) with an oscillating potential $\cos(\omega t) + 0.5 \sin(2\omega t)$ does not show such a pair-wise cancellation. In both cases, the integrated current contributed by the third eigenstate is zero.

the contribution to the current from the third eigenstate of $U(T)$ for a ring with six sites, when a static potential and an oscillating potential are applied to two different sites. The way in which the current integrates to zero is quite different depending on whether the oscillating potential is time reversal invariant or not. If the oscillating potential is time reversal invariant, the integrated current vanishes due to a pair-wise cancellation from the times t and $T - t$ as we have proved above. But if the oscillating potential is not time reversal invariant, there is apparently no simple symmetry reason for the vanishing of the integrated current.

Since the integrated current vanishes if an oscillating potential is applied to only one site, we will now study what happens when oscillating potentials are applied to two sites. In all the figures discussed below (Figs. 5-9), we will consider a six-site system in which a static potential is applied at site 2, and oscillating potentials of the forms $b \cos(\omega t + \phi_0)$ and $b \cos(\omega t + \pi/2 + \phi_0)$ are applied at sites 3 and 4 respectively.

We first study the dependence of the pumped current on the overall phase ϕ_0 of the oscillating potentials. We take $b = 0.1$, and use Eqs. (28-29) to compute the averaged current as a function of $\phi_0 = 2\pi\tau/T$. In Fig. 5, we show the dependence of the current I_{dc} on ϕ_0 when the system has three electrons which corresponds to half-filling. We find that the variation of I_{dc} from its mean

value is about 8%. When we reduce b by a factor of 2, we find that the mean value of I_{dc} decreases by a factor of 4 while its variation with ϕ_0 decreases by a factor of 16. In the Appendix, we show that the mean value of I_{dc} scales as b^2 which is in agreement with the numerical result quoted above. In addition, the numerics suggests that the variation of I_{dc} with ϕ_0 scales as b^4 . Thus, if the pumping amplitude b is small compared to the hopping amplitude γ , the variation of the pumped current with ϕ_0 becomes much smaller than the current itself.

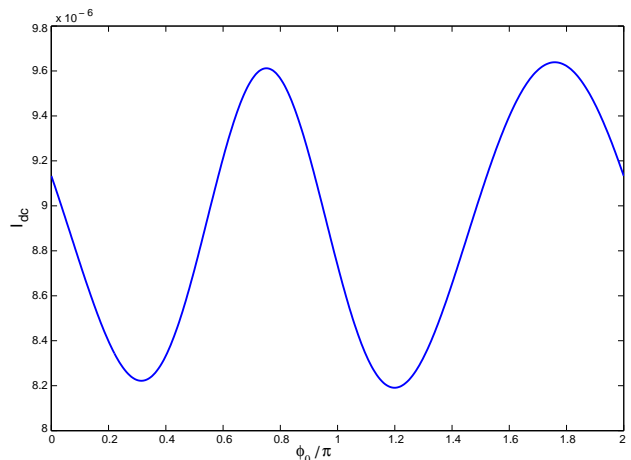


FIG. 5: (Color online) Total pumped current versus the overall phase for oscillating potentials applied at two sites, for a six-site ring with three electrons. A static potential of strength 1 is applied at site 2, while the oscillating potentials are applied at sites 3 and 4 with an amplitude $b = 0.1$, a frequency $\omega = 0.2$, and a phase difference of $\pi/2$.

Next, we consider the contributions to the averaged pumped currents, $I_j \equiv (\hat{J}_n)_{jj}$ of the different eigenstates of $U(T)$, taking the overall phase to be given by $\phi_0 = 0$. For the six-site ring, with a static potential of strength 1 applied at site 2, the eigenvalues of the static part of the Hamiltonian, H_0 , are equal to -1.8912 , -1.0000 , -0.7046 , 1.0000 , 1.3174 , and 2.2784 . In Fig. 6, we show the six contributions I_j as a function of the oscillation amplitude b , when the oscillation frequency $\omega = 0.2$ is non-resonant, i.e., it does not correspond to the difference between any two energy levels of H_0 . We see that all the curves show a quadratic dependence on b , although two of them lie very close to zero; the quadratic dependence is in accordance with the results derived in the Appendix for the non-resonant case. In Fig. 7, we show the total pumped current I_{dc} versus b when there are three electrons, where I_{dc} has been calculated using Eq. (28) and the individual pumped currents shown in Fig. 6.

In Fig. 8, we show the contributions I_j as a function of b , when the oscillation frequency $\omega = 1.7046$ is resonant; it corresponds to the difference between the third and fourth energy levels of H_0 . We see that four of the curves lie very close to zero and show a quadratic

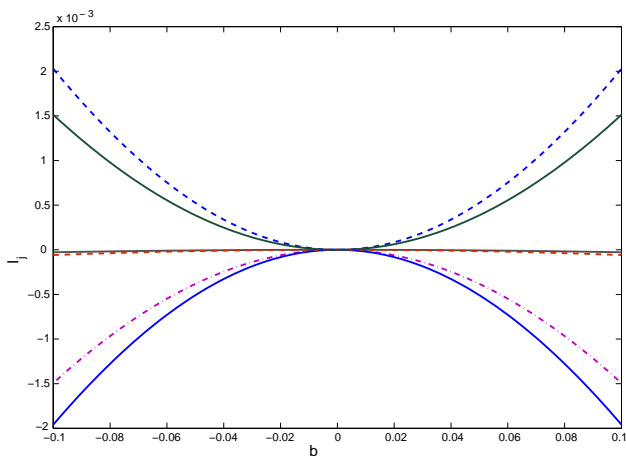


FIG. 6: (Color online) Pumped currents for all the eigenstates of $U(T)$ for oscillating potentials applied at two sites versus the oscillation amplitude b , for a six-site ring. A static potential of strength 1 is applied at site 2, while the oscillating potentials are applied at sites 3 and 4 with a phase difference of $\pi/2$ and a non-resonant frequency $\omega = 0.2$. In all cases, the current is proportional to b^2 for small b .

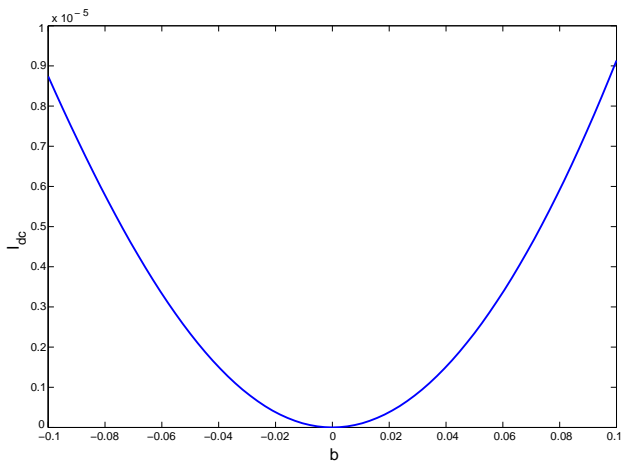


FIG. 7: (Color online) Total pumped current for oscillating potentials applied at two sites versus the oscillation amplitude b , for a six-site ring with three electrons. All the parameters are the same as in Fig. 6.

dependence on b , but the other two curves, which have large contributions from the third and fourth eigenstates of H_0 , show a linear dependence on b ; the linear dependence agrees with the results derived in the Appendix for the resonant case. In Fig. 9, we show the total current I_{dc} versus b when there are three electrons. This current varies quadratically with b for the following reasons. First, the two states which show a linear dependence on b in Fig. 8 are found to contribute with equal weight to I_{dc} . Secondly, the slopes of these two curves in Fig. 8

are equal and opposite at $b = 0$. Hence the linear dependences on b of these two curves cancel out when they are added up using Eq. (28) to calculate I_{dc} which therefore shows a quadratic dependence on b . We also observe that the currents in Fig. 9 are about 90 times those in Fig. 7, for the same values of b ; this shows the effectiveness of charge pumping at resonant versus non-resonant frequencies.

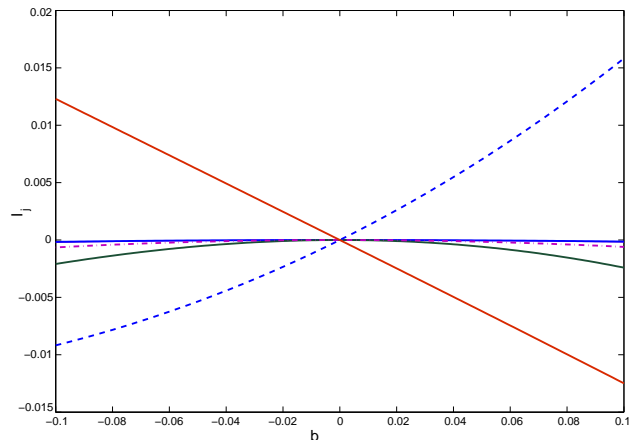


FIG. 8: (Color online) Pumped currents for all the eigenstates of $U(T)$ for oscillating potentials applied at two sites versus the oscillation amplitude b , for a six-site ring. A static potential of strength 1 is applied at site 2, while the oscillating potentials are applied at sites 3 and 4 with a phase difference of $\pi/2$ and a resonant frequency $\omega = 1.7046$. In four cases, the current is proportional to b^2 , but in two cases, the current is proportional to b for small b (see text for details).

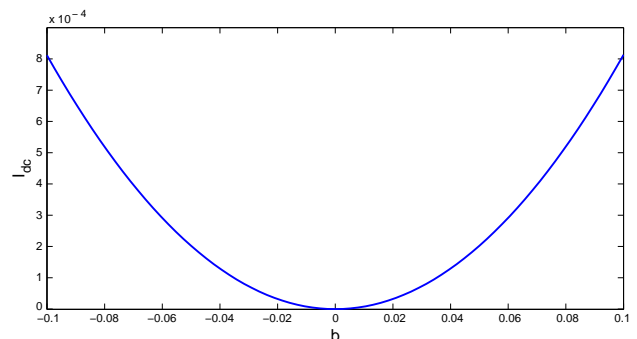


FIG. 9: (Color online) Total pumped current for oscillating potentials applied at two sites versus the oscillation amplitude b , for a six-site ring with three electrons. All the parameters are the same as in Fig. 8.

Finally, let us briefly discuss what happens if the Hamiltonian is not real. For instance, if there is a magnetic flux passing through the ring, its effects can be studied by making the hopping amplitudes γ complex in Eq. (15). In such cases, we find that there can be a net dc

current in the ground state even in the absence of any oscillating potentials; this is called a persistent current. The value of the dc current can then change even if we apply oscillating potentials which are time reversal invariant or if an oscillating potential is applied at only one site.

IV. DISCUSSION

To summarize, we have studied charge pumping both on an infinite line and on a finite ring, for a system of non-interacting electrons at zero temperature. For the infinite line with reservoirs at the same chemical potential on the two sides, we have verified, in agreement with earlier work, that oscillating potentials applied to one or two sites can pump a net dc current as long as the left-right symmetry is broken by some static potentials; the oscillating potentials do not need to break time reversal invariance [22]. As a specific example, we have studied pumping in a situation where the Fermi energy differs from the resonant energy, but the pumping frequency is equal to the difference of the those two energies. We have contrasted the cases of pumping at one site and two sites. We have also shown that the $\sin \phi$ rule, which holds in the adiabatic limit ($\omega \rightarrow 0$) for pumping by two oscillating potentials with a phase difference of ϕ , fails if ω is larger than the resonance width.

For a purely Hamiltonian evolution on a finite ring, we have shown that if both the static and time-dependent parts of the Hamiltonian are real, the net dc current is zero either if the oscillating potentials are time reversal invariant or if the oscillating potential is applied to only one site. We have presented an analytical proof of the former statement and have presented numerical evidence for the latter. It would be very useful if an analytical proof could be found for the vanishing of the current for one-site pumping with an arbitrary time dependence.

We have argued that for a purely Hamiltonian evolution, the system on a ring does not reach a steady state; the current averaged over one time period T continues to vary with time in an aperiodic manner although there is a simple expression for the current averaged over an infinitely long time. Further, the averaged current depends on the initial state and on the overall phase of the oscillating potentials since these two determine the overlap between the initial state and the eigenstates of the evolution operator $U(T)$.

The facts that a steady state is not reached and that breaking of time reversal invariance of the oscillating potentials is required for charge pumping to occur on a finite ring but not on an infinite line is due to an important difference between the models that we have assumed in the two cases. For the finite ring, we have assumed a purely Hamiltonian evolution, with no mechanisms for momentum relaxation or phase decoherence. On the other hand, the study of the infinite line assumed that there are reservoirs which are maintained at certain

chemical potentials. This implicitly assumes that there are mechanisms for energy or momentum relaxation; for instance, if an electron emerges from the double barrier with an energy equal to the resonant energy E_r , we assume that when it reaches one of the reservoirs, it will relax down to the Fermi energy E_F if $E_r > E_F$. It appears that such relaxation processes, which we have not explicitly referred to in our calculations but which are necessarily present in the reservoirs, effectively lead to a breaking of time reversal invariance which is required to have a net dc current on the infinite line. An earlier study has shown that if a finite ring is coupled to reservoirs, then charge pumping can occur even if the oscillating potentials are time reversal invariant [26].

It is also worth noting that on a finite ring, an electron which emerges to the right from the region containing the potentials (both static and oscillating) eventually comes back and enters the same region from the left. Thus the outgoing current on the right of that region must be equal to the incoming current on the left, when these currents are averaged over a long time. Similarly, the averaged outgoing current on the left of the region must be equal to the averaged incoming current on the right. These relations do not hold on the infinite line since an electron going out to the right (left) does not return to the left (right) of the region containing the potentials.

We now turn to the possible experimental implications of our results. It is possible that the dependence of the averaged pumped current on the initial state and on the overall phase of the oscillating potentials on a ring with no mechanisms for momentum and phase relaxation can be observed experimentally. For mesoscopic rings which have a large number of impurities which lead to elastic scattering, the transport is diffusive and is characterized by a diffusive round-trip time τ_d which is equal to $3L^2/(v_F l_c)$, where l_c is the mean free path and L is the circumference of the ring [65]. Another important length scale for ring systems is the phase coherence length l_ϕ which depends strongly on the temperature [64, 66, 67]. However, one may consider wires which have a sufficiently low density of scatterers and are at sufficiently low temperatures that both l_c and l_ϕ are much larger L . In such a situation, we expect that if the pumping potentials are suddenly switched on, then the averaged pumped current will initially depend on the overall phase of the potentials. Eventually, at time scales which are much longer than l_ϕ/v_F and τ_d , the averaged pumped current will no longer remember the overall phase; however, a proof of this is beyond the scope of our analysis since we have not introduced any mechanisms for momentum and phase relaxation.

Another arena where our results could possibly be tested is the field of molecular electronics [42, 68]. We would like to propose an experimental set-up as follows. The conductance properties of aromatic molecules (which typically have a ring-like structure) have been studied extensively for several years. Typically, the transport properties of such molecules are studied by depositing

the molecule on a substrate and using an scanning tunnel microscope (STM) tip from above to probe the molecule [68]. The number of electrons in the molecule can be fixed initially by bringing the STM tip close to the molecule and applying the correct potential to the tip. We propose that the distance of the STM tip from the molecule can then be increased so that electron tunneling between the STM and the molecule becomes negligible; however the STM tip can still be used to induce an on-site pumping (oscillating) potential at a particular atom. This can be used to study the effect of pumping on the electronic transport through the molecule. A theoretical analysis of this would also require us to consider the effect of interactions between the electrons.

An interesting problem for future studies may be to include the effects of interactions between the electrons [69]. In particular, one can study whether interactions modify some of the peculiar features observed on the finite ring, such as the absence of pumping for an oscillating potential which is applied to only one site. In this context, we note that interactions between electrons are believed to play a role in determining the magnitude of the persistent current in rings placed in a magnetic field [70].

Acknowledgments

We thank A. Agarwal, A. Dhar, D. Dhar, A. Jayanavar, M. Moskalets and M. Stone for stimulating discussions. A. S. thanks CSIR, India for financial support, and D. S. thanks DST, India for financial support under Project No. SR/S2/CMP-27/2006.

Appendix

We will use first order perturbation theory to derive expressions for the eigenstates of $U(T)$ on a finite ring and the integrated current in those eigenstates, for both the non-resonant and resonant cases. The treatment below will be seen to have interesting parallels with the use of first order perturbation theory to obtain the eigenstates of a time-independent Hamiltonian in the non-degenerate and degenerate cases respectively.

The Hamiltonian of interest is $H = H_0 + V(t)$, where $V(t)$ has a periodicity given by $T = 2\pi/\omega$. Let us first set $V = 0$. H_0 will have a complete set of orthonormal eigenstates ψ_j and eigenvalues E_j , where we will assume, for simplicity, that the E_j 's are non-degenerate. We will also assume that H_0 is real; hence the ψ_j 's can be chosen to be real. If a unitary evolution operator $U_0(T)$ is constructed using H_0 , its eigenstates and eigenvalues will be given by ψ_j and $e^{-iE_j T}$. Note that since the wave functions ψ_j are real and $\hat{J}_n^* = \hat{J}_n^T = -\hat{J}_n$, we have the useful

relations

$$\begin{aligned}\psi_j^\dagger \hat{J}_n \psi_j &= 0, \\ \psi_j^\dagger \hat{J}_n \psi_k &= -\psi_k^\dagger \hat{J}_n \psi_j \quad \text{for } j \neq k.\end{aligned}\quad (33)$$

We now turn on the time-dependent perturbation V which will be assumed to satisfy Eq. (17). There are two different possibilities which we will discuss separately:

- (i) Non-resonant case where $E_j - E_k$ is not an integer multiple of ω , i.e., $e^{-i(E_j - E_k)T} \neq 1$, for any pair of states j, k , and
- (ii) Resonant case where $E_j - E_k$ is an integer multiple of ω , i.e., $e^{-i(E_j - E_k)T} = 1$, but $E_j \neq E_k$, for some pair of states j, k .
- (iii) Resonant case where $E_j = E_k$ for some pair of states j, k .

Non-resonant case

We will find the eigenstate of $U(T)$, called v_1 , which differs at first order in V from a particular eigenstate of $U_0(T)$, say, ψ_1 . We assume that $v_1(t) = U(t)v_1$ has an expansion of the form

$$v_1(t) = \sum_{j=1}^N c_j(t) e^{-iE_j t} \psi_j, \quad (34)$$

where we choose $c_1(0) = 1$. (We are not worrying about the normalization of v_1 here, although we see that v_1 is normalized to 1 up to zero-th order in V). We expect that the deviation of $c_1(t)$ from 1 at different values of t and also the values of $c_j(t)$ for $j \neq 1$ will be of order V . From the Schrödinger equation

$$i \frac{dv_1(t)}{dt} = [H_0 + V(t)] v_1(t), \quad (35)$$

we find the following equations to first order in V ,

$$\begin{aligned}i \frac{dc_1(t)}{dt} &= c_1(t) \langle \psi_1 | V(t) | \psi_1 \rangle, \\ i \frac{dc_j(t)}{dt} &= c_1(t) \langle \psi_j | V(t) | \psi_1 \rangle e^{i(E_j - E_1)t}\end{aligned}\quad (36)$$

for $j \neq 1$. At first order, we can replace $c_1(t)$ by $c_1(0) = 1$ in Eqs. (36). This gives the solution

$$\begin{aligned}c_1(t) &= 1 - i \int_0^t dt' \langle \psi_1 | V(t') | \psi_1 \rangle, \\ c_j(t) &= \alpha_j - i \int_0^t dt' \langle \psi_j | V(t') | \psi_1 \rangle e^{i(E_j - E_1)t'},\end{aligned}\quad (37)$$

for $j \neq 1$, where α_j are constants of integration which can be fixed as follows. Since $c_1(T) = c_1(0)$ due to Eq. (17), we see from the ψ_1 term in Eq. (34) that $v_1(T) = e^{-iE_1 T} v_1(0)$, i.e., v_1 is an eigenstate of $U(T)$ with eigenvalue $e^{-iE_1 T}$. We therefore demand that this should also be true for all the other terms ψ_j for $j \neq 1$ in Eq. (34).

We therefore require that $c_j(T)e^{-iE_jT} = e^{-iE_1T}c_j(0)$ for all $j \neq 1$. This fixes the value of the constants α_j in Eq. (37), and we find that

$$c_j(t) = -i \frac{\int_0^T dt' \langle \psi_j | V(t') | \psi_1 \rangle e^{i(E_j - E_1)t'}}{e^{i(E_j - E_1)T} - 1} - i \int_0^t dt' \langle \psi_j | V(t') | \psi_1 \rangle e^{i(E_j - E_1)t'} \quad (38)$$

for $j \neq 1$. Combining Eqs. (34), (37) and (38), we have an expression for the eigenstate of $U(T)$ to first order in V . Note that the corresponding eigenvalue remains e^{-iE_1T} to this order; this is a consequence of the choice made in Eq. (17).

We can now calculate the current averaged over one time period for one of these eigenstates,

$$(\hat{J}_n)_{jj} = \frac{1}{T} \int_0^T dt v_j^\dagger U^\dagger(t) \hat{J}_n U(t) v_j. \quad (39)$$

Due to the fact that $\psi_j^\dagger \hat{J}_n \psi_j = 0$, the current can only get a contribution from cross-terms of the form $\psi_j^\dagger \hat{J}_n \psi_k$ for $j \neq k$ arising from Eq. (34). From Eqs. (37-38), we see that $(\hat{J}_n)_{jj}$ has no contributions of order 1, while the contributions of order V can only come from a cross-term between ψ_1 and ψ_j for $j \neq 1$. Such contributions are proportional to

$$\int_0^T dt e^{i(E_1 - E_j)t} c_j(t), \quad (40)$$

where $c_j(t)$ is given in Eq. (38). We can now do the integral in Eq. (40) explicitly and we find that it vanishes. We therefore conclude that $(\hat{J}_n)_{jj}$ only receives contributions of second order and higher in V .

Resonant case with $E_1 \neq E_2$

Let us now consider the case when two eigenstates of $U_0(T)$, say, ψ_1 and ψ_2 , have the same eigenvalue $e^{-iE_1T} = e^{-iE_2T}$ which implies that $E_1 - E_2$ is an integer multiple of ω . We will assume, however, that $E_1 \neq E_2$. We will consider only the states 1 and 2, and will study how they can be combined to form eigenstates of $U(T)$ to first order in V . Let us consider an expansion of the form

$$v(t) = c_1(t) e^{-iE_1t} \psi_1 + c_2(t) e^{-iE_2t} \psi_2, \quad (41)$$

where we now assume that both $c_1(t)$ and $c_2(t)$ are of order 1. (This is in contrast to the non-resonant case where only $c_1(t)$ was taken to be order 1). Further, let us take $c_1(0) = c_{10}$ and $c_2(0) = c_{20}$; we will assume that the deviations of $c_1(t)$ and $c_2(t)$ from c_{10} and c_{20} respectively will be of order V at all values of t . The

Schrödinger equation in Eq. (35) now gives

$$\begin{aligned} i \frac{dc_1(t)}{dt} &= c_1(t) \langle \psi_1 | V(t) | \psi_1 \rangle \\ &\quad + c_2(t) e^{i(E_1 - E_2)t} \langle \psi_1 | V(t) | \psi_2 \rangle, \\ i \frac{dc_2(t)}{dt} &= c_2(t) \langle \psi_2 | V(t) | \psi_2 \rangle \\ &\quad + c_1(t) e^{i(E_2 - E_1)t} \langle \psi_2 | V(t) | \psi_1 \rangle. \end{aligned} \quad (42)$$

At first order, we can replace $c_1(t)$ and $c_2(t)$ by c_{10} and c_{20} on the right hand sides in Eqs. (42). This gives

$$\begin{aligned} c_1(t) &= c_{10} - i c_{10} \int_0^t dt' \langle \psi_1 | V(t') | \psi_1 \rangle \\ &\quad - i c_{20} \int_0^t dt' \langle \psi_1 | V(t') | \psi_2 \rangle e^{i(E_1 - E_2)t'}, \\ c_2(t) &= c_{20} - i c_{20} \int_0^t dt' \langle \psi_2 | V(t') | \psi_2 \rangle \\ &\quad - i c_{10} \int_0^t dt' \langle \psi_2 | V(t') | \psi_1 \rangle e^{i(E_2 - E_1)t'}. \end{aligned} \quad (43)$$

Using Eq. (17), we see that

$$\begin{aligned} c_1(T) &= c_{10} - i c_{20} \int_0^T dt \langle \psi_1 | V(t) | \psi_2 \rangle e^{i(E_1 - E_2)t}, \\ c_2(T) &= c_{20} - i c_{10} \int_0^T dt \langle \psi_2 | V(t) | \psi_1 \rangle e^{i(E_2 - E_1)t}. \end{aligned} \quad (44)$$

If we now demand that the state in Eq. (41) satisfies $v(T) = e^{i\theta} v(0)$, i.e., that $v(0)$ is an eigenstate of $U(T)$ with eigenvalue $e^{i\theta}$, we find that

$$\frac{c_1(T) e^{-iE_1T}}{c_1(0)} = \frac{c_2(T) e^{-iE_2T}}{c_2(0)} = e^{i\theta}. \quad (45)$$

This implies that

$$\left(\frac{c_{20}}{c_{10}} \right)^2 = \frac{\int_0^T dt \langle \psi_2 | V(t) | \psi_1 \rangle e^{i(E_2 - E_1)t}}{\int_0^T dt \langle \psi_1 | V(t) | \psi_2 \rangle e^{i(E_1 - E_2)t}}. \quad (46)$$

Defining

$$\alpha = \frac{1}{T} \int_0^T dt \langle \psi_1 | V(t) | \psi_2 \rangle e^{i(E_1 - E_2)t}, \quad (47)$$

we see that

$$\frac{c_{20}}{c_{10}} = \pm \sqrt{\frac{\alpha^*}{\alpha}}, \quad (48)$$

so that c_{20}/c_{10} is a pure phase. Using Eqs. (44-45), we see that the \pm sign in Eq. (48) corresponds to two solutions $v_\pm(t)$ which satisfy $U(T)v_\pm(0) = e^{i\theta_\pm} v_\pm(0)$, where

$$\begin{aligned} e^{i\theta_\pm} &= e^{-iE_1T} \left[1 - i\alpha T \frac{c_{20}}{c_{10}} \right] \\ &= e^{-iT(E_1 \pm |\alpha|)} \end{aligned} \quad (49)$$

to first order in α . We thus see that the degeneracy of eigenvalues of $U_0(T)$ is broken at first order in V , with the phases θ_{\pm} being split by equal and opposite amounts.

Finally, we can compute the current averaged over one time period as defined in Eq. (39) for either one of the states, v_+ or v_- . Once again, only cross-terms of the form $\psi_1^\dagger \hat{J}_n \psi_2$ will contribute. We find that terms of order 1 vanish because they are of the form

$$\int_0^T dt [c_{10}^* c_{20} e^{i(E_1 - E_2)t} \psi_1^\dagger \hat{J}_n \psi_2 + c_{20}^* c_{10} e^{i(E_2 - E_1)t} \psi_2^\dagger \hat{J}_n \psi_1], \quad (50)$$

and $\int_0^T dt e^{i(E_1 - E_2)t} = 0$ because $E_1 - E_2$ is an integer multiple of ω but $E_1 \neq E_2$. However, unlike the non-degenerate case, there is now no reason for contributions of order V to vanish in general. Hence $(\hat{J}_n)_{jj}$ can get contributions at first order in V .

Resonant case with $E_1 = E_2$

Finally, let us consider the case when two eigenstates of H_0 , say, ψ_1 and ψ_2 , have $E_1 = E_2$. This implies that they also have the same eigenvalue $e^{-iE_1 T} = e^{-iE_2 T}$ of $U_0(T)$. As in the previous subsection, we will study how these two states can be combined to form eigenstates of $U(T)$ to first order in V .

We can check that all the discussion from Eq. (41) to (44) will remain valid in this case, except that we have to substitute $E_1 = E_2$ everywhere. We then find that

$c_1(T) = c_1(0) = c_{10}$ and $c_2(T) = c_2(0) = c_{20}$ due to Eq. (17). Further, there is now no relation between c_{10} and c_{20} ; we can choose c_{10} and c_{20} in an arbitrary way to obtain two orthonormal states v_{\pm} which are eigenstates of $U(T)$ with the same eigenvalue $e^{-iE_1 T}$. Thus the eigenvalues of $U(T)$ and their degeneracy do not change to first order in V .

When we compute the current averaged over one time period as defined in Eq. (39) for either one of the states, v_+ or v_- , we find that, depending on the choices of c_{10} and c_{20} , we can get a contribution to zero-th order in V . To be explicit, this is given by

$$\int_0^T dt [c_{10}^* c_{20} \psi_1^\dagger \hat{J}_n \psi_2 + c_{20}^* c_{10} \psi_2^\dagger \hat{J}_n \psi_1] \\ = T (c_{10}^* c_{20} - c_{20}^* c_{10}) \psi_1^\dagger \hat{J}_n \psi_2, \quad (51)$$

where we have used Eq. (33).

It may seem strange that if $E_1 = E_2$, there can be a non-zero current in the states v_+ and v_- separately even at the zero-th order in V . However, we note that an energy degeneracy usually does not occur if static potentials are present. But if there are no static potentials present, then the system is translation invariant, and we see that there are momentum eigenstates (with momenta $\pm k$) which carry equal and opposite currents even in the limit that the amplitudes of the oscillating potentials go to zero.

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