Nonadiabatic charge pumping in a one-dimensional system of noninteracting electrons
by an oscillating potential

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Using a tight-binding model, we study one-parameter charge pumping in a one-dimensional system of non-interacting electrons. An oscillating potential is applied at one site while a static potential is applied in a different region. Using Floquet scattering theory, we calculate the current up to second order in the oscillation amplitude and exactly in the oscillation frequency. For low frequency, the charge pumped per cycle is proportional to the frequency and therefore vanishes in the adiabatic limit. If the static potential has a bound state, we find that such a state has a significant effect on the pumped charge if the oscillating potential can excite the bound state into the continuum states or vice versa. Finally, we use the equation of motion for the density matrix to numerically compute the pumped current for any value of the amplitude and frequency. The numerical results confirm the unusual effect of a bound state.

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I. INTRODUCTION

The phenomenon of charge pumping and rectification by time-dependent potentials applied to certain points in a system has been extensively studied both theoretically [1-31] and experimentally [32-38]. The idea of charge pumping is that periodically oscillating potentials can transfer a net charge per cycle between two leads which are at the same chemical potential. For the case of non-interacting electrons, theoretical studies of charge pumping have used adiabatic scattering theory [9, 10, 11, 12], Floquet scattering theory [16, 17], variations of the non-equilibrium Green function formalism [18, 19, 20], and the equation of motion approach [31]. The case of interacting electrons has also been studied, using a renormalization group method for weak interactions [39], and the method of bosonization for arbitrary interactions [40-50].

Apart from a few papers [19, 20, 38], the earlier studies of charge pumping have generally studied systems in which oscillating potentials are applied to two or more sites. In such cases, it is known that if the oscillation frequency \( \omega \) is small, the dc part of the pumped current is proportional to \( \omega \); the charge pumped per cycle (with time period \( 2\pi/\omega \)) therefore has a finite value in the adiabatic limit \( \omega \to 0 \). However, an oscillating potential applied to a single site can also pump charge provided that the system has no left-right symmetry, as has been emphasized in Refs. [19, 20]. This can happen if, for instance, there is a static potential at another site. In these cases, however, the dc part of the pumped current is proportional to \( \omega^2 \), and the charge pumped per cycle is proportional to \( \omega \) if \( \omega \) is small. In this paper, we will study such a system in detail using both analytical and numerical methods. Our analysis will not be restricted to small values of \( \omega \). If \( \omega \) is large enough, we discover that a bound state (defined as a state whose energy lies outside the continuum band of the tight-binding model that we will consider) can have a significant effect on the pumped charge. Namely, although the bound state has a localized wave function and therefore cannot contribute to the current at the same energy, the electrons can be scattered from the bound state to the continuum states (lying within the band) or vice versa, and this can contribute to the current flow. This phenomenon does not seem to have received much attention in the existing literature.

The plan of the paper is as follows. In Sec. II, we will use Floquet scattering theory to obtain an expression for the pumped current produced by a single harmonically oscillating potential, when there is a static potential present at some other point in the system. Our analysis will be exact in the scattering matrix arising from the static potential and in the oscillation frequency, but it will be perturbative in the amplitude of the oscillations. The effect of a bound state produced by the static potential will also be considered using the same formalism. In Sec. III, we will use the equation of motion to numerically compute the pumped charge for the same model; this method can be used for any value of the oscillation amplitude. Our numerical results will confirm the unusual effect that a bound state can have on the pumped charge, as well as the difficulty which the equation of motion method faces in dealing with a bound state [51]. We will summarize our results in Sec. IV.

II. FLOQUET SCATTERING THEORY

Let us consider a one-dimensional system consisting of two semi-infinite leads \( a = L, R \) (denoting left and right) and a finite region called the wire which lies between the two. We will model the three regions together by a lattice model of spinless electrons governed by a one-channel tight-binding Hamiltonian with the same hopping ampli-
with energy agating modes have energies lying within the continuum where the corresponding wave function is tering matrix $p$ (right) respectively.

The static potential at the site $n = 0$ causes scattering of electrons incident from the left or right lead. If an incident electron has wave number $k$, the effect of the potential is described by a scattering matrix

$$S(k) = \begin{pmatrix} r_L & t_L \\ t_R & r_R \end{pmatrix},$$

where $r_R(k) = r_L(k) = -\frac{ia}{2γ \sin k + ia}$, $t_R(k) = t_L(k) = \frac{2γ \sin k}{2γ \sin k + ia}$. (2)

and $r_{L(R)}$ and $t_{L(R)}$ denote the reflection and transmission amplitudes for an electron coming from the left (right) respectively.

It turns out that for any value of the parameter $a \neq 0$, there is a bound state. For $a > 0$, the bound state energy $E_B = \sqrt{4γ^2 + a^2}$ lies above the continuum, and the normalized bound state wave function is

$$ψ_B(n) = (-\gamma)^n \sqrt{\tanh κ} e^{-κ|n|} \text{ for all } n, \quad (3)$$

where $κ = \sinh^{-1}(a/2γ)$. For $a < 0$, the bound state energy $E_B = -\sqrt{4γ^2 + a^2}$ lies below the continuum, and the corresponding wave function is

$$ψ_B(n) = \sqrt{\tanh κ} e^{-κ|n|} \text{ for all } n, \quad (4)$$

where $κ = \sin^{-1}(-a/2γ)$.

We now apply an oscillating potential at the site $n = r$ of the model described in Eq. 11, where we assume that $r \geq 1$. This part of the Hamiltonian is given by

$$\hat{V}(t) = b \cos(ωt) c_i^d c_r.$$

Then Floquet scattering theory works as follows [16, 17]. Incoming electrons of energy $E_0$ gain or lose energy in quanta of $ω$ on interacting with the oscillating potential. Hence, the outgoing states are characterized by energies $E_p = E_0 + pω$, where $p = 0, \pm 1, \pm 2, \ldots$; the energies with $p \neq 0$ are called the Floquet side bands. The effect of the oscillating potential can be described by a Floquet scattering matrix $S_{αβ}(E_p, E_0)$, which is the amplitude for an electron with energy $E_0$ entering through lead $β$ to leave with energy $E_p$ through lead $α$. In the leads, the propagating modes have energies lying within the continuum band $[-2γ, 2γ]$; only these modes can directly contribute to charge pumping. States with energies lying outside the continuum band have wave functions which decay exponentially into the leads and hence do not directly contribute to charge transfer. The wave function of an electron coming from the left lead with an energy $E_0$ and wave number $k_0$ (with $E_0 = -2γ \cos k_0$) is given by

$$ψ(n) = e^{i(E_0 - E_0t)} + \sum_p r_{L,p} e^{i(k_p - E_p t)} \quad (6)$$

at a site $n$ far to the left of the scattering region, and

$$ψ(n) = \sum_p t_{R,p} e^{i(k_p - E_p t)} \quad (7)$$

far to the right of the scattering region, where $E_p = -2γ \cos k_p$, and the sums over $p$ run over values such that $E_p$ lies within the continuum band of the leads. The quantities $r_{L,p}$ and $t_{R,p}$ denote reflection and transmission amplitudes in the different side bands; they respectively denote the elements $S_{LL}(E_p, E_0)$ and $S_{RL}(E_p, E_0)$ of the Floquet scattering matrix, where $L$ and $R$ denote the left and right leads. Similarly, the wave function of an electron coming from the right lead with an energy $E_0$ and wave number $k_0$ is given by

$$ψ(n) = e^{i(-k_0 - E_0 t)} + \sum_p r_{R,p} e^{i(k_p - E_p t)} \quad (8)$$

far to the right of the scattering region, and

$$ψ(n) = \sum_p t_{L,p} e^{i(k_p - E_p t)} \quad (9)$$

far to the left of the scattering region. Due to unitarity, we have the relations

$$\sum_p \frac{v_p}{v_0} \left[ |r_{L,p}|^2 + |t_{R,p}|^2 \right] = 1,$$

and

$$\sum_p \frac{v_p}{v_0} \left[ |r_{R,p}|^2 + |l_{L,p}|^2 \right] = 1 \quad (10)$$

where $v_p = 2γ \sin k_p$ is the velocity in the $p$-th side band.

The reflection and transmission amplitudes are found by writing down the wave functions in the scattering region, and matching coefficients of terms having the same $f$ at different sites. If the oscillating potentials are weak, the reflection and transmission amplitudes decrease rapidly far to the left of the scattering region. Due to unitarity, we have the relations

$$\sum_p \frac{v_p}{v_0} \left[ |r_{L,p}|^2 + |t_{R,p}|^2 \right] = 1,$$

and

$$\sum_p \frac{v_p}{v_0} \left[ |r_{R,p}|^2 + |l_{L,p}|^2 \right] = 1 \quad (10)$$

where $v_p = 2γ \sin k_p$ is the velocity in the $p$-th side band.
where \( f(E) = 1/\left[e^{(E-\mu)/k_BT} + 1\right] \) is the Fermi function, and \( q \) is the charge of an electron. The upper limit is \( 2\gamma - \omega \) in the first integral in Eq. (11) because if \( E_0 > 2\gamma - \omega \), \( E_1 \) will lie above the continuum band and will therefore not contribute to the current. Similarly, the lower limit is \(-2\gamma + \omega \) in the second integral in Eq. (11) because if \( E_0 < -2\gamma + \omega \), \( E_{-1} \) will lie below the continuum band and will not contribute to the current. Thus the wave function is given by \( \alpha_R e^{i(k_n-\mu_n+\omega t)} \) and \( \alpha_L e^{i(-k_n-\mu_n+\omega t)} \) far to the right and left of the scattering region respectively, where

\[
\alpha_R = -\frac{ib}{4\gamma \sin k_1} e^{-ik_1 r} \psi_B(r) \times [1 + r(R(k_1)) e^{i2k_1 r}],
\]

\[
\alpha_L = -\frac{ib}{4\gamma \sin k_1} e^{ik_1 r} \psi_B(r) t_L(k_1),
\]

and the function \( \psi_B \) is given in Eq. (4). The dc part of the current pumped to the right is then given by

\[
I_{RB} = q \frac{2\gamma \sin k_1}{2} \left[ |\alpha_R|^2 - |\alpha_L|^2 \right] \{ f(E_B) - f(E_1) \},
\]

where \( 2\gamma \sin k_1 \) is the electron velocity. Equation (15) has to be added to Eq. (11) in order to obtain the total pumped current. At zero temperature, \( I_{RB} \) is non-zero only if \( E_B + \omega > \mu > E_B \), and it is then independent of \( \mu \).

Similar considerations hold if there is a positive energy bound state with \( E_B > 2\gamma \) and \( E_{-1} = E_B - \omega \) lies within the continuum band. Such a bound state will then contribute to the pumped current. One can compute this contribution by applying a particle-hole transformation to the calculation given above for a negative energy bound state. Under the transformation \( c_n \to (-1)^n c_n \), the hopping term in Eq. (11) remains the same but \( c_n^\dagger c_n \) changes sign. This is equivalent to changing \( a \to -a \) in Eq. (11), and the chemical potential \( \mu \to -\mu \). Thus the filling fraction \( f = k_F/\pi \) changes as \( f \to 1 - f \), and the current changes as \( I_R \to -I_R \); the latter can be seen directly from the form of the current operator given in Eq. (17) below.

We now observe that, to second order in the amplitude \( b \), Eqs. (11) and Eqs. (14) for the pumped current remain valid for the case of a general static potential which may be extended over more than one site, as long as the oscillating potential lies outside the region of the static potential; we only have to use the appropriate expressions for the reflection and transmission amplitudes \( r_\pm(k) \) and \( t_\pm(k) \), and the bound state wave function \( \psi_B(r) \). The same derivation which was used to obtain the above equations for the case of a static potential at one site will work for a more general case. We can show this in a different way by using the idea of sum over paths. To first order in \( b \), the reflection amplitude \( r_{R,1} \) in Eq. (12) can be understood as arising from the sum of the following four paths (see Fig. 1), remembering that the oscillating potential lies to the right of the static potential. An electron incident from the far right with a wave number \( k_0 \) can be (i) reflected to the right by the oscillating potential to a wave number \( k_1 \) with an amplitude \(-ib/(4\gamma \sin k_1)\) [this
An electron incident from the far left with a wave number \( k_0 \) can be (i) transmitted to the right by the static potential with an amplitude \( t_R(k_0) \), and then transmitted to the right by the oscillating potential to a wave number \( k_1 \) with an amplitude \( -ib/(4\gamma \sin k_1) \), or (ii) transmitted to the right by the static potential with an amplitude \( t_R(k_0) \), then reflected to the left by the oscillating potential to a wave number \( k_1 \) with an amplitude \( -ib/(4\gamma \sin k_1) \), and finally reflected to the right by the static potential with an amplitude \( r_R(k_1) \).

Similar ideas can be used to derive the expressions in Eq. [14]. The amplitude \( \alpha_R \) is the sum of two terms. An electron with a wave function \( \psi_B(r) \) can either be (i) transmitted to the right by the oscillating potential to a wave number \( k_1 \) with an amplitude \( -ib/(4\gamma \sin k_1) \), or (ii) transmitted to the left by the oscillating potential to a wave number \( k_1 \) with an amplitude \( -ib/(4\gamma \sin k_1) \), and then reflected to the right by the static potential with an amplitude \( r_R(k_1) \). The amplitude \( \alpha_L \) corresponds to an electron with a wave function \( \psi_B(r) \) being transmitted to the left by the oscillating potential to a wave number \( k_1 \) with an amplitude \( -ib/(4\gamma \sin k_1) \), and then transmitted to the left by the static potential with an amplitude \( t_L(k_1) \).

We thus see that Eqs. [12] and [13] are valid to first order in \( b \) for any static potential, provided that the static and oscillating potentials are separated by a finite distance.

III. EQUATION OF MOTION METHOD

We will now discuss how the pumped current can be obtained by numerically solving the equation of motion for the density matrix of a system with a finite number of sites [51]. The density matrix of the system evolves according to the equation of motion

\[
\dot{\rho}(t + dt) = e^{-i\hat{H}(t)dt} \rho(t) e^{i\hat{H}(t)dt},
\]

where \( \hat{H}(t) = \hat{H}_0 + \hat{V}(t) \) is given in Eqs. [11] and [53].

The current across any bond is then obtained by taking the trace of the appropriate current operator with \( \hat{\rho} \). The current operator on the bond from site \( n \) to site \( n+1 \) and its expectation value at time \( t \) are given by

\[
\hat{j}_{n+1/2} = iq_\gamma (c_{n+1}^\dagger c_n - c_n^\dagger c_{n+1}),
\]

and

\[
\hat{j}_{n+1/2}(t) = Tr(\hat{\rho}(t) \hat{j}_{n+1/2}^\dagger) = iq_\gamma [\hat{\rho}_{n+1,n}(t) - \hat{\rho}_{n+1,n}(t)].
\]

The charge transferred between the left and right halves of the system \( L \) and \( R \) between two times can be found either by integrating the above expression in time, or by taking the operator

\[
\Delta \hat{Q} = \frac{q}{2} \left[ \sum_{n \in R} c_n^\dagger c_n - \sum_{n \in L} c_n^\dagger c_n \right].
\]
and computing $Tr (\hat{ρ}(t)\Delta \hat{Q})$ at the two times; these methods give the same result for the charge transferred in a cycle.

In all our calculations, we take the left and right leads to have $N_l$ sites each and the wire in the middle to have $N_w$ sites; the total number of sites is $N = 2N_l + N_w$. We take the density matrix at time $t = 0$ to be given by that of a single system governed by the Hamiltonian $\hat{H}_0$ in Eq. (1) with $N$ sites, chemical potential $\mu$, and temperature $T$. If $E_\alpha$ and $\psi_\alpha(n)$ are the eigenvalues and eigenstates of the $\hat{H}_0$ ($\alpha$ and $n$ label the states and sites respectively), the initial density matrix is given by

$$\hat{ρ}_{\text{ini}}(0) = \sum_\alpha \psi_\alpha(m) \psi_\alpha^\dagger(n) f(E_\alpha). \quad (19)$$

We then evolve the density matrix in time and compute the current and charge transferred using Eqs. (14-18).

An important point to note is that the finite length of the leads (with $N_l$ sites) implies that the system has a return time equal to $2N_l/v_F$ where the Fermi velocity $v_F = 2\gamma \sin k_F$ [51]; this is the time required for an electron to travel from the wire in the middle to the end of either of the two leads and then return to the wire. The numerical results can be trusted only for times which are less than the return time. Further, there are transient effects which last for one or two cycles; the effects of different choices of the initial density matrix get washed out after this transient period. All the numerical results presented below are therefore taken from times which are larger than the transient time but smaller than the return time; typically, we have computed the charge transferred between the times $6\pi/\omega$ and $10\pi/\omega$, where $\omega$ is the oscillation frequency. The dc part of the charge pumped per cycle should of course be independent of the location of the bond where it is measured; we have checked that this is true for all our numerical results except for the contribution of a bound state as we will discuss below.

We will now present our numerical results for the pumped charge (in units of $q$). In all cases we have set the temperature to zero, the hopping amplitude $\gamma = 1$, and $r = 5$, i.e., the static and oscillating potentials are separated by five lattice spacings.

In Fig. 2, we show the charge pumped per cycle ($\Delta Q = (2\pi/\omega)I_R$) as a function of the Fermi wave number $k_F$ for the case $a = 1.5$, $b = 0.25$, and $\omega = \pi/10$ (corresponding to a time period of 20). The dash-dot and starred lines show the numerical and analytical results obtained from Eq. (11) respectively; the agreement between the two is excellent. The pumped charge can be seen to go to zero at the band edges as expected. Although there is a positive energy bound state at $E_B = 2.5$, it does not contribute to the pumped charge because the first side band lies at an energy of $E_{-1} = E_B - \omega \approx 2.19$ which is above the continuum band.

Figure 3 shows the charge pumped per cycle as a function of $k_F$ for $a = 1$, $b = 0.25$, and $\omega = \pi/10$. The dash-dot line shows the numerical results, while the starred and dash lines show the analytical results obtained from Eq. (11) (continuum states) and Eq. (11) plus (15) (continuum and bound states) respectively. In contrast to the case shown in Fig. 1, the total pumped current does not go to zero near $k_F = \pi$. This is because of the contribution from a positive energy bound state; this has the energy $E_B \simeq 2.24$, and the first side band lies at an energy of $E_{-1} = E_B - \omega \simeq 1.92$ which lies within the continuum band. Hence, when the chemical potential exceeds $E_{-1}$, the bound state begins to contribute to the pumped charge. The above value of $E_{-1}$ corresponds to a Fermi wave vector of $k_F = \cos^{-1}(-1.92/2) = 2.86$; we can see from the figure that when $k_F/\pi \simeq 0.91$, the total pumped charge begins to deviate from the continuum contribution (which, according to Eq. (11), does go to zero as $k_F \rightarrow \pi$). Using Eq. (15), we can compute the contribution to the pumped charge from the bound state, $\Delta Q_B = (2\pi/\omega)I_{RB}$. We find that $\Delta Q_B = -0.0055$ which agrees reasonably well with the value obtained numerically when $k_F \rightarrow \pi$. However, we find that the pumped charge arising from the bound state has rather long lived transients, and the value of the dc part of the current varies significantly depending on the location of the bond where it is measured; the numerical result shown in Fig. 3 is the current measured at the bond lying midway between the static and oscillating potentials. Thus our model has a numerical difficulty in correctly computing the contribution of a bound state to the current. The reason for this difficulty will be discussed in Sec. IV.

Figure 4 shows the charge pumped per cycle as a function of the oscillation frequency $\omega$ for $a = 1.5$, $b = 0.25$, and $k_F = \pi/4$ (corresponding to $\mu \simeq -1.414$). The dash-
FIG. 3: (Color online) Charge pumped per cycle from left to right versus the Fermi wave number for a static potential separated from an oscillating potential by five sites, with $a = 1$, $b = 0.25$, and $\omega = \pi/10$; the system has 252 sites. The numerical and analytical results with and without the bound state contribution are shown by dash-dot (red), starred (blue) and dashed (black) lines, respectively.

The dot and starred lines show the numerical and analytical results obtained from Eq. (11) respectively. A noticeable change is seen to occur when $\omega$ crosses a value of about 0.59; this is because the first side band $E_{-1} = \mu - \omega$ goes below the continuum band and stops contributing to the pumped charge at that point. A less noticeable change occurs for a similar reason when $\omega$ crosses a value of about 3.41, where the first side band $E_{1} = \mu + \omega$ goes above the continuum band. We also note that the pumped charge goes to zero at $\omega = 4$, as we had commented after Eq. (11).

Finally, Fig. 5 shows the charge pumped per cycle as a function of the oscillation amplitude $b$ for $a = 1.5$, $\omega = \pi/10$, and $k_F = \pi/4$. In this case, we cannot use the analytical expression given in Eq. (11) since $b$ is not small in general and there is a substantial contribution from higher side bands with $|p| \geq 2$. It is interesting to note that the pumped charge vanishes and changes sign at certain values of $b$.

IV. DISCUSSION

In this paper, we have studied charge pumping by a single oscillating potential when the spatial left-right symmetry is broken due to the presence of a static potential at another point; this model is similar to the one used to describe some recent experiments [38]. We have used Floquet scattering theory to compute the pumped charge to second order in the oscillation amplitude. We have shown that if the oscillation frequency is larger than a threshold value, a bound state can contribute to charge pumping; this possibility does not seem to have been studied earlier.

For small amplitudes, we find that the results obtained numerically using the equation of motion method generally agree well with the analytical results. However, some
numerical problems arise when the contribution from a bound state becomes important. These problems have been observed earlier in Ref. 51 (see also Ref. 53); they are due to a difficulty in maintaining the occupation of the bound state at the correct equilibrium value. The simple model we have used for the numerical calculations has no interactions between electrons and no phonons which can lead to inelastic scattering processes and thereby maintain the occupation of the bound state at a value dictated by the Fermi function. Some ways of addressing the problem of bound states have been discussed in Refs. 51, 53.

It would be interesting to generalize our analysis to the case of an arbitrary time-dependent potential applied at one point where the potential may contain a very large number of oscillation frequencies with arbitrary amplitudes. In particular, one can consider the case of a noisy potential and study whether that can, on the average, pump charge in one direction while the left-right symmetry is broken by a static potential. The brief discussion in Sec. II of a potential consisting of a few oscillating terms with low frequencies and small amplitudes suggests that a weak noise may indeed be able to pump charge on the average, but a detailed investigation of this may be useful.

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