Heat production and energy balance in nanoscale engines driven by time-dependent fields

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We present a formalism to study the heat transport and the power developed by the local driving fields on a quantum system coupled to macroscopic reservoirs. We show that, quite generally, two important mechanisms can take place: (i) directed heat transport between reservoirs induced by the ac potentials, and (ii) at slow driving, two oscillating out of phase forces perform work against each other, while the energy dissipated into the reservoirs is negligible.

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I. INTRODUCTION

The understanding of the heat transport at the microscopic realm has attracted the attention of theoreticians for several years now. Several studies investigate this issue in the framework of one-dimensional lattice models of interacting classical oscillators.[1–5] Nowadays, the technological trend toward the fabrication of nanosize electronic devices is boosting the theoretical interest in quantum transport in a variety of setups and materials. Recently, there have been efforts to address the related problems of energy transport and heat dissipation in these small-size systems.[6–13]

Electronic quantum transport through mesoscopic systems has been traditionally analyzed as a response to dc voltages. There are, however, alternative possibilities to induce net transport by using time-dependent fields as the generating source. Interesting examples of this kind have been recently realized experimentally.[14–18] An important characteristic of these systems is that directed motion is realized by pure ac forces thanks to the convenient breaking of relevant symmetries.[19–21]

Energy transport in stationary conditions is achieved as a response to temperature and/or chemical potential gradients. The application of time-dependent fields can induce net particle transport between reservoirs at the same chemical potentials, while it brings about by itself heating of the sample. Then, it is possible that ac forces can also generate directed heat transport between those reservoirs even if they are at the same temperatures or even against a temperature gradient. If so, what determines the direction of that heat flow? In general, what is the detailed energy balance for such a system? Is it possible to transport part of this energy to develop work? The theoretical study of the underlying physical processes demands a full quantum-mechanical treatment of the problem to evaluate the heat currents through the different parts of the device, as well as the calculation of the powers developed by the external fields.

The aim of this work is to present a theoretical approach based on nonequilibrium Green's function that will allow us to address details of the energy balance in the framework of an exactly solvable model of an electronic quantum pump.[22]

In Sec. II, we present the model used and introduce an elementary unit (a bond) which stores energy. Based on a developed general formalism in Sec. III, we discuss generic features of energy flows in driven quantum systems. We conclude in Sec. IV.

II. MODEL

The device can be described in terms of a Hamiltonian with three pieces representing the electronic driven system, the contact with the reservoirs, and the reservoirs:

$$H(t) = H^{sys}(t) + H^{cont} + H^{res}. \tag{1}$$

For simplicity, we consider a two terminal setup with left (L) and right (R) reservoirs, and an N-site one-dimensional lattice model for the driven system. We assume that the latter has an energy profile ε_l^0 and nearest neighbor hopping elements w_l. At M lattice positions, ac potentials of the form $V_j(t)=V_j\cos(\Omega_0 t+\varphi_j)$ are locally applied. This system Hamiltonian can, thus, be expressed as

$$H^{sys}(t) = \sum_{l=1}^{N-1} H^{(l,l+1)}(t), \tag{2}$$

where

$$H^{(l,l+1)}(t) = \varepsilon_l(t)c_l^\dagger c_l + \varepsilon_{l+1}(t)c_{l+1}^\dagger c_{l+1} - w_l(c_l^\dagger c_{l+1} + c_{l+1}^\dagger c_l), \tag{3}$$

with $\varepsilon_l(t)=\zeta_l[\varepsilon_l^0+\Sigma_{j=1}^M \delta_{l,l_j}V_j(t)]$, where $\zeta_l=1/2$ for $1<l<N$ and $\zeta_{l_\alpha}=1$ for the sites that intervene in the connection to the reservoirs $l_\alpha \equiv 1,N$. The contacts are represented by hopping terms between the reservoirs and the latter positions:

$$H^{cont} = \sum_{\alpha,k_\alpha} w_\alpha(c_{k_\alpha}^\dagger c_{l_\alpha} + \text{H.c.}). \tag{4}$$

The reservoirs are described by free-electron models:

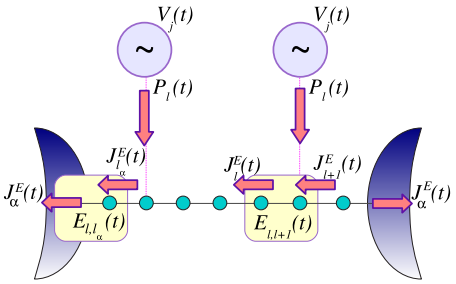

FIG. 1. (Color online) Sketch of the device. The sites of the chain described by $H^{sys}(t)$ are represented by small circles. The local harmonically time-dependent fields $V_j(t)$ develop a power $\bar{P}_j$. The right box encloses a unit of chain described by $H^{l,l+1}(t)$, where energy conservation is considered, while the left one corresponds to a unit described by $H^{(cont)}$. The arrows indicate the dc energy currents $\bar{J}^E_l$ flowing into a bond $(l,l+1)$ of the system, $\bar{J}^E_{l_\alpha}$ entering the contacts and $\bar{J}^E_\alpha$ entering the reservoirs.

$$H^{res} = \sum_{k_\alpha} \varepsilon_{k_\alpha} c^\dagger_{k_\alpha} c_{k_\alpha}, \tag{5}$$

which are assumed to remain at equilibrium with well defined chemical potentials μ_α and temperatures T_α, even after being connected to the driven structure.

A. Energetics of bonds

In order to define currents of energy, we can follow the quantum-mechanical counterpart of the procedure carried out in Refs. 2 and 5 for a classical model. We formulate the equation for the conservation of the energy $E_{l,l+1}(t) = \langle H^{(l,l+1)}(t)\rangle$ stored in a bond $(l,l+1)$. The variation in time of this mean value is calculated by recourse to Ehrenfest's theorem which casts

$$\frac{dE_{l,l+1}(t)}{dt} = J^E_{l+1}(t) - J^E_l(t) + \frac{1}{2}[P_l(t) + P_{l+1}(t)], \tag{6}$$

$$\frac{dE_{\alpha,l_\alpha}(t)}{dt} = J^E_{l_\alpha}(t) - J^E_\alpha(t) + \frac{1}{2}P_{l_\alpha}(t), \tag{7}$$

where the first equation corresponds to bonds of the system without sites in contact with reservoirs (i.e., $1<l<N-1$) (the one enclosed by the right box of Fig. 1), while the second one corresponds to the left bond that establishes the contact between system and reservoir (see left box of Fig. 1). The first two terms of Eq. (6) represent a discretized version of the divergence of the energy current flowing through the bond, while the last two terms represent the power developed by the external forces and are equal to $\langle \partial H^{(l,l+1)}(t)/\partial t\rangle$. In Eq. (7), the first current represents the flow of energy toward the system, the second one is the flow of energy entering the reservoir, and the third one is the power developed by the external forces.

Denoting $\rho_{j,j'}(t) = \langle c^\dagger_{j'}(t) c_j(t)\rangle$, the explicit expressions for the different energy currents read

$$J^E_l(t) = 2\,\mathrm{Im}\{\varepsilon_l(t)[\rho_{l,l-1}(t)w_{l-1} - \rho_{l,l+1}(t)w_l] + w_{l-1}\rho_{l-1,l+1}(t)w_l\}, \tag{8}$$

$$J^E_\alpha(t) = -2\,\mathrm{Im}\left\{\sum_{k_\alpha} w_\alpha \rho_{l_\alpha,k_\alpha}(t)\varepsilon_{k_\alpha}\right\}, \tag{9}$$

and a similar expression for $J^E_{l_\alpha}(t)$, while the power developed by the external forces is

$$P_l(t) = \sum_{j=1}^{M} \delta_{l,l_j} \frac{dV_j(t)}{dt} \rho_{l_j,l_j}(t). \tag{10}$$

In order to analyze the energy balance, we focus on the dc components of the energy currents and powers done by the external forces. The conservation of the energy (6) and (7) implies

$$\overline{dE_{l,l+1}(t)/dt} = 0,$$

$$\overline{dE_{\alpha,l_\alpha}(t)/dt} = 0, \tag{11}$$

which defines continuity equations for the dc energy currents $\bar{J}^E_l$, $\bar{J}^E_\alpha$ and powers $\bar{P}_l$, where $\bar{A} \equiv (1/\tau_0)\int_0^{\tau_0} dt A(t)$, with $\tau_0 = 2\pi/\Omega_0$ being the period of the oscillating time-dependent fields.

B. Energy currents and powers

To evaluate the different energy currents and powers, we employ the treatment based on Keldysh nonequilibrium Green's functions of Ref. 22, which has been useful to study charge transport in the kind of systems we are considering. The mean values of observables entering the corresponding expressions can be expressed in terms of lesser Green's functions as follows: $\rho_{j,j'}(t) = -iG^<_{j,j'}(t,t)$. The latter is evaluated from a Dyson equation, which for j,j' lying on the central system reads

$$G^<_{l,l'}(t,t) = \sum_{\alpha=L,R} \sum_{kk'=-\infty}^{\infty} e^{-ik\Omega_0 t} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \Gamma^<_\alpha(\omega) \times \mathcal{G}_{l,l_\alpha}(k+k',\omega)\mathcal{G}^*_{l',l_\alpha}(k',\omega), \tag{12}$$

with $\Gamma^<_\alpha(\omega) = i f_\alpha(\omega)\Gamma_\alpha(\omega)$, where the Fermi function $f_\alpha(\omega)$ depends on μ_α and T_α, and $\Gamma_\alpha(\omega) = 2\pi\Sigma_{k_\alpha}|\epsilon_{k_\alpha l_\alpha}|^2\delta(\omega-\varepsilon_{k_\alpha})$. The Green's function $\mathcal{G}_{l,l'}(k,\omega)$ is the kth Fourier coefficient of the Fourier transform of the retarded Green's function, which can be exactly evaluated with convenient methods.[22] The above expression (12) can be used in Eqs. (8) and (10) to evaluate $\bar{J}^E_l$ and $\bar{P}_{l_j}$. By using properties of the Green's function,[23] the dc component of the energy current flowing into the reservoir reads

$$\bar{J}^E_\alpha = \sum_{\beta=L,R} \sum_{k=-\infty}^{\infty} \int \frac{d\omega}{2\pi} (\omega + k\Omega_0)\Gamma_\alpha(\omega + k\Omega_0)\Gamma_\beta(\omega) \times |\mathcal{G}_{l_\alpha,l_\beta}(k,\omega)|^2[f_\beta(\omega) - f_\alpha(\omega + k\Omega_0)]. \tag{13}$$

We are interested in the case of reservoirs at the same chemical potentials $\mu_\alpha = \mu, \forall\,\alpha$. Following the same line as

in stationary transport at linear response,[11] we define the dc heat current as

$$\bar{J}^Q_\gamma = \bar{J}^E_\gamma - \mu \bar{J}^C_\gamma, \tag{14}$$

the latter term being the convective flow which depends on the dc–charge current $\bar{J}^C_\gamma$.[24] As this current is conserved, $\bar{J}^Q_\gamma$ obeys the same continuity equation satisfied by $\bar{J}^E_\gamma$.

III. DISCUSSION

We now use the above theoretical framework to analyze two generic mechanisms that can take place in quantum pumps.

A. Directed heat transport

The first one concerns the possibility of achieving *directed heat transport* between reservoirs. To this end, notice that the dc heat current along the lead α can be split into the addition of a generated and a pumped contribution:

$$\bar{J}^Q_\alpha = \bar{J}^{Q(g)}_\alpha + \bar{J}^{Q(p)}_\alpha, \tag{15}$$

where the pumped component reads explicitly as

$$\bar{J}^{Q(p)}_\alpha = \int \frac{d\omega}{2\pi}(\omega-\mu)\Bigg[2\Gamma^<_\alpha(\omega)\mathrm{Im}[\mathcal{G}_{l_\alpha,l_\alpha}(0,\omega)] + \sum_{\beta=L,R}\sum_{k=-\infty}^{\infty}\Gamma_\alpha(\omega+k\Omega_0)\Gamma^<_\beta(\omega)|\mathcal{G}_{l_\alpha,l_\beta}(k,\omega)|^2\Bigg]. \tag{16}$$

This component can be proven to satisfy

$$\sum_{\alpha=L,R}\bar{J}^{Q(p)}_\alpha = 0, \tag{17}$$

meaning that heat can be extracted from a given reservoir and injected into the other one. From the continuity equation for the dc heat current, it follows that

$$\sum_{j=1}^{M}\bar{P}_{l_j} = \sum_{\alpha=L,R}\bar{J}^{Q(g)}_\alpha, \tag{18}$$

indicating that the $\bar{J}^{Q(g)}_\alpha$ contribution accounts for the heat generated by the external forces, which is dissipated into the reservoirs.

1. Example

An example of the behavior of these two different contributions to the heat flows at the reservoirs is shown in Fig. 2 for a two-barrier setup in contact with reservoirs at the same temperature $T_L=T_R=T$. We consider $\varepsilon^0_{l_j}=E$ $(l_j=2,N-1)$ and $\varepsilon^0_{l_j}=0$ $(l\neq l_j)$, with two oscillating potentials with the same amplitude V and a phase lag $\varphi_1=\varphi$ $\varphi_2=0$ applied at the barriers. Under such conditions, a dc charge current $\bar{J}^C$ is induced, which behaves like $\bar{J}^C \propto V^2\sin(\varphi)$ at small V.[19] The pumped component of the heat current, shown in the left panel of Fig. 2, flows outward in a reservoir and inward in the other one. It exhibits a complex structure of maxima, minima, and sign inversions as a function of Ω_0. The details of these features are model dependent. They are a consequence of the electronic propagation through a structure with discrete energy levels and quantum interference that takes place when the pumping frequency Ω_0 is resonant with the energy difference between these levels.[7] The generated heat currents at the different leads $\bar{J}^{Q(g)}_{L,R}$ also display a complex landscape in the T,Ω_0 plane. Their sum is, however, always positive and equals the total developed power $\bar{P}=\bar{P}_1+\bar{P}_2$, which is a monotonous increasing function of Ω_0 and decreases with T, as shown in the right panel of Fig. 2.

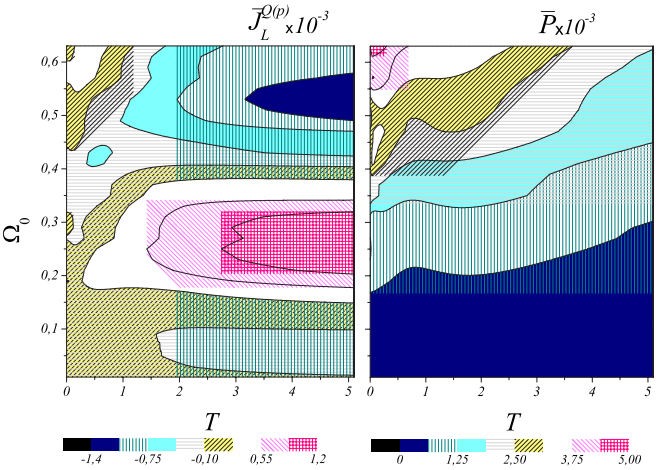

FIG. 2. (Color online) Pumped heat current (left) and total power $P=\bar{P}_1+\bar{P}_2$ developed by the forces (right) as functions of temperature and the pumping frequency. Parameters are $N=22$, $E=1$, $V=0.2$, $\varphi=\pi/2$, and $\mu=-1.5$.

At $T=0$, dissipation dominates and masks the heat pumping effect. For our example, the total heat currents $\bar{J}^Q_L,\bar{J}^Q_R$ as functions of T are plotted in Fig. 3. There it is seen that the sign of both currents is positive at $T=0$, which indicates that the flow goes from the central system toward the reservoirs. Such a behavior is the one expected from considerations based on general thermodynamics since, at $T=0$, there is no heat at the reservoirs amenable to be transported. However, the results of Fig. 3 show that at finite T a regime exists for low pumping frequencies Ω_0, where heat pumping takes place. In fact, the signs of the heat currents are different, indicating that they leave one of the reservoirs and enter the other one. For higher Ω_0, dissipation is again dominant and heat flows always from the central system into the two reservoirs.

In the inset of Fig. 3, we show that heat pumping still takes place even in the presence of a temperature gradient $\Delta T=T_R-T_L$: At low ΔT, $<1\times10^{-4}w$, the heat current flows from the reservoir with a lower temperature $(\bar{J}^Q_L<0)$ into the reservoir with higher temperature $(\bar{J}^Q_R>0)$. Instead, for $\Delta T>1\times10^{-4}w$, the direction of heat flow is opposite to the temperature gradient.

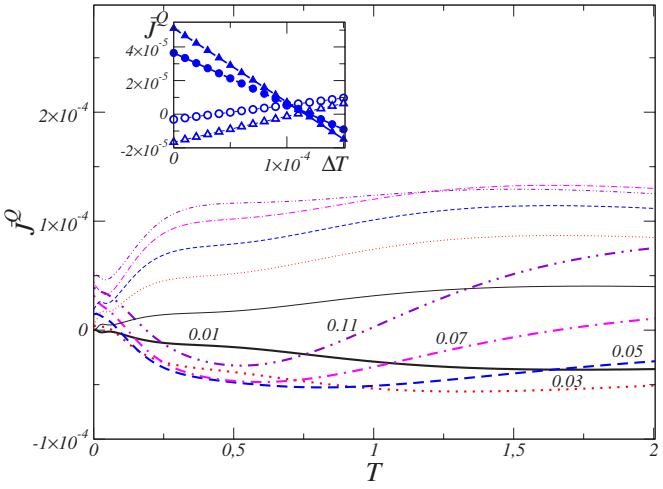

FIG. 3. (Color online) Total heat current as functions of $T=T_R=T_L$ for different pumping frequencies. Thin and thick lines correspond to $\bar{J}^Q_L$ and $\bar{J}^Q_R$, respectively. Parameters are as in Fig. 2. The values of Ω_0 are indicated in the plots. Inset: Heat currents $\bar{J}^Q_L$ (open symbols) and $\bar{J}^Q_R$ (closed symbols) for $\Omega_0=0.03$ and $T_L=0.1$ (circles) and 0.15 (triangles) as a function of a temperature gradient $\Delta T=T_R-T_L$.

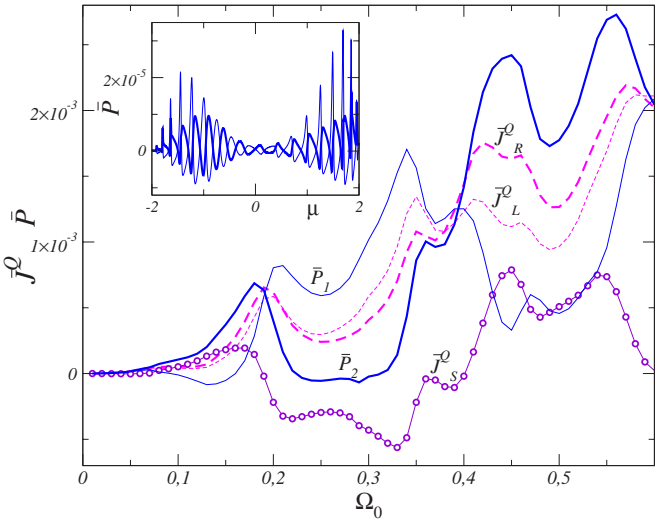

FIG. 4. (Color online) Main panel: Heat currents $\bar{J}^Q_L, \bar{J}^Q_R$ (dashed thin and thick lines, respectively) and $\bar{J}^Q_S$ (circles) along the left and right leads and the central system, respectively, for $\mu=-1.5$. Powers developed by the external fields $\bar{P}_1, \bar{P}_2$ (thin and thick solid lines, respectively). Inset: $\bar{P}_1, \bar{P}_2$ as function of μ for $\Omega_0=0.01$. Parameters are as in Fig. 2.

B. Energy exchange between external forces

The second remarkable mechanism we would like to analyze is the possibility of extracting work from the phase coherent electron system. This issue can be addressed on the basis of a perturbative solution of the Dyson equation, which allows for the evaluation of $\bar{P}_{l_j}$ at the lowest order in V_j.[21,22] It casts

$$\bar{P}_{l_j} \sim \sum_{i=1}^{M} [\lambda_{ji}^{(1)} \cos(\varphi_j - \varphi_i) + \lambda_{ji}^{(2)} \sin(\varphi_j - \varphi_i)], \quad (19)$$

where the coefficients are

$$\lambda_{ji}^{(1)} = \Omega_0 \frac{V_i V_j}{2} \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \mathrm{Im}\{\gamma_{ji}(\omega)\bar{\gamma}_{ji}(\omega)\},$$

$$\lambda_{ji}^{(2)} = \Omega_0 \frac{V_i V_j}{2} \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \mathrm{Re}\{\gamma_{ji}(\omega)\gamma_{ji}^{+}(\omega)\}, \quad (20)$$

with $\gamma_{ji}(\omega)=\Sigma_{\alpha=L,R}\Gamma_\alpha^<(\omega)[G^0_{l_j,l_\alpha}(\omega)]^* G^0_{l_i,l_\alpha}(\omega)$ and $\gamma_{ji}^{\pm}(\omega)=[G^0_{l_j,l_i}(\omega+\Omega_0)\pm G^0_{l_j,l_i}(\omega-\Omega_0)]$, where $G^0_{l,l'}(\omega)$ is the equilibrium retarded Green's function of the system in contact with the reservoirs but without the time-dependent fields. In the low frequency limit, $\lambda_{ij}^{(1)} \propto \Omega_0^2$ while $\lambda_{ij}^{(2)} \propto \Omega_0$. Thus, this solution indicates that quantum coherence in the wave function propagation along the structure, which rules the behavior of the charge current, also plays a role in the way in which energy is provided and exchanged. In particular, for more than one oscillating field, the terms $\propto\lambda_{ij}^{(2)}$ dominate at low enough Ω_0. Since these terms can be positive for some fields and negative for other ones, this enables a scenario where the total energy $\bar{P}=\Sigma_{j=1}^M \bar{P}_j$ is dissipated to the reservoirs at a ratio $\propto\Omega_0^2$, while a larger amount of energy $\propto\Omega_0$ is exchanged between the different pumping centers.

1. Example

Such an effect is, in fact, observed for some parameters in the example of the two-barrier setup. Results are shown in Fig. 4 for $T=0$ with $\varphi=\pi/2$. The dc powers are shown along with the dc heat currents $\bar{J}^Q_L, \bar{J}^Q_R$ flowing to the reservoirs and the one flowing within the system between the two barriers $\bar{J}^Q_S$. The exchange of energy between the two fields is further highlighted in the inset, where the two dc powers $\bar{P}_1$ and $\bar{P}_2$ as functions of μ are shown. It is also interesting to note that the direction of the heat flow between the two pumping centers goes from the field with the largest power toward the other one. In the reservoirs, the heat currents are always positive, indicating that they flow inward. These features are in line with the idea that the fields locally heat the sample inhomogeneously, then the heat current flows from the hottest to the coldest regions.

IV. CONCLUSION

We have investigated details of the energy transport in open quantum systems driven by time-dependent fields, after developing a method based on local conservation of energy. We identified two *generic* interesting mechanisms: First, the achievement of directed transport of heat between reservoirs at finite temperature even against a temperature gradient. Second, we showed that energy taken from one external force can be extracted to perform work against another external force. While the first mechanism opens the possibility of employing quantum pumps as cooling machines at low temperatures, the second one allows for the coupling of two or more of such devices to operate cooperatively, as well as

the use of energy gained at some point of the device to, e.g., induce ac motion in a coupled molecular transistor at a low dissipation rate. We illustrated the two effects in an exactly solvable schematic model of an electronic quantum pump. We found that, for typical values of the scale energy w,[25] heat pumping takes place at $T\sim 1-10$ K and temperature gradients up to $\Delta T/T\sim 1\times 10^{-3}$ with low driving frequencies ($\Omega_0\sim(3-30)\times 10^{-2}$ meV). At very low $T\sim 0$ and Ω_0, up to $\sim 20\%$ of the power done by one of the forces can be transferred to work against the other one. Our results for reservoirs at $T=0$ also suggest that the direction of the heat flows seems to be ruled by an effective temperature gradient[26] induced by the application of external driving.

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