Energy current magnification in coupled oscillator loops

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Motivated by studies on current magnification in quantum mesoscopic systems we consider sound and heat transmission in classical models of oscillator chains. A loop of coupled oscillators is connected to two leads through which one can either transmit monochromatic waves or white noise signal from heat baths. We look for the possibility of current magnification in this system due to some asymmetry introduced between the two arms in the loop. We find that current magnification is indeed obtained for particular frequency ranges. However the integrated current shows the effect only in the presence of a pinning potential for the atoms in the leads. We also study the effect of anharmonicity on current magnification.

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Mesoscopic systems of micron size have recently been studied extensively. In these systems, at low temperatures the mean free path of an electron can exceed the sample dimensions, thus maintaining the coherence of the single particle wave function across the entire sample. In such coherent systems several novel effects have been observed which do not have any classical analogue [1, 2]. An interesting example is that of a mesoscopic conducting loop connected through metallic leads to two separate electron reservoirs at different chemical potentials μ_L and μ_R respectively. A current is established between these two reservoirs. In the presence of this transport current it has been shown that current magnification (CM) can occur in the loop [3, 4]. In this case under appropriate conditions depending on the Fermi energy, the current in one arm of the loop exceeds the total current across the system. For current conservation at the junctions, the current in the other arm flows in the reverse direction, *i.e* opposite to the transport current in the leads. The predicted circulating current density can be very large [4] and has been termed as giant persistent current [5]. Several studies have shown the existence of CM in a variety of models including multi-channel systems [6], and systems with spin [7, 8] and thermoelectric [9] currents.

Motivated by these studies on quantum systems, in this paper we address the question as to whether CM can occur in classical models of energy transport in oscillator networks. Energy transport in such systems is by lattice vibrations which in the long wavelength limit corresponds to sound-waves. Since CM is basically a wave-phenomena, one expects that it should be observable also in oscillator networks. Heat conduction in such networks have earlier been studied by Eckmann and Zabey [10] who also discussed the possibility of circulating currents. The system we consider is schematically shown in Fig. (1). It consists of a loop formed by particles, all with masses m and connected by springs with stiffness k . Two Leads [(1) and (4) in the figure] formed by semi-infinite oscillator chains are connected to the loop in an asymmetric way such that the loop has two arms (2) and (3) of unequal lengths. We consider two situations. First we study the transmission of single frequency plane waves across this geometry. Next we consider the case where a band of frequencies are fed into the leads by connecting them to heat baths kept at different temperatures. We also look at the effect of anharmonicity on CM. Since CM is a wave-phenomena one expects it to be suppressed in the presence of any thermalizing mechanism such as arising from inelastic phonon-phonon scattering due to anharmoncity. In fact for macroscopic systems these kind of processes would lead to an Ohmic (diffusive) behavior of the wire in which case one would not get CM. In the electron case one important source of thermalization is electron-electron interactions. However

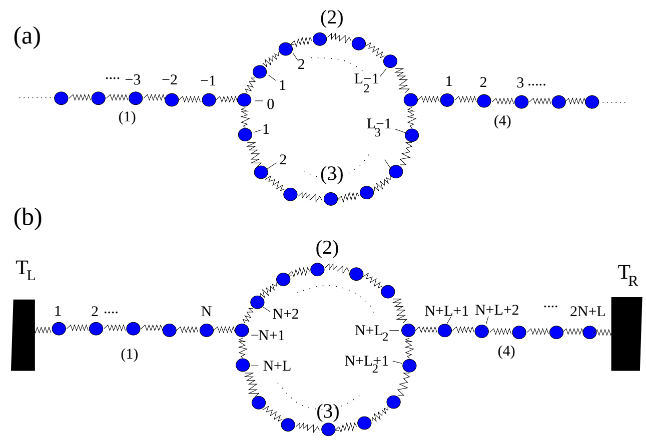

FIG. 1: (color online). Models studied: (a) Oscillator loop connected to infinite leads formed by coupled oscillators. (b) System with finite leads connected to heat reservoirs.

it is quite difficult to study its effect on CM without using approximation methods. On the other hand for the classical oscillator case, it is easy to introduce anharmonicity and numerically see its effect on CM.

We first discuss transmission of monochromatic plane waves across the system. The number of particles on the loop are $L = L_2 + L_3$ and particles in different regions are numbered as in Fig. (1a). For a wave incident from the left side the particle displacements are given by:

$$\begin{aligned} x_l^{(1)} &= Re[\ (e^{iql_1} \ + \ re^{-iql_1})\ e^{-i\omega\tau}\ ]\ ,\ \ -\infty < l_1 \leq 0 \\ x_l^{(2)} &= Re[\ (t_1\ e^{iql_2} \ + \ r_1\ e^{-iql_2})\ e^{-i\omega\tau}\ ]\ ,\ 0 \leq l_2 \leq L_2 \\ x_l^{(3)} &= Re[\ (t_2\ e^{iql_3} \ + \ r_2\ e^{-iql_3})\ e^{-i\omega\tau}\ ]\ ,\ 0 \leq l_3 \leq L_3 \\ x_l^{(4)} &= Re[\ t\ e^{iql_4}\ e^{-i\omega\tau}]\ ,\ 0 \leq l_4 < \infty, \end{aligned} \tag{1}$$

with $q \in (0, \pi)$ and $\omega = 2\sqrt{\frac{k}{m}}\ \sin(q/2)$, the usual dispersion relation for the harmonic chain. The six unknown transmission amplitudes can be found out by matching the solutions Eqns. (1) at the junctions and considering the equations of motion of the particles at the junctions. Then one gets:

$$\begin{aligned} 1 \ + \ r &= t_1 \ + \ r_1 = t_2 \ + \ r_2 \\ -m\ w^2\ (\ 1 \ + \ r\ ) &= -k\ (\ 3(1+r) - \ e^{-iq} - \ r\ e^{iq} - \ t_1\ e^{iq} - \ r_1\ e^{-iq} - \ t_2\ e^{iq} - \ r_2\ e^{-iq}) \\ t &= t_1\ e^{iq\ L_2} + \ r_1\ e^{-iq\ L_2} = \ t_2\ e^{iq\ L_3} + \ r_2\ e^{-iq\ L_3} \\ -m\ w^2\ t &= -k\ (3t\ - te^{iq} - \ t_1 e^{iq\ (L_2-1)} - \ r_1 e^{-iq\ (L_2-1)} - \ t_2 e^{iq\ (L_3-1)} - \ r_2 e^{-iq\ (L_3-1)}). \end{aligned} \tag{2}$$

These linear equations can be explicitly solved to get all the unknown amplitudes. We do not give explicit expressions here since they are quite lengthy. The instantaneous energy current from site l to $l+1$ is the product of the velocity of the $(l+1)^{\rm th}$ particle and the force on it due to the $l^{\rm th}$ particle. Thus the energy current averaged over a time period between two neighboring sites on any of the four regions ($s = 1, 2, 3, 4$) is given by: $I^{(s)} = -k\ (\omega/2\pi) \int_0^{2\pi/\omega}\ d\tau\ \dot{x}_{l+1}^{(s)}\ [\ x_{l+1}^{(s)} - x_l^{(s)}\ ]$. One then finds $I^{(s)} = (k\omega \sin q/2)\mathcal{T}^{(s)}(\omega)$ where the transmission coefficients are given by $\mathcal{T}^{(1)} = \mathcal{T}^{(4)} = 1 - |r|^2 = |t|^2$, $\mathcal{T}^{(2)} = |t_2|^2 - |r_2|^2$ and $\mathcal{T}^{(3)} = |t_3|^2 - |r_3|^2$. In Fig. (2) we plot these transmission coefficients as a function of frequency ω for a particular choice of parameters k, m, L_2, L_3 with $L_2 < L_3$. The most interesting features that we see are that, for certain values of the frequency, the transmission $\mathcal{T}^{(2)}$ [$\mathcal{T}^{(3)}$] on one of the arms of the loop can be *negative* and when this happens there is CM on the other arm, *i.e* $|\mathcal{T}^{(3)}/\mathcal{T}^{(1)}| > 1$ [$|\mathcal{T}^{(2)}/\mathcal{T}^{(1)}| > 1$]. In contrast, the inset of Fig. (2) gives results for $L_2 = L_3$ in which case all transmission coefficients are positive with magnitudes less than one. Note that current conservation implies $I^{(1)} = I^{(2)} + I^{(3)} = I^{(4)}$ and hence negative current flow on one arm necessarily implies CM on the other.

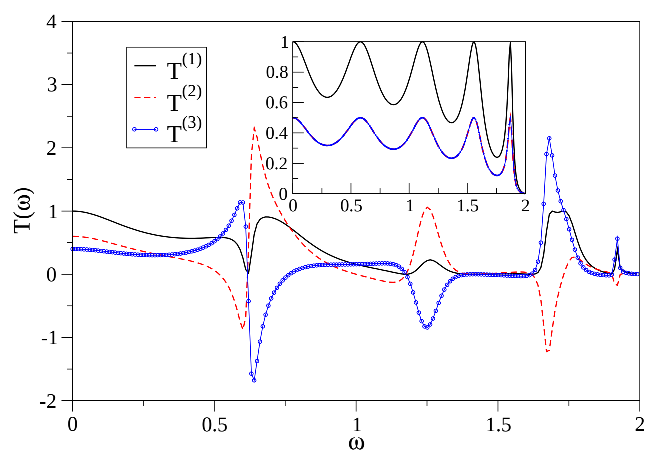

FIG. 2: (color online). Plot of transmission-versus-frequency in different regions of the network for the case of infinite leads. Parameters used are $k = 1$, $m = 1$, $L_2 = 4$ and $L_3 = 6$. Inset shows the same plots for the case where there is no asymmetry in the loop arm lengths ($L_2 = L_3 = 6$).

Next we ask the question as to what happens when the two leads are connected to white-noise heat baths at different temperatures T_L and T_R. Do we still get negative heat current flow in one of the arms and CM ? For systems with diffusive heat flow this is clearly not possible. In the nonequilibrium steady state one would expect the system to be in local thermal equilibrium which means that the local temperatures at the junctions will define the direction of heat flow and this will then be unique (high-to-low temperature). However, for ballistic heat flow, as in a harmonic system, a local temperature does not have a thermodynamic significance and there is a possibility that we can get CM. We again consider the harmonic network shown in Fig. (1b) with each lead consisting of a finite number of particles, say N. The full network of the loop and leads thus has $M = 2N + L$ particles and is described by the harmonic Hamiltonian

$$\mathcal{H} = \frac{1}{2}\,\dot{X}^T\mathbf{M}\dot{X} + \frac{1}{2}\,X^T\mathbf{\Phi}X, \qquad (3)$$

where $X = \{x_1, x_2, ..., x_M\}$, $\mathbf{M}$ is the diagonal mass matrix and $\mathbf{\Phi}$ is the force matrix. We label the particles as shown in Fig. (1b). To model the heat baths, the particles at the free ends of the leads have extra terms in their equations of motion corresponding to a Langevin dynamics. Thus the particle at the end of the left reservoir has an extra part $-\gamma_L\dot{x}_1 + \eta_L$ in its equations of motion while the particle at the right end has an extra part $-\gamma_R\dot{x}_M + \eta_R$. The noise terms are Gaussian with zero mean and variances given by the fluctuation-dissipation relations $\langle\eta_{L,R}(t)\eta_{L,R}(t')\rangle = 2k_BT_{L,R}\gamma_{L,R}\delta_{L,R}\delta(t-t')$. For the same parameter values as in Fig. (2) we computed the average heat current in the four regions. The steady state heat current on a bond between sites a and b is given by $J^{(s)} = -k\langle\dot{x}_b^{(s)}[\,x_b^{(s)} - x_a^{(s)}\,]\rangle$ where $\langle...\rangle$ now denotes a noise average. Using the methods described in Ref [11], the heat current in any part of the system can be expressed as an integral over all frequencies of the transmission function, which can be written in terms of the Green's function matrix $G(\omega) = [-\omega^2\mathbf{M}+\mathbf{\Phi}-i\omega\mathbf{\Gamma}]^{-1}$ where $\mathbf{\Gamma}$ is a dissipation matrix whose only non-vanishing elements are the two diagonal terms γ_L and γ_R occurring at positions corresponding to the two sites connected to reservoirs. Thus, assuming that a unique nonequilibrium steady-state is achieved, the heat current on any part can be written as [11]:

$$I^{(s)} = \frac{k_B(T_L - T_R)}{4\pi}\int_{-\infty}^{\infty} d\omega\;\mathcal{T}^{(s)}(\omega), \qquad (4)$$

where the transmission coefficient $\mathcal{T}^{(s)}(\omega) = 2ki\omega\,[\;G_{a,1}(\omega)G_{b,1}(-\omega) - \;G_{a,M}(\omega)G_{b,M}(-\omega)\;]$ with a, b being two adjacent sites on the region of interest. The site b is chosen to be on the right of a so that the convention used is that current is from left-to-right.

In all the calculations we set with $T_L = 10, T_R = 1$ and $N = 20$. The other parameters of the network are the same as for the data in Fig. (2). In Fig. (3) we plot the transmission coefficients in the leads and in the two arms. We see that for particular values of frequencies the value of $\mathcal{T}^{(2)}(\omega)$ is negative and whenever this occurs we have $|\mathcal{T}^{(3)}/\mathcal{T}^{(1)}| > 1$ implying CM. Next we calculate the total heat current using Eqs. (4). From our numerical calculations we find $I^{(1)} = 0.7661, I^{(2)} = 0.37968, I^{(3)} = 0.3864$. We have also verified these results from direct nonequilibrium simulations. Thus we do not get any CM. For several other choices of parameter values we find the same situation. Introducing impurities in the loop can enhance the asymmetry in the system. With this we find that while one gets CM in specific frequency ranges, the integrated current again does not show any CM.

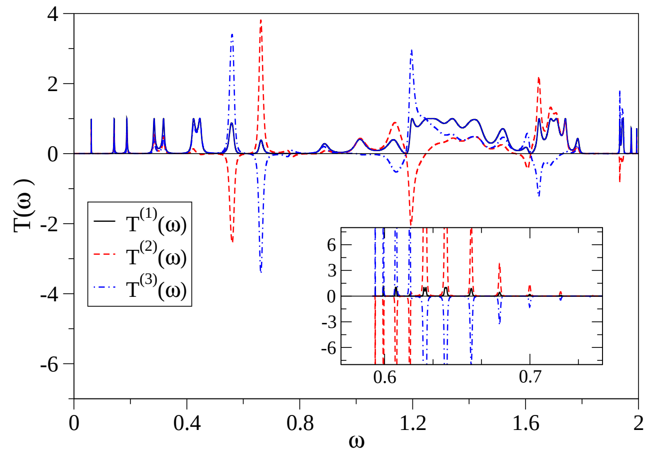

FIG. 3: (color online). Plot of transmission-versus-frequency in different regions of the network for the same system as in Fig. (2) but with finite leads ($N = 20$) connected to Langevin heat reservoirs at temperatures $T_L = 10$ and $T_R = 1$. The inset shows $\mathcal{T}(\omega)$ for the case where the parameters of the leads are chosen such that they have a narrow frequency transmission band (see text for the parameter values).

Let us now consider the effect of introducing a band-pass filter between the loop and reservoirs such that only frequencies over the range where CM occurs, are allowed to pass. It seems plausible that introduction of such a filter will allow us to observe CM in the integrated current. We now test this numerically. For this we introduce a harmonic pinning potential on all sites of the leads. Thus for particles in the leads, in addition to the interparticle potential $k(x_l - x_{l+1})^2/2$, there is also an additional onsite potential $V(x_l) = k_o x_l^2/2$. For the choice of pinning strength $k_o = 0.35$ and $k = 0.1$ (only on the leads), only frequencies in the range $\omega \approx (0.6 - 0.87)$ can pass through the leads. This is the range where, as can be seen from the plot of $\mathcal{T}(\omega)$ data for the unpinned system in Fig. (3), we expect maximum CM. In the inset of Fig. (3) we show plots of $\mathcal{T}^{(1)}, \mathcal{T}^{(2)}, \mathcal{T}^{(3)}$ for this system. As expected, we find significant transmission in a small frequency band. The values of the integrated currents in this case are: $I^{(1)} = 0.01245, I^{(2)} = 0.06681, I^{(3)} = -0.05436$. Thus in this case CM is observed even for the integrated current. Note that there is CM on both the arms and the magnification factor is more than about five times. In Fig. (4) we show the temperature profile in this network with pinning. Here we define a local temperature at any site through its mean kinetic energy, *i.e* $T_l = m\langle\dot{x}_l^2\rangle$ at the $l^{\rm th}$ site. We see that the temperature profile is non-monotonic. As mentioned earlier this is not surprising since the local temperature in this integrable system does not have the usual thermodynamic meaning.

We now consider the effect of introducing anharmonicity in the Hamiltonian of the loop. We consider a quartic onsite potential of the form $V(x) = \lambda x^4/4$ at all sites of the loop. We fix all other parameters to have the same

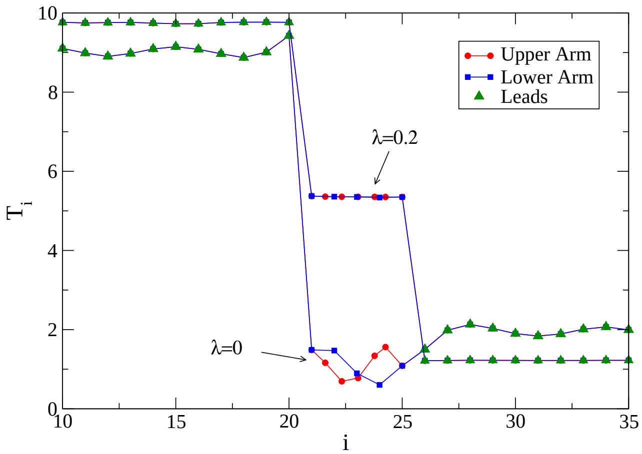

FIG. 4: (color online). Plot of the temperature profile in the network for the same system as considered in the inset of Fig. (3) without anharmonicity ($\lambda = 0$) and with anharmoncity ($\lambda = 0.2$). The temperature across the leads and the two arms of the loop are shown.

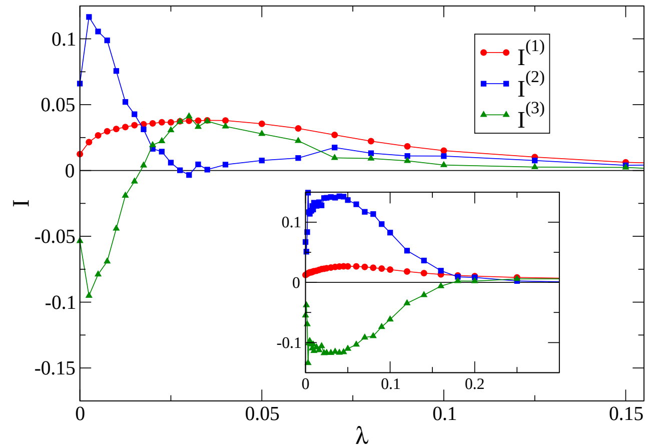

FIG. 5: (color online). Plots of currents $I^{(1)}, I^{(2)}, I^{(3)}$ as a function of strength of onsite anharmonicity λ. The inset shows the corresponding plots for inter-particle anharmonicty.

values as the pinned system studied earlier. We plot in Fig. (5) the currents $I^{(1)}, I^{(2)}, I^{(3)}$ in different regions as a function of the strength of anharmonicity λ. We see that CM decreases with anharmonicity. Interestingly we find that for some value of λ the current on the lower arm ($I^{(3)}$) becomes *exactly zero*. Note also that the current on the upper arm seems to vanish at some value of λ. The inset of Fig. (5) shows the effect of an inter-particle anharmonic potential of the form $\lambda(x_l - x_{l+1})^4/4$ between particles on the loop. We see a similar reduction of CM as in the onsite case though there are some qualitative differences. For macroscopic systems where the effective mean free path due to anharmonicity becomes much smaller than the system size it is expected that CM will not be observed. In Fig. (4) we show temperature profiles for a strongly anharmonic case. In this case, in contrast to the harmonic case, the temperature profile is *not* non-monotonic and correspondingly there is no CM.

Conclusions: Motivated by studies of CM in quantum mesoscopic systems, in this paper we have studied models of energy transmission in classical oscillator chains. We have considered an oscillator loop connected to two external leads. The system is made asymmetric by either making the two arm lengths of the loop different or by introducing impurities. For single-frequency sound waves we find that CM is obtained over particular frequency ranges. For the case where the network is connected to heat baths which send waves at all frequencies we find absence of CM. This is true for various parameter sets that we have tried, but we do not have a proof for this result. We find that CM in the presence of heat baths can be obtained if we introduce a pinning potential in the leads so that only a narrow band of frequencies are allowed to pass through the loop. While we have reported results for a small loop, we have checked that for harmonic systems CM is obtained for much larger sizes also. Finally we have looked at the effect of anharmonicity on CM. Our simulations show that CM is reduced but not completely destroyed in the presence of small anharmonic interactions. We also find the remarkable effect that with appropriate choice of parameters, the current in one arm can be made to exactly vanish. We expect that CM in phononic heat transport will be observable experimentally in mesoscopic systems such as insulating nanotubes where the effective mean free path for inelastic phonon scattering is large compared to system size.

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