Models of classical heat and particle pumps.

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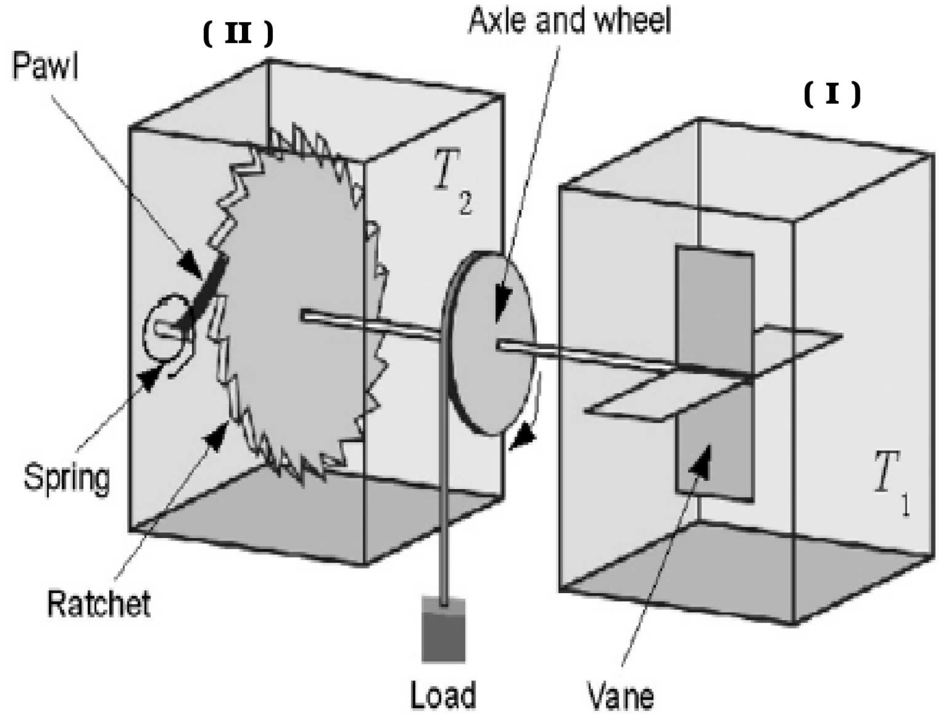
Plan of the talk.

- Introduction.
- Two models of classical heat pumps.
- Particle pumping in the symmetric exclusion process (SEP).
- Discussion.

Feynman ratchet and pawl (Feynman Lectures on Physics, chap.46)



- Two compartments with gas at temperatures T_1 and T_2.
- Apparently ratchet can move only in one direction and one gets useful work by transfer of heat between the baths at same temperature (MAXWELL DEMON).
- Mechanical model of a heat engine.

Molecular pumps and engines

- Equations of motion:

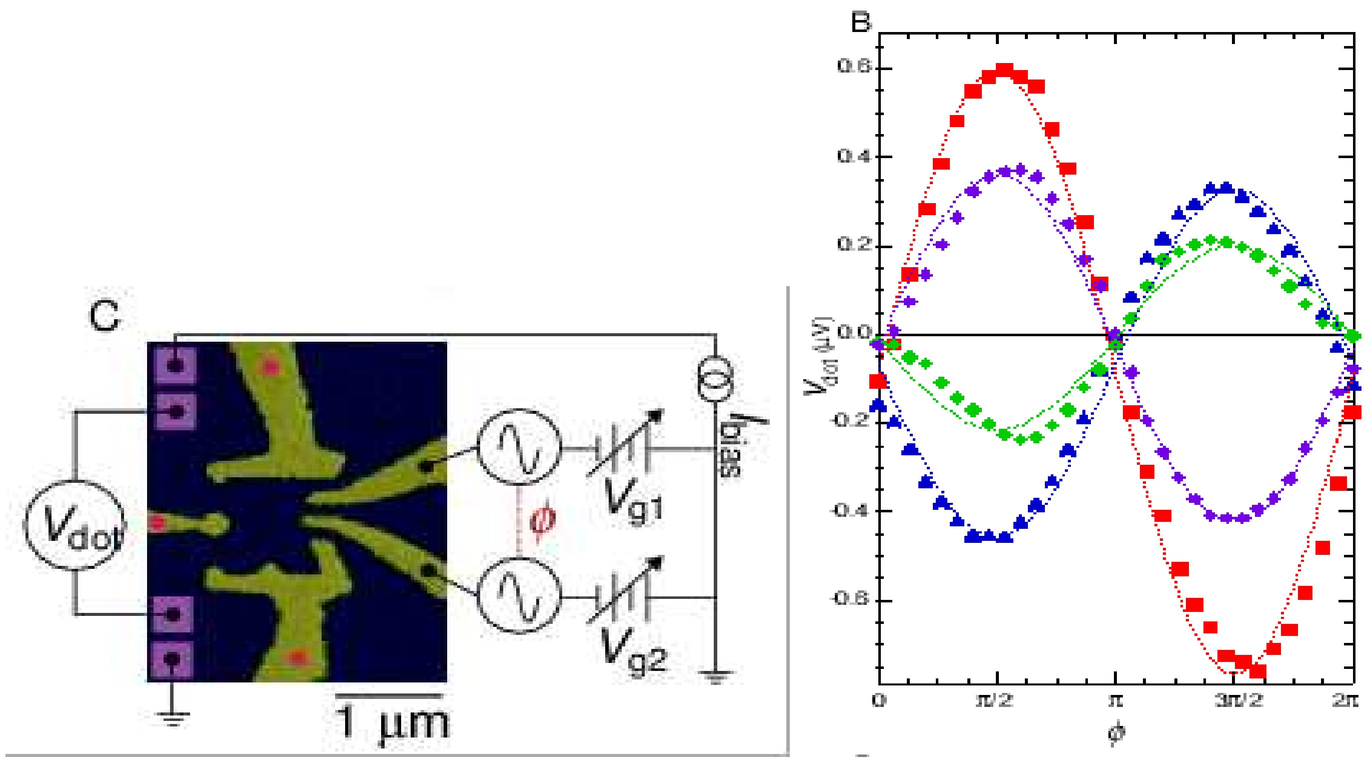
$$\ddot{x} = -\frac{\partial V(x,\theta)}{\partial x} - \gamma \dot{x} + \eta_L$$
$$\ddot{\theta} = -\frac{\partial V(x,\theta)}{\partial \theta} - \gamma \dot{\theta} + \eta_R + L$$

- Analysis nontrivial: flaws in Feynman's analysis: Parrondo, Espanol (AJP, 1996), Magnasco, Stolovitsky (JSP, 1998). System simultaneously in contact with both baths. Thermal fluctuations important.
- Particle pumps: Ratchet models for molecular motors in cells.
- We discuss pumps motivated by quantum pump models.

Quantum Pumps.

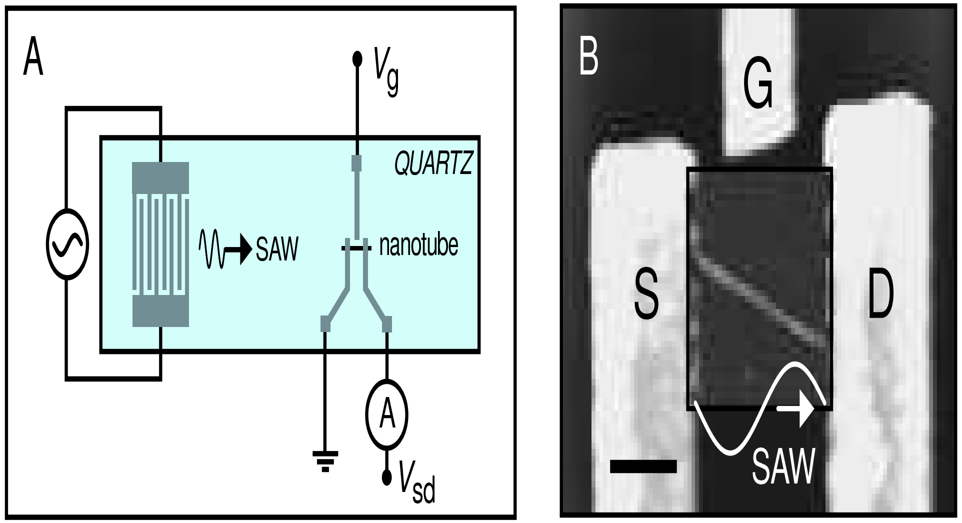
- Models of Quantum Pumps which are recently being studied theoretically and have also been experimentally realized.
- A simple example of such a device would be two coupled quantum dots each separately in contact with particle reservoirs which are at the same chemical potential. One applies ac gate voltages $V_1 = V_0 \cos(\Omega t)$ and $V_2 = V_0 \cos(\Omega t + \phi)$ to two dots respectively. This leads to a net flow of particle current between two reservoirs whose sign depends on the phase ϕ.

An adiabatic Quantum electron pump. Switkes et. al. Science, 283, 1905 (1999)



- Three gates marked with red circles control conductances of point-contact leads that connect the dot to electronic reservoirs.
- The remaining two gate voltages are varied periodically with a phase difference. Which leads to the pumping.

Charge pumping in carbon nanotubes. Leek et.al. PRL, 95, 256802 (2005)



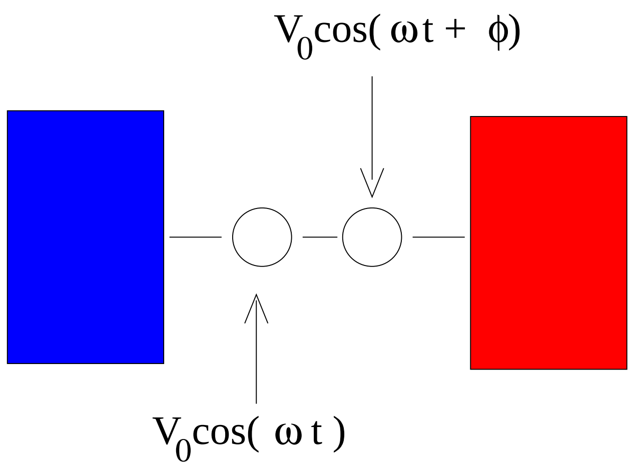
- A surface acoustic wave (SAW) produces traveling potential wells which convey packets of electrons along the channel.
- In the SAW pumps, transport of charge resembles the pumping of water by an Archimedean screw.

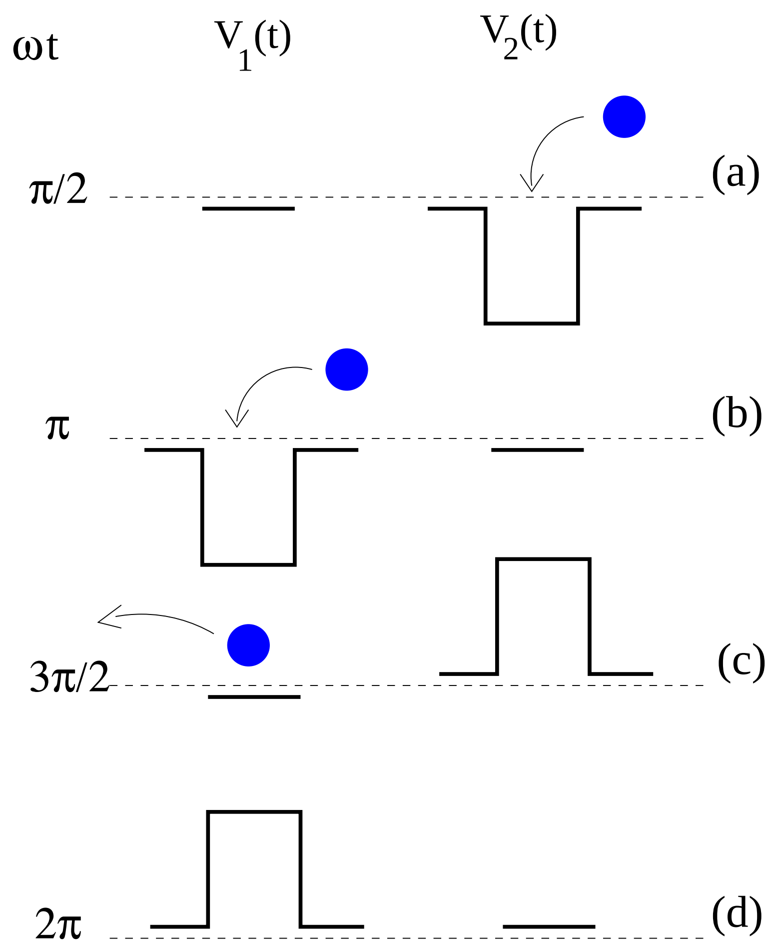
Difference between microscopic and usual heat engines

- The important difference between microscopic models (for example Feynman ratchet-and-pawl model) of heat engines, and the usual thermodynamic heat engines is that here effects of "thermal fluctuations" are important.
- Second important difference is that here system is simultaneously in contact with both the cold and hot baths.

Physical picture.

Let $\phi = \pi/2$,





This picture can not be used in all cases.

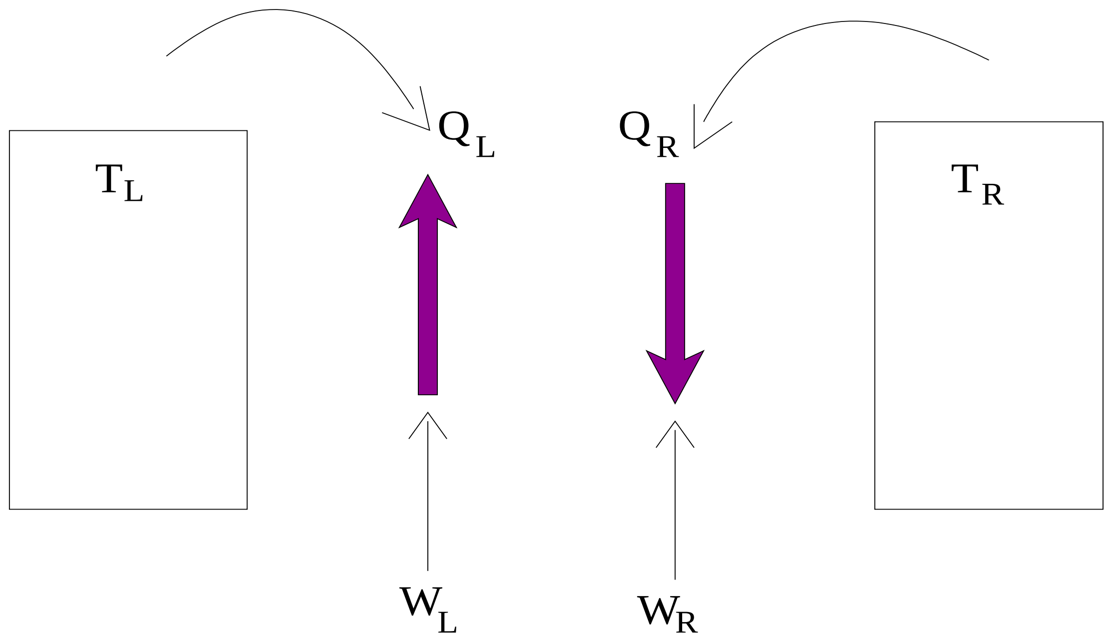
Models of heat pumps

R.M., A. Jayannavar, A. Dhar, Phys. Rev. E **75**, 030103(R) (2007).

Classical Pump Models

- Motivated by these quantum pump models, we examine classical models which have the same basic design as the quantum version.
- We consider two different models,
  - A spin system consisting of two Ising spins each driven by periodic magnetic fields with a phase difference and connected to two heat reservoirs.
  - An oscillator system of two interacting particles driven by periodic forces with a phase difference and connected to two heat reservoirs.

Model of Heat Pump with two Ising spins



- We would like to build a similar microscopic model of heat pump or engine.
- The model consists two Ising spins in contact with two heat baths.
- Spins interact separately with these heat baths.
- Spins interact with each other and are also driven by two external periodic magnetic fields $h_L(t)$ and $h_R(t)$.

- The Hamiltonian of the system is given by

$$\mathcal{H} = -J\sigma_1\sigma_2 - h_L(t)\sigma_1 - h_R(t)\sigma_2, \qquad \sigma_{1,2} = \pm 1$$

- Where J is the interaction energy between the spins. Magnetic fields have the form $h_L(t) = h_0 \cos(\Omega t)$ and $h_R(t) = h_0 \cos(\Omega t + \phi)$, where ϕ is the phase difference.
- The interaction of each spin with the heat baths is modeled by a stochastic dynamics. Here we assume that the time evolution of the spins is given by GLAUBER DYNAMICS, generalized to the case of two heat baths, with temperatures T_L and T_R.

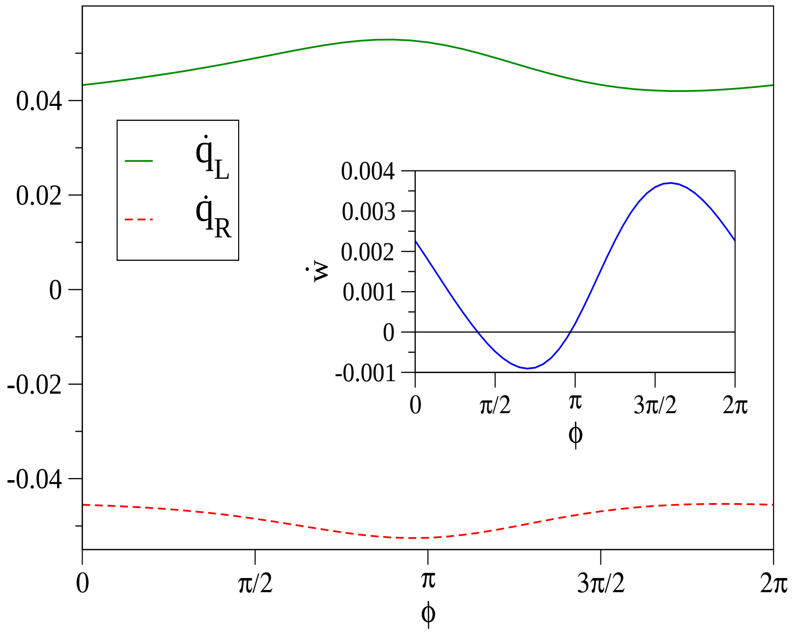
Definitions of heat currents.

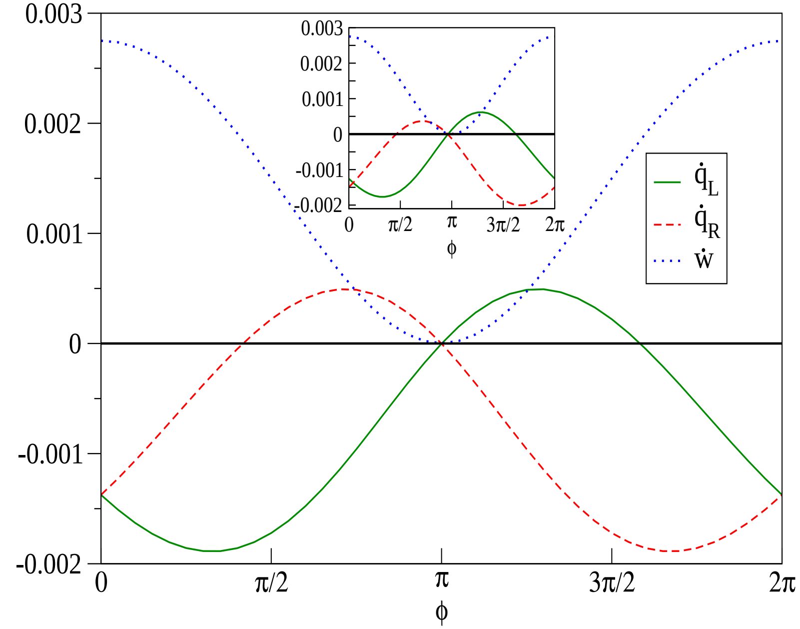
- We define $\dot{Q}_L$, $\dot{Q}_R$ to be the rates (averaged over the probability ensemble) at which heat is absorbed from the left and right baths respectively.
- And $\dot{W}_L$, $\dot{W}_R$ are the rates at which work is done on the left and right spins by the external magnetic field. These can be readily expressed in terms of the spin distribution function and the various transition rates.
- We look at time averaged heat currents,

$$\dot{q}_{L,R} = \frac{1}{\tau} \int_0^\tau \dot{Q}_{L,R}$$

$$\dot{w}_{L,R} = \frac{1}{\tau} \int_0^\tau \dot{W}_{L,R}$$

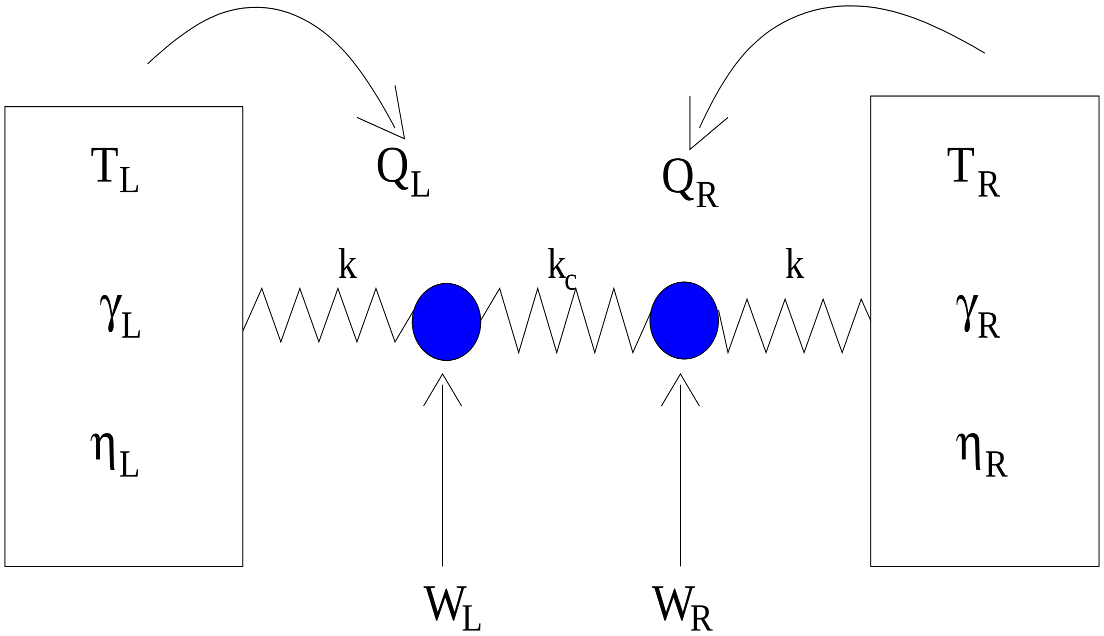
Numerical results for different energy exchange rates.





- First figure shows different energy rates for parameter values chosen such that model performs as an engine.
- Second figure shows different energy rates for parameter values chosen such that model performs as a pump. Inset shows currents for the case when right bath is slightly colder.

Model of Heat Pump with two Brownian particles



- The model consists two Brownian particle in contact with two heat baths.
- Particles interact separately with these heat baths.
- Particles interact with each other and are also driven by two external periodic forces of the form $f_L(t) = f_0 \cos(\Omega t)$ and $f_R(t) = f_0 \cos(\Omega t + \phi)$, where ϕ is the phase difference.

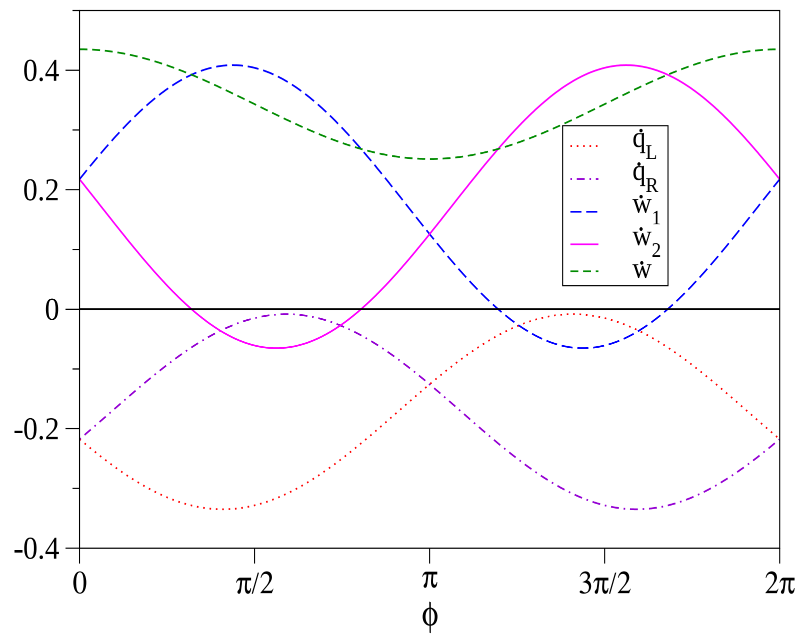
Definition of Model

- The Hamiltonian of the system is given by,
$\mathcal{H} = \frac{P_1^2}{2m} + \frac{P_2^2}{2m} + \frac{1}{2}\, k x_1^2 + \frac{1}{2}\, k x_2^2 + \frac{1}{2}\, k_c (x_1 - x_2)^2 - (f_L(t) x_1 + f_R(t) x_2)$
- The effect of the heat baths at temperatures T_L and T_R is modeled by Langevin equations.
- The two noise terms are Gaussian and uncorrelated and satisfy usual fluctuation-dissipation relations,
$$< \eta_{L,R}(t) \eta_{L,R}(t') >= 2 k_B T_{L,R} \gamma \delta_{L,R} \delta(t - t')$$
- Time averaged energy transfer rates in the steady state are $\dot{q}_L = \frac{1}{\tau} \int_0^\tau \dot{Q}_L dt$ and similarly $\dot{q}_R$, $\dot{w}_{L,R}$.

Results..

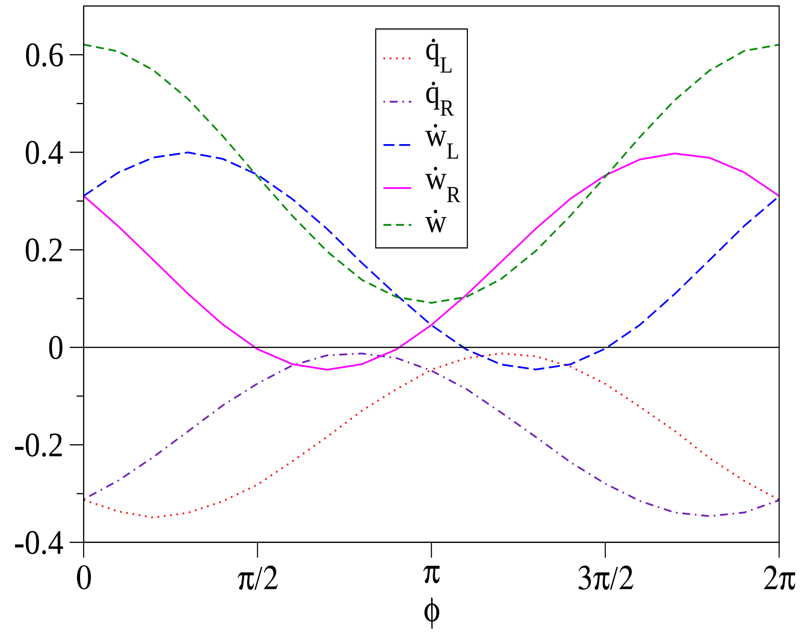
- The steady state solutions of these equations is of the form $X(t) = X_N(t) + X_D(t)$. These equations can be solved exactly.
- Heat transfer rates parts can be separated into deterministic parts (depending on driving strength f_0) and noisy parts (dependent on temperatures of two heat baths). The work terms are temperature independent.
- Also it can be shown that the deterministic parts of $\dot{q}_L$ and $\dot{q}_R$ are both negative. That means for $T_L > T_R$ we always get $\dot{q}_R < 0$, hence we can never have heat transfer from the cold to hot reservoir.
- Thus this model *"cannot"* work as heat pump.
- Also $\dot{w}_L$,$\dot{w}_R$ can individually be negative but the total work done $\dot{w}_L + \dot{w}_R$ is always positive.
- Thus this model *"cannot"* work as an engine either.
- These conclusions remain unchanged even we define work as $\dot{W}_L =< f_L \dot{x}_1 >$, $\dot{W}_R =< f_R \dot{x}_2 >$.

Plots of different energy rates vs phase difference ϕ.



- Only effect of driving in this case is to pump in energy which is asymmetrically distributed between the two reservoirs.
- This asymmetric transfer of energy into baths is an interesting effect considering that there is no built-in directional asymmetry in the system.
- In this model the heat baths and the external driving seems to act independently on the system.

Plots of different energy rates vs phase difference ϕ, with non-linearity.



- It is clear that linearity of the model leads to separability of the effects of the driving and noise forces. And this could be the reason that the model is not able to function as heat pump.
- We have numerically studied the effect of including a nonlinear part of the form $\alpha[x_1^4 + x_2^4 + (x_1 - x_2)^4]/4$ in the oscillator Hamiltonian.
- From simulations with a range of parameter values we find that the basic conclusions remain unchanged and the model does not work either as a pump or as an engine.

Conclusions

- We have studied two models which have the same ingredients as those on which recent models of quantum pump have been constructed.
- We find that first model performs as a heat pump to transfer heat from a cold to a hot reservoir. Thus pumping is not an essentially quantum mechanical phenomena.
- Also our model performs as an engine to do work on the driving force.
- One difference of Feynman's ratchet-and-pawl model from ours is that there no periodic external driving. This also means that in order for the model to work in a cyclic way, at least one of the degrees of freedom has to be a periodic (or angular) variable.
- Surprisingly, our second model though seems to have built on same principles, fails to perform either as a pump or as an engine.

Classical particle pump

Symmetric exclusion process (SEP) with time-dependent hopping rates.

Toy model for colloidal particles diffusing in symmetric time-dependent potentials.

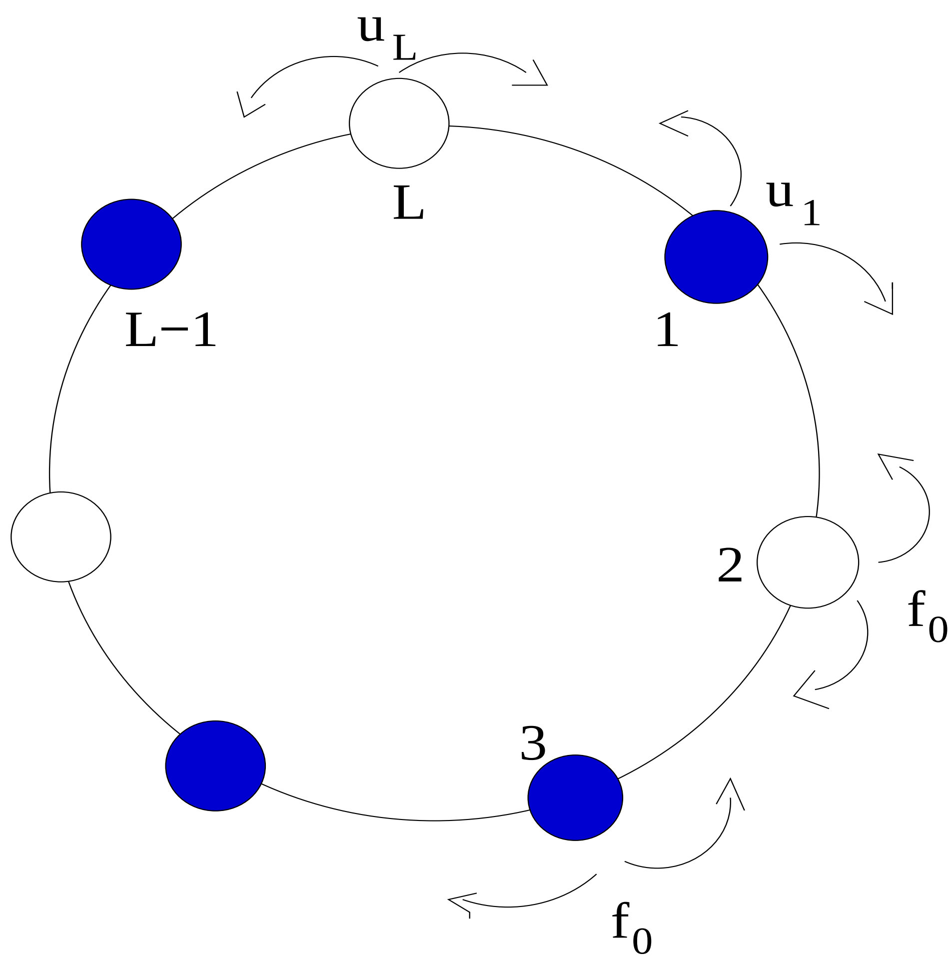
K. Jain, R.M., A. Chaudhuri, A. Dhar, Phys. Rev. Lett. 99, 190601 (2007)

R. Marathe, K. Jain, A. Dhar, cond-mat/0809.2468, Submitted to Journal of statistical mechanics.

Driving particle current through narrow channels using classical pump.

- Basic idea in all these models is that a DC current can be generated by applying an external field periodic in time but inhomogeneous in space.
- In this model we apply same designing principles as discussed before for driving classical particles such as micron-sized charged colloidal particles confined in a closed narrow tube.
- Systems of colloidal particles with excluded volume interactions diffusing in a narrow channel have been studied by one dimensional "symmetric exclusion process" (SEP).
- In this process hard-core particles attempt to hop to an empty neighbor with equal rate.
- In such models attention is given to non equilibrium steady state properties of driven SEP in which particles can enter or leave the system at boundaries.

SEP with time dependent rates at sites 1 and L.



SEP.

Usual SEP: All states occur with equal probability.

Particle density: $\langle n_l \rangle = \rho = \frac{N}{L}$

Two-point correlation: $\langle n_l n_m \rangle = \rho \frac{N-1}{L-1}$

m-point correlation: $\langle n_{l_1} n_{l_2} ... n_{l_m} \rangle = \binom{L-m}{N-m} / \binom{L}{N}$

Independent of site and time.

Zero particle current:

$$
\begin{aligned}
J_{l,l+1} &= u_l \langle n_l (1 - n_{l+1}) \rangle - u_{l+1} \langle n_{l+1} (1 - n_l) \rangle \\
&= u \langle (n_l - n_{l+1}) \rangle = -u \nabla \rho = 0
\end{aligned}
$$

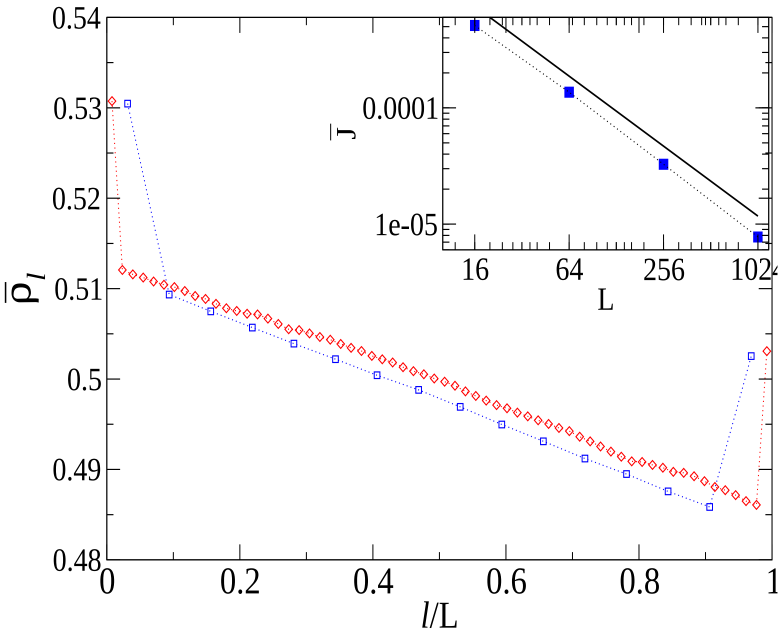
True even if u_l is site-dependent.

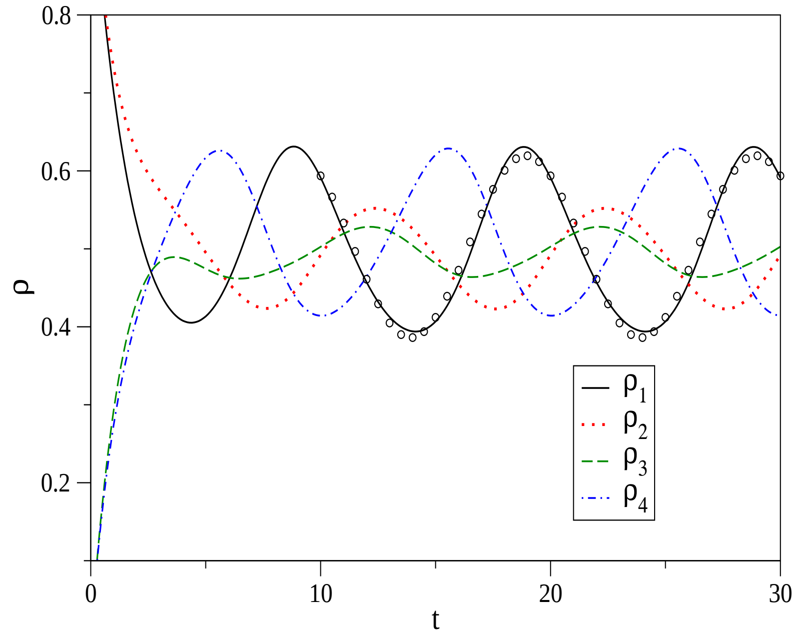
Definition of Model.

- In this model we introduce a SEP in which the hop out rates at two or more lattice sites are chosen to be time-dependent with relative phase difference between different points. (this is like modeling oscillating voltages in quantum pumps).
- The model is defined on a ring (with periodic boundary conditions) with L sites. A site $l = 1, 2, 3, ..., L$ can be occupied by $n_l = 0, 1$ particle, and the system contains a total of $N = \rho L$ particles where ρ is the density.
- A particle at site l hops to an empty site either on the left or right with rate u_l, where

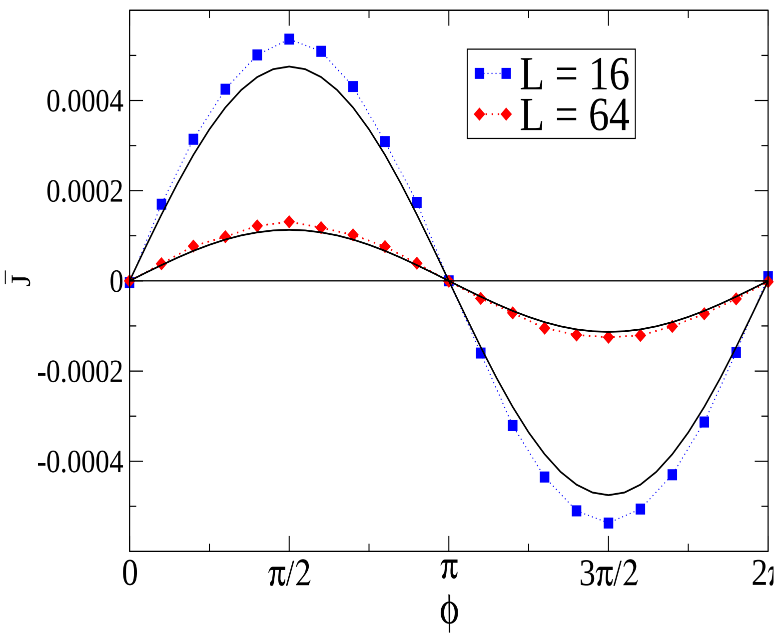
$$\begin{aligned} u_l &= f_0 && \text{if } l \neq 1, L \\ u_1 &= f_0 + f_1 \sin(\omega t) && \text{if } l = 1 \\ u_L &= f_0 + f_1 \sin(\omega t + \phi) && \text{if } l = L. \end{aligned}$$

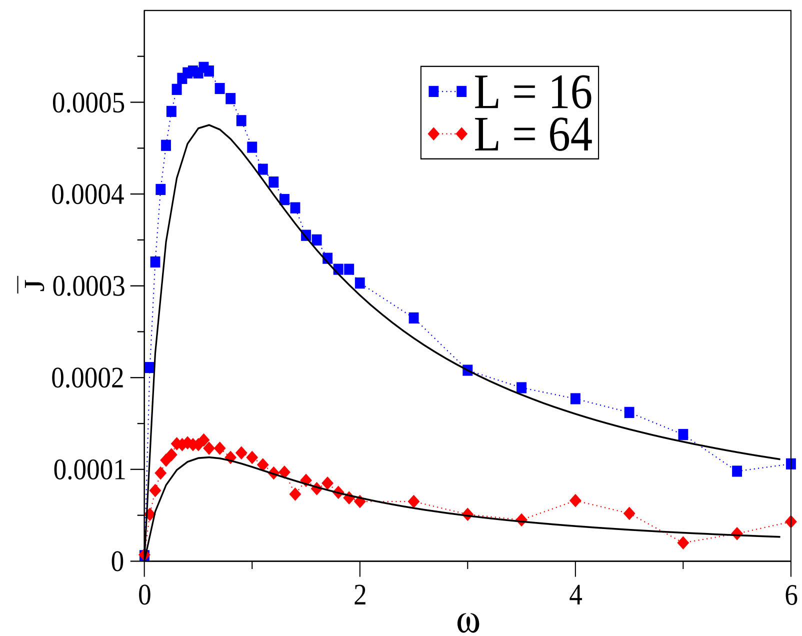
- Or all sites can have time-dependent hopping rates $u_l = f_0 + f_1 \sin(\omega t + \phi_l)$, where $\phi_l = ql$ with $q = 2\pi s/L$.
- For $f_1 = 0$ the above model reduces to SEP with periodic boundary conditions.





- First figure shows density profile ρ_l across the ring, inset shows that the current $\bar{J}$ scales as $1/L$.
- Second figure shows the time-dependent densities at the four sites of a $L = 4$ lattice.





- First figure shows current $\bar{J}$ vs phase ϕ, we get a sinusoidal dependence.
- Second figure shows current $\bar{J}$ vs driving frequency ω.

- We consider peturbative expansions of various quantities of interest with f_1 as the perturbation parameter about the homogeneous steady state corresponding to $f_1 = 0$.
- Thus we write,

$$\rho_l(t) = \langle n_l(t) \rangle = \rho + \sum_{k=1}^{\infty} f_1^k \rho_l^{(k)}(t).$$
$$C_{l,m}(t) = \langle n_l(t) n_m(t) \rangle = C_{l,m}^{(0)} + \sum_{k=1}^{\infty} f_1^k C_{l,m}^{(k)}(t)$$

  and similar expressions for higher correlations.
- The current in a bond connecting sites l and $l+1$ is given by,

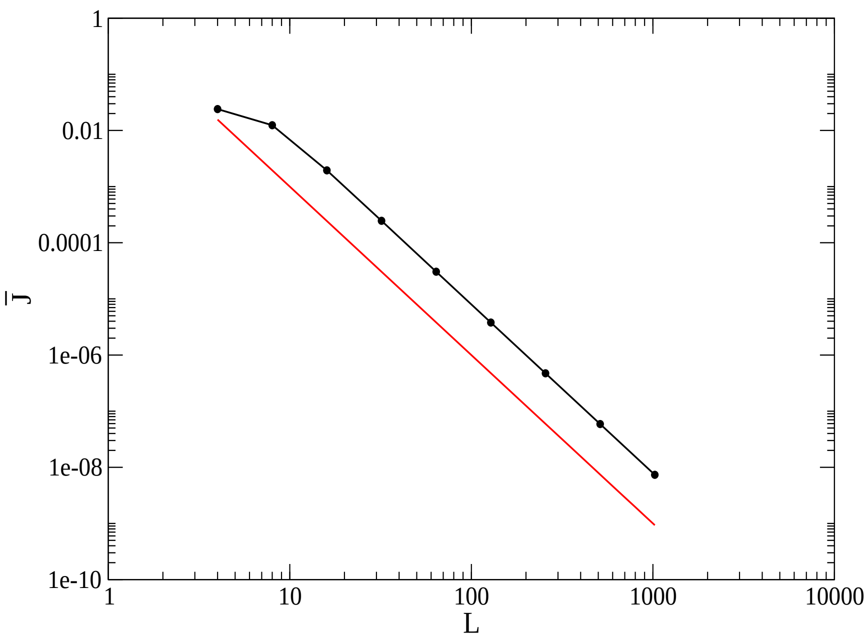
$$J_{l,l+1}(t) = u_l(\rho_l - C_{l,l+1}) - u_{l+1}(\rho_{l+1} - C_{l,l+1})$$

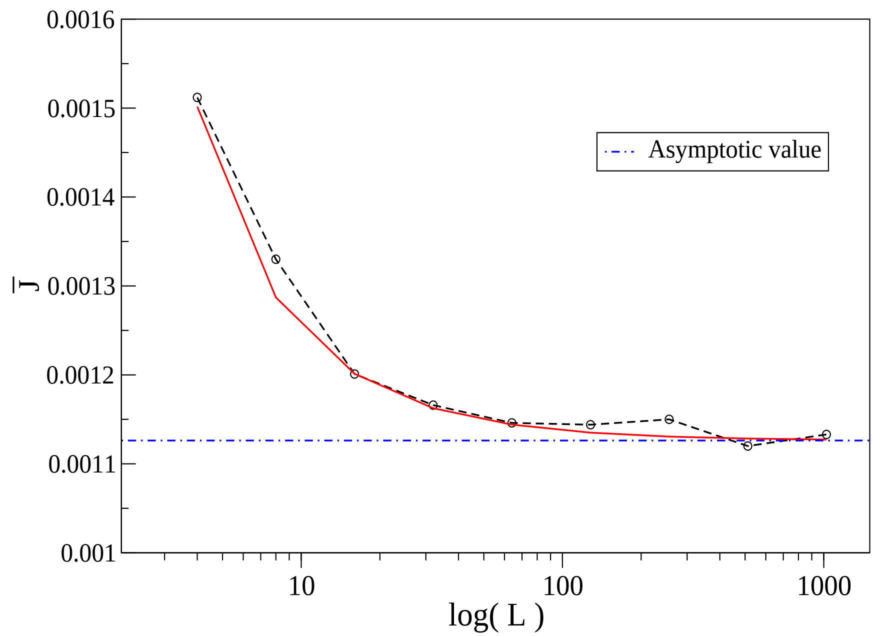
  which can also be expanded in perturbation series using above expansions.
- The final expression for the current looks like,

$$\hat{J} = (\frac{f1}{f_0})^2 \ \frac{k_0 \omega \sin(\phi)}{L} \ F(f_0, \omega) + O(f_1^3).$$

- We observe $1/L$ dependence of the DC current and its sinusoidal variation with the phase is also captured by the perturbation theory at $O(f_1^2)$.
- Also in the limits $\omega \to 0$ and $\omega \to \infty$ we get $\hat{J} \to \omega$ and $\hat{J} \to 1/\omega$ respectively from above expression.

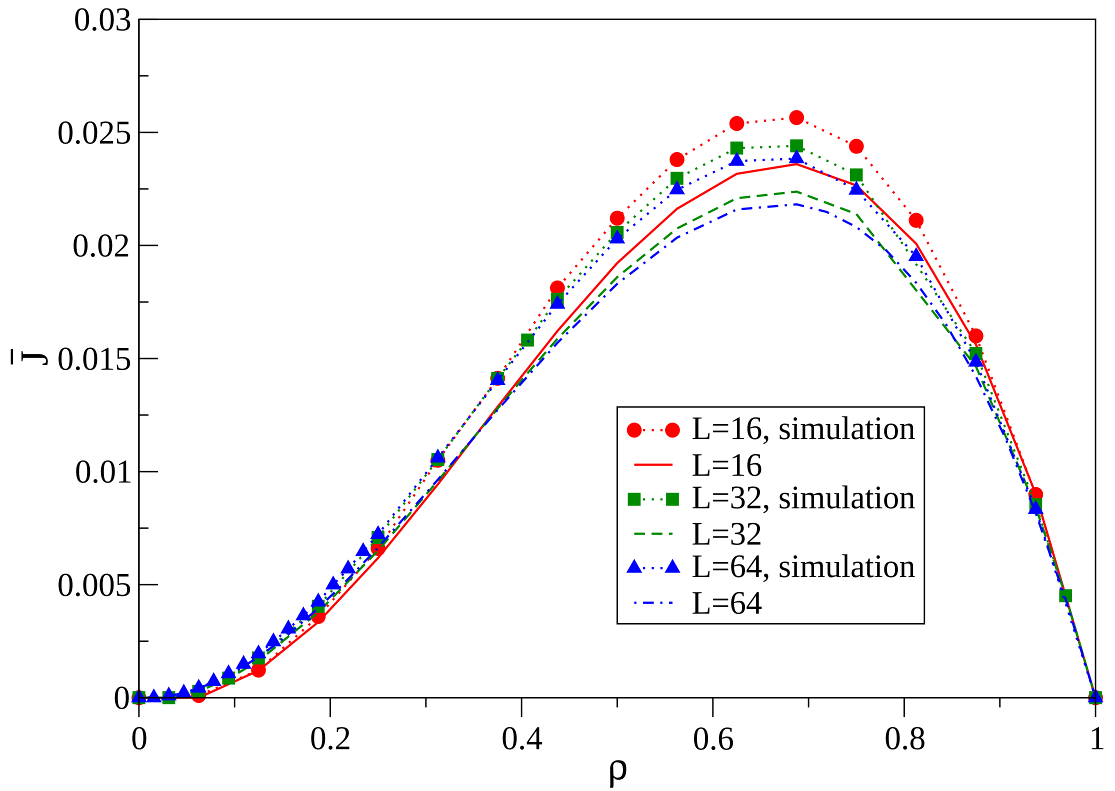
Results for pumping at all sites





$$\bar{J}^{(2)} = \frac{2\ f_1^2\ k_0\ \omega\ \sin q\ (1-\cos q)}{[\ \omega^2\ +\ 4 f_0^2\ (1-\cos q)^2\ ]}\ , q = 2\pi s/L$$

- For $q = 2\pi/L$, current $\bar{J}^{(2)} \sim L^{-3}$.
- For $q = \pi/2$, current $\bar{J}^{(2)} \sim L^0$.



- We find, $\bar{J}^{(2)} \sim \rho^2(1-\rho)$.
- No particle hole symmetry. Maximum of current occurs at $\rho = 2/3$.

Summary

- We have studied a stochastic model of hard-core particles on a ring in which periodically varying hopping rates can induce a DC current.
- Simulations and perturbative analysis shows that many of the qualitative features are similar to that seen in quantum pumps.
- Model is generalized to include several pumps, and shown that a current $\bar{J} \sim 1$ can be obtained in thermodynamic limit.
- We have also studied same model with open boundaries (model for ion channel pumps), where boundary sites are in contact with particle reservoirs. In this model also we get a non-zero DC current.
- A current can also be established between the two reservoirs against a gradient which depends upon the rates of hopping at the boundary sites.