Quantum Ratchets

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Abstract.

The concept of thermal ratchets is extended to the system governed by quantum mechanics. We study a tight-binding model with an asymmetric periodic potential contacting with a heat bath under an external oscillating field as a specific example of quantum ratchet. Dynamics of a density operator of this system is studied numerically by using the quantum Liouville equation. Finite net current is found in the non-equilibrium steady state. The direction of the current varies with parameters, in contrast with the classical thermal ratchets.

keywords:
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Brownian particles under spatially asymmetric potential attract much attention recently, which has been shown to produce nonzero net current under certain conditions\cite{1, 2}. This type of the system is called thermal ratchet because particles are subject to the thermal noise. In the context of biology, thermal ratchets has been discussed as a possible mechanism of biological motors\cite{3, 4, 5, 6}. They also can be a mechanism of actuators for micro- or nano-machines. In the field of physics, it is studied in connection with the noise induced transportation\cite{7, 8, 9, 10, 11, 12, 13, 14, 15}.

For nonzero net current to appear in thermal ratchets both the spatial and time reversal symmetries need to be broken. Otherwise, no finite net current is expected, because of the Curie’s principle\cite{16}, which states that asymmetric phenomena is caused by asymmetry (when no symmetry breaks spontaneously). Hence both (1) existence of an spatially asymmetric potential and (2) a contact with a heat bath, which breaks the time reversal symmetry of the system by energy dissipation, are required for the realization of thermal ratchets. These two requirements alone, however, can not produce finite net current due to the second law of thermodynamics. In order to make system nonequilibrium, and thus to allow steady current, we require (3) existence of an additional noise or a time correlated force. A spatially unbiased noise or force is assumed hereafter, because otherwise an occurrence of directional motion of the particle is a trivial consequence of the asymmetry. We expect a directional particle motion in a non-equilibrium steady state, if and only if above three conditions are fulfilled.

The models of thermal ratchets discussed so far in the literatures are based on classical mechanics. But there are situations in which quantum effects such as quantum tunneling play important roles in the particle motion; for instance, in small systems like mesoscopic devices at low temperature. Here we propose a new concept, quantum ratchets, which are ratchet systems governed by quantum mechanics. Quantum ratchets give rise to interesting questions about nonequilibrium quantum dynamics in the presence of interaction with environments. Moreover, by studying quantum ratchet systems, we would be able to explore the new paradigm of quantum thermodynamics such as a quantum engine or a quantum energy transducer. In addition, from the technological point of view, quantum ratchets have a potential of being used as a new quantum electronic devices or quantum motors for nano-machines in future. In this letter, we propose one possible realization of quantum ratchets and show that finite net current appear in that system, which originates from purely quantum mechanical effects.

The model investigated in this letter is a tight-binding model. Its Hamiltonian is given as follows:

\begin{equation}
H_{\text{total}}(t) = H_{\text{sys}}(t) + \gamma_0 H_{\text{int}} + H_B, \tag{1}
\end{equation}

\begin{equation}
H_{\text{sys}}(t) = \sum_n \left\{ |n\rangle \langle n + 1| + |n\rangle \langle n - 1| + \left( V_{n \text{ mod } N} + F_n(t) \right) |n\rangle \langle n| \right\}, \tag{2}
\end{equation}
\[ H_B = \sum_\alpha \hbar \omega_\alpha \left( a_\alpha^\dagger a_\alpha + \frac{1}{2} \right), \quad (3) \]
\[ H_{int} = \sum_{n,\alpha} \left\{ g_{n,n+1} |n\rangle \langle n+1| + g_{n-1,n} |n-1\rangle \langle n| \right\} \left( a_\alpha + a_\alpha^\dagger \right) \]
\[ + \gamma_2 V_{n \text{mod} N} |n\rangle \langle n| \right\} \left( a_\alpha + a_\alpha^\dagger \right) \]
\[ \equiv H_I \sum_\alpha \left( a_\alpha + a_\alpha^\dagger \right). \quad (4) \]

\( H_{total}(t) \) is Hamiltonian of the total system consisting of the ratchet part and the heat bath. The ratchet part is described by \( H_{sys}(t) \). The localized state at site \( n \) is represented by \( |n\rangle \). \( V_{n \text{mod} N} \) represents an asymmetric periodic potential with period \( N \) and \( F_n(t) \) an external time dependent field. We measure energy in unit of the hopping coefficient. The heat bath, which is described by \( H_B \), is a collection of harmonic oscillators, each of which has a frequency \( \omega_\alpha \) and is described by the creation(annihilation) operator \( a_\alpha^\dagger (a_\alpha) \). The ratchet part and the heat bath interact with each other with a coupling constant \( \gamma_0 \) via \( H_{int} \), which is factorized into the following two parts: \( H_I \) and \( \sum_\alpha \left( a_\alpha^\dagger + a_\alpha \right) \), which operate on the Hilbert space of the ratchet part and the heat bath, respectively. In \( H_I \) the function \( g_{n,m} \) is defined as \( 1 + \gamma_1 (V_{n \text{mod} N} + V_{m \text{mod} N}) \) with the coupling parameter \( \gamma_1 \); \( \gamma_2 \) is another coupling parameter. This interaction is a general form of real symmetric tridiagonal interactions up to the first order of \( V_n \) (We omit 0-th order of the diagonal part, since it is a multiple of an identity operator and does not contribute to the energy dissipation). We note that the Hamiltonian \( H_{total}(t) \) is Hermitian, because only the diagonal part of \( H_{total}(t) \) is spatially asymmetric.

Let us start with the quantum Liouville equation for the density operator of the total system \( \sigma(t) \),
\[ \frac{\partial \sigma(t)}{\partial t} = -\frac{i}{\hbar} [H_{total}(t), \sigma(t)]. \quad (5) \]

The density operator of the ratchet part \( \rho(t) \) is obtained by \( \rho(t) = \text{Tr}_B \sigma(t) \), where \( \text{Tr}_B \) means the trace operation with respect to the Hilbert space of the heat bath. Assuming that (1) the total density operator at initial time, \( t = 0 \), is decomposed into the ratchet part and the heat bath part, i.e., \( \sigma(0) = \rho(0) \rho_B \), (2) the heat bath is at its thermal equilibrium at temperature \( T_{bath} \), so that \( \rho_B = \exp(-\beta H_B) / \text{Tr}_B \exp(-\beta H_B) \), \( \beta = 1/k_B T_{bath} \), and (3) the coupling constant \( \gamma_0 \) is sufficiently small, we get the following equation for \( \rho(t) \) after standard calculations:
\[ \frac{\partial \rho(t)}{\partial t} = -\frac{i}{\hbar} [H_{sys}(t), \rho(t)] \]
\[ -\frac{\gamma_0^2}{\hbar} \int_0^t ds \left( [H_I, H_I^{t-s} \rho(t-s)^{t-s}] \Phi(s) \right) \]
where $\Phi(t)$ is the autocorrelation function of the operator $\xi(t) \equiv \exp\{(i/\hbar)H_B t\} \sum_\alpha (a_\alpha + a_\alpha^\dagger) \exp\{-i(\hbar)H_B t\}$, i.e., $\Phi(t) = \text{Tr}_B \{\rho_B \xi(t) \xi(0)\}$. We introduced the notation $A^{t,\tau}$ for an arbitrary operator $A$ as follows:

$$
A^{t,\tau} = \mathcal{T}_t \exp\left\{-\frac{i}{\hbar} \int_{\tau}^{t} H_{\text{sys}}(t') dt' \right\} A \mathcal{T}_t^\prime \exp\left\{\frac{i}{\hbar} \int_{\tau}^{t} H_{\text{sys}}(t') dt' \right\},
$$

where $\mathcal{T}_t$ and $\mathcal{T}_t^\prime$ indicate time ordering product from the right to the left, and one from the left to the right, respectively. Equation (3) is exact up to order $\gamma_0^2$.

Since we have assumed the parameter $\gamma_0$ very small, the characteristic time of the relaxation of $\rho(t)$ is very long. Moreover, if the heat bath is sufficiently large, the function $\Phi(t)$ vanishes quickly. In such situation the integrand near $s \sim 0$ mainly contributes to the integral. In addition, assuming the external field changes more slowly than the characteristic time of $\Phi(t)$, we can approximate eq. (3) as

$$
\frac{\partial \rho(t)}{\partial t} = -\frac{i}{\hbar}[H_{\text{sys}}(t), \rho(t)] - \frac{2}{\hbar} \left\{[H_I, [K(t), \rho(t)]] + i[H_I, [H(t), \rho(t)]]\right\},
$$

where $[A, B]_+ = AB + BA$. Here we introduced new operators,

$$
K(t) = \int_0^\infty ds \exp \left\{-\frac{i}{\hbar} H_{\text{sys}}(t)s\right\} H_I \exp \left\{\frac{i}{\hbar} H_{\text{sys}}(t)s\right\} \text{Re} \Phi(s) \quad (9)
$$

$$
H(t) = \int_0^\infty ds \exp \left\{-\frac{i}{\hbar} H_{\text{sys}}(t)s\right\} H_I \exp \left\{\frac{i}{\hbar} H_{\text{sys}}(t)s\right\} \text{Im} \Phi(s). \quad (10)
$$

In what follows, we study the dynamics of the system with an asymmetric parabolic potential of period 5; i.e., $V_0 \mod 5 = 0, V_1 \mod 5 = 1/9, V_2 \mod 5 = 4/9, V_3 \mod 5 = 1,$ and $V_4 \mod 5 = 1/9$. Thus an unit cell consists of five sites. For modeling of the heat bath, we use the spectral density of $\omega$ which produces the standard Ohmic dissipation with the cutoff frequency $1/\lambda$ [19, 20, 21]; then we can replace a summation over modes by an integration, i.e., $\sum_\alpha \rightarrow \int_0^\infty d\omega \exp(-\lambda \omega)$ in the evaluation of $\Phi(s)$. The external field is simply chosen as a periodically on-off type ("flushing") field of the period $T$ [3, 40]:

$$
F_n(t) = \begin{cases} 
- V_n \mod N & \text{for } t \mod T > T/2 \\
0 & \text{for } t \mod T \leq T/2.
\end{cases} \quad (11)
$$

A current is defined through the conservation of the probability; taking the diagonal element of the equation of motion (8), we can define the local current $J_n(t)$ at the site $n$, by using the conservation relation for the probability $\langle n|(\partial \rho(t)/\partial t)|n \rangle + J_{n+1}(t) - J_n(t) = 0$, as follows:

$$
J_n(t) = -\frac{2}{\hbar} \text{Im} \langle n|\rho(t)|n-1 \rangle + \frac{2\gamma_0^2}{\hbar^2} g_{n-1,n} \text{Re} \langle n|W(t)|n-1 \rangle, \quad (12)
$$

\[3\]
where $W(t) = [\mathcal{K}(t), \rho(t)] + i[\mathcal{H}(t), \rho(t)]$. We integrate numerically each matrix element of eq. (8) by the fourth-order Runge-Kutta method\cite{22} (thus we solve complex simultaneous differential equations). We use the following parameters: $\hbar = 1$, $\gamma_0 = 0.01$, $\gamma_1 = 0.14$, $\gamma_2 = 0.14$, and $\lambda = 0.01$. System size is taken to be 10 sites and the periodic boundary condition is imposed, that is, the system consists of two unit cells. All the numerical integrations are made with the time step of Runge-Kutta method to be 0.0001. The initial state of $\rho(t)$ is prepared as the thermal equilibrium state of the inverse temperature $\beta$.

In Fig. (1) we show a typical time series of the total current per unit cell $J \equiv \sum_{in	ext{ unit cell}} J_n$. Here we set $\beta = 0.8$ and $T = 500$. The first duration of 250 time corresponds to the on-potential period in which the external force is zero, and next one for 250 time is the off potential period in which the external field cancels the asymmetric periodic potential. Oscillation in the current are clearly seen in Fig. (1): in the on-potential periods, fast oscillation appears but does not contribute to the time-averaged net current. Its typical time scale is the scale of $\hbar/\Delta E$, where $\Delta E$ is the typical eigenvalue difference in the asymmetric potential. On the other hand, much slower fluctuation is observed in the off-potential period. This is originated in the interaction Hamiltonian; its time scale is the order of $1/\gamma_0$. In the off-potential periods, we recognize a synchronous appearance of the current, that is, every phase of the oscillations in each off-potential period has an almost same value. This synchronous oscillation of the current, which does not depend on initial conditions and has a positive value for the present parameters, mainly contributes to the net current when the long-time average is taken.

In Figs. (2) we show the time-averaged current $\langle J \rangle$, versus the inverse temperature $\beta$ (a), and versus the period of the external field $T$ (b), respectively. The current varies with $\beta$ and $T$ and takes negative or positive values according to the conditions. This result is in clear contrast with the classical thermal ratchets. In the latter, the direction of the current does not change with parameters. In the present case the finite value of $J$ results from the synchronous oscillation mentioned above. The direction and the magnitude of $J$ depend on the phase of the oscillation at the instance the potential is turned off, which depends on the parameters.

Contact with the heat bath is essential for the synchronous appearance of the current. In fact, such an synchronous oscillation disappear if we turn off the interaction between the ratchet system and the heat bath. Figure (3) shows the current as the function of time, as Fig. (1), but in the absence of interaction with the heat bath. In this situation, the ratchet system obeys pure quantum dynamics. The current still appears in the off-potential periods, but its magnitude and direction are random. The reason is the following: in the on-potential periods, the current oscillates according to the eigenvalue difference of the Hamiltonian. Since the period of external field and a oscillation period in the on-potential period is generally incommensurate with each other, the phase of the oscillation when the potential is turned off fluctuates almost randomly.
The mechanism of synchronous oscillation for the case of finite $\gamma_0$ is considered as follows: After large enough repeated time $n$ of the external field, the system becomes non-equilibrium steady state due to the dissipation. Then the density matrix $\rho$ at each end of the period of the external field coincides with each other. It produces the synchronous oscillation. It is to be noted that the above stationary motion does not mean the stationary motion in each duration where the potential is constant.

To summarize, we proposed a new concept, quantum ratchet, and its one possible realization. Finite net current is found in the non-equilibrium steady state, which originates from purely quantum mechanical effects. The behavior of the current is quite different from that in the classical one: in the quantum ratchet, the current flows both direction which is determined by the heat bath temperature and/or the period of the external field, though, in the classical situation, it flows to one-direction decided by asymmetry of potential and type of external field. The bidirectionality means that, in quantum ratchet devices, we can control the electric current by changing parameters.

The present model has been considered in the weak coupling situation. Thus the relaxation time of the system becomes long. Because of this, we have studied the system only in the non-adiabatic time scale. If we study in the adiabatic and strong coupling region, different phenomena like crossover between classical and quantum regimes may be observed. The present results depend strongly on the detail of the model such as the potential shape, system size, and so on. This indicates that there is a possibility to produce the current more effectively by changing details of the model. For the study of the quantum thermodynamics of the ratchet system, especially properties as a quantum engine, or a quantum energy transducer, we have to study efficiency of energy. Detailed study is now in progress.

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Figure 1: Typical time series of the total current per unit cell: initial state is chosen as a thermal equilibrium state. We take some parameters to be $\beta = 0.8$ and $T = 500$. The system in first duration for 250 time is in “on-potential” state. In next one for 250 time it is in “off-potential” state. The total current $J = \sum_{\text{in unit cell}} J_n$ in the unit cell is calculated with the time interval 5.

Figure 2: The average current $\langle J \rangle$ versus (a) the heat bath inverse temperature $\beta$ and (b) the period of the external field $T$. In a classical overdamp limit, we expect only negative current to appear.

Figure 3: Typical time series of the current under pure quantum dynamics, that is, in the absence of the interaction with the heat bath. Initial condition of the system density matrix is taken to be “thermal equilibrium” state with inverse temperature $\beta = 0.8$. All of the other conditions are same as Fig. 1.