Adiabatically Rocked Quantum Ratchets

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Abstract. We investigate quantum Brownian motion in adiabatically rocked quantum ratchet systems. Above a crossover temperature $T_c$, tunneling events are rare, yet they already substantially enhance the classical particle current. Below $T_c$, quantum tunneling prevails and the classical predictions greatly underestimate the transport. Upon approaching $T = 0$ the quantum current exhibits a tunneling induced reversal, and tends to a finite limit.

INTRODUCTION

Traditional heat engines are devices to extract useful work out of thermal fluctuations by way of transferring heat between equilibrium baths at different temperatures. More realistic set-ups, involving also non-thermal forces, have been addressed quantitatively only since a few years under the label of “Brownian motors”, “molecular motors”, or “ratchets” [1,2]. Besides their principal interest and the diverse astonishing effects they can produce, they also entail a variety of interesting technological applications [2,3], and may be of relevance for intracellular transport as well [4]. In this note we highlight the intriguing features of a Brownian motor when quantum effects start to play an important role [5]. At sufficiently low temperatures, our predictions should be observable in mesoscopic structures such as the superconducting quantum interference device (SQUID) proposed in [6]. Using recent technical developments [7], semiconductor superlattices could be designed which, too, exhibit a quantum ratchet effect. On top of that, our results are also of potential relevance for biological transport phenomena that involve transfer of light particles such as electron- or proton-reactions.

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139
MODEL

Our starting point is the system-plus-bath Hamiltonian

$$H(t) = p^2/2m + V(x) - x f(t) + H_B.$$  

where \(x\), \(p\), and \(m\) are the coordinate operator, momentum operator, and mass of the quantum particle, respectively. Furthermore, the "ratchet"-potential \(V(x)\) is assumed to be asymmetric and periodic, for instance (cf. Fig. 1)

$$V(x) = V_0 \left( \sin(2\pi x/L) - 0.29 \sin(4\pi x/L) \right).$$  

and \(f(t)\) represents an unbiased non-thermal driving force. Finally, \(H_B\) describes the heat bath interacting with the particle and we adopt its usual modelling by an ensemble of harmonic oscillators at thermal equilibrium with a coupling bilinear in the bath and particle coordinates [8]

$$H_B = \sum_{j} \left( \frac{p_j^2}{2m_j} + \frac{m_j \omega_j^2}{2} (q_j - c_j x)^2 \right),$$  

where \(q_j\) and \(p_j\) are the coordinate and momentum operators of the bath oscillators. The effect of the remaining model parameters \(m_j\), \(\omega_j\), and \(c_j\) are completely fixed in the continuum limit, \(V \to \infty\) by the spectral density.

![Figure 1](image_url)  

**Figure 1.** Solid: ratchet potential \(V(x)\) is (2). Dashed and dotted: "sawtooth" potential \(U^a(x)\) is (8) with \(FL = 0.2 V_0\), \(L = 2\pi c_0\).
\[ J(\omega) = -\frac{\omega^2}{2} \int_{-\infty}^{\infty} \frac{d^2 \omega}{d\omega^2} \delta(\omega - \omega) . \]  

(4)

Focusing on so-called Ohmic friction, \[ J(\omega) = \omega \eta , \]  

(5)

the bath oscillators can be integrated out and the dynamics of the quantum particle in \( \psi \) can be rewritten as operator-valued quantum Langevin equation

\[ m \ddot{x}(t) = -\eta \dot{x}(t) - V'(x(t)) + f(t) + \xi(t) . \]  

(6)

Here, \( \eta \) is the viscous damping coefficient and \( \xi(t) \) a self-adjoint thermal noise operator with a Gaussian statistics of vanishing mean \( \langle \xi(t) \rangle \) and a symmetrized correlation \( \langle [\xi(t), \xi(0)] \rangle = k_B T \) \( \delta(t) \) (fluctuation-dissipation theorem with \( T \), \( k_B \), and \( \delta \) representing temperature, Boltzmann’s constant, and Planck’s constant over \( 2 \pi \), respectively).

The quantity of foremost interest in our above defined ratchet dynamics is the particle current in the steady state

\[ J = \lim_{t \to \infty} \langle \dot{x}(t) \rangle . \]  

(7)

where \( \langle \cdot \rangle \) denotes the quantum statistical mechanical expectation value together with a time average over the driving force.

In general, this requires the solution of a highly non-trivial far from equilibrium problem. To simplify matters, we restrict ourselves to very slowly varying forces \( f(t) \) such that the system can always adiabatically adjust to the instantaneous thermal equilibrium state (accompanying equilibrium). We furthermore assume that \( f(t) \) is basically restricted to the values \( \pm F \), i.e., the transitions between \( \pm F \) occur on a time scale of negligible duration in comparison with the time the particles in (6) are exposed to either of the “tiled washboard” potentials

\[ U^\pm(z) = V(z) \mp F z \]  

(8)

see also Fig. 1. As a final assumption we require a positive but not too large \( F \), such that \( U^\pm(z) \) still display a local maximum and minimum within each period \( T \), but these premises, the driving \( f(t) \) can be either of stochastic or of deterministic nature. In particular, our results presented in the next section are valid both for stochastic and deterministic chains of \( f(t) \).

To completely fix the model, we still have to specify the \( 5 \) parameters \( m, \eta, V_0, F, \) and \( t = T/2 \) in (3) and (8). We do this by prescribing 5 dimensionless numbers as follows: First, we fix \( V_0, F, \) and \( t \) and then \( u^\pm(z) \) through \( F/\sqrt{V_0} = 0.2, \Delta U_{\text{max}}/V_0 = 1.423, \) and \( |U^\pm(z)|^2 = 1.390 \), where \( \Delta U_{\text{max}} \) denotes the curvature of \( U^\pm(z) \) at a local maximum and \( \Delta U_{\text{max}} \) is the smallest of the 4 different
potential barriers between adjacent local minima of $U^*(x)$ and $U^-(x)$. This choice of $V_0$, $F$, and $l = L/2\pi$ corresponds to the situation depicted in Fig. 1. Next we choose $\eta/m_0 = 1$ with $\Delta_0 = [V_0/\hbar^2m_0]^{1/2}$, meaning a moderate damping as compared to inertia effects. To see this, we notice that $\Delta_0$ approximates rather well the true ground-state frequency $\omega_0$ in the potential $U^+(x)$, $\omega_0 = 1.13a_0$, and similarly for $U^-(x)$. In particular, $\eta/m_0 = 1$ rules out the occurrence of "deterministically running classical solutions" both in $U^+(x)$ and $U^-(x)$. Before specifying our last dimensionless number we remark that the temperature $T$ will not be fixed but rather used as control parameter. We, however, will restrict ourselves to thermal energies $k_BT$ much smaller than $\Delta T_{\text{max}}$ (so-called semiclassical condition) such that meaningful transition rates between adjacent minima of $U^-(x)$ can be defined and employed to determine the transport property (7) of our ratchet dynamics [5]. It then can be shown [8] that in the potential $U^+(x)$ genuine quantum tunneling events "through" the potential barrier are rate above a crossover temperature

$$T_c = \frac{\hbar \mu^+}{2k_B}, \quad \mu^+ = \sqrt{\eta^2 + 4m[\Delta T^+ - \Delta]}.$$  \hspace{1cm} (9)

while for $T < T_c^+$ tunneling yields the dominant contribution to the transition rates. An analogous crossover temperature $T_c^-$ arises for the potential $U^-(x)$ which is typically not identical but rather close to $T_c^-$. With the definitions

$$T_{\text{max}} = \max(T_c^+, T_c^-), \quad T_{\text{min}} = \min(T_c^+, T_c^-)$$  \hspace{1cm} (10)

we now fix our last dimensionless quantity through $\Delta T_{\text{max}}/k_B T_{\text{max}} = 10$. In this way, the weak noise condition is safely fulfilled for $T \leq T_{\text{max}}^+, \text{i.e., up to temperatures well above both } T_c^+ \text{ and } T^-$. At the same time, the so-called semiclassical condition [6] can be taken for granted when evaluating the quantum mechanical transition rates for all $T \leq T_{\text{max}}^+$. Adopting a path integral approach of the full system-plus-bath problem (1) this condition allows one to work within a saddle point approximation scheme [8]. For more details regarding the calculation of those rates and their relation to the current (7) we refer to [9].

\section*{RESULTS}

We performed in our work [5] the first numerical dissipative, low-temperature calculations to tackle the involved saddle point problem arising in the determination of the exponential leading contribution (bounce action) to the transition rates in a generic ratcheting potential (2); moreover, we have evaluated the full prefactors (rations of functional determinants) which dominate the non-exponential contributions to the incoherent, dissipative quantum tunneling rates in the semiclassical approximation. Our results for the quantum
ratchet model as specified in the previous section are depicted in Fig. 2. Shown are the current $J_{qm}$ from the above sketched quantum mechanical treatment together with the result $J_d$ that one would obtain by means of a purely classical calculation. The small dashed part in $J_{qm}$ in a close vicinity of the crossover temperatures $T_{e, \text{max}}$ and $T_{e, \text{min}}$ from (10) signifies an increased uncertainty of the semiclassical rate theory in this temperature domain.

Our first observation is that even above $T_{e, \text{max}}$, quantum effects may enhance the classical transport by more than a decade. They become negligible only beyond several $T_{e, \text{max}}$. In other words, significant quantum corrections of the classically predicted particle current set in already well above the cross-over temperature $T_0$, where tunneling processes are still rare. (They can be associated to quantum effects other than genuine tunneling “through” a potential barrier.) With decreasing temperature, $T < T_{e, \text{max}}$, quantum transport is even much more enhanced in comparison with the classical results [1b,1e]. A fur-

![Diagram](image)

**FIGURE 2.** The quantum mechanical steady state current $J_{qm}$ from (7) and its classical counterpart $J_d$ for the ratchet potential from Fig. 1 in dimensionless units $J/dqL$. Note the change of sign, the finite $T \to 0$ limit, and the non-monotonicity of $J_{qm}$. For more details see main text.

143
ther remarkable feature caused by the intriguing interplay between thermal noise and quantum tunneling is the inversion of the quantum current direction at very low temperatures. In a classical description, such a reversal for adiabatically slow driving is ruled out. Finally, $J_{	ext{th}}$ approaches a finite (negative) limit when $T \to 0$, implying a finite (positive) stopping force \cite{[2]} since at $T = 0$. In contrast, the classical prediction $J_d$ remains positive but becomes arbitrarily small with decreasing $T$. A curious detail is Fig. 2 is the non-monotonicity of $J_{	ext{th}}$ around $T_{	ext{max}}/T \approx 2.5$, caused by a similar resonance-like $T$-dependence in one of the underlying quantum mechanical transition rates. A better understanding of this issue is the subject of ongoing work.

We also studied other parameter values than those used in Fig. 2 as well as somewhat modified potentials \cite{[2]}. Basically, the same qualitative results are found except that the non-monotonic temperature dependence disappears for sufficiently large $\Delta U_{\text{eff}}/k_{\text{B}} T_{\text{th}}$ values. Thus all the above described novel features appear to be typical for a large class of quantum ratchet systems. Such effects clearly become of paramount importance for applications in mesoscopic systems at low temperatures. Note that $T_{\text{th}}$ can reach values larger than $100 \text{ K}$ in some physical and chemical systems, while it is in the $\text{mK}$ region in Josephson systems \cite{[8]}.

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REFERENCES


