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Adiabatically Rocked Quantum Ratchets

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Abstract. We investigate quantum Brownian motion in adiabatically rocked ratchet systems. Above a cross-over 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 grossly 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 protons-reactions.

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MODEL

Our starting point is the system-plus-bath Hamiltonian

$$\mathbf{H}(t) = \mathbf{p}^2/2m + V(\mathbf{x}) - \mathbf{x}\, f(t) + \mathbf{H}_B \ . \tag{1}$$

where $\mathbf{x}$, $\mathbf{p}$, 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)

$$V(x) = V_0\left[\sin(2\pi x/L) - 0.22\,\sin(4\pi x/L)\right] , \tag{2}$$

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

$$\mathbf{H}_B = \sum_{j=1}^{N}\left(\frac{\mathbf{p}_j^2}{2\,m_j} + \frac{m_j\omega_j^2}{2}\left(\mathbf{q}_j - \frac{c_j\mathbf{x}}{m_j\omega_j^2}\right)^2\right) , \tag{3}$$

where $\mathbf{q}_j$ and $\mathbf{p}_j$ are the coordinate and momentum operators of the bath oscillators. The effect of the remaining model parameters m_j, ω_j, and c_j are completely fixed in the continuum limit $N \to \infty$ by the spectral density

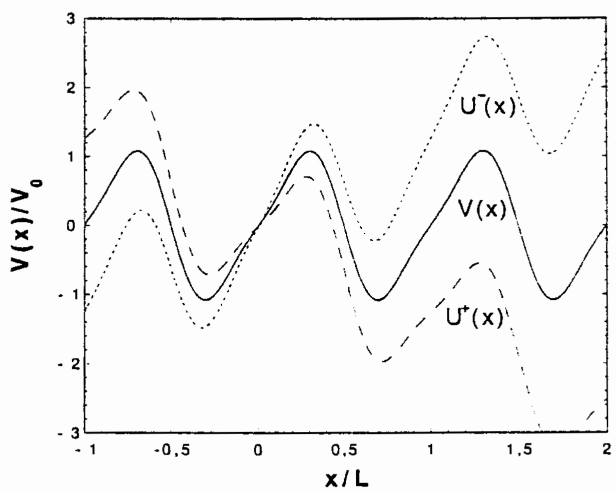

FIGURE 1. Solid: ratchet potential $V(x)$ in (2). Dashed and dotted: "tilted washboard potentials" $U^{\pm}(x)$ in (8) with $F\,l = 0.2\,V_0$, $l = L/2\pi$.

$$J(\omega) = \frac{\pi}{2} \sum_{j=1}^{\infty} \frac{c_j^2}{m_j \omega_j} \delta(\omega - \omega_j) \ . \tag{4}$$

Focusing on so-called Ohmic friction [8], *i.e.*,

$$J(\omega) = \omega \, \eta \ , \tag{5}$$

the bath oscillators can be integrated out and the dynamics of the quantum particle in (1) can be rewritten as operator-valued quantum Langevin equation

$$m \, \ddot{\mathrm{x}}(t) = -\eta \, \dot{\mathrm{x}}(t) - V'(\mathrm{x}(t)) + f(t) + \boldsymbol{\xi}(t) \ . \tag{6}$$

Here, η is the viscous damping coefficient and $\boldsymbol{\xi}(t)$ a self-adjoint thermal noise operator with a Gaussian statistics of vanishing mean $\langle \boldsymbol{\xi}(t) \rangle$ and a symmetrized correlation $\frac{1}{2}\langle \boldsymbol{\xi}(t)\boldsymbol{\xi}(0) + \boldsymbol{\xi}(0)\boldsymbol{\xi}(t)\rangle = k_B T \eta \frac{d}{dt} \coth(\pi k_B T \, t/\hbar)$ (fluctuation dissipation theorem with T, k_B, and $\hbar$ representing temperature, Boltzmann's constant, and Planck's constant over 2π, respectively).

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

$$J = \lim_{t \to \infty} \langle \dot{\mathrm{x}}(t) \rangle \ , \tag{7}$$

where $\langle \ \rangle$ 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 "tilted washboard" potentials

$$U^{\pm}(x) = V(x) \mp F \, x \tag{8}$$

see also Fig. 1. As a final assumption we require a positive but not too large F, such that $U^{\pm}(x)$ still display a local maximum and minimum within each period L. Apart from 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 choices of $f(t)$.

To completely fix the model, we still have to specify the 5 parameters m, η, V_0, F, and $l := L/2\pi$ in (2),(6),(8). We do this by prescribing 5 dimensionless numbers as follows: First, we fix V_0, F, l and thus $U^{\pm}(x)$ through $Fl/V_0 = 0.2$, $\Delta U^{min}/V_0 = 1.423$, and $|U''_{+}| \, l^2/V_0 = 1.330$, where U''_{+} denotes the curvature of $U^{+}(x)$ at a local maximum and ΔU^{min} 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 $\eta/m\Omega_0 = 1$ with $\Omega_0 := [V_0/l^2 m]^{1/2}$, meaning a moderate damping as compared to inertia effects. To see this, we notice that Ω_0 approximates rather well the true ground state frequency ω_0^+ in the potential $U^+(x)$, $\omega_0^+ = 1.153\,\Omega_0$, and similarly for $U^-(x)$. In particular, $\eta/m\Omega_0 = 1$ 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 $k_B T$ much smaller than ΔU^{min} (so-called semiclassical condition) such that meaningful transition rates between adjacent minima of $U^\pm(x)$ 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 rare above a crossover temperature

$$T_c^+ = \frac{\hbar\,\mu^+}{2\pi k_B}\,, \qquad \mu^+ = \frac{\sqrt{\eta^2 + 4m|U_+''|} - \eta}{2\,m}\,, \tag{9}$$

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

$$T_c^{max} = \max\{T_c^+, T_c^-\}\,, \qquad T_c^{min} = \min\{T_c^+, T_c^-\} \tag{10}$$

we now fix our last dimensionless quantity through $\Delta U^{min}/k_B T_c^{max} = 10$. In this way, the weak noise condition is safely fulfilled for $T \leq 2T_c^{max}$, *i.e.*, up to temperatures well above both T_c^+ and T_c^-. At the same time, the so-called semiclassical condition [8] can be taken for granted when evaluating the quantum mechanical transition rates for all $T \leq 2T_c^{max}$. Adopting a path integral treatment 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 [5].

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 exponentially leading contribution (bounce action) to the transition rates in a generic ratchet potential (2); moreover, we have evaluated the full prefactors (ratios 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_{cl} 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_c^{max} and T_c^{min} from (10) signifies an increased uncertainty of the semiclassical rate theory in this temperature domain.

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

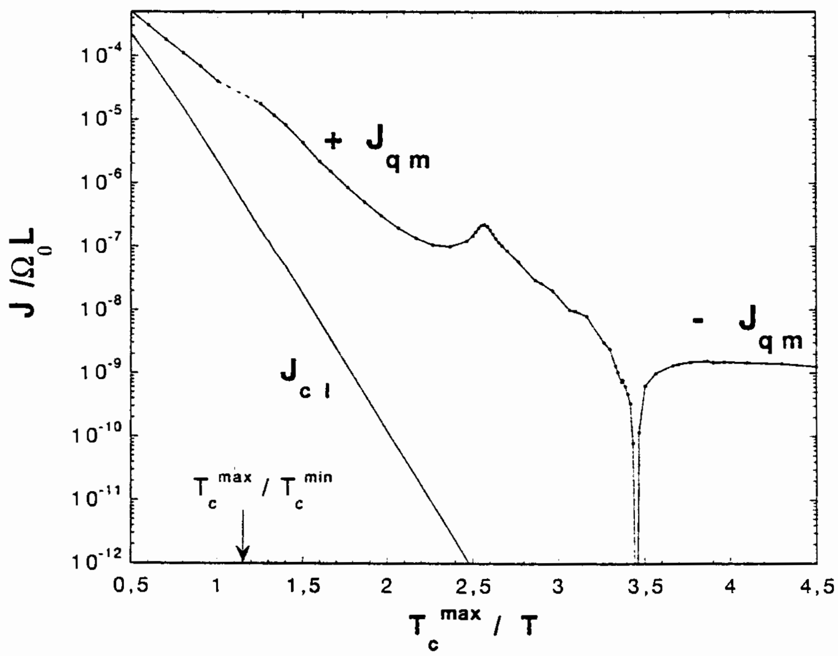

FIGURE 2. The quantum mechanical steady state current J_{qm} from (7) and its classical counterpart J_{cl} for the ratchet potential from Fig. 1 in dimensionless units $J/\Omega_0 L$. Note the change of sign, the finite $T \to 0$ limit, and the non-monotonicity of J_{qm}. For more details see main text.

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_{qm} approaches a finite (negative) limit when $T \to 0$, implying a finite (positive) stopping force [2,6] also at $T = 0$. In contrast, the classical prediction J_{cl} remains positive but becomes arbitrarily small with decreasing T. A curious detail in Fig. 2 is the non-monotonicity of J_{qm} around $T_c^{max}/T \simeq 2.5$, 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 (2). Basically, the same qualitative results are found except that the non-monotonous temperature dependence disappears for sufficiently large $\Delta U^{min}/k_B T_c^{max}$ 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_c can reach values larger than 100K in some physical and chemical systems, while it is in the mK region in Josephson systems [8].

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