Consistent description of quantum Brownian motors operating at strong friction

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A quantum Smoluchowski equation is put forward that consistently describes thermal quantum states. In particular, it notably does not induce a violation of the second law of thermodynamics. This so modified kinetic equation is applied to study *analytically* directed quantum transport at strong friction in arbitrarily shaped ratchet potentials that are driven by nonthermal two-state noise. Depending on the mutual interplay of quantum tunneling and quantum reflection these quantum corrections can induce both, a sizable enhancement or a suppression of transport. Moreover, the threshold for current reversals becomes markedly shifted due to such quantum fluctuations.

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I. INTRODUCTION

Brownian motors are small physical machines that operate far from thermal equilibrium by extracting energy fluctuations to generate work against external loads [1,2]. They present the physical analog of biomolecular motors that direct intracellular transport and control motion and sensation in cells [3]. In contrast to these molecular biomotors, however, the molecular sized physical engines necessitate—depending on the nature of particles to be transported and their operating temperature—a description that accounts as well for quantum features such as tunneling and quantum reflection. For this class of quantum Brownian motors, recent theoretical studies [4,5] have predicted that the transport becomes distinctly modified as compared to its classical counterpart. In particular, innate quantum effects such as tunneling induced current reversals, power-law-like quantum diffusion transport laws, and quantum Brownian heat engines have been observed with recent, guiding experiments that involve either arrays of asymmetric quantum dots [6] or cell arrays composed of different Josephson junctions [7].

The present field of classical Brownian motors is very well established [1–3]. In contrast, this is not the case in the quantum regime. It is mainly due to the mutual interplay of quantum mechanics, dissipation, and nonequilibrium driving that the theoretical description of such nonequilibrium, dissipative quantum Brownian motor devices is notoriously difficult. The present state of the art of the theory is characterized by specific restrictions such as, e.g., an adiabatic driving regime, a tight binding description, a semiclassical analysis, or combinations thereof [4,5]. As such, the study of quantum Brownian motors is far from being complete and there exists an urgent need of further developments. The analytic study of quantum Brownian transport for *arbitrarily shaped* spatially periodic ratchet potentials presents such a challenge. This goal is addressed here within the strong friction regime, where the underlying quantum dynamics can be modeled by a recently put forward, ingenious quantum generalization of Smoluchowski dynamics [8].

Classically, a system coupled to a thermal bath at temperature T is described in terms of Langevin equations or corresponding Fokker-Planck equations [9]. For a Brownian particle this yields the Kramers equation which in the strong friction limit reduces to the Smoluchowski equation. In quantum statistical physics the description of Brownian motion dynamics is distinctly more intricate; it has been worked out, however, in some detail within limited generality using, e.g., the assumption of a linear bath dynamics or a weak coupling limit. For the latter case, quantum master equations, e.g., of Lindblad form, have been derived [10,11].

II. QUANTUM SMOLUCHOWSKI DYNAMICS

Recent work within the strong friction limit shows that quantum Brownian motion can be described by a generalized Smoluchowski equation that accounts for leading quantum corrections [8,12]. For a particle of mass M moving in the potential $V(x)$, Ankerhold *et al.* proposed a quantum Smoluchowski equation (QSE) for the diagonal part of the density operator $\rho(t)$, i.e., the rate of change of the probability density $P(x,t)=\langle x|\rho(t)|x\rangle$ in position space x assumes the form [8]

$$\gamma M \frac{\partial}{\partial t} P(x,t) = \frac{\partial}{\partial x} V'_{\text{eff}}(x) P(x,t) + \frac{\partial^2}{\partial x^2} D_{\text{eff}}(x) P(x,t), \quad (1)$$

where γ denotes friction. The effective potential reads

$$V_{\text{eff}}(x) = V(x) + (1/2)\lambda V''(x), \quad (2)$$

wherein the prime denotes the derivative with respect to the coordinate x. The prominent parameter

$$\lambda = (\hbar/\pi M\gamma)\ln(\hbar\beta\gamma/2\pi), \quad \beta = 1/k_B T, \quad (3)$$

describes quantum fluctuations in position space and k_B is the Boltzmann constant. The effective diffusion coefficient reads [8]

$$D_{\text{eff}}(x) = D_{\text{Ank}}(x) = \beta^{-1}[1 + \lambda\beta V''(x)]. \quad (4)$$

Note that Eq. (1) is valid whenever $k_B T \ll \hbar\gamma$.

This so-derived quantum-Smoluchowski equation exhibits, however, a disturbing short-coming: In clear contradiction to the validity of the second law of thermodynamics, Eq. (1) yields for an arbitrary, *asymmetric* periodic ratchet potential $V(x)$ of period L at *zero*-external bias a *non-zero*, stationary average velocity $\langle v\rangle = JL$ (or equivalently, a nonvanishing probability current J). This is so because the expression for the current reads

$$\langle v\rangle = \frac{L}{\gamma M}\frac{1-\exp[\Psi(L)]}{\int_0^L dx D_{\mathrm{Ank}}^{-1}(x)\exp[-\Psi(x)]\int_x^{x+L} du\ \exp[\Psi(\mathrm{u})]}, \tag{5}$$

where $\Psi(x)=\int_0^x du V'_{\mathrm{eff}}(u)/D_{\mathrm{Ank}}(u)$ upon inspection is nonperiodic with $\Psi(L)\neq 0$. Thus a finite stationary drift emerges; i.e., a Maxwell demon seemingly is at work at stationary, thermal equilibrium.

III. DEMON-FREE QUANTUM-SMOLUCHOWSKI DYNAMICS

Next, we put forward a clear-cut modification of the above quantum-Smoluchowski equation which does not cause such a fake perpetual motion phenomenon. First, we observe from theory [8] that the *leading* strong friction quantum correction involves the second order derivative of the potential $V(x)$, see Eq. (4). Following prior works [8,12] we shall consistently neglect (in the high friction limit) higher order contributions in λ, which in fact would involve also higher order derivatives of the potential. This new, modified quantum Smoluchowski equation (MQSE) is derived from the following set of construction criteria: We seek a new diffusion coefficient that (i) in leading order reproduces the previous result in Refs. [8,12], and (ii) does not exhibit a Maxwell demon behavior, i.e., the modified dynamics yields in thermal equilibrium a vanishing probability current, and additionally, (iii) the dynamics reproduces the correct thermal quantum position probability for strong friction [13]. The construction criterion (ii) of zero flux together with the correct leading order result for the thermal position probability in (iii) then fixes the form of the diffusion function $F[V''(x)]=a^{-1}[1-bV''(x)]^{-1}$ *uniquely*. The two constants a and b read explicitly $a=\beta$ and $b=\lambda\beta$.

Upon an expansion of $F[V''(x)]$ into a series in λ the two diffusion functions do coincide in first order with respect to the quantity $\epsilon(x)=|\lambda\beta V''(x)|<1$, as required by the condition in (i). Therefore this improved modified quantum-Smoluchowski equation (1) is given by a modified diffusion, reading

$$D_{\mathrm{eff}}(x) = D_{\mathrm{mod}}(x) = \beta^{-1}[1-\lambda\beta V''(x)]^{-1}. \tag{6}$$

Note that from a mathematical viewpoint our thermal MQSE dynamics assumes the form of a Padé-like, nonperturbative result in place of Eq. (4). The thermal quantum-Smoluchowski stochastic dynamics in this strong friction limit is thus equivalent to classical Brownian dynamics within the effective potential (2) and the new, state-dependent diffusion coefficient given in Eq. (6). The corresponding (MQSE) Langevin equation reads in the Ito representation [10]

$$\gamma M\dot{x} = -V'_{\mathrm{eff}}(x) + \sqrt{2\gamma M D_{\mathrm{mod}}(x)}\ \xi(t), \tag{7}$$

where the dot denotes the time derivative and $\xi(t)$ is (classical) Gaussian white noise of vanishing mean and correlation $\langle\xi(t)\xi(s)\rangle=\delta(t-s)$. The above scheme is close in spirit with the approximation method of colored noise driven dynamics in terms of corresponding effective Markovian processes [14].

IV. QUANTUM BROWNIAN MOTOR TRANSPORT

A finite transport emerges when the system operates far from thermal equilibrium [2]. In the present context, we investigate overdamped, quantum Brownian motors [4,5] with the quantum fluctuations characterized by the parameter λ in Eq. (3). To this aim, we complement the thermal quantum dynamics in Eq. (7) with a slowly waggling nonthermal, deterministic, or random force $\eta(t)$, i.e.,

$$\gamma M\dot{x} = -V'_{\mathrm{eff}}(x) + \sqrt{2\gamma M D_{\mathrm{mod}}(x)}\xi(t) + \eta(t). \tag{8}$$

In dimensionless form we then obtain

$$\dot{y} = -W'_{\mathrm{eff}}(y) + \sqrt{2\mathcal{D}_{\mathrm{mod}}(y)}\hat{\xi}(s) + \hat{\eta}(s), \tag{9}$$

where the position of the Brownian motor is scaled as $y=x/L$, time is rescaled as $s=t/\tau_0$, with the characteristic time scale reading $\tau_0=M\gamma L^2/\Delta V$ [the barrier height ΔV is the difference between the maximal and minimal values of $V(x)$]. During this time span, a classical, overdamped particle moves a distance of length L under the influence of the constant force $\Delta V/L$. The effective potential is $W_{\mathrm{eff}}(y)=W(y)+(1/2)\lambda_0 W''(y)$, where the rescaled potential $W(y)=V(x)/\Delta V=W(y+1)$ possesses a unit period and a unit barrier height. The dimensionless parameter $\lambda_0=\lambda/L^2$ describes quantum fluctuations over the characteristic length L. For example, the value $\lambda_0=0.01$ means that, roughly speaking, the difference between quantum and classical fluctuations of the position of the Brownian particle is significant over distances of the order $\sqrt{\lambda_0}L=0.1L$. The rescaled diffusion function $\mathcal{D}_{\mathrm{mod}}(y)$ reads

$$\mathcal{D}_{\mathrm{mod}}(y) = \beta_0^{-1}[1-\lambda_0\beta_0 W''(y)]^{-1}. \tag{10}$$

The dimensionless, inverse temperature $\beta_0=\Delta V/k_B T$ is a ratio of the activation energy in the nonscaled potential and the thermal energy. The rescaled Gaussian white noise is $\hat{\xi}(s)=(L/\Delta V)\xi(t)$ and the rescaled, nonthermal force reads $\hat{\eta}(s)=(L/\Delta V)\eta(t)$.

As a specific realization, we next consider nonthermal fluctuations modeled by Markovian, two-state noise, $\hat{\eta}(s)=\{-a,a\}$, that switches with a rate ν between the levels a and $-a$. This problem can be solved analytically in the adiabatic limit, i.e., if $\nu\to 0$. In this limit the stationary averaged dimensionless velocity reads $\langle\dot{y}\rangle=J=(1/2)[J(a)+J(-a)]$, where

$$J(a) = \frac{1 - \exp(-\beta_0 a)}{\int_0^1 dy\ \mathcal{D}_{\mathrm{mod}}^{-1}(y)\exp[-\beta_0\Psi(y,a)]\ \int_y^{y+1} dz\ \exp[\beta_0\Psi(z,a)]} \tag{11}$$

and

$$\Psi(y,a) = W(y) + (1/2)\lambda_0 W''(y) - (1/2)\lambda_0\beta_0[W'(y)]^2 - (1/4)\lambda_0^2\beta_0[W''(y)]^2 + a\lambda_0\beta_0 W'(y) - ay. \tag{12}$$

Its classical behavior, i.e., $\lambda_0=0$, has been studied in Ref. [15].

The influence of the quantum corrections is presented in Figs. 1–4. The role of quantum noise enters via two functions: The effective potential $W_{\mathrm{eff}}(y)$ and the effective diffusion function $\mathcal{D}_{\mathrm{mod}}(y)$. The quantum correction to the potential depends logarithmically weakly on temperature. The crucial correction stems from the diffusion which increases as the temperature decreases. The prominent quantum effects appear for lower temperatures. In Figs. 1–4, we take for the rescaled quantum fluctuations a parameter value of $\lambda_0 = 10^{-4}\ln(10^3\beta_0)$. This choice assures that the quantum Smoluchowski regime is fully valid down to low temperatures of the order $\beta_0\approx 10$. In Fig. 1 we depict the current vs the dichotomic noise level a. We deduce that the quantum corrections reduce the absolute value of the current (the maximal absolute quantum correction is $|\lambda_0\beta_0 W''(y)|=0.202$). Note that the current value approaches zero for a vanishing noise amplitude $a\to 0$ (solid line) and, as well, for very large amplitude $a\to\infty$. The modification of the diffusion coefficient turns out to be essential for small amplitudes a of the nonequilibrium two-state noise; this regime describes the nearequilibrium behavior with the directed current approaching zero. In clear contrast, the use of the conventional quantum Smoluchowski equation (QSE) in Eq. (4) (dotted) yields a nonphysical, (although small) positive current value. It should be pointed out, however, that far away from equilibrium (for $a>0.5$) the two forms of quantum-Smoluchowski dynamics yield practically identical results.

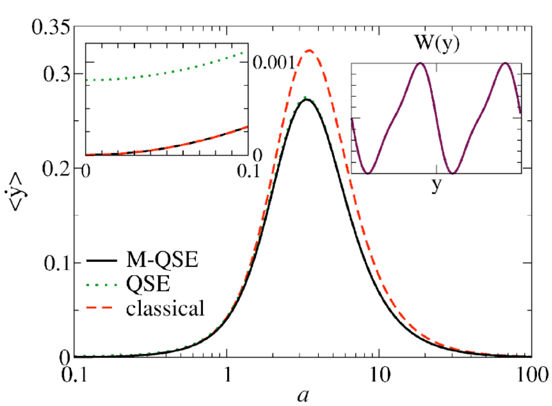

FIG. 1. Stationary velocity $\langle\dot{y}\rangle$ vs the two-state noise amplitude a for both a strongly damped quantum Brownian motor (solid line) and its classical counterpart (dashed line) is depicted for the potential (see the right inset) of unit barrier height, $W(y)=-W_0[\sin(2\pi y)+0.25\sin(4\pi y)]$, with $W_0\approx 0.454$. The theory (dotted line) in Ref. [8] yields a nonphysical (although small) quantum-Maxwell demon behavior at small noise amplitudes a (see the left inset); further away from equilibrium ($a>0.5$) the QSE and the MQSE predictions practically coincide within line thickness. The chosen dimensionless inverse temperature is $\beta_0=5$.

The analytic expression for the current allows one to study *arbitrarily shaped* ratchet profiles. As examples we consider different cases from the family of more complex shaped asymmetric periodic potentials

$$W(y) = W_0\{\sin(2\pi y) + 0.4\sin[4\pi(y-0.45)] + b\sin[6\pi(y-0.45)]\}, \tag{13}$$

where b is a shape parameter and W_0 is chosen such that the barrier height is normalized to unity. This ratchet potential exhibits an intriguing current reversal vs the noise amplitude a. The maximal absolute quantum correction is $|\lambda_0\beta_0 W''(y)|=0.06$. There occur two regimes: one regime of small noise levels a for which the amplitude of the quantum current is enhanced and one at larger noise amplitudes where the classical current exceeds its quantum counterpart. A most salient intermediate regime occurs for which the *classical current is positive while the quantum current remains negative*. The point of the physically relevant quantum current reversal is shifted towards larger noise levels. Use of the

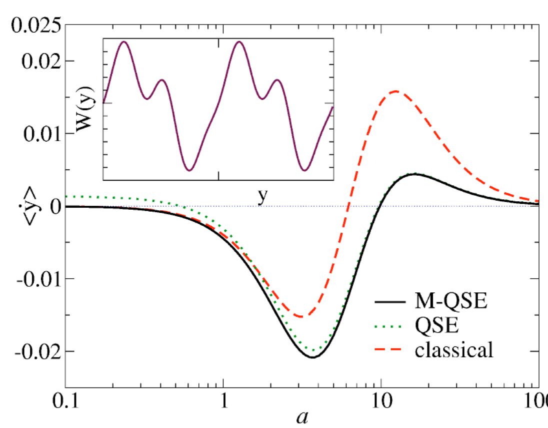

FIG. 2. The dependence of the stationary current $\langle\dot{y}\rangle$ vs the two-state noise level a is depicted for the potential (13) with $b=0.3$ (inset) for the modified quantum-Smoluchowski (MQSE) theory (solid line), the conventional quantum-Smoluchowski (QSE) theory (dotted), and the classical case (dashed line), respectively, for an inverse dimensionless temperature $\beta_0=2$. Note that the maximal absolute correction is actually rather small: $|\lambda_0\beta_0 W''(y)|=0.06$

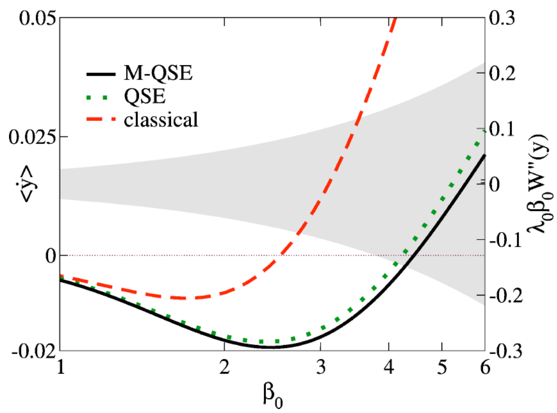

FIG. 3. The directed noise-induced transport $\langle \dot{y} \rangle$ of the quantum Brownian motor (solid line) vs the dimensionless inverse temperature β_0 for the ratchet potential (13) with $b=0.3$, see inset in Fig. 2, is compared with its classical limit (dashed line) and the conventional quantum theory in Eq. (4) (dotted line). The dichotomic noise level is set at $a=5$. The variations of the quantum corrections are depicted with the shaded background.

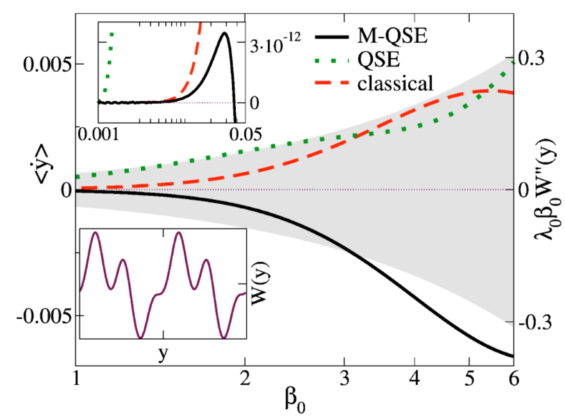

FIG. 4. Comparison of classical and quantum noise induced directed transport as in Fig. 3 vs inverse temperature for a different dichotomic noise level $a=1$ and for a different ratchet potential (13) with $b=0.62$, see the lower inset. The notation and symbols are the same as in Fig. 3. For this potential the classical current does not change the direction. The standard quantum Smoluchowski equation predicts a positive current whereas the modified quantum Smoluchowski equation leads to a positive current only for small values of β_0 and then yields a current in the opposite direction. For this current reversal see the upper inset.

quantum-Smoluchowski diffusion theory of Refs. [8,12] yields a fake, positive-valued current at small dichotomic noise strength (dotted line), being accompanied by a nonphysical (!) current reversal, see Fig. 2. We find again that the expected convergence between the two theories occurs far away from thermal equilibrium.

In Figs. 3 and 4 we elucidate the role of temperature. Equation (10) shows that the quantum corrections increase monotonically as temperature decreases. We must refrain, however, from analyzing the limit of extreme low temperature. This is so because the quantum corrections then grow too large, causing the diffusion to pass from positive to nonphysical, negative values upon exceeding the threshold value 1; clearly, the strong friction quantum theory is valid only below this threshold. In fact, for correction values close to threshold, the nondiagonal, density matrix elements assume nonzero decoherence values that can no longer be neglected with the quantum-Smoluchowski theory. Figures 3 and 4 depict these increasing quantum corrections with decreasing temperature for two different potentials and different dichotomic noise levels. For the potential (13) with $b=0.3$, see the inset in Fig. 2, for large temperatures both the classical current and the quantum current are negative. With decreasing temperature the interplay between reflection and tunneling causes a larger (in absolute value) quantum current; upon crossing the point of classical current reversal this behavior is interchanged. At even lower temperatures quantum corrections cause a smaller current value. The conventional and the modified quantum theories yield similar results, see Fig. 3. For the potential (13) with $b=0.62$, see the inset in Fig. 4, and for the dichotomic noise level $a=1$, there is no classical current reversal. For very large temperatures the quantum current agrees with the classical one and, with decreasing temperature, first increases and then changes the direction, see the upper inset in Fig. 4. The conventional theory completely misses these particular quantum features and predicts a similar current as the classical Smoluchowski equation does, see Fig. 4.

V. CONCLUSIONS

By use of a distinct modification of quantum-Smoluchowski theory we have developed a strong friction quantum approximation that is in agreement with both thermal equilibrium statistics and—above all—with the second law of thermodynamics. This so obtained, modified quantum theory can be applied to far from equilibrium transport where it facilitates closed form expressions (in terms of quadratures) for directed, quantum Brownian motor transport. Our tractable results hold true away from the semiclassical limit and, additionally, can readily be applied to experimentally, arbitrarily shaped ratchet profiles. Note that this presents an important advance over prior studies of quantum ratchets [4,5] that often require the use of manageable, stylized potential forms. Our investigation additionally manifests a rich spectrum of quantum Brownian motor behaviors, exhibiting both quantum induced enhancement and suppression of transport, as well as shifted current reversals.

These novel features can advantageously be put to work for quantum ratchets on the micro- and nanoscale [2]. Moreover, the structure of our quantum-Smoluchowski dynamics can be generalized to higher dimensional overdamped situations as, e.g., for quantum noise-induced directed transport on surfaces. In particular, our method and these quantum ratchet signatures can be utilized to optimize transport properties in superconductors by controlling the motion of vortices and magnetic flux quanta [16,17].

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