Quantum diffusion in biased washboard potentials: Strong friction limit

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(Received 24 November 2005; published 7 March 2006)

Diffusive transport properties of a quantum Brownian particle moving in a tilted spatially periodic potential and strongly interacting with a thermostat are explored. Apart from the average stationary velocity, we foremost investigate the diffusive behavior by evaluating the effective diffusion coefficient together with the corresponding Peclet number. Corrections due to quantum effects, such as quantum tunneling and quantum fluctuations, are shown to substantially enhance the effectiveness of diffusive transport if only the thermostat temperature resides within an appropriate interval of intermediate values.

DOI: 10.1103/PhysRevE.73.031105 PACS number(s): 05.40.−a, 02.50.Ey, 42.50.Lc, 05.60.Gg

I. INTRODUCTION

Brownian motion in periodic structures can describe diverse processes in many different branches of science. Within a physical context, among other phenomena, it models the dynamics of the phase difference across a Josephson junction [1,2], rotating dipoles in external fields [3,4], superionic conductors [5], charge density waves [6], particle separation by electrophoresis [7], transport on crystalline surfaces [8,9], and biophysical processes such as intracellular transport [10–13]. Yet another important area constitutes the noise-assisted transport of Brownian particles [14,15], as occurs for Brownian motors possessing ample applications in physics and chemistry [10].

In this paper, we study the one-dimensional overdamped motion of a quantum Brownian particle subjected to a tilted potential $U(x)$,

$$U(x) = V(x) - Fx, \quad V(x) = V(x+L), \tag{1}$$

where $V(x)$ denotes a periodic potential of period L and F is an external static force.

The basic quantities characterizing this motion are statistical moments of position and velocity of the Brownian particle. At least the first two moments—i.e., the average position and average velocity—and their respective dispersions are most substantial. In particular, the stationary average velocity can be defined by the relation

$$\langle v \rangle = \lim_{t\to\infty} \frac{\langle x(t) \rangle}{t}, \tag{2}$$

where $x(t)$ is the position of the Brownian particle at time t and $\langle \cdots \rangle$ is the average over all realizations of the thermal noise and initial conditions. The dispersion of the position can be characterized by the diffusion coefficient defined as [16]

$$D_{eff} = \lim_{t\to\infty} \frac{\langle x^2(t) \rangle - \langle x(t) \rangle^2}{2t}. \tag{3}$$

In the classical case, for strong friction, when only thermal equilibrium fluctuations affect the particle, the stationary average velocity and the diffusion coefficient can be expressed by exact closed formulas [17,18]. For nonequilibrium driving they can be calculated in specific cases only; see, e.g., [19–21].

Depending on the form of the potential, the magnitude of the tilt, and thermostat temperature, two interesting phenomena can be observed: A giant enhancement of the diffusion constant at a critical tilt [17,18] and a low-randomness window at subcritical tilts [22]. The influence of the shape of the potential [22,23] and of a position-dependent friction coefficient [24] on the transport has also been investigated.

However, in many cases, like for the Josephson junction at intermediate temperatures, the classical theory is insufficient; i.e., the leading quantum corrections [25] should be considered. It was shown in Refs. [26,27] that in the strong friction limit, effects of quantum Brownian fluctuations [28] are restricted not only to low temperatures; therefore, these should be incorporated for higher temperatures as well. This is so because quantum fluctuations, even if reduced for one variable, are enlarged for the conjugate variable. Quantum corrections can modify the dynamics quantitatively and sometimes even qualitatively. Physically relevant examples illustrating these features are presented in Refs. [27–29].

For the average current in Eq. (2) of the Brownian particle dynamics such quantum corrections have been studied repeatedly in the previous literature within different approaches [30]. In particular, within the quantum Smoluchowski equation these quantum corrections have been studied recently by Ankerhold in Ref. [31] for an overdamped Josephson junction.

In distinct contrast, with this work we mainly focus on the role of the quantum corrections to the diffusion of the mean squared displacement of the coordinate (or Josephson phase, respectively) as defined with Eq. (3).

The quantum diffusive dynamics in the regime of a strong interaction with a thermostat can be described by the so-called quantum Smoluchowski equation (QSE) [26,27] incorporating quantum fluctuations above the crossover temperature [14,25]. It corresponds to a classical Smoluchowski equation, in which the potential $U(x)$ and diffusion coefficient D are modified due to quantum effects. In other words, the quantum non-Markovian diffusion process of a particle position is approximated by a classical Markov process de-

scribing motion in an effective potential and with an effective, state-dependent diffusion coefficient. This leads to a quite comfortable situation because methods of analyzing Smoluchowski equations are well elaborated and can directly be applied and implemented for a wide class of systems. In this paper we demonstrate how the quantum fluctuations influence the diffusion behavior of a Brownian particle stochastically moving in washboardlike potentials.

II. CLASSICAL BROWNIAN PARTICLE IN TILTED PERIODIC POTENTIALS

The overdamped motion of a classical Brownian particle is described by the Langevin equation

$$\eta\dot{x} = -U'(x) + \sqrt{2\eta kT}\xi(t), \tag{4}$$

where η denotes the viscous friction coefficient and k is the Boltzmann constant. The overdot and prime indicate differentiation with respect to time t and to position x, respectively. The zero-mean and δ-correlated Gaussian white noise $\xi(t)$, i.e. $\langle \xi(t)\xi(s)\rangle = \delta(t-s)$, models the influence of a thermostat of temperature T on the system.

The calculation of the average velocity $\langle v\rangle$ and effective diffusion D_{eff} can be accomplished by mapping the washboard potential on a corresponding jump process. This construction procedure has been elucidated in [22]. As a result, a cumulative process with independent increments is obtained and its asymptotic mean and variance are given by the first two central moments of the escape time density [14,17,18]. In this way, the stationary average velocity [14,15,32,33] and the diffusion coefficient [17,18] for the process modeled by Eq. (4) can be expressed by closed-form relations involving quadratures only—i.e.,

$$\langle v\rangle = \frac{L}{T_1(x_0 \to x_0 + L)},$$

$$D_{eff} = \frac{L^2}{2}\frac{T_2(x_0 \to x_0 + L) - T_1^2(x_0 \to x_0 + L)}{T_1^3(x_0 \to x_0 + L)}, \tag{5}$$

where x_0 is an arbitrary, initial value and

$$T_n(x_0 \to b) = \langle t^n(x_0 \to b)\rangle \tag{6}$$

denotes the nth statistical moment of the first passage time $t(x_0 \to b)$ at which the Brownian particle arrives at the point b while starting out from the position x_0. For the case $b > x_0$, these moments are given by the recurrence relation [34]

$$T_n(x_0 \to b) = n\beta\eta\int_{x_0}^{b} \mathrm{d}x \exp[\beta U(x)] \times \int_{-\infty}^{x} \mathrm{d}y \exp[-\beta U(y)] T_{n-1}(y \to b) \tag{7}$$

for $n = 1, 2, 3\ldots$, where $T_0(y \to b) = 1$, $\beta = 1/kT$, and the product $\beta\eta = D_0^{-1}$ is the reciprocal of the Einstein diffusion coefficient D_0. Expressions (6) and (7) are rather complicated. However, they can be simplified as shown in [17,18].

III. OVERDAMPED QUANTUM BROWNIAN MOTION

To start with the investigation of quantum corrections to diffusion we consider a quantum Brownian particle moving in the tilted potential $U(x)$. The evolution of its position can be described by the respective probability density function $P(x,t) = \langle x|\rho(t)|x\rangle$, which is the diagonal part of the statistical operator $\rho(t)$. Within the strong friction limit (the quantum Smoluchowski regime), the dynamics of such a particle is described by the QSE which correctly takes into account leading quantum corrections in a temperature regime above the crossover temperature [14,25]. Above this crossover temperature the overall escape is dominated by thermal activation with corrections stemming from quantum tunneling and quantum reflection [35,36]. The corresponding theory assumes the structure of a classical Smoluchowski equation with modified drift and modified diffusion terms [26,27,29]:

$$\eta\frac{\partial}{\partial t}P(t,x) = \frac{\partial}{\partial x}\left(U'_{eff}(x) + \frac{\partial}{\partial x}D(x)\right)P(x,t). \tag{8}$$

The effective potential reads

$$U_{eff}(x) = U(x) + (1/2)\lambda U''(x). \tag{9}$$

The effective diffusion coefficient $D(x)$, being constant in the classical case—i.e., $D(x) = D = k_B T = \beta^{-1}$—becomes position dependent, assuming the unique form [29,36]

$$D(x) = \left[\beta\left[1 - \lambda\beta U''(x)\right]\right]^{-1}. \tag{10}$$

This diffusion is required to remain non-negative; i.e., within its regime of validity [29,36], the inequality $\lambda\beta U''(x) = \lambda\beta V''(x) < 1$ must be satisfied for all positions x. For smooth periodic functions $V(x)$ and sufficiently small $\lambda\beta$ this inequality holds for arbitrary x.

The prominent parameter λ characterizes quantum fluctuations in position space; it explicitly reads [26,27]

$$\lambda = (\hbar/\pi\eta)\ln(\hbar\beta\eta/2\pi M). \tag{11}$$

It depends nonlinearly on the Planck constant $\hbar$ and on the mass M of the Brownian particle, whereas, in the classical case, the overdamped dynamics neither depends on $\hbar$ nor on the mass M (note that we use the friction constant η which has units kg/s as in the classical Stokes case). Note also that this quantum correction approaches zero with the friction η growing towards infinity.

The Langevin equation corresponding to the Smoluchowski equation (8) becomes, within the Ito interpretation [37],

$$\eta\dot{x} = -U'_{eff}(x) + \sqrt{2\eta D(x)}\xi(t). \tag{12}$$

The average stationary velocity $\langle v\rangle$ and the diffusion classical coefficient D_{eff} can be calculated as in the case described by the Langevin equation (4), using relation (6) and the known formula for statistical moments of the first passage time. In comparison with Eq. (7), the statistical moments are thereby modified into the form [34]

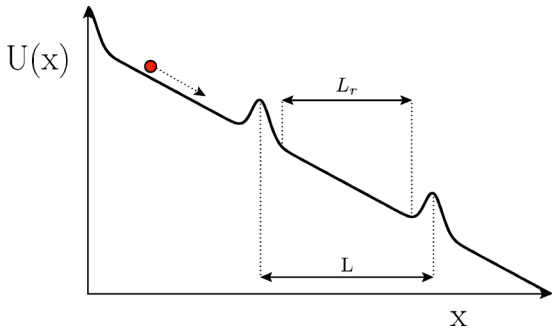

FIG. 1. (Color online) Schematic picture of the Brownian particle in the tilted periodic potential $U(x)=V(x)-Fx$, defined in Eqs. (1) and (17) below. L denotes the period of the potential $V(x)$, and L_r stands for the length of free slide between the barriers.

$$T_n(x_0 \to b) = n\eta \int_{x_0}^{b} \mathrm{d}x \exp[\phi(x)] \times \int_{-\infty}^{x} \mathrm{d}y D^{-1}(y) \exp[-\phi(y)] \times T_{n-1}(y \to b), \tag{13}$$

where

$$\phi(x) = \int^{x} \frac{U'_{eff}(z)}{D(z)} \mathrm{d}z. \tag{14}$$

Insertion of the expressions for the effective potential (9) and the effective diffusion function (10) yields

$$T_n(x_0 \to b) = n\beta\eta \int_{x_0}^{b} \mathrm{d}x \exp[\beta\psi(x)] \times \int_{-\infty}^{x} \mathrm{d}y \exp[-\beta\psi(y)][1-\lambda\beta U''(y)] \times T_{n-1}(y \to b), \tag{15}$$

where the thermodynamic potential $\psi(x)$ becomes

$$\psi(x) = U(x) + (1/2)\lambda U''(x) - (1/2)\lambda\beta[U'(x)]^2 - (1/4)\lambda^2\beta[U''(x)]^2. \tag{16}$$

We observe that quantum corrections modify the statistical moments as given by Eq. (15) compared to the classical form (7) in a two fold way: First, the physical potential $U(x)$ is replaced by the thermodynamic potential $\psi(x)$. This thermodynamic potential depends on the temperature β of the system and on the coupling constant of the Brownian particle with its surroundings via the damping constant η, which in turn enters into the parameter λ. Second, the function in the inner integral (over the variable y) on the right-hand side of Eq. (15) is modified by the factor $[1-\lambda\beta U''(y)]$, which depends on the curvature [i.e., on $U''(y)=V''(y)$] of the physical potential $U(y)$.

We will examine the quantum Brownian particle moving in a tilted washboard potential like that presented in Fig. 1. We scale the space and time in such a way that for the rescaled equation corresponding to Eq. (12) the friction coefficient equals $\eta=1$ and the temperature is represented by the dimensionless quantity $\beta_0=10\Delta V/k_BT$, where ΔV is the barrier height of the unscaled periodic potential. We choose a specific form of the dimesionless periodic part $V(x)$ of the potential $U(x)$: namely [22],

$$V(x) = \Delta \exp\{\varepsilon[\cos(x)-1]\}/\varepsilon. \tag{17}$$

The advantage of this choice is that by an appropriate manipulation of ε and Δ, the barrier height and distance between neighboring barriers can be varied independently. As a consequence, one can change two time scales independently: a first one is related to the deterministic sliding motion between neighboring barriers, and the other is related to the inverse of the activation rate over a barrier. In all numerical calculations here, we have chosen $\varepsilon=100$ and $\Delta=10$; thus, the barrier height of the dimensionless potential without the tilt is 0.1.

IV. QUANTUM DIFFUSION IN TILTED WASHBOARD POTENTIALS

In order to understand the influence of the shape of the washboard potential on the particle dynamics, in both the classical and quantum regimes, is it desirable to identify characteristic time scales. The first one is given by the time $\tau_r=L_r/F$ the particle needs to slide down the distance L_r (see Fig. 1) with a constant velocity $v=F$ (remember that the friction coefficient $\eta=1$ and the force is rescaled). This time scale is relevant if the potential has an almost constant slope between neighboring comparatively narrow barriers, as in the case considered here. The second time scale τ_e is determined by the escape time, as determined by the effective quantum Smoluchowski equation. The potential $V(x)$ has been chosen in the above-described way, so that these time scales can be "tuned" independently: τ_r by the force F and the parameter ε, and τ_e by the barrier height using both parameters ε and Δ of the potential (17).

The transport of particles is optimal if a large mean velocity goes along with small diffusion. This can be quantified by the dimensionless Peclet number [38]

$$\mathrm{Pe} = \frac{\langle v \rangle L}{D_{eff}}. \tag{18}$$

The efficiency of the diffusive transport as measured by the Peclet number can either be enhanced by an increase of the net current (i.e., the stationary mean velocity) and/or by a decrease of the effective diffusion, resulting in a maximal Peclet number Pe. The average velocity for the overdamped motion in a tilted washboard potential is limited by the free-slide speed which coincides with the value F in our case. The particle will approach this free-slide velocity when the barriers become negligible—for example, for a sufficiently high thermal energy kT or very strong tilt F. This situation, however, does not lead to an optimal transport performance in the sense of a maximal Peclet number [22,39]; see also below.

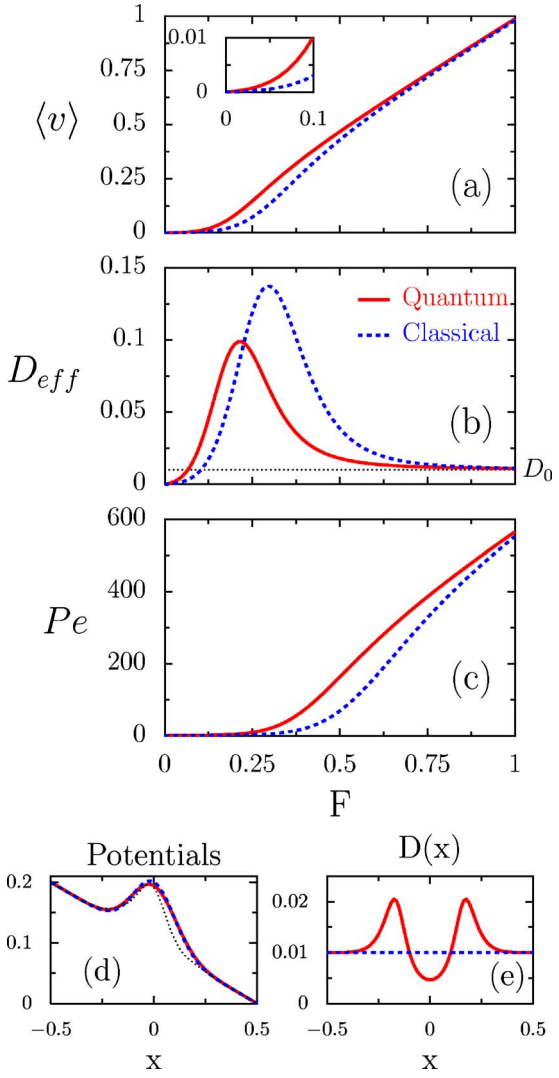

FIG. 2. (Color online) Average velocity $\langle v \rangle$ (a), effective diffusion D_{eff} (b), and Peclet number Pe (c) are drawn versus tilt F. Parameters of the potential are $\varepsilon=100$, $\Delta=10$, which result in a barrier height of $\Delta V=0.1$ in the absence of a tilt ($F=0$) and a critical tilt $F_c \simeq 0.6$ above which all barriers disappear. The rescaled inverse temperature is set to $\beta=100$, corresponding to a small quantum parameter $\lambda_0 \simeq 0.00115129$. The mean velocity and Peclet number are always larger in the quantum case, even if the classical effective diffusion is smaller (as is the case for $F \lesssim 0.25$). With panel (d) we depict the corresponding classical, $U(x)$ (dashed line), quantum effective, $U_{eff}(x)$ (solid line), and thermodynamic, $\psi(x)$ (dotted line) tilted potentials, respectively. The position-dependent diffusion coefficient is plotted in panel (e).

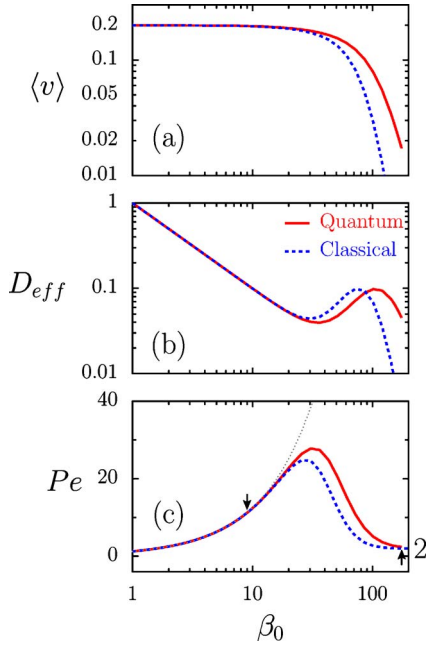

FIG. 3. (Color online) Average velocity (a), effective diffusion (b), and Peclet number (c) versus the inverse temperature β_0. The chosen parameters are bias $F=0.2$ and potential parameters $\varepsilon=100$ and $\Delta=10$. The two arrows in panel (c) mark the characteristic temperatures where the system starts to markedly deviate from the classical behavior (see text for details). The region of intermediate temperatures is located between the downward- and upward-pointing arrows. It bridges between the regions of freely sliding Brownian particle dynamics, characterized by the Peclet number $\mathrm{Pe}=FL\beta_0$ [see the thin, dotted line in (c)] and Poisson-like behavior with $\mathrm{Pe}=2$. Within this region the Peclet number assumes its maximal value.

A. Quantum renormalization of the barrier shape

We studied the influence of quantum corrections on transport in tilted periodic systems by means of a numerical analysis of the basic expressions (5) and (15). We found that the quantum current is always higher than the corresponding classical one (see Figs. 2–4). This phenomenon can be explained by comparing the potential $U(x)$, the effective quantum potential $U_{eff}(x)$, and the thermodynamic potential $\psi(x)$ with each other, as well as by analyzing the effective diffusion function $D(x)$ (which is constant in the classical case); see Fig. 2. Clearly, the effective quantum potential $U_{eff}(x)$(solid line) possesses slightly lower and thinner barriers than $U(x)$ (dashed line).

The state-dependent diffusion function $D(x)$ possesses maxima and minima. The maxima, which are shifted away from the potential barrier locations, can be interpreted as a higher effective local temperature. The minimum of $D(x)$ is located in the neighborhood of the top of the barrier [near $x \sim 0$ in panel (e)]. It means that quantum fluctuations mimic an effective temperature which is lower at the barrier and higher in the potential wells. For the escape dynamics the thermodynamic potential $\psi(x)$ is decisive: It contains the combined influences of the effective potential and the effective diffusion. In the present case, $\psi(x)$ displays both a lower and a narrower barrier than the bare potential $U(x)$ of the corresponding classical process. It is remarkable that for all cases considered, the Peclet number is always larger in the quantum case than in the classical case, thus providing a more coherent motion. This behavior is exemplified in Figs. 2–4.

B. Role of quantum corrections for diffusion

Depending on the relation between the thermal energy kT and the barrier height of the tilted potential, one can distin-

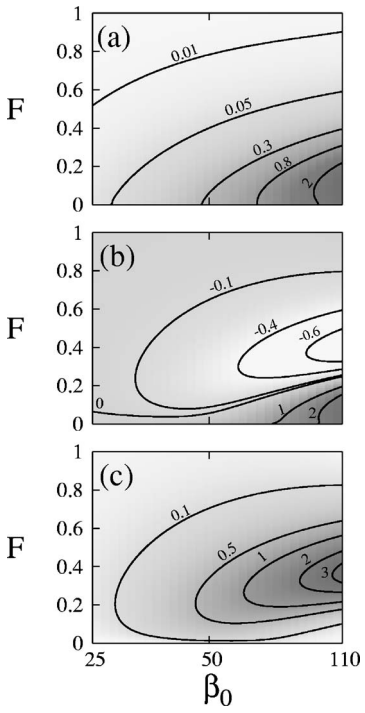

FIG. 4. The influence of quantum corrections is illustrated as a function of bias F vs inverse temperature β_0 by the relative difference between the quantum (Q) and the corresponding classical (C) values of the current $(\langle v\rangle^Q-\langle v\rangle^C)/\langle v\rangle^C$ (a), the effective diffusion $(D^Q_{eff}-D^C_{eff})/D^C_{eff}$ (b), and the Peclet number $(\mathrm{Pe}^Q-\mathrm{Pe}^C)/\mathrm{Pe}^C$ (c), respectively. The positive values of the depicted quantities indicate the relevant role of quantum effects.

guish regimes of high and low temperatures, denoted in Fig. 3 by a downward and an upward arrow, respectively. To the left of the downward arrow—i.e., for high temperatures—the particle barely feels the barriers and thus freely slides down the hill with an average velocity given by $\langle v\rangle \approx F$.

The effective diffusion coefficient D_{eff} can then be approximated by the Einstein diffusion coefficient $1/\beta_0$ in both the classical and quantum cases. The corresponding approximated values of the Peclet number, given by $\mathrm{Pe}=FL\beta_0$, are depicted as a dotted line. To the right of the upward arrow in Fig. 3(c) the relaxation time τ_r is much smaller than the time scale for barrier crossing. The time evolution in that case consists of a sequence of independent activations. Indeed, the value of the Peclet number approaches $\mathrm{Pe}=2$ which is characteristic for Poisson processes.

The most interesting region is located between the two temperatures, indicated by two oppositely directed arrows (one downwards and one upwards), where we found the optimal transport—i.e., the maximum of the Peclet number Pe. The quantum behavior significantly deviates from the classical one only within this very region. We observe that the transport quality, expressed in terms of the characterizer Pe, is never suppressed by quantum effects (see Figs. 3 and 4), even though quantum corrections may increase the effective diffusion D_{eff}.

In Fig. 4 we depict the relative value for the correction of D_{eff} and Pe, respectively, in the parameter space spanned by β_0, F. First, it is detectable that the corrected values of velocity, the effective diffusion, and Peclet number may differ up to 200% from the classical values. Second, the sign of the relative corrections of $\langle v\rangle$ and Pe is positive, but in the case of the effective diffusion D_{eff} it might assume negative values within some range of parameters.

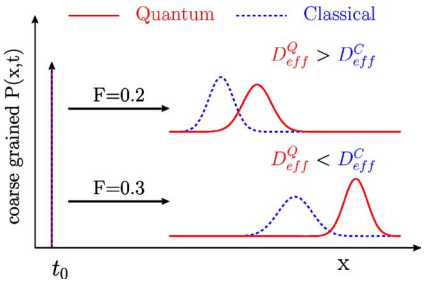

FIG. 5. (Color online) The influence of the quantum corrections on the evolution of the coarse-grained probability density function $P(x,t)$ (see discussion in [22]) is illustrated for the same set of parameters as in Fig. 2 and for different forces $F=0.2$ and 0.3. Note that in the quantum case the velocity is always *larger*; therefore, the maximum of the density is located at a more distant position as compared to the classical case. The width of the density differs depending on the driving parameters and thereby reflects the effective diffusion strength.

Finally, we illustrate the effect of quantum corrections on the transport in tilted washboard potential. In Fig. 5 we present two examples of the time evolution of the density function $P(x,t)$. The impact of quantum corrections is clearly visible. The width of $P(x,t)$ becomes larger at $F=0.2$ and smaller at $F=0.3$ when the quantum corrections are acting, but the peak of the probability density travels in the quantum case with a larger velocity in both situations.

V. CONCLUSIONS

The effect of the quantum contribution on Brownian motion, in particular on the diffusion of particles and the related transport performance, is addressed in this work. The quantum current always exceeds the corresponding classical one; quantum features like tunneling and quantum fluctuations seemingly always assist the particle to overcome barriers and to pass longer distances, resulting in a larger average stationary velocity. The diffusion coefficient D_{eff} is found to assume, generally, a nonmonotonic function of the static force F and the temperature β_0. In other words, optimal conditions exist for both directed and diffusive transport. Depending on the parameters of the system, quantum effects may either increase or decrease the effective diffusion of the particle. The Peclet number is found to be *always* larger for quantum systems; see Fig. 4(c). The most significant finding is that quantum effects always improve diffusive quantum transport for the class of systems considered in this work.

The findings of this work for quantum diffusion can be tested with experiments that are aimed at evaluating, apart from the current, also the fluctuation behavior. Ideal systems that come to mind to do so are overdamped, driven Josephson junctions for which the quantum corrections to the escape rate have been determined in the literature [40–42], vortex-Josephson quantum Brownian motors [43], or also quantum diffusion in superionic conductors [44].

ACKNOWLEDGMENTS

The authors gratefully acknowledge helpful discussions with Gerhard Schmid. This work was supported by the Deutsche Forschungsgemeinschaft via Grant No. HA 1517/13-4, the Graduiertenkolleg 283 (L.M.), collaborative research Grant No. SFB 486, and the DAAD-KBN (German-Polish project "Stochastic Complexity") (P.H. and J.Ł.).

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