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# The diffusion in the quantum Smoluchowski equation

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## Abstract

A novel quantum Smoluchowski dynamics in an external, nonlinear potential has been derived recently. In its original form, this overdamped quantum dynamics is not compatible with the second law of thermodynamics if applied to periodic, but asymmetric ratchet potentials. An improved version of the quantum Smoluchowski equation with a modified diffusion function has been put forward in L. Machura et al. (Phys. Rev. E 70 (2004) 031107) and applied to study quantum Brownian motors in overdamped, arbitrarily shaped ratchet potentials. With this work we prove that the proposed diffusion function, which is assumed to depend (in the limit of strong friction) on the second-order derivative of the potential, is uniquely determined from the validity of the second law of thermodynamics in thermal, undriven equilibrium. Put differently, no approximation-induced quantum Maxwell demon is operating in thermal equilibrium. Furthermore, the leading quantum corrections correctly render the dissipative quantum equilibrium state, which distinctly differs from the corresponding Gibbs state that characterizes the weak (vanishing) coupling limit.


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## 1. Introduction

In classical statistical physics, the description of a system coupled to thermal bath of temperature $T$ is formulated in terms of Langevin-type equations and corresponding Fokker–Planck or master equations [1,2]. This scheme models the phenomenon of Brownian motion, a phenomenon that has been described theoretically by the two ‘‘grandfathers’’ of Brownian motion: Albert Einstein and Marian von Smoluchowski [3,4]. For a classical Brownian particle moving in an external field, the statistical properties are described by the Klein–Kramers equation in the phase space of position and momentum degree of freedom [1,2,5]. In the strong friction limit it reduces to the so-called Smoluchowski equation in position space alone [6]. The issue of quantum Brownian motion is more subtle [7]. In this context, it is important to note that for a correct description of the quantum dynamics of the subsystem, the Brownian particle must at all times be consistent with the Heisenberg principle and the commutator structure of quantum dynamics; as a consequence, the reduced dynamics modeled in the form of a corresponding quantum Langevin equation must necessarily operate in the total Hilbert space of the system dynamics (i.e., the particle) and the thermal bath degrees of freedom. Given an initial preparation scheme [8], a consistent statistical description is also possible as well in terms of (generalized) quantum master equations for the *reduced* density operator of the system dynamics alone, i.e., the quantum Brownian dynamics. An example constitutes the weak coupling limit, for which quantum master equations (e.g. of Lindblad form) have been derived [9]. The strong friction limit has only recently attracted interest. Different approaches have been proposed in the recent years that are seemingly not wholly consistent with each other [10]. Here, we follow the scheme that is rigorously based on a path integral formulation of the (reduced) quantum Brownian motion [5,7].

Following Ankerhold–Pechukas–Grabert [11], the limit of strong friction can be described by a corresponding quantum Smoluchowski dynamics containing leading quantum corrections. For a particle of mass $M$ moving in the potential $V(x)$, such a quantum Smoluchowski equation has been derived for the diagonal part of the density operator $\rho(t)$, i.e., for the probability density $P(x,t) = \langle x|\rho(t)|x\rangle$ in the position space $x$. It explicitly reads [11]

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

where $\gamma$ is a friction coefficient. The effective potential reads

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

wherein the prime denotes the derivative with respect to the coordinate $x$. The effective diffusion coefficient

$$D_{eff}(x) = D_1(x) = \tfrac{1}{\beta}[1 + \lambda\beta V''(x)] \tag{3}$$