# A real-time path integral method for driven dissipative quantum systems

M. Thorwart P. Reimann P. Hänggi

Theoretische Physik I
Universität Augsburg
Universitätsstr. 1
86135 Augsburg
Germany

Email: Michael.Thorwart@physik.uni-augsburg.de

LRZ-Account: b5101bm

**Abstract**

We use an efficient real-time path integral approach to investigate general time-dependent quantum systems which are coupled to a dissipative environment. To obtain a reliable check of this method, we compare numerical results with available analytical results for a linear test system. This findings are important to justify the application of the numerical algorithm to more complex, nonlinear problems where no analytical approach is available *a priori*.

## 1 Introduction

The question how a quantum system is influenced by the interaction with its environment is of broad general interest in physics [1, 2]. Usually, no detailed microscopic knowledge of the environment is available. However, very successful methods in phenomenological modeling of the environment have become widely known (*system-bath-models*). Therefore, the central quantum system of interest is coupled bilinearly to a collection of harmonic oscillators (*heat bath, reservoir*). Due to the linearity of the bath and the coupling, the equations of motion for the bath degrees of freedom can be solved exactly. If the central quantum system itself is linear, the model describes the Brownian motion of a quantum particle in a parabolic potential. For this system, analytical solutions are available even when additionally the curvature is periodically modulated [3]. Other physical problems like the relaxation of a quantum system to equilibrium via tunneling involve in general non-linear potentials for which no simple analytical solution is at hand. For such questions, a very efficient numerical method using a *quasiadiabatic propagator path integral (QUAPI)* has been developed [4]. In this work, we review the application of this technique to the parametrically driven dissipative quantum harmonic oscillator and the comparison of the results with the known analytical results [5]. This justifies the application of the algorithm to a more complex situation of a harmonically driven double-well potential where no analytical solution is known [6, 7].

## 2 The quasiadiabatic propagator path integral

The phenomenological model of a quantum system interacting with a harmonic oscillator bath is described by the Hamiltonian

$$\mathbf{H}(t) = \mathbf{H}_{\rm S}(t) + \mathbf{H}_{\rm B}, \tag{1}$$

where

$$\mathbf{H}_{\mathrm{S}}(t) = \frac{\mathbf{p}^2}{2M} + V(\mathbf{x}, t) \tag{2}$$

is the Hamiltonian of the central system of interest, i.e. a quantum particle of mass $M$ with position operator $\mathbf{x}$ and momentum operator $\mathbf{p}$ moving in a one-dimensional potential $V(\mathbf{x}, t)$ which may be in general time-dependent due to an external driving force. The bath (including the interaction with the system) describing the environment is modeled by

$$\mathbf{H}_{\mathrm{B}} = \sum_{j=1}^{N} \mathbf{H}_j(\mathbf{q}) = \sum_{j=1}^{N} \frac{1}{2}\Big[\frac{\mathbf{p}_j^2}{m_j} + m_j\omega_j^2\Big(\mathbf{x}_j - \frac{c_j}{m_j\omega_j^2}\mathbf{x}\Big)^2\Big], \tag{3}$$

being an ensemble of $N$ harmonic oscillators of masses $m_j$ with coordinate and momentum operators $\mathbf{x}_j$ and $\mathbf{p}_j$ and potential curvatures $\omega_j$. The coupling of the system to the bath is assumed to be linear with the coupling constants $c_j$. We assume that the density operator $\mathbf{W}(t)$ of the entire system-plus-bath at initial time $t = t_0$ factorizes according to

$$\mathbf{W}(t_0) = \boldsymbol{\rho}_{\mathrm{S}}(t_0) \otimes Z^{-1}\exp(-\beta\mathbf{H}_{\mathrm{B}}) \tag{4}$$

with $\boldsymbol{\rho}_{\mathrm{S}}(t_0)$ being the density operator of the system at time $t_0$ and $Z^{-1}\exp(-\beta\mathbf{H}_{\mathrm{B}})$ being the canonical equilibrium distribution of the bath at temperature $T = (k_B\beta)^{-1}$. The bath is fully characterized by the spectral density $J(\omega)$ (for further details see e.g. [1]). Throughout this work, we assume an Ohmic bath with exponential cut-off at $\omega_c \gg \omega_0$, i. e. $J(\omega) = M\gamma\exp(-\omega/\omega_c)$, where $\gamma$ is the damping constant.

## 3 The parametrically driven quantum harmonic oscillator

The dynamics of the central system of interest is described by the time evolution of the reduced density matrix

$$\rho(x_f', x_f; t_0, t) = Tr_{bath}\langle x_f'|\mathcal{T}e^{-i/\hbar\int_{t_0}^{t} H dt'}W(t_0)e^{i/\hbar\int_{t_0}^{t} H(t')dt'}|x_f\rangle. \tag{5}$$

Here, $x_f$ and $x_f'$ are the spatial coordinates of the system at time $t$, $\mathcal{T}$ denotes the chronological operator, $W(t_0)$ the density operator of the total system at time $t_0$ and $Tr_{bath}$ the trace over the harmonic oscillator coordinates. In general, the time evolution can only be performed numerically. We use the method of the *quasi adiabatic path integral propagator* in combination with a powerful tensor multiplication scheme [4] to evaluate the quasi-adiabatic path-integral iteratively (see also [6, 7]). It is for this purpose, where we have used the high-performance computer at the LRZ.

In the case of the central quantum system being linear, the numerical findings within the QUAPI framework can be compared to analytical results obtained by real time path integral methods [5, 3]. The potential is given by

$$V(\mathbf{x}, t) = \frac{M}{2}[\omega_0^2 + \epsilon\cos\Omega t]\mathbf{x}^2. \tag{6}$$

The interesting quantities we have calculated are the autocorrelations of the position and the momentum operator, i. e. $\sigma_{xx}(t) = \langle\mathbf{x}^2\rangle - \langle\mathbf{x}\rangle^2$, $\sigma_{pp}(t) = \langle\mathbf{p}^2\rangle - \langle\mathbf{p}\rangle^2$ and their cross-correlation $\sigma_{xp}(t) = \frac{1}{2}\langle\mathbf{xp} + \mathbf{px}\rangle - \langle\mathbf{xp}\rangle$.

Fig. 1 shows two examples of parameter sets given in the figure caption. We see that the numerical QUAPI algorithm results and the analytical calculations agree very well (for further discussion, see [5]). Moreover, the dependence of the QUAPI algorithm on its free parameters (which are due to systematic approximations) can be studied in a detailed way with the analytic solution at hand. The perfect reproduction of the analytical results by this numerical algorithm fortifies for further applications like the investigation of relaxation phenomena in statically tilted or ac-driven double-well potentials [6, 7].

This work was supported by the DFG and the Freistaat Bayern within the postgraduate scheme (Graduiertenkolleg) GRK 283 „Nonlinear Problems in Analysis, Geometry and Physics“.

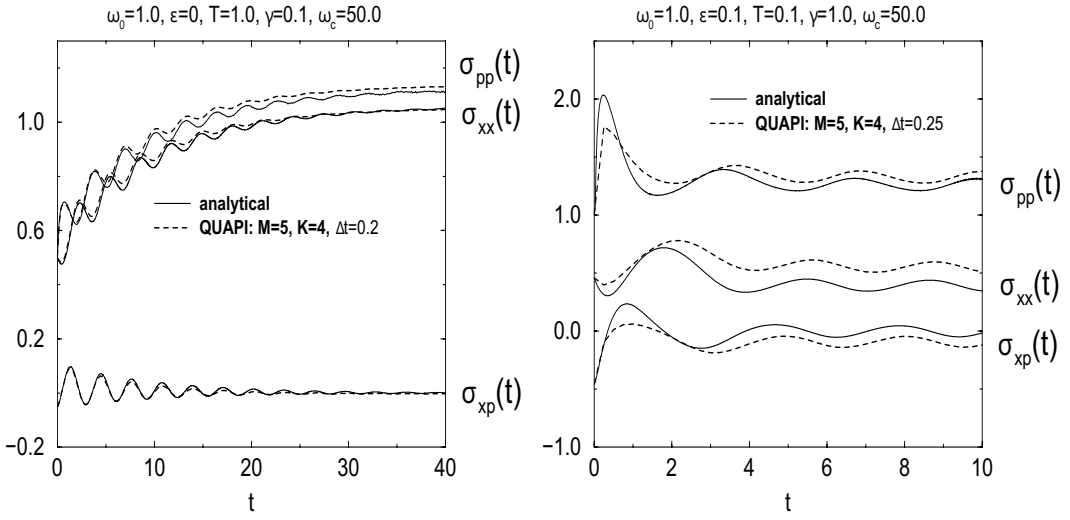


Figure 1: Left: Time-dependence of the correlations $\sigma_{xx}(t), \sigma_{xp}(t)$ and $\sigma_{pp}(t)$ for the undriven dissipative quantum harmonic oscillator ($\epsilon = 0, \omega_0 = 1.0$) with bath parameters $T = 1.0, \gamma = 0.1$ and an exponential cut-off with $\omega_c = 50.0$. In all the figures, we have used scaled quantities (see [5] for further details). The solid lines show the analytic results while the dashed lines represent the numerical solution obtained by the QUAPI algorithm with parameters $M = 5, K = 4, \Delta t = 0.2$. Right: The same for the parametrically driven dissipative quantum harmonic oscillator with a driving amplitude $\epsilon = 0.1$ ($\omega_0 = 1.0$). The bath parameters are $T = 0.1, \gamma = 1.0$ and $\omega_c = 50.0$ (exponential cut-off). Here, the QUAPI parameters are $M = 5, K = 4, \Delta t = 0.25$.

# Bibliography

[1] U. Weiss, *Quantum Dissipative Systems*, (World Scientific, Singapore, 1993; 2nd edition 1999).

[2] P. Hänggi, P. Talkner and M. Borkovec, *Reaction-rate theory: fifty years after Kramers*, Rev. Mod. Phys. **62**, 251 (1990).

[3] C. Zerbe and P. Hänggi, *Brownian parametric quantum oscillator with dissipation*, Phys. Rev. E **52**, 1533 (1995).

[4] N. Makri, *Real time path integrals with quasi-adiabatic propagators: Quantum Dynamics of a system coupled to a harmonic bath*, in *Time-Dependent Quantum Molecular Dynamics*, Proceedings of a NATO Advanced Research Workshop 1992 in Snowbird, Utah, NATO ASI Series B: Physics, Vol. 299, edited by J. Broeckhove and L. Lathouwers, (Plenum Press, New York, 1992); D. E. Makarov and N. Makri, *Path integrals for dissipative systems by tensor multiplication: condensed phase quantum dynamics for arbitrary long-times*, Chem. Phys. Lett. **221**, 482 (1994); N. Makri, *Numerical path integral techniques for long time dynamics of quantum dissipative systems*, J. Math. Phys. **36** 2430 (1995).

[5] M. Thorwart, P. Reimann and P. Hänggi, submitted for publication.

[6] M. Thorwart and P. Jung, *Dynamical Hysteresis in Bistable Quantum Systems*, Phys. Rev. Lett. **78**, 2503 (1997).

[7] M. Thorwart, P. Reimann, P. Jung and R.F. Fox, *Quantum hysteresis and resonant tunneling in bistable systems*, Chem. Phys. **235**, 61 (1998).