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Simulation of Decoherence by Averaged Semiquantum Method

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Abstract. We investigate the dynamics of a system coupled to an environment by averaged semiquantum method. The theory origins from the time-dependent variational principle (TDVP) formulation and contains nondiagonal matrix elements, thus it can be applied to study dissipation, measurement and decoherence problems in the model. In the calculation, the influence of the environment governed by differential dynamical equation is incorporated using a mean field. We have performed averaged semiquantum method for a spin-boson model, which reproduces the results from stochastic Schrodinger equation method and Hierarchical approach quite accurately. Moreover, we validate our results with noninteracting-blip approximation (NIBA) and generalized Smoluchowski equation (GSE). The problem dynamics in nonequilibrium environments has also been studied by our method. When applied to the harmonic oscillator model coupled to a heat bath with different coupling strengths and dimensionalities of the bath, we find that the loss of coherence predicted by semiquantum method is identical to the result of master equation with different initial state (Gaussian wave packet and superposed wave packets).

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Key words: Quantum chaos, spin-boson model, decoherence, harmonic oscillator system, environment, averaged semiquantum method.

1 Introduction

The system-bath dynamics of open quantum systems at finite temperatures has long been a central problem in chemistry and physics [1, 2], which is usually associated with reduced density matrix evolving in time according to the Liouville von-Neumann equation. The understanding of the nonequilibrium dynamics of open quantum systems has also

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been a main challenge in the last decades [3]. In recent years the subject has particularly gained considerable interest due to experimental progress which allows for the tailoring and manipulation of quantum matter on ever larger scales. In mesoscopic physics, for instance, superconducting circuits have been realized to observe coherent dynamics and entanglement [4]. Similar advance has been achieved on molecular scales with the detection of interferences in wave packet dynamics and the control of the population of specific molecular states [5]. These systems are in contact with a large number of environmental degrees of freedom, giving rise to decoherence and relaxation [6].

Traditional approaches treating the dynamics typically yield approximate equations of motion such as master equations. For large coupling constants and long time scales, it can be accomplished in a formally exact manner by path integrals for open quantum systems [7]. Noninteracting-blip approximation (NIBA) was originally derived by Leggett using the path-integral influence-functional method [35], and can be obtained using standard reduced density matrix perturbation theory by Aslagul *et al.* [36]. Generalized Smoluchowski equation (GSE) was introduced by Zusman [37] and later derived by Garg *et al.* [38].Very recently, it was generalized to study electron-transfer problem [39]. Furthermore, Monte Carlo wave-function techniques [8–14] are extensively used to treat master equations in the weak coupling or Markovian limit. In recent years, the quantum dynamics in nonequilibrium environments has attracted our attention. Also, stochastic equation [15–18] is used to treat the system-environment problem, which can describe the long-time evolution exactly.

In this work, we propose averaged semiquantum method to study the system environment problem. Conventional semiquantum method has a wide application in many branches of physics. Recently, this method has been used to study the nonlinear dynamics and chaos [19]. It is also named as Gaussian wave-packet dynamics [20, 21] and origins from TDVP formulation, $\Gamma=\int dt\langle\Psi(t)|i\hbar\frac{\partial}{\partial t}-\hat{H}|\Psi(t)\rangle$ with $\delta\Gamma=0$. This approach enables us to study the effects of the quantum fluctuations dynamically [22–23]. Moreover it has been proven to be very successful in the investigation of dynamical systems ranging from integrable to many-body nonintegrable systems [24], which simplifies the quantum version and gives better results than the semiclassical approach. The averaged semiquantum method may provide a significant numerical advantage over the trajectories, in particular in the case that the Hilbert space dimension$N$ of the open system is large. Moreover, to be numerically efficient (the best possible sampling), it gives good solutions with a significant weight in average.

The spin-boson model [40] and the harmonic oscillators system [41] have been the subject of considerable attention with a major review available. In this paper, at first, we focus on the spin-boson system and compare the results with that obtained by the stochastic Schrodinger equation method. Then we study the harmonic oscillator model coupled to a heat bath with different dimensionalities to find whether the loss of coherence can be predicted by the semiquantum method.

The paper is organized as follows: In Section 2 we introduce the averaged semiquantum method. In Section 3 we will use this method to study the spin-boson model and