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# Convergence Analysis on Stochastic Collocation Methods for the Linear Schrödinger Equation with Random Inputs

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**Abstract.** In this paper, we analyse the stochastic collocation method for a linear Schrödinger equation with random inputs, where the randomness appears in the potential and initial data and is assumed to be dependent on a random variable. We focus on the convergence rate with respect to the number of collocation points. Based on the interpolation theories, the convergence rate depends on the regularity of the solution with respect to the random variable. Hence, we investigate the dependence of the stochastic regularity of the solution on that of the random potential and initial data. We provide sufficient conditions on the random potential and initial data to ensure the smoothness of the solution and the spectral convergence. Finally, numerical results are presented to support our analysis.

**AMS subject classifications**: 65M12, 81Q05, 60H25

**Key words**: Schrödinger equation, stochastic collocation methods, convergence analysis, uncertainty quantification.

## 1 Introduction

The linear Schrödinger equation describes the motion of electrons in the external field, which has been studied both theoretically [17, 39] and numerically [8, 19]. Recently, the linear Schrödinger equation with a random potential [1, 30] has attracted a great deal of attention. The randomness may arise from disordered structures like amorphous solids, random alloys and non-crystalline systems, thermal fluctuation or randomly distributed impurities [2, 12, 13, 15, 21, 22, 25]. The random Schrödinger operators have been intensively studied in a theoretical way [5,6,14,23,24]. In addition, Schrödinger equations with random initial data are investigated recently [26]. However, the numerical literatures on

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them are not so abundant [7]. Indeed, this kind of problems belongs to uncertainty quantification (UQ) for PDEs with random inputs, where randomness could appear in initial conditions, boundary conditions, coefficients of the equations, etc. There have been quite a few numerical methods developed for UQ in recent years. Among them, the stochastic collocation method and the stochastic Galerkin method [28, 34–38] are two of most popular methods, both of which make use of the polynomial approximation theory. They have been successfully applied to many physical and engineering problems [16, 18, 20, 31, 40]. Convergence analyses on both methods for different kinds of differential equations have also been established [3, 4, 27, 29, 32, 41]. For the linear Schrödinger equation, Wu and Huang applied the stochastic Galerkin method to the Schrödinger equation with a periodic potential and a random external potential [33]. Nevertheless, to the best of our knowledge, there is not any convergence result on both methods for the linear Schrödinger equation with a random potential.

In this paper, we focus on the convergence analysis on the stochastic collocation method for the Schrödinger equation with a random potential and random initial data. Since the stochastic collocation method makes use of the polynomial approximation theory, the convergence rate of the stochastic method w.r.t. the number of collocation points relies on the regularity of the solution w.r.t. the random variable, which in turn depends on the smoothness of the potential and initial data w.r.t. the random variable. We first study the stochastic regularity for the Schrödinger equation where the spatial variable $x\in\mathbb{R}^d$. To study the stochastic regularity, we will make use of some well-posedness results on the Schrödinger equation in the deterministic case, for which there have been numerous results [17, 39]. The results given by Yajima [39] will be fully utilized. The well-posedness of the random Schrödinger equation will be established and two cases of sufficient conditions to ensure the stochastic regularity will be presented. As a usual practice in numerical computations for the Schrödinger equation, we compute it in a truncated domain. Hence we then consider the Schrödinger equation in a bounded domain and provide sufficient conditions on the random potential and initial data to ensure the spectral convergence of the stochastic collocations. The more smoothly the potential and initial data depend on the random variable, the faster the convergence rate will be. It turns out that the stochastic collocation method is a solid method when the magnitude of the randomness is within an appropriate range.

The outline of this paper is as follows. In Section 2, the well-posedness result in the deterministic case by Yajima is reviewed. In Section 3, we study the stochastic regularity of the random linear Schrödinger equation. Then the time splitting based stochastic collocation method and its corresponding convergence results are presented in Section 4. We give some numerical results in Section 5 to support our analyses. Finally, a conclusion is given in Section 6.

Throughout this paper, the analysis will be performed for the case where the random variable $y\in\mathbb{R}$ for simplicity. However, similar analyses can be extended to the high-dimensional cases using tensor-product rule in the parametric space, see e.g., [3].