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ANALYSIS OF A SPLITTING SCHEME FOR A CLASS OF NONLINEAR STOCHASTIC SCHRÖDINGER EQUATIONS

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ABSTRACT. We analyze the qualitative properties and the order of convergence of a splitting scheme for a class of nonlinear stochastic Schrödinger equations driven by additive Itô noise. The class of nonlinearities of interest includes nonlocal interaction cubic nonlinearities. We show that the numerical solution is symplectic and preserves the expected mass for all times. On top of that, for the convergence analysis, some exponential moment bounds for the exact and numerical solutions are proved. This enables us to provide strong orders of convergence as well as orders of convergence in probability and almost surely. Finally, extensive numerical experiments illustrate the performance of the proposed numerical scheme.

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1. INTRODUCTION

Deterministic Schrödinger equations are widely used within physics, plasma physics or nonlinear optics, see for instance [43, 1, 12, 34]. In certain physical situations it may be appropriate to incorporate some randomness into the model. One possibility is to add a driving random force and obtain a stochastic partial differential equation (SPDE) of the form

$$i\frac{\partial u}{\partial t}(x, t) = \Delta u(x, t) + F(x, u) + \xi(x, t),$$

considered for $x \in \mathbb{T}^d$, the d -dimensional torus, with periodic boundary conditions. The nonlinearity F and the white noise ξ are described in details below. See Equation (1) for

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the formulation of this problem as a stochastic evolution equation. See for example [35, 24, 21, 20, 23] and references therein for further details and applications. The nonlinearities we shall consider encompass for instance the case of an external potential or of a nonlocal interaction cubic nonlinearity. Such long-range interaction is defined as the convolution of an interaction kernel with the density function $|u|^2$ and is a smooth version of the Schrödinger–Poisson equation. Such nonlinearities are used in modeling deterministic problems arising in quantum physics, chemistry, materials sciences, and biology [5, 8]. However, the case of power-law nonlinearities cannot be treated by the techniques employed in this paper.

Let us now review the relevant literature on temporal discretizations of stochastic Schrödinger equations driven by an Itô noise. In [23], a Crank–Nicolson scheme is studied for the stochastic Schrödinger equation with regular coefficients. First order of convergence, resp. rate one half is obtained in the case of additive noise, resp. multiplicative Itô noise. In addition, convergence in probability as well as almost-surely are studied for the case of a power-law nonlinearity. Observe that the numerical scheme from [23] is implicit. The references [25, 6] present thorough numerical simulations and numerically study the effect of noise in the stochastic Schrödinger equation with a power-law nonlinearity. The work [29] provides a strong convergence analysis of a splitting strategy to the variational solution of Schrödinger’s equation with regular coefficients. The recent article [3] proves strong convergence of an exponential integrator for stochastic Schrödinger equations with regular coefficients. In addition, longtime behaviors of the numerical solutions of a linear model is investigated. The paper [32] provides a convergence rate of the weak error under noise discretizations of some Schrödinger’s equations. Finally, the work [33] shows convergence in probability of a stochastic (implicit) symplectic scheme for stochastic nonlinear Schrödinger equations with quadratic potential and an additive noise.

In the present work, we shall analyze a splitting strategy for an efficient time integration of a class of nonlinear stochastic Schrödinger equations. In a nutshell, the main idea of splitting integrators is to decompose the vector field of the original differential equation in several parts, such that the arising subsystems are exactly (or easily) integrated. We refer interested readers to [30, 9, 40] for details on splitting schemes for ordinary (partial) differential equations. The splitting scheme considered in this publication is given by equation (8).

Despite the fact that splitting schemes are widely used for an efficient time integration of deterministic Schrödinger-type equations, see for instance [10, 7, 39, 26, 28, 38, 4], we are not aware of a numerical analysis of such integrators approximating mild solutions of nonlinear stochastic Schrödinger equations driven by an additive Itô noise. In the present publication we prove

- bounds for the exponential moments of the mass of the exact and numerical solutions (Theorem 10);
- a kind of longtime stability, a so called trace formula for the mass, of the numerical solutions (Proposition 5);
- preservation of symplecticity for the exact and numerical solutions (Proposition 8);
- strong convergence estimates (with order) of the splitting scheme, as well as orders of convergence in probability and almost surely (Theorem 14 and Corollary 16).

Observe that, since the nonlinearity in the class of stochastic Schrödinger equation considered here may not be globally Lipschitz, we employ the exponential moments estimates mentioned above to obtain strong rates of convergence, see Propositions 12 and 13. In these propositions, we consider moments of the error multiplied by an exponential discounting factor, and obtain

the expected rate of convergence for this quantity. To the best of our knowledge, this quantity has not been considered elsewhere in the literature. Combining those estimates with the above exponential moment bounds to remove the exponential factor, we can then prove Theorem 14. Note finally, that the choice of a splitting strategy is crucial in obtaining exponential moment bounds for the numerical solution.

We begin the exposition by introducing some notations, present our main assumptions and provide several moment bound estimates for the exact solution to the considered SPDE. We then present the splitting scheme and study some geometric properties of the exact and numerical solutions in Section 3. The main results of this publication are presented in Section 4. In particular, exponential moments in the L^2 norm of the exact and numerical solutions are given, as well as several convergence results. More involved and technical proofs of results needed for convergence estimates are provided in Section 5. Various numerical experiments illustrating the main properties of the splitting scheme when applied to stochastic Schrödinger equations driven by Itô noise are given in Section 6. The paper ends with an appendix containing proofs of auxiliary results.

We use C to denote a generic constant, independent of the time-step size of the numerical scheme, which may differ from one place to another.

2. SETTING

In this work, we consider the following class of stochastic nonlinear Schrödinger equations

$$(1) \quad \begin{aligned} i du(t) &= \Delta u(t) dt + F(u(t)) dt + \alpha dW^Q(t), \\ u(0) &= u_0, \end{aligned}$$

where the unknown $(u(t))_{t \geq 0}$ is a stochastic process with values in the Hilbert space $L^2 = L^2(\mathbb{T}^d)$ of square integrable complex-valued functions defined on the d -dimensional torus \mathbb{T}^d . Details concerning the regularity and growth properties of the nonlinearity F and the covariance operator Q are provided below. In addition, $\alpha > 0$ is a real parameter measuring the size of the noise W^Q . The initial condition $u_0 \in L^2$ is deterministic, however the results below can be adapted to random initial conditions, satisfying appropriate integrability conditions, using a standard conditioning argument. The space L^2 is equipped with the norm $\|\cdot\|_{L^2}$, where for all $u, v \in L^2$,

$$\|u\|_{L^2}^2 = \langle u, u \rangle, \quad \langle u, v \rangle = \int_{\mathbb{T}^d} \bar{u}(x)v(x) dx.$$

The Sobolev spaces $H^1 = H^1(\mathbb{T}^d)$ and $H^2 = H^2(\mathbb{T}^d)$ are Hilbert spaces, and the associated norms are denoted by $\|\cdot\|_{H^1}$ and $\|\cdot\|_{H^2}$. The notation $H^0 = L^2$ will also be used below. For $\sigma \in \{0, 1, 2\}$, let also $\|\cdot\|_{\mathcal{C}^\sigma}$ denote the norm in the Banach space $\mathcal{C}^\sigma = \mathcal{C}^\sigma(\mathbb{T}^d)$ of functions of class \mathcal{C}^σ defined in \mathbb{T}^d .

Solutions of (1) are understood in the mild sense:

$$(2) \quad u(t) = S(t)u_0 - i \int_0^t S(t-s)F(u(s)) ds - i\alpha \int_0^t S(t-s) dW^Q(s),$$

where $S(t) = e^{-it\Delta}$. Let us state the following result (see e.g. [37, Lemma 3.1] and [23, Appendix A1]).

Lemma 1. *The linear operator $-i\Delta$ generates a group $(S(t))_{t \in \mathbb{R}}$ of isometries of L^2 , such that for all $\sigma \in \{0, 1, 2\}$, all $u \in H^\sigma$, and all $t \geq 0$, one has*

$$\|S(t)u\|_{H^\sigma} = \|u\|_{H^\sigma}.$$

In addition, for $\sigma \in \{1, 2\}$, there exists $C_\sigma \in (0, \infty)$ such that for all $u \in H^\sigma$ and all $t \geq 0$,

$$\|(S(t) - I)u\|_{L^2} \leq C_\sigma t^{\frac{\sigma}{2}} \|u\|_{H^\sigma}.$$

The Wiener process W^Q , with covariance operator Q , in the SPDE (1) is defined by

$$W^Q(t) = \sum_{k \in \mathbb{N}} \gamma_k \beta_k(t) e_k,$$

where $(e_k)_{k \in \mathbb{N}}$ is a complete orthonormal system of L^2 , $(\beta_k)_{k \in \mathbb{N}}$ is a sequence of independent real-valued standard Wiener processes on a stochastic basis $(\Omega, \mathcal{F}, \mathbb{P}, (\mathcal{F}(t))_{t \geq 0})$, and $(\gamma_k)_{k \in \mathbb{N}}$ is a sequence of complex numbers such that $\sum_{k \in \mathbb{N}} |\gamma_k|^2 < \infty$. The linear operators Q and $Q^{\frac{1}{2}}$

are defined by $Qe_k = \gamma_k^2 e_k$ and $Q^{\frac{1}{2}}e_k = \gamma_k e_k$, for all $k \in \mathbb{N}$.

For a linear operator Ψ from H^σ to H^σ , and any complete orthonormal system $(\varepsilon_k)_{k \in \mathbb{N}}$ of H^σ , we define

$$\|\Psi\|_{\mathcal{L}_2^\sigma}^2 = \sum_{k \in \mathbb{N}} \|\Psi \varepsilon_k\|_{H^\sigma}^2.$$

This definition is independent of the choice of the orthonormal system.

With this notation, $\|Q^{\frac{1}{2}}\|_{\mathcal{L}_2^\sigma}^2 = \sum_{k \in \mathbb{N}} |\gamma_k|^2 \|e_k\|_{H^\sigma}^2$ (whenever the sum is finite).

We now set the assumptions on the spatial Sobolev regularity of the noise as well as on the nonlinearity in the stochastic Schrödinger equation (1) required to prove well-posedness for the SPDE (1), to prove H^1 -regularity of the solution, and to show strong convergence of order 1/2 of the proposed splitting integrator in Section 4.

Assumption 1. *One has*

$$\|Q^{\frac{1}{2}}\|_{\mathcal{L}_2^1}^2 = \sum_{k \in \mathbb{N}} |\gamma_k|^2 \|e_k\|_{H^1}^2 < \infty.$$

The nonlinearity F satisfies $F(u) = V[u]u$ for all $u \in L^2$, where $V: u \in L^2 \mapsto V[u] \in \mathbb{R}$ is a real-valued mapping. Furthermore, it is assumed that $V[u_1] = V[u_2]$ if $|u_1| = |u_2|$ (i. e. the potential V is a function of the modulus).

In addition to the above, assume that the mapping F is locally Lipschitz continuous with at most cubic growth: there exists $C_F \in (0, \infty)$ and $K_F \in (0, \infty)$ such that for all $u_1, u_2 \in L^2$, one has

$$(3) \quad \|F(u_2) - F(u_1)\|_{L^2} \leq \left(C_F + K_F (\|u_1\|_{L^2}^2 + \|u_2\|_{L^2}^2) \right) \|u_2 - u_1\|_{L^2}.$$

Finally, there exists $C_1 \in (0, \infty)$ and a polynomial mapping P_1 , such that for all $u \in H^1$, one has

$$(4) \quad \begin{aligned} \|F(u)\|_{H^1} &\leq C_1 \|u\|_{H^1} \left(1 + \|u\|_{L^2}^2 \right) \\ |\operatorname{Im}(\langle \nabla u, \nabla F(u) \rangle)| &\leq C_1 \|\nabla u\|_{L^2}^2 + P_1 \left(\|u\|_{L^2}^2 \right). \end{aligned}$$

Note that assuming that $V[u]$ is real-valued implies that the equality $\text{Im}(\langle u, F(u) \rangle) = 0$ holds for all $u \in L^2$.

The value of K_F appearing in the right-hand side of (3) plays a crucial role in the convergence analysis below.

Let us recall the definition of the stochastic integral in the mild form (2) and the associated Itô isometry property. If for all $t \geq 0$, $\Psi(t)$ is a linear operator from H^σ to H^σ , the stochastic integral $\int_0^T \Psi(t) dW^Q(t)$ is understood as $\sum_{k \in \mathbb{N}} \gamma_k \int_0^T \Psi(t) e_k d\beta_k(t)$, and the Itô isometry formula is given by

$$\mathbb{E} \left[\left\| \int_0^T \Psi(t) dW^Q(t) \right\|_{H^\sigma}^2 \right] = \int_0^T \left\| \Psi(t) Q^{\frac{1}{2}} \right\|_{\mathcal{L}_2^\sigma}^2 dt.$$

Under Assumption 1, the stochastic convolution $-i \int_0^t S(t-s) dW^Q(s)$ is thus well-defined and takes values in H^1 . It solves the linear stochastic Schrödinger equation driven by additive noise

$$i du(t) = \Delta u(t) dt + dW^Q(t), \quad u(0) = 0.$$

Most of the analysis can be performed when Assumption 1 is satisfied, in particular we will prove below that (1) admits a unique global solution, and that the splitting scheme has a strong convergence order 1/2. To get strong convergence order 1 of the proposed splitting integrator for the semilinear problem (1), we need further assumptions.

Assumption 2. *On top of Assumption (1), let us assume that one has*

$$\left\| Q^{\frac{1}{2}} \right\|_{\mathcal{L}_2^2}^2 = \sum_{k \in \mathbb{N}} |\gamma_k|^2 \|e_k\|_{H^2}^2 < \infty.$$

Furthermore, let us assume that the nonlinearity F is twice differentiable, and there exists $C \in (0, \infty)$ such that for all $u, h, k \in L^2$, one has

$$(5) \quad \begin{aligned} \|F'(u) \cdot h\|_{L^2} &\leq C(1 + \|u\|_{L^2}^2) \|h\|_{L^2} \\ \|F''(u) \cdot (h, k)\|_{L^2} &\leq C(1 + \|u\|_{L^2}) \|h\|_{L^2} \|k\|_{L^2}. \end{aligned}$$

Finally, let us assume that there exists $C_2 \in (0, \infty)$ and a polynomial mapping P_2 , such that for all $u \in H^2$, one has

$$(6) \quad \begin{aligned} \|F(u)\|_{H^2} &\leq C_\sigma \|u\|_{H^2} \left(1 + \|u\|_{L^2}^2\right) \\ |\text{Im}(\langle \nabla^2 u, \nabla^2 F(u) \rangle)| &\leq C_2 \|\nabla^2 u\|_{L^2}^2 + P_2 \left(\|u\|_{L^2}^2, \|\nabla u\|_{L^2}^2\right). \end{aligned}$$

We next give examples of nonlinearities verifying Assumption 1 or 2. First, the conditions in Assumption 1 or 2 are satisfied in the case of a linear mapping $F(u) = Vu$, where the external potential function $V: \mathbb{T}^d \rightarrow \mathbb{R}$ is a real-valued mapping of class \mathcal{C}^σ , with $\sigma = 1$ (resp. $\sigma = 2$) to satisfy Assumption 1 (resp. Assumption 2). In that case, the mapping F is globally Lipschitz continuous, and (3) holds with $C_F = \|V\|_{\mathcal{C}^0}$ and $K_F = 0$. Second, the conditions in Assumption 1 or 2 also hold for the following class of nonlocal interaction cubic nonlinearities. Note that $K_F > 0$ in this case.

Proposition 2. *Let $\sigma \in \{1, 2\}$ and let $V : \mathbb{T}^d \rightarrow \mathbb{R}$ be a real-valued mapping of class \mathcal{C}^σ . For every $u \in L^2$, set*

$$V[u] = V \star |u|^2 = \int V(\cdot - x) |u(x)|^2 dx,$$

where \star denotes the convolution operator.

Then Assumption 1 (resp. Assumption 2) is satisfied for the nonlinearity $F(u) = V[u]u = (V \star |u|^2)u$ when $\sigma = 1$ (resp. when $\sigma = 2$).

Proof. Observe that for any $u \in L^2$, the mapping $V[u]$ is of class \mathcal{C}^σ , with $\nabla^\sigma V[u] = \nabla^\sigma V \star |u|^2$. It thus follows that $\|V[u]\|_{\mathcal{C}^\sigma} \leq \|V\|_{\mathcal{C}^\sigma} \|u\|_{L^2}^2$ for all $u \in L^2$.

First, assume that $\sigma = 1$. Let us check that (3) holds. Let $u_1, u_2 \in L^2$, then one has

$$\begin{aligned} \|F(u_2) - F(u_1)\|_{L^2} &\leq \|V[u_2](u_2 - u_1)\|_{L^2} + \|(V[u_2] - V[u_1])u_1\|_{L^2} \\ &\leq \|V[u_2]\|_{\mathcal{C}^0} \|u_2 - u_1\|_{L^2} + \|V[u_2] - V[u_1]\|_{\mathcal{C}^0} \|u_1\|_{L^2} \\ &\leq \|V\|_{\mathcal{C}^0} \left(\|u_2\|_{L^2}^2 + \|u_1 + u_2\|_{L^2} \|u_1\|_{L^2} \right) \|u_2 - u_1\|_{L^2} \\ &\leq \frac{3}{2} \|V\|_{\mathcal{C}^0} \left(\|u_1\|_{L^2}^2 + \|u_2\|_{L^2}^2 \right) \|u_2 - u_1\|_{L^2}. \end{aligned}$$

Thus (3) holds with $C_F = 0$ and $K_F = \frac{3}{2} \|V\|_{\mathcal{C}^0}$. The conditions in (4) follow from straightforward computations.

Second, assume that $\sigma = 2$. The conditions in (5) follow from writing, for all $u, h, k \in L^2$,

$$\begin{aligned} F'(u).h &= V[u]h + 2(V \star \operatorname{Re}(\bar{u}h))u \\ F''(u).(h, k) &= 2(V \star \operatorname{Re}(\bar{u}h))k + 2(V \star \operatorname{Re}(\bar{k}u))h + 2(V \star \operatorname{Re}(\bar{h}k))u. \end{aligned}$$

The conditions in (6) follow from straightforward computations.

This concludes the proof of the Proposition. \square

Note that the conditions in Assumption 1 or 2 are not satisfied in the standard cubic nonlinear Schrödinger case, where $V[u] = \pm|u|^2$, or for other (non-trivial) power-law nonlinearities.

To conclude this section, let us state a well-posedness result for the stochastic Schrödinger equation (1) in terms of mild solutions (2), and several moment bound estimates. Note that additional bounds for the exponential moments in L^2 of the exact solution are given in Section 4.

Proposition 3. *Let Assumption 1 be satisfied.*

For any initial condition $u_0 \in L^2$, there exists a unique mild solution $(u(t))_{t \geq 0}$ of the stochastic Schrödinger equation (1), which satisfies (2) for all $t \geq 0$. In addition, for every $T \in (0, \infty)$, $\sigma \in \{0, 1, 2\}$, $u_0 \in H^\sigma$, and $p \in [1, \infty)$, there exists $C_p(T, \alpha, Q, u_0) \in (0, \infty)$ such that one has a moment bound in H^σ

$$\sup_{0 \leq t \leq T} \mathbb{E}[\|u(t)\|_{H^\sigma}^{2p}] \leq C_p(T, \alpha, Q, u_0),$$

with $\sigma = 1$, resp. $\sigma = 2$, when Assumption 1, resp. Assumption 2, is satisfied.

Finally one has the following temporal regularity estimate: for all $t_1, t_2 \in [0, T]$,

$$\mathbb{E} \left[\|u(t_2) - u(t_1)\|_{L^2}^{2p} \right] \leq C_p(T, \alpha, Q, u_0) |t_2 - t_1|^p.$$

The proof uses standard arguments and is postponed to the appendix.

3. SPLITTING SCHEME

In this section we define a splitting integrator for the stochastic Schrödinger equation (1) and show some geometric properties of this time integrator. The main idea of splitting schemes is to decompose the original problem, equation (1) in our case, into subsystems that can be solved explicitly (or efficiently numerically). Splitting schemes are widely used for time discretization of deterministic cubic Schrödinger equations, see, e.g. the key early reference [31].

The definition of the splitting scheme studied in this article relies on the flow associated with the differential equation $i\dot{u} = F(u) = V[u]u$. For all $u \in L^2$ and $t \in \mathbb{R}$, define

$$(7) \quad \Phi_t(u) = e^{-itV[u]}u.$$

Since $V[u] \in \mathbb{R}$, one has $|\Phi_t(u)| = |u|$ for all $t \geq 0$, which gives $V[\Phi_t(u)] = V[u]$ using Assumption 1 or 2. It is then straightforward to check that $(\Phi_t)_{t \in \mathbb{R}}$ is the flow associated with the differential equation $i\dot{u} = F(u)$. Indeed, for all $u \in L^2$ and all $t \in \mathbb{R}$, one has

$$i \frac{d}{dt} \Phi_t(u) = F(\Phi_t(u)).$$

Observe that the flow of the above ODE preserves the L^2 -norm: $\|\Phi_t(u)\|_{L^2} = \|u\|_{L^2}$ for all $t \geq 0$ and all $u \in L^2$.

The splitting scheme for the stochastic Schrödinger equation (1) considered in this article is then defined by the explicit recursion

$$(8) \quad u_{n+1} = S(\tau) (\Phi_\tau(u) - i\alpha \delta W_n^Q),$$

where τ denotes the time-step size, and $\delta W_n^Q = W^Q((n+1)\tau) - W^Q(n\tau)$ are Wiener increments. Recall that $S(\tau) = e^{-i\tau\Delta}$. Without loss of generality, it is assumed that $\tau \in (0, 1)$. The scheme is obtained using a splitting strategy: at each time step, first one may write $\tilde{u}_n = \Phi_\tau(u_n)$, *i. e.* the equation $i\dot{u} = F(u)$ with initial condition u_n is solved exactly, second one has $u_{n+1} = S(\tau)\tilde{u}_n - i\alpha S(\tau)\delta W_n^Q$, which comes from applying an exponential Euler scheme to the stochastic differential equation $idu = \Delta u dt + \alpha dW^Q(t)$. Observe that bounds for the exponential moments in L^2 of the numerical solution are given in Section 4.

Remark 4. *Alternatively, solving exactly the stochastic differential equation $idu = \Delta u dt + \alpha dW^Q(t)$ yields the following numerical scheme for the SPDE (1)*

$$(9) \quad u_{n+1} = S(\tau)\Phi_\tau(u) - i\alpha \int_{n\tau}^{(n+1)\tau} S((n+1)\tau - t) dW^Q(t).$$

Generalizing the results obtained below to this numerical scheme is straightforward.

The error analysis for the splitting scheme (8) presented in the next section will make use of the following additional assumption.

Assumption 3. *There exists $C \in (0, \infty)$ such that for all $t \in [0, 1]$ and $u \in L^2$ one has*

$$\|\Phi_t(u) - u\|_{L^2} \leq C|t| \left(1 + \|u\|_{L^2}^3\right).$$

Note that Assumption 3 is satisfied for the two examples of nonlinearities described in Section 2. Indeed, $\|\Phi_t(u) - u\|_{L^2} \leq t \|V[u]\|_{C^0} \|u\|_{L^2}$, with $\|V[u]\|_{C^0} = \|V\|_{C^0}$ in the external potential case ($V[u] = V$) and $\|V[u]\|_{C^0} \leq \|V\|_{C^0} \|u\|_{L^2}^2$ in the nonlocal interaction case ($V[u] = V \star |u|^2$).

We now present some geometric properties of the splitting scheme (8).

3.1. Trace formula for the mass. It is well known that, under periodic boundary conditions for instance, the mass, or L^2 -norm or density

$$M(u) := \|u\|_{L^2}^2 = \int |u|^2 dx$$

of the deterministic Schrödinger equation $i\frac{\partial u}{\partial t} - \Delta u - V[u]u = 0$, where $V[u] = V$ (external potential) or $V[u] = V \star |u|^2$ (nonlocal interaction) or $V[u] = |u|^2$ (cubic), is a conserved quantity. In the stochastic case under consideration, one immediately gets a trace formula for the mass of the exact solution of equation (1) as well as for the numerical solution given by the splitting scheme (8).

Proposition 5. *Consider the stochastic Schrödinger equation (1) with a trace class covariance operator Q and an initial value satisfying $\mathbb{E}[M(u_0)] < \infty$. We assume that the nonlinearity in (1) is such that $F(u) = V[u]u$, where $V[u]$ is real-valued and a function of the modulus $|u|$. Furthermore, we assume that an exact global solution exists and that the differential equation in the splitting scheme can be solved exactly. This is the case for instance when one considers an external potential, a nonlocal interaction, a cubic or power-law nonlinearity.*

Then, the exact solution (2) satisfies a trace formula for the mass:

$$\mathbb{E}[M(u(t))] := \mathbb{E}\left[\|u(t)\|_{L^2}^2\right] = \mathbb{E}[M(u_0)] + t\alpha^2 \text{Tr}(Q) \quad \text{for all time } t.$$

Furthermore, the numerical solution (8) to the nonlinear stochastic Schrödinger equation (1) satisfies the exact same trace formula for the mass:

$$\mathbb{E}[M(u_n)] = \mathbb{E}[M(u_0)] + t_n\alpha^2 \text{Tr}(Q) \quad \text{for all time } t_n = n\tau.$$

Observe that the above result for the exact solution is already available in the literature in different settings, for instance in [22, 3]. However, to the best of our knowledge, the result for the numerical solution is one of the first results in the literature on a longtime qualitative behavior of the numerical solution to nonlinear SPDEs driven by Itô noise. Such a longtime behavior is not satisfied for classical time integrators like the (semi-implicit) Euler–Maruyama schemes, see the numerical experiments below.

Proof. We apply Itô's formula to the mass $M(u(t))$ and get

$$(10) \quad \begin{aligned} M(u(t)) &= M(u(0)) + \int_0^t \langle M'(u(s)), -i\alpha dW(s) \rangle + \int_0^t \langle M'(u(s)), -i\Delta u(s) - iV[u]u(s) \rangle ds \\ &\quad + \int_0^t \frac{1}{2}\alpha^2 \text{Tr} \left[M''(u(s)) \left(Q^{1/2} \right) \left(Q^{1/2} \right)^* \right] ds. \end{aligned}$$

An integration by part and the hypothesis on the potential V show that the third term on the right-hand side is zero. Taking expectation now gives

$$\mathbb{E}[M(u(t))] = \mathbb{E}[M(u(0))] + t\alpha^2 \text{Tr}(Q)$$

which concludes the proof of the trace formula for the mass of the exact solution.

We next show that the above trace formula is also satisfied for the numerical solution given by the splitting integrator (8). Using the definition of the numerical scheme (8), properties of the Wiener increments δW_n^Q , as well as the isometry property of $S(\tau)$, one gets

$$\mathbb{E}[M(u_{n+1})] = \mathbb{E}\left[\|S(\tau)\Phi_\tau(u_n)\|_{L^2}^2\right] + \alpha^2 \mathbb{E}\left[\|\delta W_n^Q\|_{L^2}^2\right] = \mathbb{E}\left[\|\Phi_\tau(u_n)\|_{L^2}^2\right] + \tau\alpha^2 \text{Tr}(Q).$$

The definition of the flow Φ_τ yields

$$\mathbb{E}[M(u_{n+1})] = \mathbb{E}[M(u_n)] + \tau\alpha^2 \text{Tr}(Q)$$

and a recursion completes the proof of the proposition. \square

Remark 6. *The same trace formula for the mass holds for the numerical solution given by the time integrator (9). Indeed, using the definition of the numerical scheme (9), Itô's isometry, as well as the isometry property of the operator $S(\tau)$, one gets*

$$\mathbb{E}[M(u_{n+1})] = \mathbb{E}\left[\|\Phi_\tau(u_n)\|_{L^2}^2\right] + \tau\alpha^2 \text{Tr}(Q).$$

Employing the definition of the flow Φ_τ followed by a recursion shows the trace formula for the mass of the splitting scheme (9).

Remark 7. *It may also be possible to study the longtime behavior of the exact and numerical solutions along the expected value of the Hamiltonian of (1) with $\alpha \neq 0$. However, in general, the drift in the expected Hamiltonian will depend on the solution u , see for example [25, Equation (11)] for the cubic case. In particular, the evolution of this quantity will not be linear in time. Such a trace formula for the energy will thus unfortunately not be as simple as the one for the mass. Very recent studies have been carried on for (mainly) the Crank–Nicolson scheme in the preprint [41]. In particular, it is observed that this numerical scheme does not verify an exact trace formula for the mass, see also the numerical experiments below. We leave the question of investigating such trace formula for the Hamiltonian of the splitting scheme for future work.*

3.2. Stochastic symplecticity. Symplectic schemes are known to have excellent longtime properties when applied to Hamiltonian (partial) differential equations, see for instance [36, 30, 15, 19, 17, 18, 27] and references therein. These particular integrators have thus naturally come into the realm of stochastic (partial) differential equations, see for example [11, 13, 2, 42, 14, 33, 16] and references therein.

The next result shows that the exact flow of the SPDE (1) as well as the proposed splitting scheme (8) are stochastic symplectic.

Proposition 8. *Consider the stochastic Schrödinger equation (1) and assume that a global solution exists. Under the same assumptions as in the previous proposition, the exact flow of this SPDE is stochastic symplectic in the sense that it preserves the symplectic form*

$$\bar{\omega}(t) = \int_{\mathbb{T}^d} dp \wedge dq dx \quad a.s.,$$

where the overbar on ω is a reminder that the two-form $dp \wedge dq$ (with differentials made with respect to the initial value) is integrated over the torus. Here, p and q denote the real and imaginary parts of u .

Furthermore, the splitting scheme (8) applied to the stochastic Schrödinger equation (1) is stochastic symplectic in the sense that it possesses the discrete symplectic structure:

$$\bar{\omega}^{n+1} = \bar{\omega}^n \quad a.s.,$$

for the symplectic form $\bar{\omega}^n := \int_{\mathbb{T}^d} dp_n \wedge dq_n dx$, where p_n , resp. q_n denoting the real and imaginary parts of u_n , and d denotes differentials in the phase space.

Proof. The symplecticity of the phase flow of the stochastic Schrödinger equation (1) can be shown using similar arguments as in [33, Theorem 3.1] for a stochastic cubic Schrödinger equation with quadratic potential, see also [14].

In order to show that the numerical solution is stochastic symplectic as well, we use the same argument as in the proof of [16, Prop. 4.3]. Taking the differential of the numerical solution yields

$$du_{n+1} = d\left(S(\tau)\left(\Phi_\tau(u_n) - i\alpha\delta W_n^Q\right)\right) = d\left(S(\tau)\Phi_\tau(u_n)\right) = du_n,$$

where in the last equality we have used the fact that the composition of exact flows is symplectic. This concludes the proof. \square

Remark 9. *The exact same proof shows that the splitting scheme (9) possesses a discrete symplectic structure.*

4. CONVERGENCE RESULTS

In this section, we study various types of convergence (strong, in probability and almost-surely) of the splitting scheme (8) when applied to the stochastic Schrödinger equation (1). In order to do this, we first show bounds for the exponential moments in the L^2 norm of the exact and numerical solutions as well as two auxiliary results. The proofs of these results are given in Section 5 for the reader's convenience.

Theorem 10. *Let us apply the splitting scheme (8) to the stochastic Schrödinger equation (1) with a trace class covariance operator Q and deterministic initial value $u_0 \in L^2$. Assume that the nonlinearity in (1) satisfies $F(u) = V[u]u$, where $V[u] = V[\bar{u}]$ is real-valued, and that the exact and numerical solutions are well defined on the interval $[0, T]$. One then has the following bounds for the exponential moments: there exists $\kappa > 0$ and τ^* such that if $\mu\alpha^2 T < \frac{\kappa}{\text{Tr}(Q)}$, then one has:*

$$\sup_{0 \leq t \leq T} \mathbb{E} \left[\exp \left(\mu \|u(t)\|_{L^2}^2 \right) \right] \leq C(\mu, T, \alpha, Q, u_0) < \infty$$

for the exact solution and

$$\sup_{\tau \in (0, \tau^*)} \sup_{0 \leq n\tau \leq T} \mathbb{E} \left[\exp \left(\mu \|u_n\|_{L^2}^2 \right) \right] \leq C(\mu, T, \alpha, Q, u_0) < \infty$$

for the numerical solution.

In the proof of this theorem, the lower bound $\kappa \geq \frac{\epsilon^{-1}}{2}$ is obtained, note that it does not depend on the nonlinearity. Furthermore, observe that the condition $\mu\alpha^2 T < \frac{\kappa}{\text{Tr}(Q)}$ gets more restrictive when α and T increase.

It is immediate to deduce the following moment estimates for the exact and numerical solutions from Theorem 10.

Corollary 11. *Under the assumptions of the previous theorem, for any $p \in [1, \infty)$ and $T \in (0, \infty)$, one has the following moment estimates for the L^2 norm of the exact and numerical solutions: for any $u_0 \in L^2$, there exists $C_p(T, \alpha, Q, u_0) \in (0, \infty)$ such that*

$$\sup_{0 \leq t \leq T} \mathbb{E} [\|u(t)\|_{L^2}^{2p}] \leq C_p(T, \alpha, Q, u_0)$$

and

$$\sup_{\tau \in (0, \tau^*)} \sup_{0 \leq n\tau \leq T} \mathbb{E} [\|u_n\|_{L^2}^{2p}] \leq C_p(T, \alpha, Q, u_0).$$

Observe that one could show this statement for $\tau \in (0, 1)$ directly without using the exponential moments estimates given in Theorem 10.

In order to show the main convergence result of this article, we will make use of the following two propositions. Each one of these propositions are used to show strong convergence order $1/2$, resp. 1 , of the numerical solution given by the splitting scheme.

Proposition 12. *Consider the time discretization of the stochastic Schrödinger equation (1) by the splitting scheme (8). Let Assumptions 1 and 3 be satisfied. Assume that $u_0 \in H^1$.*

Let $T \in (0, \infty)$. For every $q \in [1, \infty)$, there exists $C_q(T, u_0) \in (0, \infty)$ (which depends on F , Q and on α), such that for every $\tau \in (0, \tau^)$, one has*

$$\sup_{0 \leq n\tau \leq T} \mathbb{E} \left[\exp(-qK_F S_n) \|u_n - u(t_n)\|_{L^2}^q \right] \leq C_q(T, u_0) \tau^{\frac{q}{2}},$$

where K_F is given in (3) (see Assumption 1), and $S_n = \tau \sum_{k=0}^{n-1} \left(\|u(k\tau)\|_{L^2}^2 + \|u_k\|_{L^2}^2 \right)$.

Proposition 13. *Consider the time discretization of the stochastic Schrödinger equation (1) by the splitting scheme (8). Let Assumptions 2 and 3 be satisfied. Assume that $u_0 \in H^2$.*

Let $T \in (0, \infty)$. For every $q \in [1, \infty)$, there exists $C_q(T, u_0) \in (0, \infty)$ (which depends on F , Q and on α), such that for every $\tau \in (0, \tau^)$, one has*

$$\sup_{0 \leq n\tau \leq T} \mathbb{E} \left[\exp(-qK_F S_n) \|u_n - u(t_n)\|_{L^2}^q \right] \leq C_q(T, u_0) \tau^q,$$

where K_F is given in (3) (see Assumption 1) and $S_n = \tau \sum_{k=0}^{n-1} \left(\|u(k\tau)\|_{L^2}^2 + \|u_k\|_{L^2}^2 \right)$.

The proofs of the technical results, Theorem 10 and Propositions 12 and 13, are postponed to Section 5.

We are now in position to state the main convergence result of this article.

Theorem 14. *Let $u(t)$ denote the exact solution to the stochastic Schrödinger equation (1) and u_n the numerical solution given by the splitting scheme (8). Let Assumption 3 be satisfied. Let also $\sigma = 1$, resp. $\sigma = 2$, if Assumption 1, resp. Assumption 2, is satisfied. Assume that $u_0 \in H^\sigma$.*

Recall the notation $S_n = \tau \sum_{k=0}^{n-1} \left(\|u(k\tau)\|_{L^2}^2 + \|u_k\|_{L^2}^2 \right)$. Let $T \in (0, \infty)$. Assume that $\bar{\mu} \in (0, \infty)$ and $\tau_0 \in (0, \tau^)$ are chosen such that*

$$(11) \quad \sup_{\tau \in (0, \tau_0)} \sup_{0 \leq n\tau \leq T} \mathbb{E} [\exp(\bar{\mu} S_n)] = C(T, u_0, \alpha, Q, \tau_0, \bar{\mu}) < \infty.$$

Then, for all $r \in (0, \infty)$ and all $\mu \in (0, \bar{\mu})$, there exists $C_r(T, u_0, \alpha, Q, \tau_0, \mu) < \infty$ such that for all $\tau \in (0, \tau_0)$ one has

$$(12) \quad \sup_{0 \leq n\tau \leq T} (\mathbb{E} [\|u_n - u(t_n)\|_{L^2}^r])^{\frac{1}{r}} \leq C_r(T, u_0, \alpha, Q, \tau_0, \mu) \tau^{\frac{\sigma}{2} \min(1, \frac{\mu}{rK_F})}.$$

As a consequence of this theorem, the convergence is polynomial in $L^r(\Omega)$, for all $r \in [1, \infty)$. The rate of convergence of the splitting scheme depends on r in (12), and vanishes when $r \rightarrow \infty$. Note that for sufficiently small $r > 0$, one has $\min(1, \frac{\mu}{rK_F}) = 1$, thus the convergence

rate of the splitting scheme is $\frac{\sigma}{2}$ when r is sufficiently small. Observe also that a sufficient condition for condition (11) to be verified is that

$$\bar{\mu} < \frac{\kappa}{\alpha^2 T^2 \text{Tr}(Q)},$$

where $\kappa > 0$ is some positive constant (see Remark 15 below). Thus the value of $\min(1, \frac{\mu}{rK_F})$ depends on the quantity $\alpha^2 T^2 K_F$ (considering that $\text{Tr}(Q)$ is fixed and that the size of the noise is given by α). The larger this quantity, the more restrictive the condition to have $\min(1, \frac{\mu}{rK_F}) = 1$ becomes.

In the external potential case $V[u] = Vu$, one has $K_F = 0$, thus there is no restrictions and the order of convergence is $\frac{\sigma}{2}$ in $L^r(\Omega)$ for all $r \in [1, \infty)$.

Remark 15. *Owing to Theorem 10 concerning exponential moments of the exact and numerical solutions, the set of parameters $\bar{\mu}, \tau_0$ such that (11) holds is non-empty. Indeed, recalling*

that $S_n = \tau \sum_{k=0}^{n-1} (\|u(k\tau)\|_{L^2}^2 + \|u_k\|_{L^2}^2)$ and using Cauchy-Schwarz inequality, one has

$$\begin{aligned} \mathbb{E} [\exp(\mu S_n)] &= \mathbb{E} \left[\prod_{k=0}^{n-1} \left(\exp(\mu\tau \|u(t_k)\|_{L^2}^2) \exp(\mu\tau \|u_k\|_{L^2}^2) \right) \right] \\ &\leq \prod_{k=0}^{n-1} \left(\mathbb{E} \left[\exp(2n\tau\mu \|u(t_k)\|_{L^2}^2) \right] \mathbb{E} \left[\exp(2n\tau\mu \|u_k\|_{L^2}^2) \right] \right)^{\frac{1}{2n}} \\ &\leq \sup_{0 \leq k \leq n} \mathbb{E} \left[\exp(2T\mu \|u(t_k)\|_{L^2}^2) \right] \sup_{0 \leq k \leq n} \mathbb{E} \left[\exp(2T\mu \|u_k\|_{L^2}^2) \right] \\ &\leq C(\mu, T, \alpha, Q, u_0), \end{aligned}$$

if $\mu < \frac{\kappa}{\alpha^2 T^2 \text{Tr}(Q)}$ and $\tau < \tau^*$, where κ and τ^* are given in Theorem 10. The value of μ obtained by the argument above (as well as the values of $\kappa = \frac{e^{-1}}{2}$ and τ^*) may not be optimal.

Proof of Theorem 14. Set $e_n = \|u_n - u(t_n)\|_{L^2}$. For every $R \in (0, \infty)$, let $\chi_{n,R} = 1_{S_n \leq R}$. Then

$$\mathbb{E}[e_n^r] = \mathbb{E}[e_n^r \chi_{n,R}] + \mathbb{E}[e_n^r (1 - \chi_{n,R})].$$

For a given $\mu \in (0, \bar{\mu})$, let $p \in (1, \infty)$ such that $\mu = (1 - \frac{1}{p})\bar{\mu}$.

On the one hand, applying the Cauchy-Schwarz and Markov inequalities yields

$$\begin{aligned} \mathbb{E}[e_n^r (1 - \chi_{n,R})] &\leq (\mathbb{E}[e_n^{rp}])^{\frac{1}{p}} (\mathbb{E}[1 - \chi_{n,R}])^{1 - \frac{1}{p}} \leq (\mathbb{E}[e_n^{rp}])^{\frac{1}{p}} \mathbb{P}(S_n > R)^{1 - \frac{1}{p}} \\ &\leq (\mathbb{E}[e_n^{rp}])^{\frac{1}{p}} \mathbb{P}(\exp(\bar{\mu} S_n) > \exp(\bar{\mu} R))^{1 - \frac{1}{p}} \leq (\mathbb{E}[e_n^{rp}])^{\frac{1}{p}} \left(\frac{\mathbb{E}[\exp(\bar{\mu} S_n)]}{\exp(\bar{\mu} R)} \right)^{1 - \frac{1}{p}}. \end{aligned}$$

Using moment bounds for the exact and the numerical solution (Corollary 11) and the exponential moment estimate (11) for S_n , then yield (for a constant C that does not depend on R)

$$\mathbb{E}[e_n^r (1 - \chi_{n,R})] \leq C e^{-\mu R}.$$

On the other hand, let $q = pr$ for p introduced above. Applying the Cauchy–Schwarz inequality yields

$$\mathbb{E}[e_n^r \chi_{n,R}] = \mathbb{E}[e_n^r e^{-rK_F S_n} e^{rK_F S_n} \chi_{n,R}] \leq (\mathbb{E}[e_n^q e^{-qK_F S_n}])^{\frac{1}{p}} \left(\mathbb{E} \left[e^{\frac{rK_F p}{p-1} S_n} \chi_{n,R} \right] \right)^{1-\frac{1}{p}}.$$

Using Proposition 12 with $\sigma = 1$, or Proposition 13 with $\sigma = 2$, and the relation $q = pr$, for the first factor one has

$$(\mathbb{E}[e_n^q e^{-qK_F S_n}])^{\frac{1}{p}} \leq C \tau^{\frac{r\sigma}{2}}.$$

For the second factor, using the exponential moment estimates and the upper bound $S_n \leq R$ when $\chi_{n,R} \neq 0$, one obtains

$$\begin{aligned} \left(\mathbb{E} \left[e^{\frac{rK_F p}{p-1} S_n} \chi_{n,R} \right] \right)^{1-\frac{1}{p}} &\leq \left(\mathbb{E} [e^{\bar{\mu} S_n}] \exp(\max(0, \frac{rK_F p}{p-1} - \bar{\mu})R) \right)^{1-\frac{1}{p}} \\ &\leq C \exp(\max(0, rK_F - \mu)R), \end{aligned}$$

using the identity $\mu = (1 - \frac{1}{p})\bar{\mu}$.

Finally, for all $R \in (0, \infty)$, one has

$$\mathbb{E}[e_n^r] \leq C \left(\tau^{\frac{r\sigma}{2}} \exp(\max(0, rK_F - \mu)R) + \exp(-\mu R) \right).$$

It remains to optimize the choice of R in terms of τ . If $rK_F \leq \mu$, there is no condition and passing to the limit $R \rightarrow \infty$ yields $\mathbb{E}[e_n^r] \leq C \tau^{\frac{r\sigma}{2}}$. If $rK_F > \mu$, the right-hand side is minimized when $\tau^{\frac{r\sigma}{2}} e^{rK_F R} = 1$, *i. e.* $e^{-R} = \tau^{\frac{r\sigma}{2K_F}}$ and one obtains

$$\mathbb{E}[e_n^r] \leq C \tau^{\frac{r\sigma\mu}{2K_F}}.$$

This concludes the proof of the theorem. \square

To conclude this section, let us state results concerning convergence in probability, with order of convergence equal to $\frac{\sigma}{2}$, and almost sure convergence with order of convergence $\frac{\sigma}{2} - \varepsilon$ for all $\varepsilon \in (0, \frac{1}{2})$, with $\sigma \in \{1, 2\}$.

Corollary 16. *Consider the stochastic Schrödinger equation (1) on the time interval $[0, T]$ with solution denoted by $u(t)$. Let u_n be the numerical solution given by the splitting scheme (8) with time-step size τ . Under the assumptions of Theorem 14, one has convergence in probability of order $\frac{\sigma}{2}$*

$$\lim_{C \rightarrow \infty} \mathbb{P} \left(\|u_N - u(T)\|_{L^2} \geq C \tau^{\frac{\sigma}{2}} \right) = 0,$$

where $T = N\tau$.

Moreover, consider the sequence of time-step sizes given by $\tau_M = \frac{T}{2^M}$, $M \in \mathbb{N}$. Then, for every $\varepsilon \in (0, \frac{\sigma}{2})$, there exists an almost surely finite random variable C_ε , such that for all $M \in \mathbb{N}$ one has

$$\|u_{2^M} - u(T)\|_{L^2} \leq C_\varepsilon \left(\frac{T}{2^M} \right)^{\frac{\sigma}{2} - \varepsilon}.$$

Proof. Let r be chosen sufficiently small, such that applying Theorem 14 yields

$$\mathbb{E} [\|u_N - u(T)\|_{L^2}^r] \leq C(r, T) \tau^{\frac{r\sigma}{2}}.$$

Then the convergence in probability result is a straightforward consequence of Markov's inequality:

$$\mathbb{P}\left(\|u_N - u(T)\|_{L^2} \geq C\tau^{\frac{\sigma}{2}}\right) = \mathbb{P}\left(\|u_N - u(T)\|_{L^2}^r \geq C^r \tau^{\frac{r\sigma}{2}}\right) \leq \frac{\mathbb{E}\left[\|u_N - u(T)\|_{L^2}^r\right]}{C^r \tau^{\frac{r\sigma}{2}}} = \frac{C(r, T)}{C^r} \xrightarrow{C \rightarrow \infty} 0.$$

To get the almost sure convergence result, it suffices to observe that (again by applying Theorem 14)

$$\sum_{m=0}^{\infty} \frac{\mathbb{E}\left[\|u_{2^m} - u(T)\|_{L^2}^r\right]}{\tau_m^{\frac{r(\frac{\sigma}{2}-\varepsilon)}}} < \infty,$$

thus $\frac{\|u_{2^M} - u(T)\|_{L^2}^r}{\tau_M^{\frac{r(\frac{\sigma}{2}-\varepsilon)}}} \xrightarrow{M \rightarrow \infty} 0$ almost surely. \square

5. PROOFS OF TECHNICAL RESULTS

This section is devoted to giving the proofs to Theorem 10 and Propositions 12 and 13.

To simplify notation, we let $Q_\alpha = \alpha^2 Q$, where we recall that Q is the covariance operator of the noise in the SPDE (1).

5.1. Proof of Theorem 10. We start with the proof of Theorem 10.

Proof. Set $\lambda = \frac{1}{2T\text{Tr}(Q_\alpha)}$ and define the stochastic process $X(t) = e^{-t/T} \|u(t)\|_{L^2}^2$. An application of Itô's formula gives

$$d\left(e^{\lambda X(t)}\right) = e^{\lambda X(t)} \left(-\lambda/T X(t) dt + \lambda e^{-t/T} \text{Tr}(Q_\alpha) dt + \frac{\lambda^2}{2} d\langle X \rangle_t\right) + 2\lambda e^{\lambda X(t)} e^{-t/T} \langle u(t), dW^{Q_\alpha}(t) \rangle,$$

where the quadratic variation $\langle X \rangle_t$ satisfies

$$d\langle X \rangle_t \leq e^{-2t/T} 4\text{Tr}(Q_\alpha) \|u(t)\|_{L^2}^2 dt \leq 4\text{Tr}(Q_\alpha) e^{-t/T} X(t) dt.$$

Taking expectation in the first equation above and observing that $X(t) \geq 0$ a.s, one gets

$$\begin{aligned} \frac{d\mathbb{E}[e^{\lambda X(t)}]}{dt} &\leq \lambda \text{Tr}(Q_\alpha) \mathbb{E}[e^{\lambda X(t)}] + \mathbb{E}[e^{\lambda X(t)} (2\lambda^2 \text{Tr}(Q_\alpha) - \lambda/T) X(t)] \\ &\leq \lambda \text{Tr}(Q_\alpha) \mathbb{E}[e^{\lambda X(t)}] \end{aligned}$$

by definition of λ .

By definition of the stochastic process $X(t)$, the above reads

$$\frac{d\mathbb{E}\left[\exp\left(\lambda e^{-t/T} \|u(t)\|_{L^2}^2\right)\right]}{dt} \leq \lambda \text{Tr}(Q_\alpha) \mathbb{E}\left[\exp\left(\lambda e^{-t/T} \|u(t)\|_{L^2}^2\right)\right]$$

and applying Gronwall's lemma provides the following estimate

$$\mathbb{E}\left[\exp\left(\lambda e^{-t/T} \|u(t)\|_{L^2}^2\right)\right] \leq \exp\left(\lambda \|u_0\|_{L^2}^2\right) e^{\lambda \text{Tr}(Q_\alpha)t},$$

Finally, let $\mu \leq \frac{e^{-1}}{2T\text{Tr}(Q_\alpha)} = e^{-1}\lambda$. Then for all $t \in [0, T]$,

$$\begin{aligned} \mathbb{E}\left[\exp\left(\mu \|u(t)\|_{L^2}^2\right)\right] &\leq \mathbb{E}\left[\exp\left(\lambda e^{-t/T} \|u(t)\|_{L^2}^2\right)\right] \\ &\leq \exp\left(\lambda \|u_0\|_{L^2}^2\right) e^{\lambda \text{Tr}(Q_\alpha)t}, \end{aligned}$$

where we recall that $\lambda = \frac{1}{2T\text{Tr}(Q_\alpha)} = \frac{1}{2\alpha^2 T\text{Tr}(Q)}$. This concludes the proof of the exponential moment estimates for the exact solution of the stochastic Schrödinger equation (1).

Let us now prove the exponential moment estimates for the numerical solution (8). Let $p, q > 1$ such that $1/p + 1/q = 1$, and set $\lambda = \frac{1}{2Tp\text{Tr}(Q_\alpha)}$. Define $r_n = \lambda \exp(-\frac{n}{N})$ for $n = 1, \dots, N$, where $N\tau = T$, and introduce the filtration $\mathcal{F}_n = \sigma\{\delta W_k^{Q_\alpha}; k \leq n-1\}$. Note that u_n is \mathcal{F}_n -measurable. Let also $\tau^* \in (0, p(p-1))$.

Using the definition of the scheme (8) and Hölder's inequality, one has

$$\begin{aligned} & \mathbb{E}[\exp(r_{n+1} \|u_{n+1}\|_{L^2}^2) \mid \mathcal{F}_n] \\ & \leq \mathbb{E}[\exp(r_{n+1} \|u_n\|_{L^2}^2)] \left(\mathbb{E}[\exp(2pr_{n+1} \text{Im}(\langle \Phi_\tau(u_n), \delta W_n^{Q_\alpha} \rangle)) \mid \mathcal{F}_n] \right)^{\frac{1}{p}} \left(\mathbb{E}[\exp(qr_{n+1} \|\delta W_n^{Q_\alpha}\|_{L^2}^2)] \right)^{\frac{1}{q}}. \end{aligned}$$

On the one hand, since $\delta W_n^{Q_\alpha}$ is a centered Gaussian random variable and by definition of r_n , one has

$$\begin{aligned} \mathbb{E} \left[\exp \left(qr_{n+1} \|\delta W_n^{Q_\alpha}\|_{L^2}^2 \right) \right] & \leq \left(1 - 2qr_{n+1} \mathbb{E} \left[\|\delta W_n^{Q_\alpha}\|_{L^2}^2 \right] \right)^{-\frac{1}{2}} \\ & \leq (1 - 2q\lambda\tau\text{Tr}(Q_\alpha))^{-\frac{1}{2}}, \end{aligned}$$

under the condition that $\tau < \frac{1}{2q\lambda\text{Tr}(Q_\alpha)} = \frac{p^2}{q}$. This condition thus holds when $\tau < \tau^*$.

On the other hand, conditional on \mathcal{F}_n , the random variable $\langle \Phi_\tau(u_n), \delta W_n^{Q_\alpha} \rangle$ is also Gaussian and centered, thus

$$\begin{aligned} \mathbb{E} \left[\exp \left(2pr_{n+1} \text{Im}(\langle \Phi_\tau(u_n), \delta W_n^{Q_\alpha} \rangle) \right) \mid \mathcal{F}_n \right] & \leq \exp \left(2p^2 r_{n+1}^2 \text{Var}[\langle \Phi_\tau(u_n), \delta W_n^{Q_\alpha} \rangle] \right) \\ & \leq \exp \left(2p^2 \lambda r_{n+1} \tau \text{Tr}(Q_\alpha) \|u_n\|_{L^2}^2 \right). \end{aligned}$$

Gathering these estimates and taking expectation yield

$$\mathbb{E} \left[\exp \left(r_{n+1} \|u_{n+1}\|_{L^2}^2 \right) \right] \leq \mathbb{E} \left[\exp \left(r_{n+1} (1 + 2p\lambda\tau\text{Tr}(Q_\alpha)) \|u_n\|_{L^2}^2 \right) \right] (1 - 2q\lambda\tau\text{Tr}(Q_\alpha))^{-\frac{1}{2q}}.$$

Having chosen $\lambda = \frac{1}{2pT\text{Tr}(Q_\alpha)}$, one then gets $r_{n+1}(1 + 2p\lambda\tau\text{Tr}(Q_\alpha)) = r_n e^{-\frac{\tau}{T}} (1 + \frac{\tau}{T}) \leq r_n$.

A recursion on n then gives the following estimate

$$\sup_{0 \leq n\tau \leq T} \mathbb{E} \left[\exp \left(r_n \|u_n\|_{L^2}^2 \right) \right] \leq \exp(\lambda \|u_0\|_{L^2}^2) (1 - 2q\lambda\tau\text{Tr}(Q_\alpha))^{-\frac{N}{2q}} \leq C(\lambda, u_0) < \infty,$$

for $\tau < \tau^*$, where the quantity $C(\lambda, u_0)$ does not depend on τ .

We are now in position to conclude the proof of exponential moments estimates for the numerical solution. Let μ such that $\mu < \frac{e^{-1}}{2T\text{Tr}(Q_\alpha)}$. Note that $r_N = \lambda e^{-1}$, thus there exists $p > 1$ such that $\mu \leq r_N \leq r_n$ for all $n \in \{0, \dots, N\}$. This then implies that

$$\sup_{0 \leq n\tau \leq T} \mathbb{E} \left[\exp \left(\mu \|u_n\|_{L^2}^2 \right) \right] \leq C(\mu, T, Q, u_0) < \infty,$$

for all $\tau \in (0, \tau^*)$.

This concludes the proof of Theorem 10. \square

5.2. Proofs of Propositions 12 and 13. Before we start with these proofs, it is convenient to introduce some auxiliary notation and provide the steps that are common for both proofs.

Define $w(t) = -\alpha i \int_0^t S(t-s) dW^Q(s)$ for all $t \geq 0$ and $w_n = -\alpha i \sum_{k=0}^{n-1} S(\tau)^{n-k} \delta W_k^Q$ for all $n \geq 0$. Introduce also $v(t) = u(t) - w(t)$ and $v_n = u_n - w_n$. Let $t_k = k\tau$. Recall that $S_n = \tau \sum_{k=0}^{n-1} \left(\|u(k\tau)\|_{L^2}^2 + \|u_k\|_{L^2}^2 \right)$.

Define $\epsilon_n = \|v(t_n) - v_n\|_{L^2}$ and $e_n = \|u(t_n) - u_n\|_{L^2}$. Then the error between the numerical and exact solution reads $e_n \leq \epsilon_n + \|w_n - w(t_n)\|_{L^2}$.

Let us first deal with the error term $\|w_n - w(t_n)\|_{L^2}$ for the stochastic convolution: employing the Itô isometry formula, with $\sigma = 1$ (resp. $\sigma = 2$) if Assumption 1 (resp. Assumption 2) is satisfied, one has

$$\begin{aligned} \mathbb{E} \left[\|w_n - w(t_n)\|_{L^2}^2 \right] &= \alpha^2 \mathbb{E} \left[\left\| \sum_{k=0}^{n-1} \int_{t_k}^{t_{k+1}} \left(S(\tau)^{n-k} - S(t_n - t) \right) dW^Q(t) \right\|_{L^2}^2 \right] \\ &= \alpha^2 \sum_{k=0}^{n-1} \int_{t_k}^{t_{k+1}} \left\| \left(S(\tau)^{n-k} - S(t_n - t) \right) Q^{\frac{1}{2}} \right\|_{\mathcal{L}_2^0}^2 dt \\ &\leq \alpha^2 \sum_{k=0}^{n-1} \int_{t_k}^{t_{k+1}} |t - t_k|^\sigma dt \left\| Q^{\frac{1}{2}} \right\|_{\mathcal{L}_2^\sigma}^2 \leq C(T, \alpha, Q) \tau^\sigma, \end{aligned}$$

using properties of the semigroup S . Since the distribution of $w_n - w(t_n)$ is Gaussian, for every $q \in [1, \infty)$, there exists $C_q(T, Q) \in (0, \infty)$ such that one has

$$(13) \quad \mathbb{E}[\|w_n - w(t_n)\|_{L^2}^q] \leq C_q(T, \alpha, Q) \tau^{\frac{q\sigma}{2}}.$$

It remains to treat the error term $\epsilon_n = \|v_n - v(t_n)\|_{L^2}$.

Using the mild formulation (2) of the solution $u(t_n)$ and the definition of the splitting scheme (8) for u_n , one obtains

$$\begin{aligned} (14) \quad v_{n+1} - v(t_{n+1}) &= \left(S(\tau)v_n - i \int_{t_n}^{t_{n+1}} S(\tau)F(\Phi_{t-t_n}(u_n)) dt \right) - \left(S(\tau)v(t_n) - i \int_{t_n}^{t_{n+1}} S(t_{n+1}-t)F(u(t)) ds \right) \\ &= S(\tau)(v_n - v(t_n)) - i \int_{t_n}^{t_{n+1}} (S(\tau)F(\Phi_{t-t_n}(u_n)) - S(t_{n+1}-t)F(u(t))) dt \\ &= S(\tau)(v_n - v(t_n)) + E_n^1 + E_n^2 + E_n^3 + E_n^4, \end{aligned}$$

where

$$\begin{aligned} E_n^1 &= i \int_{t_n}^{t_{n+1}} (S(t_{n+1}-t) - S(\tau)) F(u(t)) dt \\ E_n^2 &= i \int_{t_n}^{t_{n+1}} S(\tau) (F(u(t)) - F(u(t_n))) dt \\ E_n^3 &= i\tau S(\tau) (F(u(t_n)) - F(u_n)) \\ E_n^4 &= i \int_{t_n}^{t_{n+1}} S(\tau) (F(u_n) - F(\Phi_{t-t_n}(u_n))) dt. \end{aligned}$$

For the first term, using properties of the semigroup S (see Lemma 1), for $\sigma \in \{1, 2\}$, one has

$$\|E_n^1\|_{L^2} \leq C\tau^{\frac{\sigma}{2}} \int_{t_n}^{t_{n+1}} \|F(u(t))\|_{H^\sigma} dt.$$

The treatment of the second term E_n^2 is different for the two propositions, details are provided below.

For the third term, recall that $\|u_n - u(t_n)\|_{L^2} \leq \epsilon_n + \|w_n - w(t_n)\|_{L^2}$. Using (3), one obtains

$$\begin{aligned} \|E_n^3\|_{L^2} &\leq \tau \left(C_F + K_F(\|u(t_n)\|_{L^2}^2 + \|u_n\|_{L^2}^2) \right) \|u_n - u(t_n)\|_{L^2} \\ &\leq \tau \left(C_F + K_F(\|u(t_n)\|_{L^2}^2 + \|u_n\|_{L^2}^2) \right) \epsilon_n + \tau \left(C_F + K_F(\|u(t_n)\|_{L^2}^2 + \|u_n\|_{L^2}^2) \right) \|w_n - w(t_n)\|_{L^2}. \end{aligned}$$

For the fourth term, using (3), the equality $\|\Phi_{t-t_n}(u_n)\|_{L^2} = \|u_n\|_{L^2}$, and Assumption 3, one obtains

$$\begin{aligned} \|E_n^4\|_{L^2} &\leq C \int_{t_n}^{t_{n+1}} \left(1 + \|u_n\|_{L^2}^2 + \|\Phi_{t-t_n}(u_n)\|_{L^2}^2 \right) \|u_n - \Phi_{t-t_n}(u_n)\|_{L^2} dt \\ &\leq C \left(1 + 2\|u_n\|_{L^2}^5 \right) \int_{t_n}^{t_{n+1}} |t - t_n| dt \\ &\leq C\tau^2 \left(1 + \|u_n\|_{L^2}^5 \right). \end{aligned}$$

At this stage, it is necessary to treat separately the proofs for Proposition 12 and 13.

Proof of Proposition 12. Assume that $\sigma = 1$. For the second error term E_n^2 , using the assumption on F and Cauchy–Schwarz inequality, one has

$$\|E_n^2\|_{L^2}^2 \leq C \int_{t_n}^{t_{n+1}} \left(1 + \|u(t)\|_{L^2}^2 + \|u(t_n)\|_{L^2}^2 \right)^2 dt \int_{t_n}^{t_{n+1}} \|u(t) - u(t_n)\|_{L^2}^2 dt.$$

Gathering all the estimates, and using the isometry property $\|S(\tau)(v_n - v(t_n))\|_{L^2} = \|v_n - v(t_n)\|_{L^2} = \epsilon_n$, from (14) one obtains

$$\epsilon_{n+1} \leq (1 + C_F\tau + K_F\tau\Gamma_n)\epsilon_n + R_n,$$

where we define $\Gamma_n = \|u(t_n)\|_{L^2}^2 + \|u_n\|_{L^2}^2$ and $R_n = \|E_n^1\|_{L^2} + \|E_n^2\|_{L^2} + \|E_n^4\|_{L^2} + K_F\tau\Gamma_n \|w_n - w(t_n)\|_{L^2}$. Using a discrete Gronwall inequality and the equality $\epsilon_0 = 0$, one gets for all $n \in \{0, \dots, N\}$

$$\exp \left(-C_F n\tau - K_F\tau \sum_{k=0}^{n-1} \Gamma_k \right) \epsilon_n \leq \sum_{k=0}^{n-1} R_k.$$

Rewriting $\tau \sum_{k=0}^{n-1} \Gamma_k = S_n$ and $\|u_n - u(t_n)\|_{L^2} \leq \epsilon_n + \|w_n - w(t_n)\|_{L^2}$, applying Minkowski's inequality yields for $q \in [1, \infty)$

$$\mathbb{E} \left[\exp(-qK_F S_n) \|u_n - u(t_n)\|_{L^2}^q \right]^{\frac{1}{q}} \leq e^{C_F T} \sum_{k=0}^{n-1} \left(\mathbb{E} [R_k^q] \right)^{\frac{1}{q}} + e^{C_F T} \left(\mathbb{E} [\|w_n - w(t_n)\|_{L^2}^q] \right)^{\frac{1}{q}}.$$

We now estimate each of the terms above. Let us first recall that $R_k = \|E_k^1\|_{L^2} + \|E_k^2\|_{L^2} + \|E_k^4\|_{L^2} + K_F\tau\Gamma_k \|w_k - w(t_k)\|_{L^2}$. Using the triangle inequality, followed by Cauchy–Schwarz's

inequality, the assumption on the nonlinearity F as well as moment estimates in the L^2 and H^1 norms for the exact solution (Corollary 11 and Proposition 3), one obtains

$$\begin{aligned} \mathbb{E} [\|E_k^1\|_{L^2}^q]^{1/q} &\leq C\tau^{1/2} \int_{t_k}^{t_{k+1}} \mathbb{E} [\|F(u(t))\|_{H^1}^q]^{1/q} dt \\ &\leq C\tau^{1/2} \int_{t_k}^{t_{k+1}} \mathbb{E} [\|u(t)\|_{H^1}^{2q}]^{1/(2q)} \mathbb{E} [(1 + \|u(t)\|_{L^2}^2)^{2q}]^{1/(2q)} dt \\ &\leq C\tau^{1/2} \int_{t_k}^{t_{k+1}} dt \leq C\tau^{3/2}. \end{aligned}$$

For the second term, we use Cauchy–Schwarz’s inequality and moment bounds and regularity properties of the exact solution from Proposition 3 to get

$$\begin{aligned} \mathbb{E} [\|E_k^2\|_{L^2}^q]^{1/q} &\leq C \left(\int_{t_k}^{t_{k+1}} \mathbb{E} \left[\left(1 + \|u(t)\|_{L^2}^2 + \|u(t_k)\|_{L^2}^2\right)^{2q} \right]^{1/q} dt \right)^{1/2} \left(\int_{t_k}^{t_{k+1}} \mathbb{E} [\|u(t) - u(t_k)\|_{L^2}^{2q}]^{1/q} dt \right)^{1/2} \\ &\leq C\tau^{1/2} \left(\int_{t_k}^{t_{k+1}} |t - t_k| dt \right)^{1/2} \leq C\tau^{3/2}. \end{aligned}$$

Similarly, using the Cauchy–Schwarz’s inequality and the moment estimates in the L^2 norm for the numerical solution (Corollary 11), we obtain

$$\begin{aligned} \mathbb{E} [\|E_k^4\|_{L^2}^q]^{1/q} &\leq C\tau^2 \mathbb{E} \left[\left(1 + 2\|u_n\|_{L^2}^2\right)^{2q} \right]^{1/(2q)} \mathbb{E} [\|u_n\|_{L^2}^{10q}]^{1/(2q)} \\ &\leq C\tau^2. \end{aligned}$$

Thanks to the bounds for the moments in the L^2 norm given by Corollary 11, as well as to the error estimate (13) for the stochastic convolution proved above, we obtain the estimate

$$\begin{aligned} \mathbb{E} [(K_F\tau\Gamma_k \|w_k - w(t_k)\|_{L^2})^q]^{1/q} &\leq C\tau \mathbb{E} [\Gamma_k^{2q}]^{1/(2q)} \mathbb{E} [\|w_k - w(t_k)\|_{L^2}^{2q}]^{1/(2q)} \\ &\leq C\tau \mathbb{E} [\|w_k - w(t_k)\|_{L^2}^{2q}]^{1/(2q)} \leq C\tau\tau^{1/2} \leq C\tau^{3/2}. \end{aligned}$$

With all these estimates at hand, we arrive at

$$\sum_{k=0}^{n-1} (\mathbb{E} [R_k^q])^{1/q} \leq C_q(T, u_0, \alpha, Q)\tau^{1/2}.$$

Finally, we obtain

$$\begin{aligned} \mathbb{E} [\exp(-qK_F S_n) \|u_n - u(t_n)\|_{L^2}^q]^{1/q} &\leq e^{C_F T} \sum_{k=0}^{n-1} (\mathbb{E} [R_k^q])^{1/q} + e^{C_F T} (\mathbb{E} [\|w_n - w(t_n)\|_{L^2}^q])^{1/q} \\ &\leq C_q(T, u_0, \alpha, Q)\tau^{1/2} + C_q(T, \alpha, Q)\tau^{1/2}, \end{aligned}$$

using (13) in the last step.

This concludes the proof of Proposition 12. \square

We now turn to the proof of the second auxiliary result.

Proof of Proposition 13. Assume that $\sigma = 2$. As explained above, one requires to substantially modify the treatment of the error term E_n^2 . As will be clear below, some changes in the analysis of the error ϵ_n are required too.

Using a second-order Taylor expansion of the nonlinearity F and equation (5) (assumption on F''), one obtains the decomposition $E_n^2 = E_n^{2,1} + E_n^{2,2}$ where

$$E_n^{2,1} = i \int_{t_n}^{t_{n+1}} S(\tau) F'(u(t_n)) \cdot (u(t) - u(t_n)) dt$$

$$\|E_n^{2,2}\|_{L^2} \leq C \int_{t_n}^{t_{n+1}} (1 + \|u(t_n)\|_{L^2} + \|u(t)\|_{L^2}) \|u(t) - u(t_n)\|_{L^2}^2 dt.$$

In addition, using the mild formulation of the exact solution (2), one has the decomposition $E_n^{2,1} = E_n^{2,1,1} + E_n^{2,1,2} + E_n^{2,1,3}$, where

$$E_n^{2,1,1} = i \int_{t_n}^{t_{n+1}} S(\tau) F'(u(t_n)) \cdot (S(t - t_n) - I) u(t_n) dt$$

$$E_n^{2,1,2} = i \int_{t_n}^{t_{n+1}} S(\tau) F'(u(t_n)) \cdot \left(\int_{t_n}^t S(t - s) F(u(s)) ds \right) dt$$

$$E_n^{2,1,3} = i\alpha \int_{t_n}^{t_{n+1}} S(\tau) F'(u(t_n)) \cdot \left(\int_{t_n}^t S(t - s) dW^Q(s) \right) dt.$$

Owing to Lemma 1 and to equation (5) in Assumption 2, the first and second terms above are treated as follows: one has

$$\|E_n^{2,1,1}\|_{L^2} \leq C\tau^2 \left(1 + \|u(t_n)\|_{L^2}^2\right) \|u(t_n)\|_{H^2},$$

and

$$\|E_n^{2,1,2}\|_{L^2} \leq C \left(1 + \|u(t_n)\|_{L^2}^2\right) \tau \int_{t_n}^{t_{n+1}} \|F(u(s))\|_{L^2} ds.$$

Using the stochastic Fubini Theorem, the third term is written as

$$E_n^{2,1,3} = i\alpha \int_{t_n}^{t_{n+1}} S(\tau) F'(u(t_n)) \cdot \left(\int_{t_n}^t S(t - s) dW^Q(s) \right) dt$$

$$= i\alpha \int_{t_n}^{t_{n+1}} \left(S(\tau) F'(u(t_n)) \cdot \int_s^{t_{n+1}} S(t - s) dt \right) dW^Q(s)$$

$$= i\alpha \int_{t_n}^{t_{n+1}} \Theta_n(s) dW^Q(s),$$

where we have defined the quantity $\Theta_n(s) = S(\tau) F'(u(t_n)) \cdot \int_s^{t_{n+1}} S(t - s) dt$.

Applying Itô's formula, one gets

$$(15) \quad \mathbb{E} \left[\|E_n^{2,1,3}\|_{L^2}^2 \right] = \alpha^2 \int_{t_n}^{t_{n+1}} \mathbb{E} \left[\left\| \Theta_n(s) Q^{\frac{1}{2}} \right\|_{\mathcal{L}_2^0}^2 \right] ds \leq C\tau^3$$

using again (5) from Assumption 2 and the moment estimates in the L^2 norm of the exact solution from Corollary 11.

However the estimate (15) is not sufficient to directly obtain the required error estimate for ϵ_n as in the proof of Proposition 12. Improving this estimate requires to exploit the

orthogonality property $\mathbb{E} \left[\langle E_n^{2,1,3}, E_m^{2,1,3} \rangle \right] = 0$ if $n \neq m$, and to modify the approach used above to deal with the error.

Starting from (14), one obtains for all $n \geq 0$

$$v_n - v(t_n) = \sum_{k=0}^{n-1} S(\tau)^{n-k-1} (E_k^1 + E_k^2 + E_k^3 + E_k^4).$$

Recalling the decomposition $E_k^{2,1} = E_k^{2,1,1} + E_k^{2,1,2} + E_k^{2,1,3}$ and using the above bounds for the term E_k^3 then yields

$$\begin{aligned} \epsilon_n &\leq \tau \sum_{k=0}^{n-1} (C_F + K_F \Gamma_k) \epsilon_k \\ &\quad + \tau \sum_{k=0}^{n-1} (C_F + K_F \Gamma_k) \|w(t_k) - w_k\|_{L^2} \\ &\quad + \sum_{k=0}^{n-1} (\|E_k^1\|_{L^2} + \|E_k^4\|_{L^2}) \\ &\quad + \sum_{k=0}^{n-1} \|E_k^2 - E_k^{2,1,3}\|_{L^2} + \left\| \sum_{k=0}^{n-1} S(\tau)^{n-1-k} E_k^{2,1,3} \right\|_{L^2}. \end{aligned}$$

Applying the Gronwall inequality to get an almost sure inequality, then using the Cauchy–Schwarz and Minkowski's inequalities, one obtains for all $n \geq 0$ and all $q \in [1, \infty)$

$$\begin{aligned} e^{-C_F n \tau} (\mathbb{E}[e^{-q K_F S_n} \epsilon_n^q])^{1/q} &\leq \tau \sum_{k=0}^{n-1} \left(\mathbb{E} \left[(C_F + K_F \Gamma_k)^{2q} \right] \right)^{1/(2q)} \left(\mathbb{E} \left[\|w(t_k) - w_k\|_{L^2}^{2q} \right] \right)^{1/(2q)} \\ &\quad + \sum_{k=0}^{n-1} \left((\mathbb{E} [\|E_k^1\|_{L^2}^q])^{1/q} + (\mathbb{E} [\|E_k^4\|_{L^2}^q])^{1/q} \right) \\ &\quad + \sum_{k=0}^{n-1} \left(\mathbb{E} \left[\|E_k^2 - E_k^{2,1,3}\|_{L^2}^q \right] \right)^{1/q} + \left(\mathbb{E} \left[\left\| \sum_{k=0}^{n-1} S(\tau)^{n-1-k} E_k^{2,1,3} \right\|_{L^2}^{2q} \right] \right)^{1/(2q)}, \end{aligned}$$

where in the last term, we have used the inclusion $L^{2q}(\Omega) \subset L^q(\Omega)$. Using the same arguments as in the proof of Proposition 12 (in particular moment estimates of Proposition 3 and Corollary 11, and the error estimate (13) for the stochastic convolution), the treatment of the error terms in the right-hand side is straightforward, except for the last one which requires more details that we now present.

First, note that using the Burkholder–Davis–Gundy inequality one has

$$\left(\mathbb{E} \left[\left\| \sum_{k=0}^{n-1} S(\tau)^{n-1-k} E_k^{2,1,3} \right\|_{L^2}^{2q} \right] \right)^{1/(2q)} \leq C_q \left(\mathbb{E} \left[\left\| \sum_{k=0}^{n-1} S(\tau)^{n-1-k} E_k^{2,1,3} \right\|_{L^2}^2 \right] \right)^{1/2},$$

thus it is sufficient to deal with the case $q = 1$. Second, one has

$$\mathbb{E} \left[\left\| \sum_{k=0}^{n-1} S(\tau)^{n-1-k} E_k^{2,1,3} \right\|_{L^2}^2 \right] = \sum_{k=0}^{n-1} \mathbb{E} \left[\|E_k^{2,1,3}\|_{L^2}^2 \right] \leq C \tau^2,$$

using the orthogonality property $\mathbb{E} \left[\langle E_n^{2,1,3}, E_m^{2,1,3} \rangle \right] = 0$ if $n \neq m$ mentioned above, and the estimate (15).

Finally, recalling that $\|u_n - u(t_n)\|_{L^2} \leq \epsilon_n + \|w_n - w(t_n)\|_{L^2}$, gathering all these estimates and using the bounds on the error in the stochastic convolution (13), we obtain

$$\mathbb{E} \left[\exp(-qK_F S_n) \|u_n - u(t_n)\|_{L^2}^q \right]^{\frac{1}{q}} \leq C_q(T, u_0, Q)\tau.$$

This concludes the proof of Proposition 13. □

6. NUMERICAL EXPERIMENTS

We present some numerical experiments in order to support and illustrate the above theoretical results. In addition, we shall compare the behavior of the splitting scheme (8) (denoted by SPLIT below) with the following time integrators

- the classical Euler–Maruyama scheme (denoted EM)

$$u_{n+1} = u_n - i\tau\Delta u_n - i\tau F(u_n) - i\alpha\delta W_n^Q.$$

- the classical semi-implicit Euler–Maruyama scheme (denoted sEM)

$$u_{n+1} = u_n - i\tau\Delta u_{n+1} - i\tau F(u_n) - i\alpha\delta W_n^Q.$$

- the stochastic exponential integrator from [3] (denoted sEXP)

$$u_{n+1} = S(\tau) (u_n - i\tau F(u_n) - i\alpha\delta W_n^Q).$$

- the Crank–Nicolson–Euler–Maruyama (denoted CN)

$$u_{n+1} = u_n - i\tau\Delta u_{n+1/2} - i\tau F(u_n) - i\alpha\delta W_n^Q,$$

where $u_{n+1/2} = \frac{1}{2}(u_n + u_{n+1})$. This is a slight modification of the Crank–Nicolson from [23].

6.1. Trace formulas for the mass. We consider the stochastic Schrödinger equation (1) on the interval $[0, 2\pi]$ with periodic boundary condition, the coefficient $\alpha = 1$, and a covariance operator with $(\gamma_k)_{k \in \mathbb{Z}} = \left(\frac{1}{1+k^2} \right)_{k \in \mathbb{Z}}$ and $(e_k(x))_{k \in \mathbb{Z}} = \left(\frac{1}{\sqrt{2\pi}} e^{ikx} \right)_{k \in \mathbb{Z}}$. We consider the initial value $u_0 = \frac{2}{2-\cos(x)}$ and the following nonlinearities: $V(x)u = \frac{3}{5-4\cos(x)}u$ (external potential), $(V \star |u|^2)u$ with $V(x) = \cos(x)$ (nonlocal interaction), $F(u) = +|u|^2u$ (cubic). We refer to [22, Theorem 3.4] for a result on global existence of solutions to the cubic case. We use a pseudo-spectral method with $N_x = 2^8$ modes and the above time integrators with time-step size $\tau = 0.1$.

Figure 1 displays the evolution of the expected value of the mass on the time intervals $[0, 1]$ (external potential) and $[0, 25]$ (other cases). The expected values are approximated using $M = 75000$ samples. The exact trace formulas for the splitting scheme, shown in Proposition 5, can be observed. The growth rates of the other schemes are qualitatively different than this linear rate of the exact solution: observe for instance the exponential drift of EM in the first plot, the fact that sEXP seems to overestimate the linear drift and the fact that sEM underestimates it. The CN scheme performs relatively well, except in the cubic case (not displayed), where it should use a much smaller step-size in order not to explode.

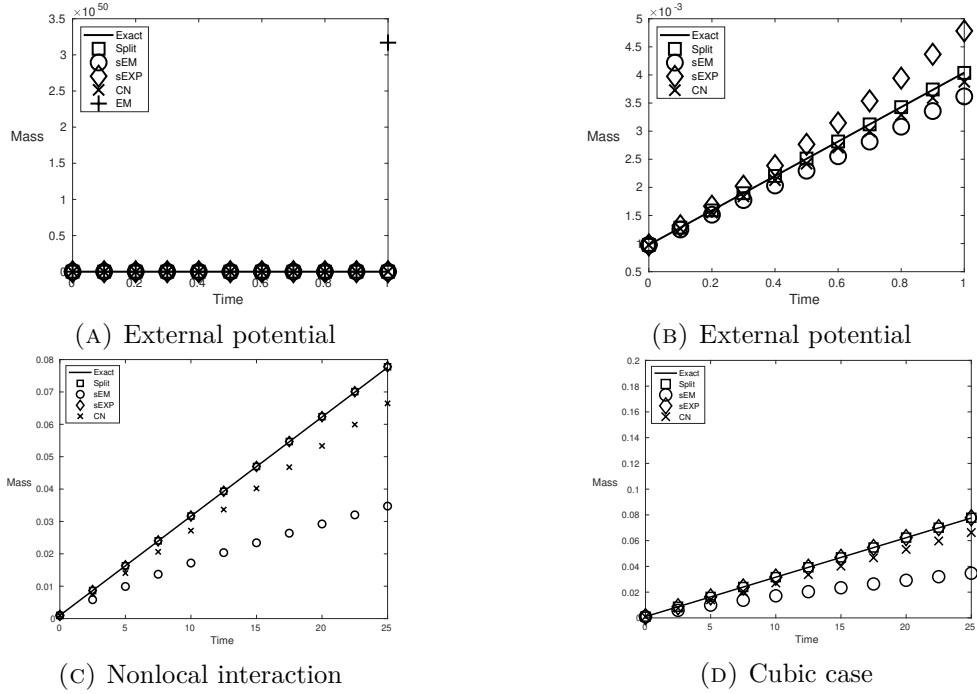


FIGURE 1. Trace formulas for mass of the splitting scheme (Split), the Euler–Maruyama scheme (EM), the semi-implicit Euler–Maruyama scheme (sEM), the exponential integrator (sEXP), and the Crank–Nicolson (CN) schemes.

6.2. Strong convergence. In this subsection, we illustrate the strong convergence of the splitting scheme (8) as stated in Theorem 14.

To do this, we consider the stochastic Schrödinger equation (1) on the interval $[0, 2\pi]$ with periodic boundary condition, and a covariance operator with $(\gamma_k)_{k \in \mathbb{Z}} = \left(\frac{1}{1+k^2}\right)_{k \in \mathbb{Z}}$. We consider the external potential $V(x) = \frac{3}{5-4 \cos(x)}$ and nonlocal interaction given by the potential $V(x) = \cos(x)$. We take the initial value $u_0 = \frac{2}{2-\cos(x)}$ (external potential) and $u_0 = \frac{1}{1+\sin(x)^2}$ (nonlocal interaction). Additional parameters are: coefficient in front of the noise $\alpha = 1.5$, time interval $[0, 1]$, 250 samples used to approximate the expectations. We use a pseudo-spectral method with $N_x = 2^{10}$ modes and the above time integrators. Strong errors, measured with $r = 1$ at the end point, are presented in Figure 2. In this numerical experiment, the splitting and exponential integrators give very close results. For clarity, only some of the values for the exponential integrator are displayed. An order 1/2 of convergence for the splitting scheme is observed. Note that, the strong order of convergence of the other time integrators are not known in the case of the nonlocal interaction potential.

In order to illustrate the higher order of convergence for the splitting scheme, we consider a smoother noise with covariance operator with $(\gamma_k)_{k \in \mathbb{Z}} = \left(\frac{1}{1+k^4}\right)_{k \in \mathbb{Z}}$ (the other parameters for the simulation are as above). Results are presented in Figure 3, where a strong order of convergence 1 is observed for the proposed time integrator, in agreement with Theorem 14.

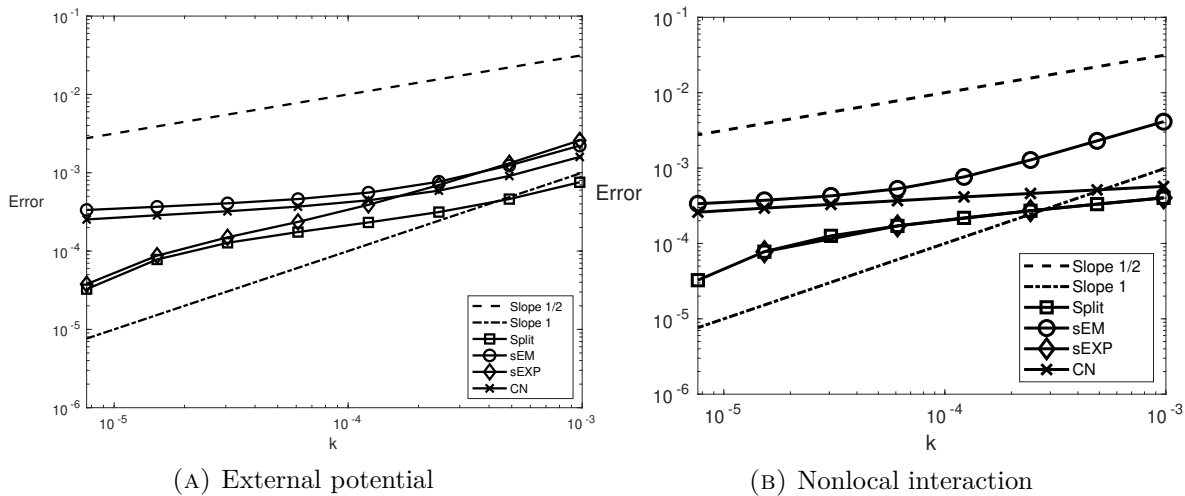


FIGURE 2. Strong errors for the stochastic Schrödinger equations.

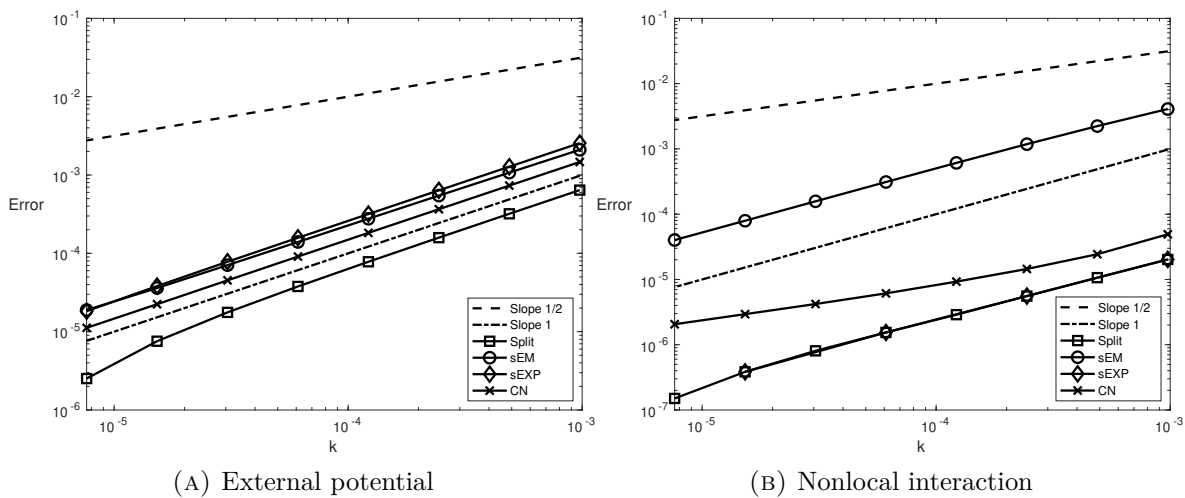


FIGURE 3. Strong errors for the stochastic Schrödinger equations with a smoother noise.

6.3. Convergence in probability. In this subsection we numerically demonstrate the order of convergence in probability for the splitting scheme (8). This order has been shown to be $1/2$ in Corollary 16 above.

Numerically, we investigate the order in probability by using the equation

$$(16) \quad \max_{n \in \{1, 2, \dots, N\}} \|u_n - u_{ref}(t_n)\|_{L^2} \geq C\tau^\delta,$$

where u_{ref} denotes a reference solution computed using the splitting scheme with step-size $\tau_{ref} = 2^{-16}$. We then study the proportion of samples, P , fulfilling equation (16) for given C and δ and observe whether $P \rightarrow 0$ for the given δ as $\tau \rightarrow 0$ and C increases.

We simulate 50 samples of the splitting scheme applied to the SPDE (1) with the initial value $u_0 = \frac{2}{2 - \cos(x)}$, the nonlocal interaction and the same noise as in the previous subsection

(non-smooth case). In addition, we take the following parameters: $t \in [0, 1]$, $N_x = 2^8$ Fourier modes and $\tau = 2^n$ where $n = -6, -7, \dots, -14$. We then estimate the proportion P of samples fulfilling (16) for each given τ , $\delta = 0.4, 0.5, 0.6$, and $C = 10^c$ for $c = 1, 2, 3$. The results are presented in Figure 4.

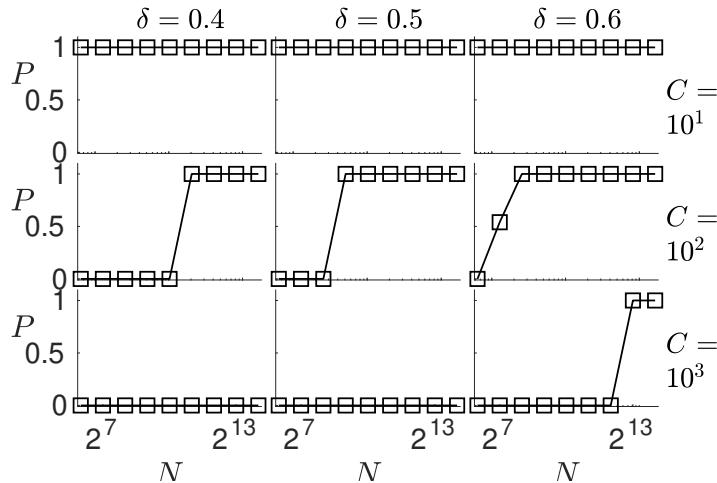


FIGURE 4. Proportion of samples fulfilling (16) for the splitting scheme (N denotes the number of step-sizes).

In this figure, one sees how the proportion of samples P quickly goes to zero for $\delta \leq 1/2$ and an increasing C . Furthermore, this property does not hold for $\delta > 1/2$. This numerical experiment thus confirms that the order of convergence in probability of the splitting scheme is $1/2$, as stated in Corollary 16.

6.4. Computational times. In this numerical experiment, we compare the computational costs of the above time integrators (expect the classical Euler–Maruyama scheme). To do this, we consider the SPDE (1) with the above nonlocal interaction potential for times $t \in [0, 2]$. We discretize this SPDE using $N_x = 2^{10}$ Fourier modes in space. We run 100 samples for each numerical scheme. For each scheme and each sample, we run several time steps and compare the L^2 error at the final time with a reference solution provided for the same sample by the same scheme for a very small time-step $\tau = 2^{-13}$. Figure 5 displays the total computational time for all the samples, for each numerical scheme and each time-step, as a function of the averaged final error. One observes better performance for the splitting scheme.

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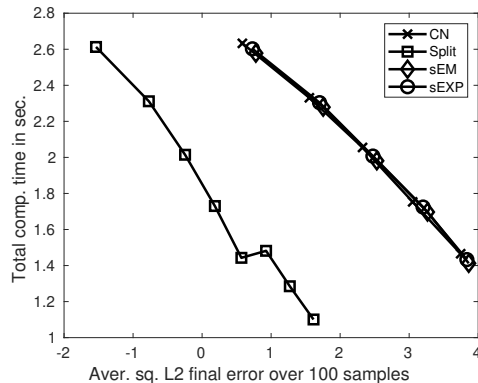


FIGURE 5. Computational time as a function of the averaged final error for the four numerical methods.

APPENDIX A. PROOF OF PROPOSITION 3

This appendix provides the proofs of properties of the exact solution to (1).

Global well-posedness. Let Assumption 1 be satisfied. Since the nonlinearity F is only locally Lipschitz continuous, a truncation argument is used to prove global well-posedness. Let us stress that the key property of (1) used in the argument below is the fact that $V[u]$ is real-valued.

Let $\theta: [0, \infty) \rightarrow [0, 1]$ be a compactly supported Lipschitz continuous function, such that $\theta(x) = 1$ for $x \in [0, 1]$. For any $R \in (0, \infty)$, set $V^R(u) = \theta(R^{-1}\|u\|_{L^2})V[u]$ and $F^R(u) = V^R(u)u$. The mapping F^R is globally Lipschitz continuous, and the SPDE

$$du^R(t) = \Delta u^R(t) dt + F^R(u^R(t)) dt + \alpha dW^Q(t),$$

with initial condition $u^R(0) = u_0$, thus admits a unique global solution $(u^R(t))_{t \in [0, T]}$. Since the mapping V^R is real-valued, the trace formula holds, see (10): indeed, one obtains

$$d\|u^R(t)\|_{L^2}^2 = \alpha^2 \text{Tr}(Q) + 2\alpha \text{Im}(\langle u^R(t), dW^Q(t) \rangle).$$

Taking expectation, one obtains the trace formula $\mathbb{E}[\|u^R(t)\|_{L^2}^2] = \|u_0\|_{L^2}^2 + 2t\alpha^2 \text{Tr}(Q)$, where the right-hand side does not depend on truncation index R . Using the Burkholder–Davis–Gundy inequality, one obtains

$$\begin{aligned} \mathbb{E}\left[\sup_{0 \leq t \leq T} \|u^R(t)\|_{L^2}^2\right] &\leq 3\left(\|u_0\|_{L^2}^2 + \alpha^2 T \text{Tr}(Q)\right) + 3\alpha^2 \int_0^T \sum_{k \in \mathbb{N}} |\gamma_k|^2 \mathbb{E}[\langle u^R(s), e_k \rangle^2] ds \\ &\leq 3\left(\|u_0\|_{L^2}^2 + \alpha^2 T \text{Tr}(Q)\right) + 3\alpha^2 \left\|Q^{\frac{1}{2}}\right\|_{\mathcal{L}_2^0}^2 \int_0^T \mathbb{E}[\|u^R(s)\|_{L^2}^2] ds \\ &\leq C(T, Q, u_0), \end{aligned}$$

where one observes that $C(T, Q, u_0)$ does not depend on R , using the trace formula above for the term in the integral $\|u^R(s)\|_{L^2}^2$.

Setting the truncation argument is then straightforward. Let $\tau^R = \inf\{t \geq 0; \|u^R(t)\|_{L^2} > R\}$. If $R_1, R_2 \geq R$, then $u^{R_1}(t) = u^{R_2}(t)$ for all $t \leq \tau^R$, by construction of F^R . This allows us

to define $u(t)$ solving (1) for all $t \in [0, \tau)$, where $\tau = \lim_{R \rightarrow \infty} \tau^R$. Finally, $\tau = \infty$ almost surely, indeed for every $T \in (0, \infty)$,

$$\mathbb{P}(\tau \leq T) = \lim_{R \rightarrow \infty} \mathbb{P}(\tau^R \leq T) = \lim_{R \rightarrow \infty} \mathbb{P}\left(\sup_{0 \leq t \leq T} \|u^R(t)\|_{L^2}^2 \geq R^2\right) \leq \lim_{R \rightarrow \infty} \frac{C(T, Q, u_0)}{R^2} = 0,$$

using the moment estimate above. This concludes the proof of the global well-posedness of (1).

Moment estimates in H^1 . Next, let us prove the moment bounds for the exact solution to (1). We provide details only for the moment estimates in the H^1 norm (under Assumption 1)

$$\sup_{0 \leq t \leq T} \mathbb{E}[\|\nabla u(t)\|_{L^2}^{2p}] \leq C_p(T, Q, u_0).$$

Indeed, the moment estimates for the L^2 norm, namely

$$\sup_{0 \leq t \leq T} \mathbb{E}[\|u(t)\|_{L^2}^{2p}] \leq C_p(T, Q, u_0),$$

can either be obtained using similar arguments, or be deduced from the exponential moment estimates for which a detailed proof is provided above. Likewise, the proof of moment estimates

$$\sup_{0 \leq t \leq T} \mathbb{E}[\|\nabla u(t)\|_{H^2}^{2p}] \leq C_p(T, Q, u_0)$$

under Assumption 2 would follow from similar arguments.

Let us first consider $\psi(u) = \|\nabla u\|_{L^2}^2$ for all $u \in H^1$. Its first and second order derivatives are given by

$$\begin{aligned} \psi'(u).h &= 2\operatorname{Re}(\langle \nabla u, \nabla h \rangle) \\ \psi''(u).(h, k) &= 2\operatorname{Re}(\langle \nabla h, \nabla k \rangle) \end{aligned}$$

for $h, k \in H^1$. Using Itô's formula, one gets

$$\begin{aligned} d\|\nabla u(t)\|_{L^2}^2 &= d\psi(u(t)) \\ &= \psi'(u(t)).du(t) + \frac{\alpha^2}{2} \sum_{k \in \mathbb{N}} \psi''(u(t)).(\gamma_k e_k, \gamma_k e_k) dt \\ &= 2\operatorname{Im}(\langle \nabla \bar{u}(t), \nabla \Delta u(t) \rangle) dt + 2\operatorname{Im}(\langle \nabla \bar{u}(t), \nabla F(u(t)) \rangle) dt \\ &\quad + 2\alpha \operatorname{Im}(\langle \nabla u(t), \nabla dW^Q(t) \rangle) + \alpha^2 \sum_{k \in \mathbb{N}} |\gamma_k|^2 \|\nabla e_k\|_{L^2}^2. \end{aligned}$$

The first term in the last equality vanishes, and when taking expectation the third term also vanishes. Using the condition (4) to deal with the second term, one obtains

$$\frac{d\mathbb{E}[\|\nabla u(t)\|_{L^2}^2]}{dt} \leq C \left(1 + \mathbb{E}[\|\nabla u(t)\|_{L^2}^2] + \mathbb{E}[P_1(\|u(t)\|_{L^2}^2)]\right),$$

where P_1 is a polynomial mapping. Note that $\sup_{0 \leq t \leq T} \mathbb{E}[P_1(\|u(t)\|_{L^2}^2)] \leq C(T, Q, u_0)$ due to moment bounds in the L^2 norm. Using the Gronwall Lemma then yields

$$\sup_{0 \leq t \leq T} \mathbb{E}[\|\nabla u(t)\|_{L^2}^2] \leq C(T, Q, u_0).$$

Let $p \geq 1$, then applying Itô's formula for $\psi_p(u) = \psi(u)^p$ yields

$$\begin{aligned} \frac{d\mathbb{E}[\|\nabla u(t)\|_{L^2}^{2p}]}{dt} &\leq C_p \|\nabla u(t)\|_{L^2}^{2(p-1)} \operatorname{Im}(\langle \nabla u(t), \nabla F(u(t)) \rangle) + C_p \alpha^2 \sum_{k \in \mathbb{N}} |\gamma_k|^2 \|\nabla e_k\|_{L^2}^2 \mathbb{E}[\|\nabla u(t)\|_{L^2}^{2(p-1)}] \\ &\leq C \left(1 + \mathbb{E}[\|\nabla u(t)\|_{L^2}^{2p}] + C\mathbb{E}[P_1(\|u(t)\|_{L^2}^2)^p] \right) \end{aligned}$$

using (4) and Young's inequality. Using Gronwall's lemma then concludes the proof of the moment bounds in the H^1 norm.

Temporal regularity. It remains to deal with the temporal regularity estimate. Using the mild formulation (2), for any $0 \leq t_1 < t_2 \leq T$, one has

$$\begin{aligned} u(t_2) - u(t_1) &= S(t_1)(S(t_2 - t_1) - I)u_0 \\ &\quad - i \int_0^{t_1} S(t_1 - s)(S(t_2 - t_1) - I)F(u(s)) ds - i \int_{t_1}^{t_2} S(t_2 - s)F(u(s)) ds \\ &\quad - i\alpha \int_0^{t_1} S(t_1 - s)(S(t_2 - t_1) - I) dW^Q(s) - i\alpha \int_{t_1}^{t_2} S(t_2 - s) dW^Q(s). \end{aligned}$$

Using Lemma 1, the first estimate of (4) and the moment bounds in the L^2 and H^1 norms, one obtains

$$\begin{aligned} \|S(t_1)(S(t_2 - t_1) - I)u_0\|_{L^2} &\leq C|t_2 - t_1|^{\frac{1}{2}} \|u_0\|_{H^1} \\ \mathbb{E} \left[\left\| \int_0^{t_1} S(t_1 - s)(S(t_2 - t_1) - I)F(u(s)) ds \right\|_{L^2}^{2p} \right] &\leq T^{2p-1} |t_2 - t_1|^p \int_0^T \mathbb{E} \left[\|F(u(s))\|_{H^1}^{2p} \right] ds \leq C|t_2 - t_1|^{\frac{2p}{2}} \\ \mathbb{E} \left[\left\| \int_{t_1}^{t_2} S(t_2 - s)F(u(s)) ds \right\|_{L^2}^{2p} \right] &\leq |t_2 - t_1|^{2p} \int_0^T \mathbb{E} \left[\|F(u(s))\|_{L^2}^{2p} \right] ds \leq C|t_2 - t_1|^{2p}. \end{aligned}$$

Using Itô's isometry formula and Lemma 1, one has

$$\begin{aligned} \mathbb{E} \left[\left\| \int_0^{t_1} S(t_1 - s)(S(t_2 - t_1) - I) dW^Q(s) \right\|_{L^2}^2 \right] &= t_1 \left\| (S(t_2 - t_1) - I)Q^{\frac{1}{2}} \right\|_{\mathcal{L}_2^0}^2 \leq Ct_1 |t_2 - t_1| \left\| Q^{\frac{1}{2}} \right\|_{\mathcal{L}_2^1}^2 \\ \mathbb{E} \left[\left\| \int_{t_1}^{t_2} S(t_2 - s) dW^Q(s) \right\|_{L^2}^2 \right] &= |t_2 - t_1| \left\| Q^{\frac{1}{2}} \right\|_{\mathcal{L}_2^0}^2. \end{aligned}$$

Since the stochastic integrals have Gaussian distribution, gathering the estimates above yields

$$\mathbb{E} \left[\|u(t_2) - u(t_1)\|_{L^2}^{2p} \right] \leq C_p(T, Q, u_0) |t_2 - t_1|^p,$$

for all $p \geq 1$ and $t_1, t_2 \in [0, T]$. This concludes the proof of Proposition 3.

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