Symplectic Runge-Kutta Semi-discretization for Stochastic Schrödinger Equation *

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Abstract

The stochastic Schrödinger equation in Stratonovich sense is an infinite-dimensional stochastic Hamiltonian system, whose phase flow preserves symplecticity. In this paper we propose a general class of stochastic symplectic Runge-Kutta methods in temporal direction to the stochastic Schrödinger equation in Stratonovich sense and show that the methods preserve the charge conservation law. We present a convergence theorem on the relationship between the mean-square convergence order of a semi-discrete method and its local accuracy order. Taking stochastic midpoint scheme as an example of stochastic symplectic Runge-Kutta methods in temporal direction, based on the theorem we show that the mean-square convergence order of the semi-discrete scheme is 1 under appropriate assumptions.

AMS subject classification: 65C20, 65C30, 65C50.

Key Words: stochastic Schrödinger equation, infinite-dimensional stochastic Hamiltonian system, symplectic structure, symplectic Runge-Kutta method, semi-discretization, mean-square convergence order

1 Introduction

More attention has been paid to the study of stochastic Schrödinger equation (see [1, 3, 15, 19] and references therein). The local and global existences of solution in space $H^1(R^n)$ for stochastic Schrödinger equation are investigated in [3]. There are some conservation laws for

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deterministic Schrödinger equation, for example, charge conservation law and energy conservation law. The evolution of these invariant quantities in the case of stochastic Schrödinger equation also are considered in [3]. It is well known that the deterministic Schrödinger equation is an infinite-dimensional Hamiltonian system, that is to say, its phase flow preserves symplecticity, see [8,12] for details. [15] establishes the theory about stochastic multisymplectic conservation law for stochastic Hamiltonian partial differential equations, the stochastic Schrödinger equation as a concrete example is investigated for this property. As far as we know, there has been no work concerning the infinite-dimensional stochastic Hamiltonian system, its stochastic symplecticity and symplectic semi-discretization up to now. In this paper we present the general formula of infinite-dimensional stochastic Hamiltonian system via a variational principle and investigate the stochastic symplecticity of stochastic Schrödinger equation in Stratonovich sense, which is shown to be an infinite-dimensional stochastic Hamiltonian system.

Finding solutions of stochastic partial differential equations (SPDEs) numerically is an active ongoing research area. Semi-discretizations in temporal direction are developed in [24] for parabolic SPDEs and in [18] for SPDEs of Zakai type driven by square integrable martingales. For space semi-discretizations, we refer to [25,31] for finite difference method and to [5,30] for Galerkin approach and to [16] for finite element method. Also plenty of works are devoted to full discrete schemes. The monograph [13] investigates Taylor approximations for SPDEs. Lattice approximations are proposed in [9,10] for finite difference method and finite elements are used in [6,17]. Combined with spectral Galerkin method, a Milstein type scheme is proposed in [14] and a Runge-Kutta type scheme is proposed in [29].

Specifically, for the numerical approximations of stochastic Schrödinger equation, a semi-discrete scheme for stochastic nonlinear Schrödinger equation in Stratonovich sense is proposed in [1]. Authors also obtain the convergence of the discrete solution in various topologies. For stochastic nonlinear Schrödinger equation in Itô sense with power nonlinearity, [2] analyzes the error of a semi-discrete scheme and proves that the numerical scheme has strong order $\frac{1}{2}$ in general and order 1 if the noise is additive. Using the integral representation idea, [19] proposes splitting schemes to stochastic nonlinear Schrödinger equation in Stratonovich sense and proves the first order convergence in non-global Lipschitz case. It is important to design a numerical scheme which preserves the properties of the original problems as much as possible. For Hamiltonian system, symplectic methods are shown to be superior to non-symplectic ones especially in long time computation, owing to their preservation of the qualitative property, the symplecticity of the underlying continuous differential equation systems; see [21,27] and references therein. Since the stochastic Schrödinger equation in Stratonovich sense is an infinite-dimensional stochastic Hamiltonian system, we investigate numerical methods to preserve symplecticity.

In the present paper, we present a general class of Runge-Kutta methods in temporal direction for stochastic Schrödinger equation firstly and then obtain the symplectic conditions for Runge-Kutta methods in temporal direction. Under the symplectic conditions of Runge-Kutta methods, we show that they preserve the charge conservation law. Adopting the idea of the work [21], which establishes the mean-square order of convergence of a method resting on properties of its one-step approximation only for stochastic ordinary differential equations, we
propose a convergence theorem on the mean-square orders of a class of semi-discrete schemes for stochastic Schrödinger equation allowing sufficient spatial regularity. As a special case of stochastic symplectic Runge-Kutta methods applied to temporal discretization, the mean-square convergence order of midpoint scheme is analyzed. Based on the convergence theorem, it is shown that the mean-square convergence order of the stochastic midpoint scheme is 1 under appropriate assumptions.

In section 2, we present some preliminaries on stochastic Schrödinger equation. We derive the general formula of infinite-dimensional stochastic Hamiltonian system and show that the phase flow of stochastic Schrödinger equation preserves symplecticity. In section 3, we propose a general class of stochastic symplectic Runge-Kutta methods in temporal direction for stochastic Schrödinger equation and show that they also preserve the charge conservation law. The midpoint scheme as an example of stochastic symplectic Runge-Kutta methods in temporal direction is analyzed. In section 4 a convergence theorem on the mean-square orders of a class of semi-discrete schemes for stochastic Schrödinger equation is proposed. Based on the theorem, we show that the mean-square convergence order of the midpoint scheme is 1 under appropriate conditions.

2 Stochastic Schrödinger equation

We are interested in one-dimensional stochastic Schrödinger equation with multiplicative noise in the sense of Stratonovich in the domain $[t_0, T] \times [-L, L]$,

$$
\begin{align*}
\text{i}d_t \psi(x, t) + \left( \frac{\partial^2 \psi}{\partial x^2} + \Psi'(|\psi|^2, x, t)\psi(x, t) \right) dt &= \varepsilon \psi(x, t) \circ dW(t), \\
\psi(-L, t) &= \psi(L, t) = 0, \\
\psi(x, t_0) &= \varphi(x),
\end{align*}
$$

(2.1)

where $\text{i}$ is the imaginary unit, $\Psi(|\psi|^2, x, t)$ is a real function of $(\psi, x, t)$ and $W(t)$ is an infinite-dimensional $Q$-Wiener process which will be specified below.

We rewrite equation (2.1) as a stochastic evolution equation in abstract form

$$
\begin{align*}
\text{i}d\psi + (A\psi + F(\psi))dt &= G(\psi) \circ dW(t), \\
\psi(t_0) &= \varphi,
\end{align*}
$$

(2.2)

where $F(\psi)(x) = \Psi'(|\psi|^2, x, t)\psi(x, t)$ and $G(\psi)(x) = \varepsilon \psi(x, t)$. From [14] we know that the equation (2.2) satisfies the condition of commutative noise in infinite dimension. The unbounded operator $A$ on the classical Lebesgue space of complex valued functions $L^2([-L, L], \mathbb{C})$, is defined by

$$
\mathcal{D}(A) = \{ \psi \in L^2([-L, L], \mathbb{C}) : \psi(-L) = \psi(L) = 0 \}
$$

$$
A\psi = \frac{\partial^2 \psi}{\partial x^2}, \quad \forall \psi \in \mathcal{D}(A).
$$
$W(t)$ denotes a $Q$-Wiener process on the Hilbert space $U = L^2([-L, L], \mathbb{R})$ which is the subspace of $L^2([-L, L], \mathbb{C})$ consisting of real valued integrable functions. Here $Q \in L(U)$ is nonnegative, symmetric and with finite trace. Let $\{e_k\}_{k \in \mathbb{N}}$ be an orthonormal basis of $U$ consisting of eigenvectors of $Q$. Then there is a sequence of independent real-valued Brownian motions $\{\beta_k\}_{k \in \mathbb{N}}$ on the probability space $(\Omega, \mathcal{F}, P)$ such that

$$W(t) = \sum_{k \in \mathbb{N}} \beta_k(t) Q^{\frac{1}{2}} e_k,$$

with covariance operator $Q = Q^{\frac{1}{2}} \circ Q^{\frac{1}{2}}$.

In addition, $Q^{\frac{1}{2}}$ is a Hilbert-Schmidt operator (the space of all Hilbert-Schmidt operators from $H$ to $U$ is denoted by $HS(H, U)$).

$$|Q^{\frac{1}{2}}|_{HS(U, U)} = \sum_{k \in \mathbb{N}} <Q^{\frac{1}{2}} e_k, Q^{\frac{1}{2}} e_k>_U = \sum_{k \in \mathbb{N}} <Qe_k, e_k>_U = tr(Q) <\infty.$$ 

Here we mention an important property of the infinite dimensional stochastic integral, which contributes a lot in the mean-square error estimation:

$$E \left| \int_0^T G_s dW_s \right|^2_H = \int_0^T |G_s|^2_{HS(Q^{\frac{1}{2}}(U), H)} ds,$$

where the subspace $Q^{\frac{1}{2}}(U) \subset U$ with the inner product given by

$$<u, v>_{Q^{\frac{1}{2}}(U)} = <Q^{-\frac{1}{2}} u, Q^{\frac{1}{2}} v>_U,$$

for $u, v \in Q^{\frac{1}{2}}(U)$, is again a separable Hilbert space with $Q^{-\frac{1}{2}}$ is the pseudo inverse of $Q^{\frac{1}{2}}$ in case $Q$ is not one-to-one.

Note that $Q^{\frac{1}{2}} e_k, k \in \mathbb{N}$ is an orthonormal basis of $Q^{\frac{1}{2}}(U)$, if $e_k, k \in \mathbb{N}$ is an orthonormal basis of $(KerQ^{\frac{1}{2}})^\perp$. This basis can be supplemented to a basis of $U$ by elements of $KerQ^{\frac{1}{2}}$. Thus we obtain that

$$|T|_{HS(Q^{\frac{1}{2}}(U), H)} = |T \circ Q^{\frac{1}{2}}|_{HS(U, H)}$$

for each $T \in HS(Q^{\frac{1}{2}}(U), H)$.

As pointed out in [3], there is an equivalent Itô form of equation (2.2)

$$i d\psi + (A \psi + \tilde{F}(\psi)) dt = G(\psi) dW(t),$$

$$\psi(t_0) = \varphi,$$  (2.3)

where $\tilde{F}(\psi) = F(\psi) + \frac{1}{2} \xi^2 \psi Q$ with $Q(x) = \sum_{k \in \mathbb{N}} (Q^{\frac{1}{2}} e_k(x))^2$, for $x \in [-L, L]$.

The mild solution of equation (2.3) is

$$\psi(t) = S(t) \varphi + i \int_{t_0}^t S(t-r) \tilde{F}(\psi(r)) dr - i \int_{t_0}^t S(t-r) G(\psi(r)) dW(r),$$  (2.4)
where \( S(t)_{t \in \mathbb{R}} \) denotes the semigroup of solution operator of the deterministic linear differential equation
\[
\frac{d\psi}{dt} = \Delta \psi.
\]

If the size of the noise \( \varepsilon \) equals to 0, i.e., the noise term is eliminated, we get the deterministic Schrödinger equation. It possesses some global conservation laws, for example, charge conservation law
\[
\mathcal{E}_1(\psi) = \int_{-L}^{L} |\psi|^2 dx = \mathcal{E}_1(\varphi),
\]
and energy conservation law if \( \Psi \) is independent of \( t \)
\[
\mathcal{E}_2(\psi) = \int_{-L}^{L} (|\psi_x|^2 - \Psi(\psi, x)) dx = \mathcal{E}_2(\varphi).
\]

We refer to [8, 12] for further understanding. These quantities have been important criteria of measuring whether a numerical simulation is good or not.

In the Stratonovich sense, the charge conservation law is still preserved by the solution of equation (2.1). In general, there is no energy conservation law for stochastic Schrödinger equation. One only can obtain the relationship satisfied by the average energy [3].

**Proposition 2.1.** The stochastic nonlinear Schrödinger equation (2.1) possesses the charge conservation law
\[
\mathcal{E}_1(\psi) = \int_{-L}^{L} |\psi|^2 dx = \mathcal{E}_1(\varphi).
\]

**Proposition 2.2.** The averaged energy \( \mathbb{E}(\mathcal{E}_2(\psi)) \) satisfies
\[
\mathbb{E}(\mathcal{E}_2(\psi)) = \mathbb{E}(\mathcal{E}_2(\varphi)) + \frac{\varepsilon^2}{2} \int_{0}^{t} \int_{-L}^{L} |\psi(x, t)|^2 \sum_{k \in \mathbb{N}} |\partial_{x} Q_{c_k}(x)|^2 dx dt
\]
if \( \Psi \) is independent of \( t \). Here \( \mathbb{E}(\cdot) \) means the expectation.

**2.1 Preserving symplectic structure**

The Hamilton equations of motion for stochastic ordinary differential equations are derived in [28]. We present the case of infinite-dimensional stochastic system here.

All the constructions done in the finite dimensional case could go over to the infinite-dimensional ones. We begin with the variational principle, and then pass to the infinite-dimensional Hamilton equations via some transformations as in finite-dimensional case. The action is
\[
\bar{S} = \int_{t_0}^{T} \left( \mathcal{L}(P, Q, \dot{P}, \dot{Q}) - \mathcal{H}_2(P, Q) \circ \dot{\chi} \right) dt,
\]
where \( \dot{\chi} \) is a time-space noise, and considered as the temporal derivative of an infinite-dimensional Wiener process \( W(t) \), i.e. \( \dot{\chi} = \frac{dW(t)}{dt} \).
The variation of the action follows as
\[
\delta \bar{S} = \delta \int_{t_0}^T \left( \mathcal{L}(P, Q, \dot{P}, \dot{Q}) - \mathcal{H}_2(P, Q) \circ \dot{\chi} \right) dt
\]
\[
= \int \left( \frac{\delta \mathcal{L}}{\delta P} \delta P + \frac{\delta \mathcal{L}}{\delta Q} \delta Q + \frac{\delta \mathcal{L}}{\delta P} \dot{\delta P} + \frac{\delta \mathcal{L}}{\delta Q} \dot{\delta Q} - \frac{\delta \mathcal{H}_2}{\delta P} \delta P \circ \dot{\chi} - \frac{\delta \mathcal{H}_2}{\delta Q} \delta Q \circ \dot{\chi} \right) dt dx
\]
\[
= \int \left[ \left( \frac{\delta \mathcal{L}}{\delta P} - \frac{d}{dt} \left( \frac{\delta \mathcal{L}}{\delta P} \right) - \frac{\delta \mathcal{H}_2}{\delta P} \circ \dot{\chi} \right) \delta P + \left( \frac{\delta \mathcal{L}}{\delta Q} - \frac{d}{dt} \left( \frac{\delta \mathcal{L}}{\delta Q} \right) - \frac{\delta \mathcal{H}_2}{\delta Q} \circ \dot{\chi} \right) \delta Q \right] dt dx. \quad (2.6)
\]
Here an integration by parts is performed and the boundary conditions \( \delta P(T, x) = \delta P(t_0, x) = 0, \delta Q(T, x) = \delta Q(t_0, x) = 0 \) were used.

Thus the Hamilton’s principle
\[
\delta \bar{S} = \delta \int_{t_0}^T \left( \mathcal{L}(P, Q, \dot{P}, \dot{Q}) - \mathcal{H}_2(P, Q) \circ \dot{\chi} \right) dt = 0
\]
leads to
\[
\begin{align*}
\frac{d}{dt} \left( \frac{\delta \mathcal{L}}{\delta P} \right) &= \frac{\delta \mathcal{L}}{\delta P} - \frac{\delta \mathcal{H}_2}{\delta P} \circ \dot{\chi}, \\
\frac{d}{dt} \left( \frac{\delta \mathcal{L}}{\delta Q} \right) &= \frac{\delta \mathcal{L}}{\delta Q} - \frac{\delta \mathcal{H}_2}{\delta Q} \circ \dot{\chi}.
\end{align*} \quad (2.7)
\]
Introduce the Hamiltonian \( \mathcal{H}_1(P, Q) \) and the generator \( \mathcal{G} \) which are defined according to the equation
\[
\mathcal{L}(P, Q, \dot{P}, \dot{Q}) - \int_{-L}^L P \dot{Q} dx + \mathcal{H}_1(P, Q) - \frac{dG}{dt} = 0. \quad (2.8)
\]
As in [28], using this equation, we find
\[
\begin{align*}
\dot{P} &= -\frac{\delta \mathcal{H}_1}{\delta Q} - \frac{\delta \mathcal{H}_2}{\delta Q} \circ \dot{\chi}, \\
\dot{Q} &= \frac{\delta \mathcal{H}_1}{\delta P} + \frac{\delta \mathcal{H}_2}{\delta P} \circ \dot{\chi},
\end{align*} \quad (2.9)
\]
which can be rewritten in the form
\[
\begin{align*}
dP &= -\frac{\delta \mathcal{H}_1}{\delta Q} dt - \frac{\delta \mathcal{H}_2}{\delta Q} \circ dW(t), \\
dQ &= \frac{\delta \mathcal{H}_1}{\delta P} dt + \frac{\delta \mathcal{H}_2}{\delta P} \circ dW(t). \quad (2.10)
\end{align*}
\]

**Remark 2.1.** If \( \mathcal{H}_1 = \mathcal{H}_2 = \mathcal{H} \), then \( \mathcal{H} \) is an invariant of system (2.10). In fact,
\[
\begin{align*}
d\mathcal{H} &= \int_{-L}^{L} \left( \frac{\delta \mathcal{H}}{\delta P} dP + \frac{\delta \mathcal{H}}{\delta Q} dQ \right) dx \\
&= \int_{-L}^{L} \left( -\frac{\delta \mathcal{H}}{\delta P} \delta P dt - \frac{\delta \mathcal{H}}{\delta Q} \delta Q \circ dW + \frac{\delta \mathcal{H}}{\delta P} \delta P dt + \frac{\delta \mathcal{H}}{\delta Q} \delta Q \circ dW \right) dx \\
&= 0.
\end{align*}
\]
The stochastic Schrödinger equation (2.1) can be written as a canonical infinite dimensional Hamiltonian system. Denote the real and imaginary part of the solution of stochastic Schrödinger equation (2.1) by $\Re(\psi) = P(t)$ and $\Im(\psi) = Q(t)$, respectively. Then we have

\[
\begin{align*}
\frac{dP}{dt} &= -\frac{\delta H_1}{\delta Q} dt - \frac{\delta H_2}{\delta Q} \circ dW(t) \\
&= -(AQ + \Psi^2|\psi|^2(P^2 + Q^2, x, t))dt + \varepsilon Q \circ dW(t), \\
\frac{dQ}{dt} &= \frac{\delta H_1}{\delta P} dt + \frac{\delta H_2}{\delta P} \circ dW(t) \\
&= (AP + \Psi^2|\psi|^2(P^2 + Q^2, x, t))dt - \varepsilon P \circ dW(t),
\end{align*}
\]

(2.11)

with initial conditions

\[
P(0) = p = \Re(\varphi), \quad Q(0) = q = \Im(\varphi),
\]

and Hamiltonians

\[
\mathcal{H}_1(P, Q) = \frac{1}{2} \int_{-L}^{L} \left( (P_x^2 + Q_x^2) - \Psi(P^2 + Q^2, x, t) \right) dx
\]

and

\[
\mathcal{H}_2(P, Q) = -\frac{\varepsilon}{2} \int_{-L}^{L} (P^2 + Q^2) dx.
\]

The general formula of stochastic ordinary differential equation of Stratonovich sense is

\[
\begin{align*}
\frac{dP}{dt} &= -\frac{\partial H(P, Q)}{\partial Q} dt - \sum_{k=1}^{m} \frac{\partial H_k(P, Q)}{\partial Q} \circ dW_k(t), \\
\frac{dQ}{dt} &= \frac{\partial H(P, Q)}{\partial P} dt + \sum_{k=1}^{m} \frac{\partial H_k(P, Q)}{\partial P} \circ dW_k(t),
\end{align*}
\]

(2.12)

It is well known that (2.12) is a stochastic Hamiltonian system with Hamiltonian functions $H(P, Q), H_k(P, Q), k = 1, 2, \cdots, m$. The preservation of symplectic structure $dP \wedge dQ$ by system (2.12) was proved in [21].

The symplectic form for system (2.11) is given by

\[
\bar{\omega}(t) = \int_{-L}^{L} dP \wedge dQ dx,
\]

where the overbar on $\omega$ is a reminder that the two-form $dP \wedge dQ$ is integrated over all space.

Using the formula of change of variables in differential forms, we obtain

\[
\bar{\omega}(t) = \int_{-L}^{L} dP \wedge dQ dx \\
= \int_{-L}^{L} \left( \frac{\partial P}{\partial p} \frac{\partial Q}{\partial q} - \frac{\partial P}{\partial q} \frac{\partial Q}{\partial p} \right) dp \wedge dq dx.
\]
Hence, the phase flow of (2.11) preserves symplectic structure if and only if
\[
\frac{d\bar{\omega}(t)}{dt} = \int_{-L}^{t} \left( \frac{\partial P}{\partial p} \frac{\partial Q}{\partial q} - \frac{\partial P}{\partial q} \frac{\partial Q}{\partial p} \right) dp \wedge dq \ dx = 0. \tag{2.13}
\]

Introduce notations
\[
P_p = \frac{\partial P}{\partial p}, \quad P_q = \frac{\partial P}{\partial q}, \quad Q_p = \frac{\partial Q}{\partial p}, \quad Q_q = \frac{\partial Q}{\partial q}.
\]

and let \( H_1(P, Q) = \frac{1}{2} \Psi(P^2 + Q^2, x, t) \). We know that \( P_p, Q_p, P_q \) and \( Q_q \) obey the following system
\[
\begin{align*}
dP_p &= - \left( AQ_p + \frac{\partial^2 H_1}{\partial P \partial Q} P_p + \frac{\partial^2 H_1}{\partial Q^2} Q_p \right) dt + \varepsilon Q_p \circ dW(t), \\
P_p(t_0) &= 1, \\
dQ_p &= \left( AP_p + \frac{\partial^2 H_1}{\partial P \partial Q} P_p + \frac{\partial^2 H_1}{\partial P \partial Q} Q_p \right) dt - \varepsilon P_p \circ dW(t), \\
Q_p(t_0) &= 0, \\
dP_q &= - \left( AQ_q + \frac{\partial^2 H_1}{\partial P \partial Q} P_q + \frac{\partial^2 H_1}{\partial Q^2} Q_q \right) dt + \varepsilon Q_q \circ dW(t), \\
P_q(t_0) &= 0, \\
dQ_q &= \left( AP_q + \frac{\partial^2 H_1}{\partial P \partial Q} P_q + \frac{\partial^2 H_1}{\partial P \partial Q} Q_q \right) dt - \varepsilon P_q \circ dW(t), \\
Q_q(t_0) &= 1. \tag{2.14}
\end{align*}
\]

Due to (2.14), we get
\[
\begin{align*}
d\left( \frac{\partial P}{\partial p} \frac{\partial Q}{\partial q} - \frac{\partial P}{\partial q} \frac{\partial Q}{\partial p} \right) &= d\left( P_p Q_q - P_q Q_p \right) \\
&= d(P_p)Q_q + d(Q_p)P_p - d(Q_p)P_p - d(P_p)Q_q \\
&= \left[ - \left( AQ_p + \frac{\partial^2 H_1}{\partial P \partial Q} P_p + \frac{\partial^2 H_1}{\partial Q^2} Q_p \right) Q_q + \left( AQ_q + \frac{\partial^2 H_1}{\partial P \partial Q} P_q + \frac{\partial^2 H_1}{\partial Q^2} Q_p \right) P_q \\
&\quad \quad + \left( AP_p + \frac{\partial^2 H_1}{\partial P \partial Q} P_p + \frac{\partial^2 H_1}{\partial P \partial Q} Q_p \right) P_p - \left( AP_q + \frac{\partial^2 H_1}{\partial P \partial Q} P_q + \frac{\partial^2 H_1}{\partial P \partial Q} Q_p \right) Q_p \right] dt \\
&\quad + \varepsilon \left( Q_p Q_q - Q_q Q_p - P_p P_q + P_q P_p \right) \circ dW(t) \\
&= \left( - AQ_p Q_q + AQ_q P_p + AP_q P_p - AP_p Q_q \right) dt. \tag{2.15}
\end{align*}
\]
Then we have
\[
\frac{d}{dt} \bar{\omega} = \int_{-L}^{L} \frac{d}{dt} \left( \frac{\partial P}{\partial p} \frac{\partial Q}{\partial q} - \frac{\partial P}{\partial q} \frac{\partial Q}{\partial p} \right) dp \wedge dq dx
\]
\[
= \int_{-L}^{L} \left( -AQ_pQ_q + AQ_qP_p + AP_qP_p - AP_pP_q \right) dp \wedge dq dx
\]
\[
= -\int_{-L}^{L} \left[ d(AQ) \wedge dQ + d(AP) \wedge dP \right] dx
\]
\[
= -\int_{-L}^{L} \frac{\partial}{\partial x} \left[ d(Q_x) \wedge dQ + d(P_x) \wedge dP \right] dx. \tag{2.16}
\]

Under the boundary condition \( \psi(-L,t) = \psi(L,t) = 0 \), which means \( P(-L,t) = P(L,t) = 0 \) and \( Q(-L,t) = Q(L,t) = 0 \), we obtain that
\[
\frac{d}{dt} \bar{\omega}(t) = 0.
\]

Thus we have the following theorem:

**Theorem 2.1.** The phase flow of stochastic Schrödinger equation
\[
\text{i} d\psi + (A \psi + F(\psi)) dt = G(\psi) \circ dW,
\]
with \( F(\psi) = \Psi_{|\psi|^2}(|\psi|^2, x, t) \psi \) and \( G(\psi) = \varepsilon \psi \), preserves the symplectic structure
\[
\bar{\omega}(t) = \int_{-L}^{L} dP \wedge dQ dx
\]
with \( P \) (resp. \( Q \)) being the real (resp. imaginary) part of the solution \( \psi \).

### 3 Symplectic Runge-Kutta semi-discretization in temporal direction

For stochastic ordinary differential equation, stochastic Runge-Kutta method is an important class of numerical methods, which has been widely investigated, see [4, 20, 21, 26, 27] and references therein for instance.

Here we introduce the uniform partition \( 0 = t_0 < t_1 < \cdots < t_N = T, \) let \( \Delta t = t_{k+1} - t_k, \) \( k = 0, 1, \cdots, N - 1 \) for simplicity and \( \Delta W_n = W(t_{n+1}) - W(t_n) \) and apply s-stage stochastic
Runge-Kutta methods to the equation (2.11) in the temporal direction, we get that

\[ P_i = P^n - \Delta t \sum_{j=1}^{s} a_{ij}^{(0)} (AQ_j + \Psi_j' Q_j) + \Delta W_n \sum_{j=1}^{s} a_{ij}^{(1)} \epsilon_j, \]

\[ Q_i = Q^n + \Delta t \sum_{j=1}^{s} a_{ij}^{(0)} (AP_j + \Psi_j' P_j) - \Delta W_n \sum_{j=1}^{s} a_{ij}^{(1)} \epsilon_j, \]

\[ P^{n+1} = P^n - \Delta t \sum_{i=1}^{s} b_i^{(0)} (AQ) + \Psi_i' Q_i) + \Delta W_n \sum_{i=1}^{s} b_i^{(1)} \epsilon_i, \]

\[ Q^{n+1} = Q^n + \Delta t \sum_{i=1}^{s} b_i^{(0)} (AP_i + \Psi_i' P_i) - \Delta W_n \sum_{i=1}^{s} b_i^{(1)} \epsilon_i, \] (3.1)

where \( \Psi_i' = \Psi_i' |_{x_0} (P^2_i + Q^2, x, t_n + \sum_{j=1}^{s} a_{ij}^{(0)} \Delta t). \)

**Theorem 3.1.** Methods (3.1) preserve the discrete symplectic structure, i.e.,

\[ \tilde{\omega}^{n+1} = \int_{-L}^{L} dP^{n+1} \wedge dQ^{n+1} \, dx = \int_{-L}^{L} dP^n \wedge dQ^n \, dx = \tilde{\omega}^n, \]

if coefficients satisfy the following conditions: \( \forall i, j = 1, \cdots, s, \)

\[
\begin{align*}
\dot{b}_i^{(0)} b_j^{(0)} = b_i^{(0)} a_{ij}^{(0)} + b_j^{(0)} a_{ji}^{(0)}, \\
\dot{b}_i^{(0)} b_j^{(1)} = b_i^{(0)} a_{ij}^{(1)} + b_j^{(1)} a_{ji}^{(0)}, \\
\dot{b}_i^{(1)} b_j^{(1)} = b_i^{(1)} a_{ij}^{(1)} + b_j^{(1)} a_{ji}^{(1)}. 
\end{align*}
\] (3.2)

*Proof.* Introduce the functions

\[ f_j = \Psi_j' Q_j, \quad \tilde{f}_j = \epsilon Q_j, \quad g_j = \Psi_j' P_j, \quad \tilde{g}_j = \epsilon P_j. \]

It is convenient to write stochastic Runge-Kutta methods (3.1) as follows:

\[ P_i = P^n - \Delta t \sum_{j=1}^{s} a_{ij}^{(0)} AQ_j - \Delta t \sum_{j=1}^{s} a_{ij}^{(0)} f_j + \Delta W_n \sum_{j=1}^{s} a_{ij}^{(1)} \tilde{f}_j, \]

\[ Q_i = Q^n + \Delta t \sum_{j=1}^{s} a_{ij}^{(0)} AP_j + \Delta t \sum_{j=1}^{s} a_{ij}^{(0)} g_j - \Delta W_n \sum_{j=1}^{s} a_{ij}^{(1)} \tilde{g}_j, \]

\[ P^{n+1} = P^n - \Delta t \sum_{i=1}^{s} b_i^{(0)} AQ_i - \Delta t \sum_{i=1}^{s} b_i^{(0)} f_i + \Delta W_n \sum_{i=1}^{s} b_i^{(1)} \tilde{f}_i, \]

\[ Q^{n+1} = Q^n + \Delta t \sum_{i=1}^{s} b_i^{(0)} AP_i + \Delta t \sum_{i=1}^{s} b_i^{(0)} g_i - \Delta W_n \sum_{i=1}^{s} b_i^{(1)} \tilde{g}_i. \]
We have
\[
dP^{n+1} \land dQ^{n+1}
\]
\[
= \left( dP^n - \Delta t \sum_{i=1}^s b_i^{(0)} d(AQ_i) - \Delta t \sum_{i=1}^s b_i^{(0)} df_i + \Delta W_n \sum_{i=1}^s b_i^{(1)} df_i \right)
\]
\[
\land \left( dQ^n + \Delta t \sum_{i=1}^s b_i^{(0)} d(AP_i) + \Delta t \sum_{i=1}^s b_i^{(0)} dg_i - \Delta W_n \sum_{i=1}^s b_i^{(1)} dg_i \right)
\]
\[
= dP^n \land dQ^n - \Delta W_n^2 \sum_{i,j=1}^s b_i^{(1)} b_j^{(1)} d\tilde{f}_i \wedge \tilde{g}_j - \Delta W_n \sum_{i=1}^s b_i^{(1)} \left( dP^n \land dg_i - d\tilde{f}_i \land dQ^n \right)
\]
\[
+ \Delta t \sum_{i=1}^s b_i^{(0)} \left( dP^n \land d(AP_i + g_i) - d(AQ_i + f_i) \land dQ^n \right)
\]
\[
+ \Delta t \Delta W_n \sum_{i,j=1}^s b_i^{(0)} b_j^{(1)} \left( d(AQ_i + f_i) \land d\tilde{g}_j + d\tilde{f}_j \land d(AP_i + g_i) \right)
\]
\[
- \Delta t^2 \sum_{i,j=1}^s b_i^{(0)} b_j^{(0)} \left( d(AQ_i) \land d(AP_j + g_j) + df_i \land d(AP_j + g_j) \right). \quad (3.3)
\]
Further
\[
dP^n = dP_i + \Delta t \sum_{j=1}^s a_{ij}^{(0)} d(AQ_j) + \Delta t \sum_{j=1}^s a_{ij}^{(0)} df_j - \Delta W_n \sum_{j=1}^s a_{ij}^{(1)} df_j,
\]
\[
dQ^n = dQ_i - \Delta t \sum_{j=1}^s a_{ij}^{(0)} d(AP_j) - \Delta t \sum_{j=1}^s a_{ij}^{(0)} dg_j + \Delta W_n \sum_{j=1}^s a_{ij}^{(1)} dg_j. \quad (3.4)
\]
Substituting (3.4) into (3.3), we obtain
\[
dP^{n+1} \land dQ^{n+1} - dP^n \land dQ^n
\]
\[
= \Delta W_n \sum_{i=1}^s b_i^{(1)} \left( d\tilde{f}_i \land dQ_i - dP_i \land d\tilde{g}_i \right)
\]
\[
+ \Delta t \sum_{i=1}^s b_i^{(0)} \left( dP_i \land d(AP_i) + dP_i \land dg_i - d(AQ_i) \land dQ_i \right)
\]
\[
+ \Delta W_n^2 \sum_{i,j=1}^s \left( b_i^{(1)} a_{ij}^{(1)} + b_j^{(1)} a_{ij}^{(1)} - b_i^{(1)} b_j^{(1)} \right) d\tilde{f}_i \land \tilde{g}_j
\]
\[
+ \Delta t \Delta W_n \sum_{i,j=1}^s \left( b_i^{(0)} b_j^{(1)} - b_i^{(0)} a_{ij}^{(1)} + b_j^{(1)} b_j^{(0)} \right) \left( d(AQ_i) \land d\tilde{g}_j + d\tilde{f}_i \land d\tilde{g}_j + d\tilde{f}_j \land d(AP_i) + d\tilde{f}_j \land dg_i \right)
\]
\[
+ \Delta t^2 \sum_{i,j=1}^s \left( b_i^{(0)} a_{ij}^{(0)} + b_j^{(0)} a_{ij}^{(0)} - b_i^{(0)} b_j^{(0)} \right) \left( d(AQ_i) \land d(AP_j) + d(AQ_i) \land dg_j + df_i \land d(AP_j) + df_i \land dg_j \right).
\]
Recalling the conditions (3.2) and the expressions of functions $f_i$, $\tilde{f}_i$, $g_i$, $\tilde{g}_i$, we have

\[
\int_{-L}^{L} dP^{n+1} \wedge dQ^{n+1} \, dx = \int_{-L}^{L} dP^n \wedge dQ^n \, dx + \Delta t \sum_{i=1}^{s} b_i^{(0)} \int_{-L}^{L} \frac{\partial}{\partial x} (dP_i \wedge d(P_i)_x - d(Q_i)_x \wedge dQ_i) \, dx
\]

\[
= \int_{-L}^{L} dP^n \wedge dQ^n \, dx.
\]

Thus the proof of the theorem is completed.  

The stochastic symplectic Runge-Kutta methods (3.1) preserve the discrete charge conservation law.

**Proposition 3.1.** The symplectic methods (3.1)-(3.2) possess the discrete charge conservation law, i.e.,

\[
\int_{-L}^{L} |\phi^{n+1}|^2 \, dx = \int_{-L}^{L} |\phi^n|^2 \, dx, \quad \forall n = 0, 1, \ldots, N.
\]

**Proof.** Recall that $\phi^n = P^n + iQ^n$ and let $\phi_i = P_i + iQ_i$, then methods (3.1) can be rewritten as

\[
\phi_i = \phi_i^n - i\Delta t \sum_{j=1}^{s} a_{ij}^{(0)} h_j - i\Delta W^n \sum_{j=1}^{s} a_{ij}^{(1)} \tilde{h}_j,
\]

(3.5)

\[
\phi_i^{n+1} = \phi_i^n - i\Delta t \sum_{i=1}^{s} b_i^{(0)} h_i - i\Delta W^n \sum_{i=1}^{s} b_i^{(1)} \tilde{h}_i,
\]

(3.6)

with $h_i = A\phi_i + \Psi_i^t \phi_i$ and $\tilde{h}_i = \varepsilon \phi_i$.

Multiplying equation (3.6) with $\bar{\phi}^{n+1} + \bar{\phi}^n$ and taking real part, we get

\[
|\phi^{n+1}|^2 = |\phi^n|^2 + \Re \left\{ i\Delta t \sum_{i=1}^{s} b_i^{(0)} h_i (\bar{\phi}^{n+1} + \bar{\phi}^n) - i\Delta W^n \sum_{i=1}^{s} b_i^{(1)} \bar{h}_i (\bar{\phi}^{n+1} + \bar{\phi}^n) \right\}.
\]

(3.7)

From equation (3.5), we have the expression of $\phi^n$,

\[
\phi^n = \phi_i - i\Delta t \sum_{j=1}^{s} a_{ij}^{(0)} h_j + i\Delta W^n \sum_{j=1}^{s} a_{ij}^{(1)} \tilde{h}_j.
\]

Combining this together with equation (3.6) leads to

\[
\bar{\phi}^{n+1} + \bar{\phi}^n = 2\bar{\phi}_i + i2\Delta t \sum_{j=1}^{s} a_{ij}^{(0)} \bar{h}_j - i2\Delta W^n \sum_{j=1}^{s} a_{ij}^{(1)} \bar{h}_j + i\Delta t \sum_{j=1}^{s} b_j^{(0)} \bar{h}_j + i\Delta W^n \sum_{j=1}^{s} b_j^{(1)} \bar{h}_j.
\]
Therefore the second term of the right hand side of equation (3.7) becomes
\[
\Re \left\{ i\Delta t \sum_{i=1}^{s} b_i^{(0)} h_i(\bar{\psi}^{n+1} + \bar{\phi}^n) - i\Delta W_n \sum_{i=1}^{s} b_i^{(1)} \bar{h}_i(\bar{\psi}^{n+1} + \bar{\phi}^n) \right\}
\]
\[
= \Im \left\{ 2\Delta t \sum_{i=1}^{s} b_i^{(0)} A\phi_i \bar{\phi}_i \right\} + \Delta t^2 \sum_{ij=1}^{s} \left( b_i^{(0)} b_j^{(1)} - b_i^{(1)} a_{ij}^{(0)} - b_j^{(1)} a_{ji}^{(0)} \right) \Re(h_i \bar{h}_j)
\]
\[
- 2\Delta t \Delta W_n \sum_{ij=1}^{s} \left( b_i^{(0)} b_j^{(1)} - b_i^{(1)} a_{ij}^{(0)} - b_j^{(1)} a_{ji}^{(0)} \right) \Re(h_i \bar{h}_j)
\]
\[
+ \Delta W_n^2 \sum_{ij=1}^{s} \left( b_i^{(1)} b_j^{(1)} - b_i^{(1)} a_{ij}^{(1)} - b_j^{(1)} a_{ji}^{(1)} \right) \Re(h_i \bar{h}_j),
\]
since \( \Re\phi = \Re\bar{\phi} \). Recalling the symplectic condition (3.2), we have
\[
|\phi^{n+1}|^2 = |\phi^n|^2 + \Im \left\{ 2\Delta t \sum_{i=1}^{s} b_i^{(0)} A\phi_i \bar{\phi}_i \right\}.
\]
Integrating the above equation from \(-L\) to \(L\) with respect to \(x\) leads to the conclusion of the proposition.

3.1 Midpoint scheme

In the sequel, we consider a special case of symplectic Runge-Kutta methods. Let coefficients be
\[
a^{(0)} = a^{(1)} = \frac{1}{2} \quad \text{and} \quad b^{(0)} = b^{(1)} = 1.
\]
Obviously, coefficients satisfy symplectic conditions (3.2), and we obtain the midpoint scheme:
\[
P^{n+1} = P^n - \Delta t A Q^{n+\frac{1}{2}} - \Delta t (\Psi')^{n+\frac{1}{2}} Q^{n+\frac{1}{2}} + \varepsilon Q^{n+\frac{1}{2}} \Delta W_n,
\]
\[
Q^{n+1} = Q^n + \Delta t A P^{n+\frac{1}{2}} + \Delta t (\Psi')^{n+\frac{1}{2}} P^{n+\frac{1}{2}} - \varepsilon P^{n+\frac{1}{2}} \Delta W_n.
\] (3.8)

Denote the approximation of \(\psi(t_n)\) by \(\phi^n\), and recall that \(\phi^n = P^n + iQ^n\), we have
\[
\phi^{n+1} = \phi^n + i\Delta t A \phi^{n+\frac{1}{2}} + i\Delta t F(t_{n+\frac{1}{2}}, \phi^{n+\frac{1}{2}}) - i\varepsilon \phi^{n+\frac{1}{2}} \Delta W_n.
\] (3.9)

Of course, (3.9) is formal and has to be understood in the following sense
\[
\phi^{n+1} = \hat{S}_{\Delta t} \phi^n + i\Delta t T_{\Delta t} F(t_{n+\frac{1}{2}}, \phi^{n+\frac{1}{2}}) - i\varepsilon T_{\Delta t} \phi^{n+\frac{1}{2}} \Delta W_n,
\] (3.10)

where
\[
F(t_{n+\frac{1}{2}}, \phi^{n+\frac{1}{2}}) := \Psi'|(\phi^{n+\frac{1}{2}})^2, x, t_{n+\frac{1}{2}}) \phi^{n+\frac{1}{2}},
\]
the operators are
\[
\hat{S}_{\Delta t} = (Id - \frac{i\Delta t}{2} A)^{-1}(Id + \frac{i\Delta t}{2} A)
\]
and
\[ T_{\Delta t} = (Id - \frac{i \Delta t}{2} A)^{-1}. \]

As in [21], we truncate the noise \( \Delta W_n = \sum \Delta \beta_i Q e_i = \sum \xi_i Q^2 e_i \sqrt{\Delta t} \), where \( \xi_i \) is \( \mathcal{N}(0,1) \)-distributed random variable, by another random variable
\[ \Delta \bar{W}_n = \sum \zeta_i Q^2 e_i \sqrt{\Delta t}. \]

For \( A_{\Delta t} = \sqrt{2k|\ln \Delta t|} \), let
\[ \zeta_i = \begin{cases} \xi_i & \text{if } |\xi_i| \leq A_{\Delta t}, \\ A_{\Delta t} & \text{if } \xi_i > A_{\Delta t}, \\ -A_{\Delta t} & \text{if } \xi_i < -A_{\Delta t}. \end{cases} \] (3.11)

The solution of \( \phi^{n+1} \) of (3.10) can be assured by contraction mapping principle (see [2, 21]).

As we can let \( k \) large enough to satisfy our numerical analysis, we denote \( \Delta \bar{W}_n \) by \( \Delta W_n \) below.

Since midpoint scheme is a special case of symplectic Runge-Kutta methods, it also preserves the discrete charge conservation law.

**Corollary 3.1.** For midpoint scheme (3.8), the discrete charge conservation law is preserved, i.e.,
\[ \int_{-L}^{L} |\phi^{n+1}|^2 dx = \int_{-L}^{L} |\phi^n|^2 dx, \quad \forall n = 0, 1, \ldots, N. \] (3.12)

The following propositions are discrete versions of the evolutionary relationship of average energy for midpoint scheme. For the general Runge-Kutta methods, it is an open problem.

**Proposition 3.2.** If \( \Psi_{|\psi|^2}(|\psi|^2, x, t) = V(x) \), then
\[ \mathbf{E}(\mathcal{E}_2(\phi^{n+1})) + \frac{\varepsilon}{\Delta t} \int_{-L}^{L} \mathbf{E}(|\phi^{n+1}|^2 \Delta W_n) dx = \mathbf{E}(\mathcal{E}_2(\phi^n)), \] (3.13)
where
\[ \mathcal{E}_2(\phi^n) = \int_{-L}^{L} |\nabla \phi^n|^2 dx - \int_{-L}^{L} V(x)|\phi^n|^2 dx. \]

**Proof.** Since scheme (3.10) can be rewritten as
\[ \frac{i}{\Delta t} (\phi^{n+1} - \phi^n) + A \phi^{n+\frac{1}{2}} + \Psi'_{|\psi|^2}(|\phi^{n+\frac{1}{2}}|^2, x, t^{n+\frac{1}{2}}) \phi^{n+\frac{1}{2}} = \frac{\varepsilon}{\Delta t} \phi^{n+\frac{1}{2}} \Delta W_n, \]
multiplying it with \( \bar{\phi}^{n+1} - \bar{\phi}^n \), taking the real part and integrating with respect to \( x \) in the space \([-L, L]\), the first term in the left hand side of the above equation becomes
\[ \Im \int_{-L}^{L} \frac{1}{\Delta t} (\phi^{n+1} - \phi^n)(\bar{\phi}^{n+1} - \bar{\phi}^n) dx = -\frac{1}{\Delta t} \Im \int_{-L}^{L} (\phi^{n+1} \bar{\phi}^n + \phi^n \bar{\phi}^{n+1}) dx = 0, \]

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the second term has the form
\[ \mathbb{R} \int_{-L}^{L} A \phi^{n+\frac{1}{2}} (\bar{\phi}^{n+1} - \bar{\phi}^{n}) dx = \frac{1}{2} \mathbb{R} \int_{-L}^{L} \left( - |\nabla \phi^{n+1}|^2 + |\nabla \phi^n|^2 + \nabla \phi^{n+1} \nabla \bar{\phi}^{n} - \nabla \phi^n \nabla \bar{\phi}^{n+1} \right) dx \]
\[ = -\frac{1}{2} \int_{-L}^{L} |\nabla \phi^{n+1}|^2 dx + \frac{1}{2} \int_{-L}^{L} |\nabla \phi^n|^2 dx, \]
the third term acquires the form
\[ \frac{1}{2} \mathbb{R} \int_{-L}^{L} V(x)(\phi^{n+1} + \phi^n)(\bar{\phi}^{n+1} - \bar{\phi}^{n}) dx = \frac{1}{2} \int_{-L}^{L} V(x)|\phi^{n+1}|^2 dx - \frac{1}{2} \int_{-L}^{L} V(x)|\phi^n|^2 dx, \]
at last, the term turns into
\[ \mathbb{R} \int_{-L}^{L} \left( \frac{\varepsilon}{\Delta t} \Delta W_n \phi^{n+\frac{1}{2}} (\bar{\phi}^{n+1} - \bar{\phi}^{n}) \right) dx = \frac{\varepsilon}{2\Delta t} \int_{-L}^{L} |\phi^{n+1}|^2 \Delta W_n dx - \frac{\varepsilon}{2\Delta t} \int_{-L}^{L} |\phi^n|^2 \Delta W_n dx. \]
Combine the above equations, the result of the proposition is obtained. \( \Box \)

**Proposition 3.3.** For the general \( \Psi'(|\psi|^2, x, t) \), we have the implicit relationship
\[ \int_{-L}^{L} |\nabla \phi^{n+1}|^2 dx - \int_{-L}^{L} |\nabla \phi^n|^2 dx - \int_{-L}^{L} (\psi^{n+\frac{1}{2}} (|\phi^{n+1}|^2 - |\phi^n|^2) dx = -\varepsilon \int_{-L}^{L} (|\phi^{n+1}|^2 - |\phi^n|^2) \Delta W_n dx. \]
(3.14)

**Proof.** The proof of this proposition is the same as that of Proposition 3.2 \( \Box \)

### 4 Convergence theorem

To investigate the mean-square convergence order of semi-discrete approximations to stochastic Schrödinger equation, we establish a convergence theorem on the relationship between local accuracy order and global mean-square order of a semi-discrete method.

In this subsection, we consider stochastic Schrödinger equation in Itô sense
\[ i d\psi + (A\psi + F(\psi)) dt = G(\psi) dW, \]
(4.1)
whose mild solution is
\[ \psi(t_{n+1}) = S(\Delta t)\psi(t_n) + i \int_{t_n}^{t_{n+1}} S(t_{n+1} - r) F(\psi(r)) dr - i \int_{t_n}^{t_{n+1}} S(t_{n+1} - r) G(\psi(r)) dW(r) \]
\[ := S(\Delta t)\psi(t_n) + \Upsilon(\psi(r)). \]
(4.2)

Denote the approximation of the solution \((\psi(t_n), \mathcal{F}_{t_n})\) for equation (4.1) by \((\phi^n, \mathcal{F}_{t_n})\), which means that the numerical approximation \(\phi^n\) is also \(\mathcal{F}_{t_n}\)-measurable. Here \(\mathcal{F}_t\) is the filtration generated by Wiener process and initial value. Define \(\phi^n\) recurrently by
\[ \phi^{n+1} = \hat{S}_{\Delta t} \phi^n + \Gamma(\phi^n, \phi^{n+1}, \Delta t, \Delta W_n, T_{\Delta t}), \]
(4.3)
where $\hat{S}_{\Delta t}$ and $T_{\Delta t}$ are two operators with $|\hat{S}_{\Delta t}| \leq 1$.

If $s \in \mathbb{R}$, the usual Sobolev space $H^s := H^s([-L, L]; \mathbb{C})$ is the space of tempered distributions $u \in S'([-L, L]; \mathbb{C})$ whose Fourier transform $\hat{u}$ satisfies $(1 + |x|^2)^{s/2} \hat{u} \in L^2([-L, L]; \mathbb{C})$. We write $| \cdot |_s = | \cdot |_{H^s}$ and make the following Hypotheses for equation (4.1) with $F$ : $H^\alpha \to H^\alpha$ and $G : H^\alpha \to HS(L^2([-L, L], \mathbb{R}); H^\alpha)$ are globally Lipschitz functions.

Hypothesis 4.1. There exist constants $K > 0$ and $q > 0$ such that

$$|S(t_k) - \hat{S}_{\Delta t}^k|_{L(H^\beta, H^\alpha)} \leq K \Delta t^q.$$  

[21] establishes the mean-square order of convergence of a method resting on properties of its one-step approximation only for stochastic ordinary differential equations. The most successful point in the proof of Milstein’s mean-square convergence theorem is the usage of conditional expectation. Properties of stochastic partial differential equations are different from those of stochastic ordinary differential equations. We have to separate operator term and integral term apart. Here we solve it by introducing a temporary process $\hat{\psi}(r)$, $t_n \leq r \leq t_{n+1}$, which is a continuous approximation of $\psi(r)$:

$$\hat{\psi}(r) = \hat{S}_{r-t_n} \psi(t_n) + i \int_{t_n}^r S(r - \rho) F(\hat{\psi}(\rho)) d\rho - i \int_{t_n}^r S(r - \rho) G(\hat{\psi}(\rho)) dW(\rho)$$

$$\hat{\psi}(x, 0) = \varphi(x). \quad (4.4)$$

If $r = t_{n+1}$, $\hat{\psi}(t_{n+1}) = \hat{S}_{\Delta t} \hat{\psi}(t_n) + \hat{Y}(\hat{\psi}(r))$.

Let $\phi$ be an $\mathcal{F}_{t_n}$-measurable random variable. $\tilde{\psi}_{t_n, \phi}(t)$ denotes the solution of the system (4.4) for $t_n \leq t \leq T$ satisfying the initial condition at $t = t_n$: $\tilde{\psi}(t_n) = \phi$.

Proposition 4.1. There is a representation

$$\tilde{\psi}_{t_n, \phi}(t_n) - \psi_{t_n, \phi}(t_{n+1}) = \hat{S}_{\Delta t}(\hat{\psi}(t_n) - \phi^n) + Z,$$

for which

$$\mathbb{E}|\tilde{\psi}_{t_n, \phi}(t_n) - \psi_{t_n, \phi}(t_{n+1})|^2 \leq \mathbb{E}|\tilde{\psi}(t_n) - \phi^n|^2 (1 + K \Delta t),$$

$$\mathbb{E}|Z|^2 \leq K \Delta t \mathbb{E}|\tilde{\psi}(t_n) - \phi^n|^2.$$
Proof. Since 
\[
\psi_{t_n,\psi(t_n)}(t_{n+1}) = \bar{S}_{\Delta t} \psi(t_n) + \Upsilon(\psi_{t_n,\psi(t_n)}(r)),
\]
\[
\psi_{t_n,\phi^n}(t_{n+1}) = \bar{S}_{\Delta t} \phi^n + \Upsilon(\psi_{t_n,\phi^n}(r)),
\]
we have
\[
\psi_{t_n,\psi(t_n)}(t_{n+1}) - \psi_{t_n,\phi^n}(t_{n+1}) = \bar{S}_{\Delta t}(\psi(t_n) - \phi^n) + Z.
\]
Then
\[
E|\psi_{t_n,\psi(t_n)}(t_{n+1}) - \psi_{t_n,\phi^n}(t_{n+1})|^2 = E|\bar{S}_{\Delta t}(\psi(t_n) - \phi^n)|^2 + 2E < \bar{S}_{\Delta t}(\psi(t_n) - \phi^n), Z >_{\alpha}
\]
\[
E|\bar{S}_{\Delta t}(\psi(t_n) - \phi^n)|^2 = E\int_{t_n}^{t_{n+1}} E|\psi_{t_n,\psi(t_n)}(r) - \psi_{t_n,\phi^n}(r)|^2 dr,
\]
where $E^\alpha(\cdot)$ denotes the conditional expectation with respect to $F_{t_n}$. From Gronwall’s Lemma, the lemma is proved.

We now propose the mean-square convergence theorem for numerical method (4.3).

**Theorem 4.1.** Suppose that the method (4.3) satisfies the following conditions
\[
\left| E(\Upsilon(\psi_{t_n,u}(r)) - \Gamma(u, \phi^{n+1}, \Delta t, \Delta W_n, T_{\Delta t})) \right|^2_{\alpha} \leq K \Delta t^{p+1}, \tag{4.5}
\]
\[
\left| E(\Upsilon(\psi_{t_n,u}(r)) - \Gamma(u, \phi^{n+1}, \Delta t, \Delta W_n, T_{\Delta t})) \right|^2_{\alpha} \leq K \Delta t^{p+\frac{1}{2}}. \tag{4.6}
\]
Then for $n = 1, 2, \cdots, N$, we have
\[
\left( E|\psi(t_n) - \phi^n|^2 \right)^{1/2} \leq K \Delta t^{\min\{q,p\}}.
\]
Since the numerical solution $\phi^n$ is $F_{t_n}$-measurable, the conditional version of the inequalities (4.5) and (4.6) are
\[
\left( E|E^n(\Upsilon(\psi_{t_n,\phi^n}(r)) - \Gamma(\phi^n, \phi^{n+1}, \Delta t, \Delta W_n, T_{\Delta t}))|^2_{\alpha} \right)^{1/2} \leq K \Delta t^{p+1}, \tag{4.7}
\]
\[
\left( E|E^n|\Upsilon(\psi_{t_n,\phi^n}) - \Gamma(\phi^n, \phi^{n+1}, \Delta t, \Delta W_n, T_{\Delta t}))|^2_{\alpha} \right)^{1/2} \leq K \Delta t^{p+\frac{1}{2}}. \tag{4.8}
\]
Before the proof of theorem 4.1, we firstly present a lemma which deals with the mean-square bound of numerical solution under the conditions (4.7)–(4.8).

**Lemma 4.1.** For all natural number $N$ and all $n = 0, 1, \cdots, N$, the following inequality holds:
\[
E|\phi^n|^2 \leq K(1 + E|\phi|^2) \leq K.
\]
Proof. From the definition of $\tilde{\psi}_{t_n, \phi^n}(t_{n+1})$

$$\tilde{\psi}_{t_n, \phi^n}(t_{n+1}) = \hat{S}\Delta t \phi^n + \Upsilon(\tilde{\psi}_{t_n, \phi^n}(r)),$$

one easily obtains

$$E|\tilde{\psi}_{t_n, \phi^n}(t_{n+1})|^2_{\alpha} \leq E|\phi^n|^2_{\alpha} + 2E\left[\int_{t_n}^{t_{n+1}} S(t_{n+1} - r) F(\tilde{\psi}_{t_n, \phi^n}(r)) dr \right]^2_{\alpha}$$

$$+ 2E\left[\int_{t_n}^{t_{n+1}} S(t_{n+1} - r) G(\tilde{\psi}_{t_n, \phi^n}(r)) dW(r) \right]^2_{\alpha}$$

$$+ 2E < \hat{S}\Delta t \phi^n, E^{t_n} \int_{t_n}^{t_{n+1}} S(t_{n+1} - r) G(\tilde{\psi}_{t_n, \phi^n}(r)) dW(r) >_{\alpha}$$

and functions $F$ and $G$ are global Lipchitz, we have

$$E|\tilde{\psi}_{t_n, \phi^n}(t_{n+1})|^2_{\alpha} \leq (1 + K\Delta t)E|\phi^n|^2_{\alpha} + K E \int_{t_n}^{t_{n+1}} |\tilde{\psi}_{t_n, \phi^n}(r)|^2_{\alpha} dr.$$

Then Gronwall’s inequality leads to

$$E|\tilde{\psi}_{t_n, \phi^n}(t_n)|^2_{\alpha} \leq (1 + K\Delta t)E|\phi^n|^2_{\alpha}.$$

Similarly, one has the estimations

$$E|\tilde{\psi}_{t_n, \phi^n}(t_{n+1}) - \hat{S}\Delta t \phi^n|^2_{\alpha} \leq K\Delta t (1 + E|\phi^n|^2_{\alpha}),$$

$$E|E^{t_n}(\tilde{\psi}_{t_n, \phi^n}(t_{n+1}) - \hat{S}\Delta t \phi^n)|^2_{\alpha} \leq K\Delta t^2 (1 + E|\phi^n|^2_{\alpha}).$$

Suppose that $E|\phi^n|^2_{\alpha} < \infty$, then

$$E|\phi^{n+1}|^2_{\alpha} \leq K E|\tilde{\psi}_{t_n, \phi^n}(t_{n+1})|^2_{\alpha} + K E|\phi^{n+1} - \tilde{\psi}_{t_n, \phi^n}(t_{n+1})|^2_{\alpha} < \infty.$$  \hspace{1cm} (4.9)

Since $E|\phi|^2_{\alpha} < \infty$, we have proved the existence of $E|\phi^n|^2_{\alpha}$, $\forall n \in \{0, 1, \ldots, N\}$. Thus we have

$$E|\phi^{n+1}|^2_{\alpha} \leq E|\phi^n|^2_{\alpha} + 2E|\Upsilon(\tilde{\psi}_{t_n, \phi^n}(r)) - \Gamma(\phi^n, \phi^{n+1}, \Delta t, \Delta W_n, T_{\Delta t})|^2_{\alpha}$$

$$+ E < \hat{S}\Delta t \phi^n, E^{t_n}(\Upsilon(\tilde{\psi}_{t_n, \phi^n}(r)) - \Gamma(\phi^n, \phi^{n+1}, \Delta t, \Delta W_n, T_{\Delta t})) >_{\alpha}$$

$$+ E < \hat{S}\Delta t \phi^n, E^{t_n}(\tilde{\psi}_{t_n, \phi^n}(t_{n+1}) - \hat{S}\Delta t \phi^n) >_{\alpha} + 2E|\tilde{\psi}_{t_n, \phi^n}(t_{n+1}) - \hat{S}\Delta t \phi^n|^2_{\alpha}$$

$$\leq (1 + K\Delta t)E|\phi^n|^2_{\alpha} + K\Delta t.$$
Hence
\[ E|\phi^n|_\alpha^2 \leq K(1 + E|\varphi|_\alpha^2) \leq K \]
is obtained. \hfill \Box

Now we are in the position of the proof of Theorem 4.1.

Proof. First we consider the mean-square error between \( \tilde{\psi}(t_{n+1}) \) and \( \phi^{n+1} \). Since
\[
\tilde{\psi}(t_{n+1}) - \phi^{n+1} = \tilde{\psi}_{t_n, \psi(t_n)}(t_{n+1}) - \phi^{n+1}
= \left( \tilde{\psi}_{t_n, \psi(t_n)}(t_{n+1}) - \tilde{\psi}_{t_n, \phi^n}(t_{n+1}) \right) + \left( \tilde{\psi}_{t_n, \phi^n}(t_{n+1}) - \phi^{n+1} \right)
= \left( \tilde{\psi}_{t_n, \psi(t_n)}(t_{n+1}) - \tilde{\psi}_{t_n, \phi^n}(t_{n+1}) \right) + \left( \Theta(\tilde{\psi}_{t_n, \phi^n}(r)) - \Gamma(\phi^n, \phi^{n+1}, \Delta t, \Delta W_n, T_{\Delta t}) \right),
\]
then
\[
E|\tilde{\psi}(t_{n+1}) - \phi^{n+1}|_\alpha^2
= E|\tilde{\psi}_{t_n, \psi(t_n)}(t_{n+1}) - \tilde{\psi}_{t_n, \phi^n}(t_{n+1})|_\alpha^2 + E|\Theta(\tilde{\psi}_{t_n, \phi^n}(r)) - \Gamma(\phi^n, \phi^{n+1}, \Delta t, \Delta W_n, T_{\Delta t})|_\alpha^2
+ 2E < \tilde{\psi}_{t_n, \psi(t_n)}(t_{n+1}) - \tilde{\psi}_{t_n, \phi^n}(t_{n+1}), \Theta(\tilde{\psi}_{t_n, \phi^n}(r)) - \Gamma(\phi^n, \phi^{n+1}, \Delta t, \Delta W_n, T_{\Delta t}) >_\alpha.
\]
From Lemma 4.1, we have
\[
E|\tilde{\psi}_{t_n, \psi(t_n)}(t_{n+1}) - \tilde{\psi}_{t_n, \phi^n}(t_{n+1})|_\alpha^2 \leq (1 + K\Delta t)E|\tilde{\psi}(t_n) - \phi^n|_\alpha^2,
\]
and from condition (4.8), we have
\[
E|\Theta(\tilde{\psi}_{t_n, \phi^n}(r)) - \Gamma(\phi^n, \phi^{n+1}, h, \Delta W_n, T_{\Delta t})|_\alpha^2 \leq K\Delta t^{2p+1}.
\]
We split \( \tilde{\psi}_{t_n, \psi(t_n)}(t_{n+1}) - \tilde{\psi}_{t_n, \phi^n}(t_{n+1}) \) as \( \tilde{S}_{\Delta t}(\tilde{\psi}(t_n) - \phi^n) + Z \) and use the trick of conditional expectation with respect to \( F_n \),
\[
E < \tilde{\psi}_{t_n, \psi(t_n)}(t_{n+1}) - \tilde{\psi}_{t_n, \phi^n}(t_{n+1}), \Theta(\tilde{\psi}_{t_n, \phi^n}(r)) - \Gamma(\phi^n, \phi^{n+1}, \Delta t, \Delta W_n, T_{\Delta t}) >_\alpha
\leq K\Delta tE|\tilde{\psi}(t_n) - \phi^n|_\alpha^2 + K\Delta t^{2p+1}.
\]
Therefore
\[
E|\tilde{\psi}(t_{n+1}) - \phi^{n+1}|_\alpha^2 \leq (1 + K\Delta t)E|\tilde{\psi}(t_n) - \phi^n|_\alpha^2 + K\Delta t^{2p+1}.
\]
Hence by Gronwall’s lemma, we obtain
\[
E|\tilde{\psi}(t_{n+1}) - \phi^{n+1}|_\alpha^2 \leq K\Delta t^{2p}. \tag{4.10}
\]
Next we consider the estimate between \( \psi(t_{n+1}) \) and \( \tilde{\psi}(t_{n+1}) \), since
\[
\psi(t_{n+1}) = S(t_{n+1})\varphi + i \sum_{k=0}^n \int_{t_k}^{t_{k+1}} S(t_{n+1} - r)F(\psi(r))dr - i \sum_{k=0}^n \int_{t_k}^{t_{k+1}} S(t_{n+1} - r)G(\psi(r))dW(r)
\]
From Hypothesis 4.3, then we have

\[ \hat{\psi}(t_{n+1}) = \hat{S}_{\Delta t} \tilde{\psi}(t_n) + i \int_{t_n}^{t_{n+1}} S(t_{n+1} - r) F(\tilde{\psi}(r)) dr - i \int_{t_n}^{t_{n+1}} S(t_{n+1} - r) G(\tilde{\psi}(r)) dW(r) \]

\[ = \ldots \ldots \]

\[ = \hat{S}_{\Delta t}^{n+1} \varphi + i \sum_{k=0}^{n} \int_{t_k}^{t_{k+1}} \hat{S}_{\Delta t}^{n-k} S(t_{k+1} - r) F(\tilde{\psi}(r)) dr - i \sum_{k=0}^{n} \int_{t_k}^{t_{k+1}} \hat{S}_{\Delta t}^{n-k} S(t_{k+1} - r) G(\tilde{\psi}(r)) dW(r) \]

then

\[ \psi(t_{n+1}) - \tilde{\psi}(t_{n+1}) = (S(t_{n+1}) - \hat{S}_{\Delta t}^{n+1}) \varphi \]

\[ + i \sum_{k=0}^{n} \int_{t_k}^{t_{k+1}} \left( S(t_{n+1} - r) F(\psi(r)) - \hat{S}_{\Delta t}^{n-k} S(t_{k+1} - r) F(\tilde{\psi}(r)) \right) dr \]

\[ - i \sum_{k=0}^{n} \int_{t_k}^{t_{k+1}} \left( S(t_{n+1} - r) G(\psi(r)) - \hat{S}_{\Delta t}^{n-k} S(t_{k+1} - r) G(\tilde{\psi}(r)) \right) dW(r) \]

\[ := T_1 + T_2 + T_3. \]

From Hypothesis 4.3, then we have

\[ E|\psi(t_{n+1}) - \tilde{\psi}(t_{n+1})|^2_\alpha \leq K E|T_1|^2_\alpha + E|T_2|^2_\alpha + E|T_3|^2_\alpha \]

\[ \leq K \Delta t^{2q} + K \int_0^{t_{n+1}} E|\psi(r) - \tilde{\psi}(r)|^2_\alpha dr. \]

Hence by Gronwall’s lemma

\[ E|\psi(t_{n+1}) - \tilde{\psi}(t_{n+1})|^2_\alpha \leq K \Delta t^{2q}. \quad (4.11) \]

At last, we estimate the mean-square error between \( \psi(t_{n+1}) \) and \( \phi^{n+1} \)

\[ E|\psi(t_{n+1}) - \phi^{n+1}|^2_\alpha \leq 2E|\psi(t_{n+1}) - \tilde{\psi}(t_{n+1})|^2_\alpha + 2E|\tilde{\psi}(t_{n+1}) - \phi^{n+1}|^2_\alpha \]

\[ \leq K \Delta t^{2q} + K \Delta t^{2p} \]

\[ \leq K \Delta t^{\min(2q,2p)}. \]

The proof of the convergence theorem is completed. \( \square \)

**Remark 4.1.** Consider the stochastic Schrödinger equation in Stratonovich sense

\[ id\psi + (A\psi + F(\psi)) dt = G(\psi) \circ dW. \quad (4.12) \]

It is well known that this equation is equivalent to the following equation in the sense of Itô

\[ id\psi + (A\psi + \tilde{F}(\psi)) dt = G(\psi) dW \]

where \( \mathcal{R}_\psi = \sum_{i \in \ell} (Q^i e_i(x))^2 \) and \( \tilde{F}(\psi) = F(\psi) + \frac{i}{2} G'(\psi) G(\psi) \mathcal{R}_\psi. \) We assume that the coefficients \( \tilde{F} \) and \( G \) of the equation satisfy the hypothesis 4.1 and 4.2, then it is not difficult to understand that Theorem 4.1 remains true for equation understood in the sense of Stratonovich.
4.1 Mean-square convergence order of the midpoint scheme

Here we use the convergence theorem 4.1 to obtain the mean-square convergence order of the symplectic semi-discrete scheme (3.10). For midpoint scheme (3.8), we have \( \hat{S}_{\Delta t} = (I - \frac{1}{2} \Delta t A)^{-1}(I + \frac{1}{2} \Delta t A) \) and \( T_{\Delta t} = (I - \frac{1}{2} \Delta t A)^{-1} \). As in [2], we set \( \alpha = s, \beta = s + 3 \) with \( s \in \mathbb{R} \). Obviously, \( |\hat{S}_{\Delta t}| \leq 1 \) and Hypothesis 4.3 is fulfilled with parameter \( q = 1 \).

From [24], we know that

\[
\Upsilon(\tilde{\psi}_{n+1}, u) = \int_{t_n}^{t_{n+1}} S(t_{n+1} - r) F(r, \tilde{\psi}_{t_n, u}(r)) dr - i \varepsilon \int_{t_n}^{t_{n+1}} S(t_{n+1} - r) \tilde{\psi}_{t_n, u}(r) dW(r)
\]

and from (3.10) we have

\[
\Gamma(u, \phi^{n+1}, \Delta t, \Delta W_n, T_{\Delta t}) = i \Delta t T_{\Delta t} F \left( t_{n+\frac{1}{2}}, \frac{1}{2}(u + \phi^{n+1}) \right) - i \varepsilon T_{\Delta t} u \Delta W_n - \frac{i \varepsilon}{2} T_{\Delta t} (\phi^{n+1} - u) \Delta W_n.
\]

Then

\[
\mathbb{E} \left( \Upsilon(\tilde{\psi}_{t_n, u}(r)) - \Gamma(u, \phi^{n+1}, \Delta t, \Delta W_n, T_{\Delta t}) \right) = \mathbb{E} \left( i \int_{t_n}^{t_{n+1}} S(t_{n+1} - r) F(r, \tilde{\psi}_{t_n, u}(r)) dr - i \varepsilon T_{\Delta t} F \left( t_{n+\frac{1}{2}}, \frac{1}{2}(u + \phi^{n+1}) \right) \right)
\]

\[
+ \mathbb{E} \left( \frac{i \varepsilon}{2} T_{\Delta t} (\phi^{n+1} - u) \Delta W_n - \frac{\varepsilon^2}{2} \int_{t_n}^{t_{n+1}} S(t_{n+1} - r) \tilde{\psi}_{t_n, u}(r) dW(r) \right)
\]

\[
:= \mathcal{A} + \mathcal{B}.
\]

We split \( \mathcal{A} \) further

\[
\mathcal{A} = \mathbb{E} \int_{t_n}^{t_{n+1}} (S(t_{n+1} - r) - T_{\Delta t}) F(r, \tilde{\psi}_{t_n, u}(r)) dr
\]

\[
+ \mathbb{E} \int_{t_n}^{t_{n+1}} T_{\Delta t} F(r, \tilde{\psi}_{t_n, u}(r)) - F(t_{n+\frac{1}{2}}, u) dr
\]

\[
- i \Delta t T_{\Delta t} \mathbb{E} \left( F(t_{n+\frac{1}{2}}, \frac{1}{2}(u + \phi^{n+1})) - F(t_{n+\frac{1}{2}}, u) \right)
\]

\[
:= \mathcal{A}^1 + \mathcal{A}^2 + \mathcal{A}^3. \tag{4.13}
\]

Suppose that \( F(t, u) \) is globally Lipschitz function with respect to \( t \) and \( u \), i.e.,

\[
|F(t, u) - F(r, v)|_{s+3} \leq K(|t - r| + |u - v|_s).
\]

One can obtain the estimate of \( \mathcal{A}^1 \) easily

\[
|\mathcal{A}^1|_s \leq K \Delta t^2.
\]
In addition, we assume that the derivatives $\frac{\partial F}{\partial u}(t, u)$ and $\frac{\partial^2 F}{\partial u^2}(t, u)$ are uniformly bounded. We write

$$F(r, \tilde{\psi}_{t, n, u}(r)) - F(t_{n+\frac{1}{2}}, u) = \left( F(r, \tilde{\psi}_{t, n, u}(r)) - F(r, u) \right) + \left( F(r, u) - F(t_{n+\frac{1}{2}}, u) \right) = \frac{\partial F}{\partial u}(r, u)(\tilde{\psi}_{t, n, u}(r) - r) + \rho_1 + \rho_2; \tag{4.14}$$

where

$$|\rho_1| \leq K|\tilde{\psi}_{t, n, u}(r) - r|^2$$

and

$$|\rho_2| \leq K \Delta t.$$

It is not difficult to obtain the estimate

$$\int_{t_n}^{t_{n+1}} |E(\tilde{\psi}_{t, n, u}(r) - r)|_s dr \leq K \Delta t^2.$$

The above implies that

$$|A^2|_s \leq K \Delta t^2.$$

Similarly as the estimate of $A^2$, one has

$$|A^3|_s \leq K \Delta t^2.$$

The estimate of $B$ is more technical. First inserting the expression of $\phi^{n+1} - u$ into $B$, we have

$$B = E\left[ \frac{i \varepsilon}{2} T_{\Delta t} \left( (\hat{S}_{\Delta t} - I)u + i \Delta t T_{\Delta t} F(t_{n+\frac{1}{2}}, \frac{1}{2}(u + \phi^{n+1})) - i \varepsilon T_{\Delta t} u \Delta W_n \right) - \frac{i \varepsilon}{2} T_{\Delta t} T_{\Delta t} F(t_{n+\frac{1}{2}}, \frac{1}{2}(u + \phi^{n+1})) \Delta W_n - \frac{\varepsilon^2}{4} \int_{t_n}^{t_{n+1}} S(t_{n+1} - r) \tilde{\psi}_{t, n, u}(r) \mathbb{N}_Q dr \right]$$

$$= - \frac{\varepsilon}{2} \Delta t T_{\Delta t}^2 E \left( F(t_{n+\frac{1}{2}}, \frac{1}{2}(u + \phi^{n+1})) \Delta W_n \right) + \frac{\varepsilon^2}{4} T_{\Delta t}^2 E \left( (\phi^{n+1} - u)(\Delta W_n)^2 \right)$$

$$+ \frac{\varepsilon^2}{2} T_{\Delta t}^2 u \mathbb{N}_Q \Delta t - \int_{t_n}^{t_{n+1}} E S(t_{n+1} - r) \tilde{\psi}_{t, n, u}(r) \mathbb{N}_Q dr \right] := B^1 + B^2 + B^3. \tag{4.15}$$

Using the Lipschitz property of $F$, the estimate of $B^1$ is as follows

$$|B^1|_s = \left| - \frac{\varepsilon}{2} \Delta t T_{\Delta t}^2 E \left( (F(t_{n+\frac{1}{2}}, \frac{1}{2}(u + \phi^{n+1})) - F(t_{n+\frac{1}{2}}, u)) \Delta W_n \right) \right|^2_s \leq K \Delta t^2.$$
Inserting the expression of $\phi^{n+1} - u$ into the term $B^2$, one can obtain that
\[
(E |B^2|_s^2)^{\frac{1}{2}} \leq K \Delta t^2.
\]

We split $B^3$ further
\[
B^3 = \frac{\varepsilon^2}{2} E \int_{t_n}^{t_{n+1}} (T_\Delta t - S(t_{n+1} - r)) \tilde{\psi}_{t_n,u}(r) dr + \frac{\varepsilon^2}{2} \int_{t_n}^{t_{n+1}} (T_\Delta t^2 - T_\Delta t S(r - t_n)) u \mathbb{N}_Q dr
- \frac{i \varepsilon^2}{2} E \int_{t_n}^{t_{n+1}} \int_{t_n}^{r} S(r - \rho) \tilde{F}(\tilde{\psi}_{t_n,u}(\rho)) d\rho \mathbb{N}_Q dr,
\]
where
\[
\tilde{F}(\psi) = F(\psi) + \frac{i \varepsilon^2}{2} \tilde{\psi}_{t_n,u}(\rho) \mathbb{N}_Q.
\]

Hence, we have the estimate of $B^3$
\[
(E |B^3|_s^2)^{\frac{1}{2}} \leq K \Delta t^2.
\]

Therefore, we have
\[
\left| E(Y(\tilde{\psi}_{t_n,u}(r)) - \Gamma(u, \phi^{n+1}, \Delta t, \Delta W_n, T_\Delta t)) \right|_s \leq K \Delta t^2.
\]

Next, let’s compute the value of $E|Y(\tilde{\psi}_{t_n,u}(r)) - \Gamma(u, \phi^{n+1}, \Delta t, \Delta W_n, T_\Delta t)|_s^2$.
\[
Y(\tilde{\psi}_{t_n,u}(r)) - \Gamma(u, \phi^{n+1}, \Delta t, \Delta W_n, T_\Delta t)
= i \int_{t_n}^{t_{n+1}} \left( S(t_{n+1} - r) F(r, \tilde{\psi}_{t_n,u}(r)) - T_\Delta t F(t_n^{1/2}, \frac{1}{2}(u + \phi^{n+1})) \right) dr
- i \varepsilon \int_{t_n}^{t_{n+1}} (S(t_{n+1} - r) - T_\Delta t) \tilde{\psi}_{t_n,u}(r) dW(r)
- \left[ i \varepsilon \int_{t_n}^{t_{n+1}} T_\Delta t (\tilde{\psi}_{t_n,u}(r) - u) dW(r) + \frac{\varepsilon^2}{2} \int_{t_n}^{t_{n+1}} S(t_{n+1} - r) \tilde{\psi}_{t_n,u}(r) \mathbb{N}_Q dr
- \frac{i \varepsilon}{2} T_\Delta t (\phi^{n+1} - u) \Delta W_n \right]
:= \mathcal{L} + \mathcal{M} - \mathcal{N}.
\]

It’s easy to obtain the estimates of $\mathcal{L}$ and $\mathcal{M}$,
\[
E|\mathcal{L} + \mathcal{M}|_s^2 \leq K \Delta t^3.
\]
Inserting the expression of $\tilde{\psi}(r) - u$ and $\phi^{n+1} - u$ into $\mathcal{N}$ and splitting $\mathcal{N}$ further

$$\mathcal{N} = \varepsilon \int_{t_n}^{t_{n+1}} T_{\Delta t}\left((\hat{S}(r - t_n) - I)u + i \int_{t_n}^{r} S(r - \rho)\tilde{F}(\tilde{\psi}_{t_n,u}(\rho))d\rho\right)dW(r)$$

$$- \frac{i\varepsilon}{2} T_{\Delta t}\left((S_{\Delta t} - I)u + i\Delta t T_{\Delta t}F(t_{n+1}, \frac{1}{2}(u + \phi^{n+1}))\right)\Delta W_n$$

$$+ \varepsilon^2 \int_{t_n}^{t_{n+1}} \int_{t_n}^{r}(T_{\Delta t}S(r - \rho)\tilde{\psi}_{t_n,u}(\rho) - T_{\Delta t}^2 u)dW(\rho)dW(r)$$

$$+ \frac{\varepsilon^2}{4} T_{\Delta t}^2(\phi^{n+1} - u)(\Delta W_n)^2 + \frac{\varepsilon^2}{2} \int_{t_n}^{t_{n+1}} (S(t_{n+1} - r)\tilde{\psi}_{t_n,u}(r) - T_{\Delta t}^2 u)\mathbb{Q} dr,$$

we have that

$$\mathbb{E}|\mathcal{N}|_2^2 \leq K\Delta t^3.$$ 

That is

$$\left(\mathbb{E}|\mathbb{Y}(\tilde{\psi}_{t_n,u}(r)) - \Gamma(u, \phi^{n+1},\Delta t, \Delta W_n, T_{\Delta t})|^2\right)^{\frac{1}{2}} \leq K\Delta t^2.$$ 

Therefore the mean-square order of the method is $p = 1$ according to Theorem 4.1.

**Remark 4.2.** For stochastic Schrödinger equation in Stratonovich sense, the mean-square convergence order of the semi-discrete midpoint scheme is 1 under appropriate assumptions. It seems like the same as the case of stochastic ordinary differential equations. However, the convergence order here depends on the values of $p$ and $q$, where $p$ and $q$ are from estimations of the one-step deviation between exact solution and numerical solution. As we take parameters $\alpha = s$ and $\beta = s + 3$, which require more regularity conditions on the solution $\psi$, the estimation of operators is $|S(t_k) - \hat{S}_{\Delta t}^k|_{L(H^\beta, H^\alpha)} \leq K\Delta t$ with $p = 1$. Together with $q = 1$, we have that the convergence order of the semi-discrete midpoint scheme is 1. If we put less regularity on the solution, which means $p < 1$, then the convergence order is less than 1. For the general stochastic Runge-Kutta methods in temporal direction, the mean-square convergence order is an open problem.

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