ASYMPTOTIC ANALYSIS OF TIME-FRACTIONAL QUANTUM DIFFUSION

PETER D. HISLOP AND ÉRIC SOCCORSI

ABSTRACT. We study the large-time asymptotics of the mean-square displacement for the time-fractional Schrödinger equation in $\mathbb{R}^d$. We define the time-fractional derivative by the Caputo derivative. We consider the initial-value problem for the free evolution of wave packets in $\mathbb{R}^d$ governed by the time-fractional Schrödinger equation $i^\beta \partial_t^\alpha u = -\Delta u,\ u(t=0) = u_0$, parameterized by two indices $\alpha, \beta \in (0,1]$. We show distinctly different long-time evolution of the mean square displacement according to the relation between α and β. In particular, asymptotically ballistic motion occurs only for $\alpha = \beta$.

1. Introduction and statement of the problem

The Schrödinger equation with fractional spatial derivatives has been the object of many studies. It is proposed as a model for anomalous quantum transport. In this article, and companion articles [6], we study the effect of replacing the time derivative in the Schrödinger equation by a fractional time derivative. We study the behavior of the mean-square displacement (MSD) of a wave packet evolving according to the time-fractional Schrödinger equation (TFSE):

$$i^\beta \partial_t^\alpha u = -\Delta u,\ u(t=0) = u_0, \tag{1.1}$$

parameterized by two indices $\alpha, \beta \in (0,1]$. We show that the MSD $D_2(u_0,t)$ (see (3.1)) exhibits different asymptotic behavior depending on these parameters. These models generalize the time-fractional Schrödinger equations (TFSE) introduced by Naber [16], with $\alpha = \beta \in (0,1)$, and by Narahari Achar, Yale, and Hanneken [1], with $\beta = 1$ and $\alpha \in (0,1)$. For our two-parameter generalization of these models, we compute the asymptotics in time of the MSD.

In particular, we find that the MSD exhibits distinctly different behavior in each of three parameter regimes. Asymptotic ballistic evolution for which $D_2(u_0,t) \sim t^2$ occurs only when $\alpha = \beta$. A summary of the main results is as follows. We refer to Theorem 3.1 and section 3 for the details. Let us consider $0 < \beta \leq 1$ fixed, and take $0 < \alpha \leq 1$. For the first two regimes, we have

$$0 < \alpha < \beta \leq 1: \quad D_2(u_0,t) = C_\alpha(u_0) t^{-2\alpha} + \mathcal{O}(t^{-3\alpha}), \tag{1.2}$$

$$0 < \alpha = \beta \leq 1: \qquad D_2(u_0,t) = C_\alpha(u_0) t^2 + \mathcal{O}(t), \tag{1.3}$$

where $C_\alpha(u_0) > 0$ is a finite, positive constant whose value may change line-to-line. In particular, result (1.2) shows how the MSD varies for the TFSE with $\beta = 1$ as α varies in $(0,1)$. For this regime, the MSD tends to zero as $t \to \infty$. On the other hand, (1.3) shows asymptotic ballistic behavior of the MSD when the parameters are equal $\alpha = \beta$. The third regime is characterized by a MSD satisfying upper and lower bounds:

$$0 < \beta < \alpha \leq 1: \tag{1.4}$$

$$e^{2t\cos\left(\frac{\pi\beta}{2\alpha}\right)\Lambda_-^{\frac{2}{\alpha}}} \left(c_\alpha(u_0) + \mathcal{O}(t^{-1})\right) \ \leq\ D_2(u_0,t) \ \leq e^{2t\cos\left(\frac{\pi\beta}{2\alpha}\right)\Lambda_+^{\frac{2}{\alpha}}} \left(C_\alpha(u_0) + \mathcal{O}(t^{-1})\right),$$

where the finite, positive, constants $\Lambda_\pm \geq 0$ are determined by the initial condition u_0, see Theorem 3.1 and (3.17). In particular, u_0 may be chosen so that $\Lambda_- > 0$, so that the MSD exhibits exponential growth. We remark that Naber [16] stated that he considered the model with $\alpha = \beta$ because the solutions to the TFSE with these parameters behave similarly to the solutions of the Schrödinger equation. Our result that the MSD is asymptotically ballistic for $\alpha = \beta$ supports this statement.

In our companion article, [6], we studied the effect of replacing $i\partial_t$ by by $i^\beta \partial_t^\alpha$, in the Schrödinger equation, on the time evolution of the edge current of a half-plane quantum Hall model. We proved the existence of a similar transition in the long-time asymptotic behavior of the edge current depending on the relation between α and β.

We mention several works on the Schrödinger equation with a time fractional derivative, such as [2, 3, 5, 4, 8, 9, 10, 11, 13, 14, 15, 18]. We refer to [6, section 1] for a description of their contributions and the relation to our work. We have found the books by Kilbas, Srivastava, and Trujillo [12], and by Podlubny [17], to be useful references.

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2. Existence and well-posedness for the TFSE

Let $H_0 := -\Delta$ be the Laplace operator in $\mathbb{R}^d$, $d \geq 1$, with domain $\mathrm{D}(H_0) := H^2(\mathbb{R}^d)$, where $H^j(\mathbb{R}^d)$ denotes the Sobolev space of order $j \in \mathbb{N}$. The operator H_0 is self-adjoint on this domain in $L^2(\mathbb{R}^d)$. We set $\mathbb{R}_+ := (0, \infty)$. Given $\alpha \in (0, 1]$, and $\beta \in (0, 1]$, we consider the generalized time-fractional Schrödinger equation (TFSE)

$$-i^\beta \partial_t^\alpha u(x,t) + H_0 u(x,t) = 0, \ (x,t) \in \mathbb{R}^d \times \mathbb{R}_+, \tag{2.1}$$

with initial state u_0, in an appropriate subspace of $L^2(\mathbb{R}^d)$, see (2.5), so that

$$u(x,0) = u_0(x), \quad x \in \mathbb{R}^d. \tag{2.2}$$

The fractional time derivative ∂_t^α, for $\alpha \in (0,1)$, is the Caputo fractional derivative of order α defined by

$$\partial_t^\alpha u(t) := \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{u'(s)}{(t-s)^\alpha} \mathrm{d}s, \ u \in W^{1,1}_{\mathrm{loc}}(\mathbb{R}_+). \tag{2.3}$$

We note that $\partial_t^\alpha u \to \partial_t u$, as $\alpha \to 1$, if, for example, $u \in C^2(\mathbb{R})$. This follows from the formula (2.3) by an integration by parts.

We define a solution to the system (2.1)-(2.2) as any function

$$u \in L^1_{\mathrm{loc}}(\mathbb{R}_+, \mathrm{D}(H_0)) \cap W^{1,1}_{\mathrm{loc}}(\mathbb{R}_+, L^2(\mathbb{R}^d)),$$

satisfying the two following conditions simultaneously:

(1) $-i^\beta \partial_t^\alpha u(x,t) + H_0 u(x,t) = 0$ for a.e. $(x,t) \in \mathbb{R}^d \times \mathbb{R}_+$,

(2) $\lim_{t \downarrow 0} \|u(\cdot,t) - u_0\| = 0$,

where $\|\cdot\|$ denotes the usual norm in $L^2(\mathbb{R}^d)$.

2.1. **Existence and uniqueness result.** Prior to stating the existence and uniqueness result for the solution to (2.1)-(2.2), we introduce some notation. First, we define the Mittag-Leffler function as

$$E_{\alpha,\gamma}(z) := \sum_{n=0}^\infty \frac{z^n}{\Gamma(\alpha n + \gamma)}, \ \alpha \in (0,1), \ \gamma \in \mathbb{R}, \ z \in \mathbb{C}, \tag{2.4}$$

where Γ is the usual Gamma function. We refer to [12] and [17] for comprehensive discussions of these functions.

We write $\mathcal{F}$ for the Fourier transform in $\mathbb{R}^d$, i.e.,

$$\mathcal{F}u(\xi) = \hat{u}(\xi) := (2\pi)^{-d/2} \int_{\mathbb{R}^d} e^{-ix\cdot\xi} u(x) \mathrm{d}x, \ u \in L^2(\mathbb{R}^d), \ \xi \in \mathbb{R}^d,$$

where $x \cdot \xi$ is the Euclidean scalar product of $x, \xi \in \mathbb{R}^d$. We recall that the Fourier transform operator $\mathcal{F}$ is a unitary operator on $L^2(\mathbb{R}^d)$. Its inverse satisfies $\mathcal{F}^{-1} = \mathcal{F}^*$, where $\mathcal{F}^*$ is the adjoint of $\mathcal{F}$. We recall that for any $s \geq 0$, H_0^s is the operator unitarily equivalent to $\hat{H}_0^s := \mathcal{F} H_0^s \mathcal{F}^*$, where $\hat{H}_0^s$ is the operator of multiplication by $|\xi|^{2s}$. We note that H_0^0 is the identity operator. Consequently, the domain $D(H_0^s) = \{f \in L^2(\mathbb{R}^d) \mid |\xi|^{2s} \hat{f}(\xi) \in L^2(\mathbb{R}^d)\}$.

We denote by $\mathcal{C}_0(\mathbb{R}^d)$ the space of compactly supported continuous functions in $\mathbb{R}^d$. Let us introduce the set

$$\mathcal{U}_{\alpha,\beta} := \begin{cases} \mathrm{D}(H_0) & \text{if } \beta > \alpha \\ \mathrm{D}(H_0^{\frac{1}{\alpha}}) & \text{if } \beta = \alpha \\ \mathcal{F}^*\mathcal{C}_0(\mathbb{R}^d) & \text{if } \beta < \alpha, \end{cases} . \tag{2.5}$$

Since $\mathcal{F}^*\mathcal{C}_0(\mathbb{R}^d) \subset \mathrm{D}(H_0^{\frac{1}{\alpha}})$, we notice that $\mathcal{U}_{\alpha,\beta} \subset \mathrm{D}(H_0^{\frac{1}{\alpha}})$ when $\beta \le \alpha$. As above, we denote by $\|\cdot\|$ the usual norm in $L^2(\mathbb{R}^d)$, and we set $\|v\|_{\mathrm{D}(H_0^\gamma)} := \left(\|v\|^2 + \|H_0^\gamma v\|^2\right)^{1/2}$, for all $v \in \mathrm{D}(H_0^\gamma)$, $\gamma \ge 1$. We equip $\mathcal{U}_{\alpha,\beta}$ with the norm:

$$\|u\|_{\mathcal{U}_{\alpha,\beta}} := \begin{cases} \|u\|_{\mathrm{D}(H_0)} & \text{if } \beta > \alpha \\ \|u\|_{\mathrm{D}(H_0^{\frac{1}{\alpha}})} & \text{if } \beta \le \alpha. \end{cases}$$

Then, the existence and uniqueness result for the system (2.1)-(2.2) can be stated as follows.

Proposition 2.1. *Pick $u_0 \in \mathcal{U}_{\alpha,\beta}$. Then, for all $T \in \mathbb{R}_+$, the system* (2.1)-(2.2) *admits a unique solution $u \in \mathcal{C}([0,T], \mathrm{D}(H_0)) \cap W^{1,1}_{\mathrm{loc}}(0,T; L^2(\mathbb{R}^d))$, which is expressed by*

$$u(x,t) = \mathcal{F}^*\left(E_{\alpha,1}((-i)^\beta |\cdot|^2 t^\alpha)\hat{u}_0\right)(x),\ (x,t) \in \mathbb{R}^d \times \mathbb{R}_+.$$

There exists a unique positive constant C, depending only on α, β and d, such that for $\beta \ge \alpha$,

$$\|u\|_{\mathcal{C}([0,T],D(H_0))} + \|u\|_{W^{1,1}(0,T;L^2(\mathbb{R}^d))} \le C(1+T)\|u_0\|_{\mathcal{U}_{\alpha,\beta}}, \tag{2.6}$$

whereas for $\beta < \alpha$,

$$\|u\|_{\mathcal{C}([0,T],\mathrm{D}(H_0))} + \|u\|_{W^{1,1}(0,T;L^2(\mathbb{R}^d))} \le C(1+T)\mathrm{e}^{\cos\left(\frac{\pi\beta}{2\alpha}\right)\Lambda_+^{\frac{2}{\alpha}}T}\|u_0\|_{\mathcal{U}_{\alpha,\beta}}, \tag{2.7}$$

where $\Lambda_+ := \max\{|\xi|,\ \xi \in \mathrm{supp}(\hat{u}_0)\}$.

2.2. **Proof of Proposition 2.1.** We start by establishing the two following technical results.

Lemma 2.2. *Let $t \in \mathbb{R}_+$, let $\xi \in \mathbb{R}^d \setminus \{0\}$ and put $\kappa := (-i)^\beta |\xi|^2 t^\alpha$. Then, for all $\gamma \in \mathbb{R}$, there exists a constant $C > 0$, depending only on α and γ such that we have*

$$|E_{\alpha,\gamma}(\kappa)| \le \frac{C}{1+|\kappa|},\ \alpha < \beta, \tag{2.8}$$

and

$$E_{\alpha,\gamma}(\kappa) \le C\left((1+|\kappa|)^{\frac{1-\gamma}{\alpha}} \mathrm{e}^{\mathrm{Re}\left(\kappa^{\frac{1}{\alpha}}\right)} + \frac{1}{1+|\kappa|}\right),\ \alpha \ge \beta. \tag{2.9}$$

Proof. When $\alpha < \beta$, we pick $\mu \in (\pi\alpha/2, \min(\pi\alpha, \pi\beta/2))$ and apply [17, Theorem 1.6]. Since $|\arg(\kappa)| \in [\mu, \pi]$, we get (2.8) directly from [17, Eq. (1.148)]. Similarly, for $\alpha \ge \beta$, we apply [17, Theorem 1.5] with $\mu \in (\pi\alpha/2, \pi\alpha)$. As $|\arg(\kappa)| \le \mu$, we see that [17, Eq. (1.147)] yields (2.9). □

Lemma 2.3. *We have $\mathrm{D}(H_0^{\frac{1}{\alpha}}) \subset \mathrm{D}(H_0)$ and the embedding is continuous. More precisely, there exists a constant, $C_\alpha > 0$, depending only on α, such that*

$$\forall u \in \mathrm{D}(H_0^{\frac{1}{\alpha}}),\ \|u\|_{\mathrm{D}(H_0)} \le C_\alpha \|u\|_{\mathrm{D}(H_0^{\frac{1}{\alpha}})}.$$

Proof. Let $v \in \mathrm{D}(H_0^{\frac{1}{\alpha}})$. We have $\hat{v}$ in $L^2(\mathbb{R}^d)$ and $\xi \mapsto |\xi|^{\frac{2}{\alpha}}\hat{v}(\xi) \in L^2(\mathbb{R}^d)$. Thus, $\xi \mapsto |\xi|^2|\hat{v}(\xi)|^\alpha \in L^{\frac{2}{\alpha}}(\mathbb{R}^d)$ and $|\hat{v}|^{1-\alpha} \in L^{\frac{2}{1-\alpha}}(\mathbb{R}^d)$. Since

$$\frac{1}{\frac{2}{\alpha}} + \frac{1}{\frac{2}{1-\alpha}} = \frac{\alpha}{2} + \frac{1-\alpha}{2} = \frac{1}{2}$$

and

$$|\xi|^2|\hat{v}(\xi)| = |\xi|^2|\hat{v}(\xi)|^\alpha |v(\xi)|^{1-\alpha},\ \xi \in \mathbb{R}^d,$$

we have $\xi \mapsto |\xi|^2\hat{v}(\xi) \in L^2(\mathbb{R}^d)$ and

$$\left\||\xi|^2\hat{v}(\xi)\right\| \le \left\||\xi|^2|\hat{v}(\xi)|^\alpha\right\|_{L^{\frac{2}{\alpha}}(\mathbb{R}^d)} \left\||\hat{v}(\xi)|^{1-\alpha}\right\|_{L^{\frac{2}{1-\alpha}}(\mathbb{R}^d)}, \tag{2.10}$$

by Hölder's inequality. Recalling that $\mathcal{F}H_0\mathcal{F}^* = \hat{H}_0$, the multiplication operator by $|\xi|^2$, inequality (2.10) can be equivalently rewritten as

$$\left\|\hat{H}_0\hat{v}\right\| \leq \left\|\hat{H}_0^{\frac{1}{\alpha}}\hat{v}\right\|^{\alpha}\|\hat{v}\|^{1-\alpha}.$$

Applying Young's inequality, we obtain

$$\left\|\hat{H}_0\hat{v}\right\| \leq \alpha\left\|\hat{H}_0^{\frac{1}{\alpha}}\hat{v}\right\| + (1-\alpha)\|\hat{v}\|,$$

which proves the desired result. □

Armed with these two lemmas, we are now in position to prove Proposition 2.1.

Proof. Let u be a solution to (2.1)-(2.2) in the sense of Section 2. We apply the Fourier transform $\mathcal{F}$ to both sides of the equations (2.1) and (2.2). Since $\mathcal{F}H_0\mathcal{F}^* = \hat{H}_0$, the multiplication operator by $|\xi|^2$ on $L^2(\mathbb{R}^d)$, we obtain

$$\begin{cases} -i^{\beta}\partial_t^{\alpha}\hat{u}(\xi,t) + |\xi|^2\hat{u}(\xi,t) = 0, & (\xi,t) \in \mathbb{R}^d \times \mathbb{R}_+ \\ \hat{u}(\xi,0) = \hat{u}_0, & \xi \in \mathbb{R}^d, \end{cases} \tag{2.11}$$

where $\hat{u}(\xi,t) := (\mathcal{F}u(\cdot,t))(\xi)$.

For each $\xi \in \mathbb{R}^d$, the system (2.11) admits a unique solution

$$\hat{u}(\xi,t) = E_{\alpha,1}((-i)^{\beta}|\xi|^2 t^{\alpha})\hat{u}_0(\xi),\ (\xi,t) \in \mathbb{R}^d \times \mathbb{R}_+, \tag{2.12}$$

according to [12, Theorem 4.3]. We now analyze the three cases in the proposition.
First case: $\alpha < \beta$. We have

$$\left|\hat{H}_0^{\,j}\hat{u}(\xi,t)\right| \leq C\left|(\hat{H}_0^{\,j}\hat{u}_0)(\xi)\right|,\ j=0,1,\ (\xi,t) \in \mathbb{R}^d \times \mathbb{R}_+,$$

from (2.8) and (2.12), whence

$$\|\hat{u}(\cdot,t)\|_{\mathrm{D}(\hat{H}_0)} \leq C\|\hat{u}_0\|_{\mathrm{D}(\hat{H}_0)},\ t \in \mathbb{R}_+, \tag{2.13}$$

and

$$\|\hat{u}\|_{L^1(0,T;L^2(\mathbb{R}^d))} \leq CT\|\hat{u}_0\|. \tag{2.14}$$

Further, since $\frac{\mathrm{d}}{\mathrm{d}z}E_{\alpha,1}(z) = \alpha^{-1}E_{\alpha,\alpha}(z)$ for all $z \in \mathbb{C}$, which follows from (2.4) by direct computation, we deduce from (2.12) that

$$\partial_t\hat{u}(\xi,t) = (-i)^{\beta}|\xi|^2 t^{\alpha-1}E_{\alpha,\alpha}((-i)^{\beta}|\xi|^2 t^{\alpha})\hat{u}_0(\xi),\ (\xi,t) \in \mathbb{R}^d \times \mathbb{R}_+. \tag{2.15}$$

It follows from this and (2.8) that

$$|\partial_t\hat{u}(\xi,t)| \leq C\frac{|\xi|^2 t^{\alpha-1}}{1+|\xi|^2 t^{\alpha}}|\hat{u}_0(\xi)|,\ (\xi,t) \in \mathbb{R}^d \times \mathbb{R}_+.$$

Thus, integrating with respect to t over $(0,T)$, we get that

$$\begin{aligned} \|\partial_t\hat{u}(\xi)\|_{L^1(0,T)} &\leq C\ln\left(1+|\xi|^2T^{\alpha}\right)|\hat{u}_0(\xi)| \\ &\leq CT^{\alpha}\left|(\hat{H}_0\hat{u}_0)(\xi)\right|,\ \xi \in \mathbb{R}^d, \end{aligned}$$

where we used that $\ln(1+s) \leq s$ for all $s \geq 0$, and we substituted C for $\alpha^{-1}C$. Therefore, we have

$$\|\partial_t\hat{u}\|_{L^1(0,T;L^2(\mathbb{R}^d))} \leq CT^{\alpha}\left\|\hat{H}_0\hat{u}_0\right\|,$$

and (2.6) follows readily from this and (2.13)-(2.14).

Second case: $\alpha = \beta$. This time, it follows from (2.9) and (2.12) that

$$\begin{aligned} \left|\hat{H}_0^{\,j}\hat{u}(\xi,t)\right| &\leq C\left(1+\frac{1}{1+|\xi|^2t^{\alpha}}\right)\left|(\hat{H}_0^{\,j}\hat{u}_0)(\xi)\right| \\ &\leq C\left|(\hat{H}_0^{\,j}\hat{u}_0)(\xi)\right|,\ j=0,1,\ (\xi,t) \in \mathbb{R}^d \times \mathbb{R}_+, \end{aligned}$$

where we replaced $2C$ by C in the last line. Hence the estimates (2.13) and (2.14) are still valid.

Next, with reference to (2.15), we infer from (2.9) that

$$\begin{aligned} |\partial_t \hat{u}(\xi,t)| &\leq C|\xi|^2 t^{\alpha-1}\left((1+|\xi|^2 t^\alpha)^{\frac{1-\alpha}{\alpha}} + \frac{1}{1+|\xi|^2 t^\alpha}\right)|\hat{u}_0(\xi)| \\ &\leq C|\xi|^2 t^{\alpha-1}(1+|\xi|^2 t^\alpha)^{\frac{1-\alpha}{\alpha}}|\hat{u}_0(\xi)|,\ (\xi,t)\in\mathbb{R}^d\times\mathbb{R}_+, \end{aligned}$$

where we substituted C for $2C$ in the last line. Thus, by integrating with respect to t over $(0,T)$, and then using that $(1+s)^{\frac{1}{\alpha}} \leq 2^{\frac{1}{\alpha}}(s^{\frac{1}{\alpha}}+1)$ for all $s \geq 0$, we obtain that

$$\begin{aligned} \|\partial_t \hat{u}(\xi,\cdot)\|_{L^1(0,T)} &\leq C\left((1+|\xi|^2 T^\alpha)^{\frac{1}{\alpha}}-1\right)|\hat{u}_0(\xi)| \\ &\leq C\left(1+|\xi|^{\frac{2}{\alpha}}T\right)|\hat{u}_0(\xi)|,\ \xi\in\mathbb{R}^d, \end{aligned}$$

where C was substituted for $2^{\frac{1}{\alpha}}C$ in the last line. Therefore, integrating with respect to ξ over $\mathbb{R}^d$, we find that

$$\|\partial_t \hat{u}\|_{L^1(0,T;L^2(\mathbb{R}^d))} \leq C(1+T)\|\hat{u}_0\|_{\mathrm{D}(\hat{H}_0^{\frac{1}{\alpha}})}.$$

Now, putting this together with (2.13)-(2.14) and Lemma 2.3, we get (2.6).

Third case: $\alpha > \beta$. It follows readily from (2.9) and (2.12) that,

$$\begin{aligned} \left|\hat{H}_0^{\,j}\hat{u}(\xi,t)\right| &\leq C\mathrm{e}^{\cos\left(\frac{\pi\beta}{2\alpha}\right)|\xi|^{\frac{2}{\alpha}}t}\left|(\hat{H}_0^{\,j}\hat{u}_0)(\xi)\right| \\ &\leq C\mathrm{e}^{\cos\left(\frac{\pi\beta}{2\alpha}\right)\Lambda_+^{\frac{2}{\alpha}}t}\left|(\hat{H}_0^{\,j}\hat{u}_0)(\xi)\right|,\ j=0,1,\ (\xi,t)\in\mathrm{supp}(\hat{u}_0)\times\mathbb{R}_+, \end{aligned}$$

where we replaced the constant $2C$ by C in the last line. As a consequence we have

$$\|\hat{u}(\cdot,t)\|_{\mathrm{D}(\hat{H}_0)} \leq C\mathrm{e}^{\cos\left(\frac{\pi\beta}{2\alpha}\right)\Lambda_+^{\frac{2}{\alpha}}t}\|\hat{u}_0\|_{\mathrm{D}(\hat{H}_0)},\ t\in\mathbb{R}_+. \tag{2.16}$$

Next, with reference to (2.15), we infer from (2.9) that

$$\begin{aligned} |\partial_t \hat{u}(\xi,t)| &\leq C|\xi|^2 t^{\alpha-1}\left((1+|\xi|^2 t^\alpha)^{\frac{1-\alpha}{\alpha}}\mathrm{e}^{\cos\left(\frac{\pi\beta}{2\alpha}\right)|\xi|^{\frac{2}{\alpha}}t} + \frac{1}{1+|\xi|^2 t^\alpha}\right)|\hat{u}_0(\xi)| \\ &\leq C|\xi|^2 t^{\alpha-1}(1+|\xi|^2 t^\alpha)^{\frac{1-\alpha}{\alpha}}\mathrm{e}^{\cos\left(\frac{\pi\beta}{2\alpha}\right)\Lambda_+^{\frac{2}{\alpha}}t}|\hat{u}_0(\xi)|,\ (\xi,t)\in\mathrm{supp}(\hat{u}_0)\times\mathbb{R}_+, \end{aligned}$$

where C was substituted for $2C$ in the penultimate line. Thus, by integrating with respect to t over $(0,T)$, and then using that $(1+s)^{\frac{1}{\alpha}} \leq 2^{\frac{1}{\alpha}}(s^{\frac{1}{\alpha}}+1)$ for all $s \geq 0$, we obtain that

$$\begin{aligned} \|\partial_t \hat{u}(\xi,\cdot)\|_{L^1(0,T)} &\leq C\left((1+|\xi|^2 T^\alpha)^{\frac{1}{\alpha}}-1\right)\mathrm{e}^{\cos\left(\frac{\pi\beta}{2\alpha}\right)\Lambda_+^{\frac{2}{\alpha}}T}|\hat{u}_0(\xi)| \\ &\leq C\left(1+|\xi|^{\frac{2}{\alpha}}T\right)\mathrm{e}^{\cos\left(\frac{\pi\beta}{2\alpha}\right)\Lambda_+^{\frac{2}{\alpha}}T}|\hat{u}_0(\xi)|,\ \xi\in\mathrm{supp}(\hat{u}_0), \end{aligned}$$

where $2^{\frac{1}{\alpha}}C$ was replaced by C. It follows from this, that

$$\|\partial_t \hat{u}\|_{L^1(0,T;L^2(\mathbb{R}^d))} \leq C(1+T)\mathrm{e}^{\cos\left(\frac{\pi\beta}{2\alpha}\right)\Lambda_+^{\frac{2}{\alpha}}T}\|\hat{u}_0\|_{\mathrm{D}(\hat{H}_0^{\frac{1}{\alpha}})},$$

which, together with (2.16) and Lemma 2.3, yields (2.7) with $\beta < \alpha$. □

3. Diffusion properties of the TFSE

We compute the time-asymptotic behavior of the MSD for solutions of the TFSE with initial conditions in an appropriate subspace of $L^2(\mathbb{R}^d)$. These asymptotics depend on the parameters $\alpha, \beta \in (0,1)$.

3.1. **Mean square displacement.** For $s \in \mathbb{R}_+$, we define weighted L^2-spaces

$$L^{2,s}(\mathbb{R}^d) = L^2(\mathbb{R}^d, (1+|x|^2)^{\frac{s}{2}} \mathrm{d}x) := \{v \in L^2(\mathbb{R}^d),\ (1+|x|^2)^{\frac{s}{2}} v \in L^2(\mathbb{R}^d)\},\ s > 0.$$

The mean square displacement (MSD) of $\varphi \in \mathcal{C}(\overline{\mathbb{R}_+}, L^{2,2}(\mathbb{R}^d))$ at time $t \in \overline{\mathbb{R}_+}$, is defined by

$$\begin{aligned} D_2(\varphi, t) &:= \int_{\mathbb{R}^d} |x|^2 |\varphi(x,t)|^2 \mathrm{d}x \\ &= \langle |\cdot|^2 \varphi(\cdot, t), \varphi(\cdot, t) \rangle, \end{aligned} \tag{3.1}$$

where the notation $\langle \cdot, \cdot \rangle$, and $\| \cdot \|$, stands for the usual scalar product, respectively, norm, in $L^2(\mathbb{R}^d)$ or $L^2(\mathbb{R}^d)^d$. The scalar product is linear in the first entry. As $\mathcal{F}$ is unitary in $L^2(\mathbb{R}^d)$ and $\mathcal{F}(|\cdot|^2 \varphi)(\xi, t) = -\Delta \hat{\varphi}(\xi, t)$, for a.e. $\xi \in \mathbb{R}^d$ and all $t \in \overline{\mathbb{R}_+}$, integration by parts in (3.1) yields

$$\begin{aligned} D_2(\varphi, t) &= \langle -\Delta \hat{\varphi}(\cdot, t), \hat{\varphi}(\cdot, t) \rangle \\ &= \| \nabla \hat{\varphi}(\cdot, t) \|^2. \end{aligned} \tag{3.2}$$

Since the right hand side of (3.2) is well defined whenever $\hat{\varphi} \in \mathcal{C}(\overline{\mathbb{R}_+}, H^1(\mathbb{R}^d))$, we can use formula (3.2) to extend the MSD to functions $\varphi \in \mathcal{C}(\overline{\mathbb{R}_+}, L^{2,1}(\mathbb{R}^d))$ as

$$D_2(\varphi, t) := \| \nabla \hat{\varphi}(\cdot, t) \|^2. \tag{3.3}$$

3.2. **Time-fractional quantum diffusion.** We obtain the final form of the MSD (3.3) in terms of Mittag-Leffler functions (3.4)-(3.5), and derive the large time asymptotics.

3.2.1. *Settings.* We choose the initial condition $u_0 \in \mathcal{H}_{\alpha,\beta}$, where we have set

$$\mathcal{H}_{\alpha,\beta} := \begin{cases} \mathcal{S}(\mathbb{R}^d) & \text{if } \beta \geq \alpha \\ \mathcal{F}^* \mathcal{C}_0^1(\mathbb{R}^d) & \text{if } \beta < \alpha, \end{cases}$$

where $\mathcal{S}(\mathbb{R}^d)$ is the Schwartz space on $\mathbb{R}^d$, and $\mathcal{C}_0^1(\mathbb{R}^d)$ is the space of continuously differentiable, compactly supported functions in $\mathbb{R}^d$. Since it is clear that $\mathcal{H}_{\alpha,\beta} \subset \mathcal{U}_{\alpha,\beta}$, the system (2.1)-(2.2) admits a unique solution u according to Proposition 2.1, whose Fourier transform is expressed by

$$\hat{u}(\xi, t) = E_{\alpha,1}(\kappa) \hat{u}_0(\xi),\ (\xi, t) \in \mathbb{R}^d \times \mathbb{R}_+,$$

where we recall that $\kappa = (-i)^\beta |\xi|^2 t^\alpha$. Next, using that $\frac{\mathrm{d}}{\mathrm{d}z} E_{\alpha,1}(z) = \alpha^{-1} E_{\alpha,\alpha}(z)$, $z \in \mathbb{C}$, we deduce from (2.12) that

$$\nabla \hat{u}(\xi, t) = 2\alpha^{-1} (-i)^\beta t^\alpha E_{\alpha,\alpha}(\kappa) \xi \hat{u}_0(\xi) + E_{\alpha,1}(\kappa) \nabla \hat{u}_0(\xi),\ (\xi, t) \in \mathbb{R}^d \times \mathbb{R}_+. \tag{3.4}$$

Thus, in light of Lemma 2.2, we see that $\hat{u}(\cdot, t) \in H^1(\mathbb{R}^d)$ for all $t \in \overline{\mathbb{R}^+}$, and hence that the MSD of u, denoted by $D_2(u_0, t)$ in the sequel, is well defined by (3.3) when φ is replaced by $u$so that

$$D_2(u_0, t) = \| \nabla \hat{u} \|^2, t \in \mathbb{R}_+. \tag{3.5}$$

We will compute the asymptotics of $D_2(u_0, t)$ using the form of $\hat{u}$ in (3.4).

3.2.2. *Asymptotics.* We shall examine the three cases $\alpha < \beta$, $\alpha = \beta$, and $\alpha > \beta$ separately.
We first state the main theorem that was summarized in section 1.

Theorem 3.1. *We choose the initial condition $u_0 \in \mathcal{H}_{\alpha,\beta}$ as in* (2.5) *according to* (α, β). *Then, the MSD $D_2(u_0, t)$, defined in* (3.4) *and* (3.5), *has the following asymptotic behavior:*

(1) First case: $0 < \alpha < \beta \leq 1$. *The MSD is asymptotically vanishing as $t \to \infty$ and satisfies:*

$$D_2(u_0, t) = C_\alpha(u_0) t^{-2\alpha} + O(t^{-3\alpha}), \tag{3.6}$$

where the constant $C_\alpha(u_0)$ is given by

$$C_\alpha(u_0) := \left\| |\xi|^{-2} \left(\frac{\nabla \hat{u}_0}{\Gamma(1-\alpha)} + \frac{2|\xi|^{-2} \xi \hat{u}_0}{\alpha \Gamma(-\alpha)} \right) \right\|^2. \tag{3.7}$$

(2) Second case: $0 < \alpha = \beta \leq 1$. *The MSD is asymptotically ballistic as $t \to \infty$ and satisfies:*

$$D_2(u_0, t) = \left(\frac{4}{\alpha^4} \left\| |\xi|^{\frac{2-\alpha}{\alpha}} \hat{u}_0 \right\|^2 \right) t^2 + O(t). \tag{3.8}$$

(3) Third case: $0 < \beta < \alpha \le 1$. *The MSD is asymptotically bounded by exponential factors depending on the support of $\hat{u}_0$. There are finite constants $\Lambda_\pm \ge 0$, defined in (3.17), so that:*

$$\frac{4}{\alpha^2}e^{2\cos(\frac{\pi\beta}{2\alpha})\Lambda_-^{\frac{2}{\alpha}}t}t\left(\left\||\xi|^{\frac{2-\alpha}{\alpha}}\hat{u}_0\right\|^2+O(t^{-1})\right)$$
$$\le \quad D_2(u_0,t)\le\frac{4}{\alpha^2}e^{2\cos(\frac{\pi\beta}{2\alpha})\Lambda_+^{\frac{2}{\alpha}}t}t\left(\left\||\xi|^{\frac{2-\alpha}{\alpha}}\hat{u}_0\right\|^2+O(t^{-1})\right),$$

We note that for initial conditions $\hat{u}_0$ with $\Lambda_- > 0$, the upper and lower bounds on the MSD in case 3 grow exponentially in time.

Proof. First case: $\alpha < \beta$. Taking $\mu \in (\pi\alpha/2, \min(\pi\alpha, \pi\beta/2))$ in [17, Theorem 1.4], we have $\mu \le |\arg\kappa| \le \pi$, whence

$$E_{\alpha,1}(\kappa) = -\frac{1}{\Gamma(1-\alpha)}\kappa^{-1}+O(|\kappa|^{-2}),\ |\kappa|\to\infty, \tag{3.9}$$

and

$$E_{\alpha,\alpha}(\kappa) = -\frac{1}{\Gamma(-\alpha)}\kappa^{-2}+O(|\kappa|^{-3}),\ |\kappa|\to\infty, \tag{3.10}$$

according to [17, Eq. (1.143)]. Thus, substituting $\kappa = (-i)^\beta|\xi|^2t^\alpha$ into (3.9)-(3.10) and recalling (3.4), we infer from (3.5) that

$$D_2(u_0,t) = C_\alpha(u_0)t^{-2\alpha}+O(t^{-3\alpha}),\ t\to\infty, \tag{3.11}$$

where

$$C_\alpha(u_0) := \left\||\xi|^{-2}\left(\frac{\nabla\hat{u}_0}{\Gamma(1-\alpha)}+\frac{2|\xi|^{-2}\xi\hat{u}_0}{\alpha\Gamma(-\alpha)}\right)\right\|^2. \tag{3.12}$$

Second case: $\alpha = \beta$. Taking $\mu \in (\pi\alpha/2, \min(\pi, \pi\alpha))$ in [17, Theorems 1.3], we have $|\arg\kappa| \le \mu$, whence

$$E_{\alpha,1}(\kappa) = \frac{1}{\alpha}e^{\kappa^{\frac{1}{\alpha}}}-\frac{1}{\Gamma(1-\alpha)}\kappa^{-1}+O(|\kappa|^{-2}),\ |\kappa|\to\infty, \tag{3.13}$$

$$E_{\alpha,\alpha}(\kappa) = \frac{1}{\alpha}\kappa^{\frac{1-\alpha}{\alpha}}e^{\kappa^{\frac{1}{\alpha}}}-\frac{1}{\Gamma(-\alpha)}\kappa^{-2}+O(|\kappa|^{-3}),\ |\kappa|\to\infty, \tag{3.14}$$

by [17, Eq. (1.135)]. Substituting (3.13)-(3.14) into (3.4), and using that $\kappa = (-i)^\alpha|\xi|^2t^\alpha$, we infer from (3.5) that

$$D_2(u_0,t) = \frac{4\left\||\xi|^{\frac{2-\alpha}{\alpha}}\hat{u}_0\right\|^2}{\alpha^4}t^2+O(t),\ t\to\infty. \tag{3.15}$$

Third case: $\alpha > \beta$. Taking μ as in the *Second case*, we still have $|\arg(\kappa)| \le \mu$, whence (3.13)-(3.14) remain valid. In light of this, and (3.4), this implies the large t-asymptotic expansion

$$\begin{aligned}\nabla\hat{u}(\xi,t) \quad &= \quad e^{\left(\cos(\frac{\pi\beta}{2\alpha})-i\sin(\frac{\pi\beta}{2\alpha})\right)|\xi|^{\frac{2}{\alpha}}t}\left(\frac{2}{\alpha^2}(-i)^{\frac{\beta}{\alpha}}|\xi|^{\frac{2(1-\alpha)}{\alpha}}t\xi\hat{u}_0(\xi)+\frac{1}{\alpha}\nabla\hat{u}_0(\xi)\right)\\ &\quad -i^\beta|\xi|^{-2}\left(\frac{2}{\alpha\Gamma(-\alpha)}|\xi|^{-2}\xi\hat{u}_0(\xi)+\frac{1}{\Gamma(1-\alpha)}\nabla\hat{u}_0(\xi)\right)t^{-\alpha}+O(t^{-2\alpha}).\end{aligned} \tag{3.16}$$

For any $u_0 \in \mathcal{F}^*C_0^1(\mathbb{R}^d)$, that is, $\hat{u}_0 \in C_0^1(\mathbb{R}^d)$, there exist finite constants $\Lambda_\pm \ge 0$, so that

$$\operatorname{supp}(\hat{u}_0) \subset \{\xi\in\mathbb{R}^d,\ \Lambda_- \le |\xi| \le \Lambda_+\}. \tag{3.17}$$

Substituting (3.16) into (3.5), and using $\Lambda_\pm$ defined in (3.17), we get the follow bounds as $t\to\infty$:

$$\frac{4}{\alpha^2}e^{2\cos(\frac{\pi\beta}{2\alpha})\Lambda_-^{\frac{2}{\alpha}}t}t\left(\left\||\xi|^{\frac{2-\alpha}{\alpha}}\hat{u}_0\right\|^2+O(t^{-1})\right)$$
$$\le \quad D_2(u_0,t)\le\frac{4}{\alpha^2}e^{2\cos(\frac{\pi\beta}{2\alpha})\Lambda_+^{\frac{2}{\alpha}}t}t\left(\left\||\xi|^{\frac{2-\alpha}{\alpha}}\hat{u}_0\right\|^2+O(t^{-1})\right),\ t\to\infty.$$

□

Remark 3.2. *In recent work* [7], *the authors prove that the three different asymptotic behaviors exhibited by the MDS $D_2(u_0, t)$ in Theorem 3.1 are stable with respect to a large family of potential perturbations. That is, if the TFSE in* (1.1) *is replaced by*

$$i^\beta \partial_t^\alpha u = (-\Delta + V)u, \; u(t = 0) = u_0, \tag{3.18}$$

for real-valued potentials $V \in C^1(\mathbb{R}^d)$ that are relatively H_0-bounded (with relative bound less than one), then the MSD exhibits the same asymptotic behaviors as in Theorem 3.1 for the same ranges of the parameters (α, β).

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Department of Mathematics, University of Kentucky, Lexington, Kentucky 40506-0027, USA
E-mail address: peter.hislop@uky.edu

Aix Marseille Univ, Université de Toulon, CNRS, CPT, Marseille, France
E-mail address: eric.soccorsi@univ-amu.fr