

Subdiffusion in the nonlinear Schrödinger equation with disorder

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The nonlinear Schrödinger equation in the presence of disorder is considered. The dynamics of an initially localized wave packet is studied. A subdiffusive spreading of the wave packet is explained in the framework of a continuous time random walk. A probabilistic description of subdiffusion is suggested, and a transport exponent of subdiffusion is obtained to be $2/5$.

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In this work the dynamics of an initially localized wave function is considered in the framework of the nonlinear Schrödinger equation in the presence of disorder. The wave function is governed by the following equation:

$$i\partial_t\psi = -\partial_x^2\psi + \beta|\psi|^2\psi + V\psi, \quad (1)$$

where β is a nonlinearity parameter. The variables are chosen in dimensionless units and the Planck constant is $\hbar=1$. The random potential $V=V(x)$, $x \in (-\infty, +\infty)$ is such that for the linear case ($\beta=0$) the Anderson localization takes place [1,2], and the system is described by the exponentially localized Anderson modes (AMs) $\Psi_{\omega_k} \equiv \Psi_k(x)$, where $\Psi_{\omega_k}(x)$ are real functions and the eigenspectrum ω_k is discrete and dense [2]. The problem in question is an evolution of an initially localized wave function $\psi(t=0)=\psi_0(x)$.

This problem is relevant to experiments in nonlinear optics, for example disordered photonic lattices [3,4], where Anderson localization was found in the presence of nonlinear effects, as well as to experiments on Bose-Einstein condensates in disordered optical lattices [5–10]. A discrete analog of Eq. (1) is extensively studied numerically [11–14], and a subdiffusive spreading of the initially localized wave packet has been observed, such that $\langle x^2(t) \rangle = \int |\psi(t)|^2 x^2 dx \sim t^\alpha$, where a transport exponent α was found in the range $0.3 \div 0.4$ [13,14].

A subdiffusive spreading of the wave packet was also obtained analytically [15] in the limit of the large times asymptotic dynamics of the tails of the wave packet, where the transport exponent was found to be $\alpha < 1$. In that case the dynamics of the wave packet has been approximated by the fractional Fokker-Planck equation (FFPE) due to the arguments of a so-called continuous time random walk (CTRW).

The concept of the CTRW was originally developed for mean first passage time in a random walk on a lattice with further application to a semiconductor electronic motion [16]. The mathematical apparatus of the fractional CTRW is well established for many applications in physics, see, e.g., [17–21].

The primary purpose of the present analysis is to develop the physical mechanism of the wave-packet spreading and to obtain the transport exponent α . The analysis is based on mapping nonlinear Eq. (1) to the linear Liouville equation for the probability amplitude $|\psi(x,t)|^2$, where the transition elements in the Liouville operator are determined by the nonlinear term in Eq. (1). Therefore we proceed to developing

the analysis further by application of the CTRW approach to the corresponding Liouville equation [22].

First we obtain the linear Liouville equation for $|\psi(x,t)|^2$ [15]. Projecting Eq. (1) on the basis of the AMs,

$$\psi(x,t) = \sum_{\omega_k} C_{\omega_k}(t)\Psi_{\omega_k}(x) \equiv \sum_k C_k(t)\Psi_k(x), \quad (2)$$

we obtain a system of equations for coefficients of the expansion C_k

$$i\partial_t C_k = \omega_k C_k + \beta \sum_{k_1, k_2, k_3} A_{k_2, k_3}^{k, k_1} C_{k_1}^* C_{k_2} C_{k_3}. \quad (3)$$

Here $A(\mathbf{k}) \equiv A_{k_2, k_3}^{k, k_1}$ is an overlapping integral of the four AMs,

$$A_{k_2, k_3}^{k, k_1} = \int \Psi_k(x)\Psi_{k_1}(x)\Psi_{k_2}(x)\Psi_{k_3}(x)dx. \quad (4)$$

The initial conditions for the system of Eq. (3) are such that $\psi_0(x) = \sum_k a_k \Psi_k(x)$. Equations (3) correspond to a system of interacting nonlinear oscillators with the Hamiltonian

$$H = \sum_k \omega_k C_k^* C_k + \beta \sum_{\mathbf{k}} A_{k_2, k_3}^{k_1, k_4} C_{k_1}^* C_{k_4}^* C_{k_2} C_{k_3}. \quad (5)$$

Therefore, Eq. (3) is produced by the Poisson brackets $\{H, \dots\}_{PB}$ by means of the Liouville operator

$$\hat{L} = \frac{1}{i} \{H, \dots\}_{PB} = \frac{1}{i} \sum_k \left(\frac{\partial H}{\partial C_k^*} \frac{\partial}{\partial C_k} - \frac{\partial H}{\partial C_k} \frac{\partial}{\partial C_k^*} \right). \quad (6)$$

Since $\hat{L}H=0$ and $H(\{C, C^*\})=H(\{a, a^*\})$, we obtain that the Liouville operator is an operator function of the initial values,

$$\hat{L} = \frac{1}{i} \sum_k \left[\frac{\partial H}{\partial a_k^*} \frac{\partial}{\partial a_k} - \frac{\partial H}{\partial a_k} \frac{\partial}{\partial a_k^*} \right] \quad (7)$$

and corresponds to an infinite system of linear equations $\partial_t \mathbf{C} = \hat{L} \mathbf{C}$, where $\mathbf{C} = \mathbf{C}(\{a_k, a_k^*\}) = (\dots, C_{k-1}, C_k, C_{k+1}, \dots)$ is an infinite vector. Thus, the Liouville operator reads as

$$\hat{L} = -i \sum_k \omega_k \left(a_k \frac{\partial}{\partial a_k} - \text{c.c.} \right) - i\beta \sum_{\mathbf{k}} A_{k_2, k_3}^{k_1, k_4} \times \left[a_{k_1}^* a_{k_2} a_{k_3} \frac{\partial}{\partial a_{k_4}} - \text{c.c.} \right], \quad (8)$$

where c.c. denotes the complex conjugation. The Liouville equation is valid for any functions of the initial conditions $\{a_k, a_k^*\}$. In particular, introducing the function $F_{k,k'}(t) = C_k(t) \cdot C_{k'}^*(t)$, one has the Liouville equation

$$\partial_t F_{k,k'}(t) = \hat{L} F_{k,k'}(t), \quad F_{k,k'}(t=0) = F_{k,k'}^{(0)} = a_k a_{k'}^*.$$

Therefore, the probability amplitude

$$\mathcal{P}(x, t) = |\psi|^2 = \sum_{k,k'} F_{k,k'}(t) \Psi_k(x) \Psi_{k'}(x),$$

as a function of the initial conditions, satisfies the Liouville equation as well,

$$\partial_t \mathcal{P} = \hat{L} \mathcal{P}. \quad (9)$$

Here the initial condition is

$$\mathcal{P}(x, t=0) = \mathcal{P}_0(x) = \sum_{k,k'} F_{k,k'}^{(0)} \Psi_k(x) \Psi_{k'}(x). \quad (10)$$

Finally, we obtain that nonlinear Schrödinger equation (NLSE) (1) is replaced by Liouville Eq. (9), which is the *linear* equation with a formal solution in the exponential form,

$$\mathcal{P}(x, t) = e^{\hat{L}t} \mathcal{P}_0(x) = \sum_{k,k'} \Psi_k(x) \Psi_{k'}(x) \sum_{n=0}^{\infty} \left[\frac{t^n}{n!} \hat{L}^n \right] F_{k,k'}^{(0)}. \quad (11)$$

In what follows we consider the dynamics of the initial wave packet $\mathcal{P}_0(x)$ in the framework of the probabilistic approach, where the dynamics of the wave packet is considered as the CTRW. Since the dynamics of the probability distribution function (PDF) $\mathcal{P}(x, t)$ is governed by the same Liouville operator in Eqs. (9) and (11), the overlapping integrals $A(\mathbf{k})$ play the dominant role in the wave-packet spreading. As follows from Eq. (11), the overlapping integrals determine the spread of the initially localized wave packet $\mathcal{P}_0(x)$ over all the Anderson modes as transitions from one mode to another. Since all states are localized, these transitions between states determine the transitions (or jumps) in the coordinate space as well.

According to the values of the overlapping integrals, we divide the transitions between the localized states into two main groups. The first one corresponds to the exponentially small overlapping integrals and the second one corresponds to the strong overlapping between four AMs when the overlapping integrals are on the order of 1. In the case of strong overlapping, the AMs form clusters, where the wave functions have the same averaged coordinates for each cluster. Consequently, all transitions inside one cluster do not lead to any appreciable differences in the coordinate space, and we regard these transitions as *trapping* of the wave packet, or a

particle, inside this cluster. Contrary to that, transitions due to the exponentially small overlapping integrals between the AMs belonging to different clusters lead to a change of the space coordinates that can be accounted for. We call these processes *jumps*. Contributions of trappings and jumps to the wave-packet spreading described by Eqs. (9) and (11) are different, and correspond to different probabilistic interpretations.

In the sequel we follow the CTRW approach [16] and paraphrase it from [18,20] in a form suitable for the present analysis. First, we consider a process of jumps. Let $P_n(x)$ be the PDF of being at x after n jumps. It is reasonable to assume that the transitions between different states are independent of each other; therefore, the jumps are independent and obey the Markov property

$$P_{n+1}(x) = \int P_n(x') p(x-x') dx', \quad (12)$$

where $P_0(x) = \mathcal{P}_0(x)$ and $p(x)$ is the PDF of a jump determined by the overlapping integrals as $p(x) = \xi \exp(-\xi|x|)/2$, and $\xi = 1/R$ is an inverse localization length.

The trapping is associated with clusters with effective lengths Δ . Due to the exponential localization, these values are distributed by the exponential law $P_{cl}(\Delta) = \Delta_0^{-1} \exp(-\Delta/\Delta_0)$, where Δ_0 is the mean length of a cluster. The effective lengths are determined by overlapping integrals; therefore, the minimum length of the cluster is $\Delta = R$, while the maximum one is $\Delta = 4R$. As a result, one obtains $\Delta_0 = 5R/2$. Now the probability that a particle exits this cluster and jumps to another one is of the order of $\sim \exp(-\Delta/R)$. This value is also proportional to the inverse waiting time, $t \sim \exp(\Delta/R)$. The probability to find the waiting time in the interval $(t, t+dt)$ is equal to the probability to find the corresponding trapping length in the interval $(\Delta, \Delta+d\Delta)$, namely, $w(t)dt = P_{cl}(\Delta)d\Delta$. Therefore, after simple calculations one obtains that the PDF of the waiting times is

$$w(t) = P_{cl}(\Delta) \frac{d\Delta}{dt} \sim \frac{1}{(t/\tau)^{1+\alpha}}, \quad (13)$$

where $\alpha = R/\Delta = 2/5$ and τ is a time scale related to the trapping [23]. It follows that the mean waiting time is infinite. Taking into account that the waiting time PDF is normalized we have

$$w(t) = \frac{w_0}{1 + (t/\tau)^{1+\alpha}}, \quad (14)$$

such that $\int_0^\infty w(t)dt = 1$ and $\int_0^\infty tw(t)dt = \infty$. Here $w_0 = \frac{2\alpha \sin(\pi/2\alpha)}{\pi(1+\alpha)^{2\alpha}}$ is a normalization constant.

Now let us consider the PDF $w(t)$ taking into account the dynamics of the jumps. Again, since transitions between different states are statistically independent, waiting times for different jumps are statistically independent as well. Therefore, indexing the waiting time PDF by the jump number, we define that $w_n(t)$ is the probability density that n th jump occurs at time t (see e.g., [20], p. 42). Due to the reasonable assumption that jumps are independent transitions, we also introduce the Markov property for $w_n(t)$, which reads as

$$w_{n+1}(t) = \int_0^\infty w_n(t')w(t-t')dt', \quad (15)$$

where $w_1(t) \equiv w(t)$. Now we introduce the PDF $P(x, t) = \sum_n P_n(x)w_n(t)$ of arriving at coordinate x at time t . From Eqs. (12) and (15) we introduce the equation [18]

$$P(x, t) = \int_{-\infty}^\infty p(x-x') \int_0^\infty w(t-t')P(x', t')dx'dt' + \mathcal{P}_0(x)\delta(t), \quad (16)$$

which relates the PDF $P(x, t)$ of just having arrived at position x at time t to the PDF $P(x', t')$ of just arriving at x' at time t' . The last term in Eq. (16) is the initial condition. Thus the PDF $\mathcal{P}(x, t)$ of being at position x at time t is given by arrival at x' at time t' and not having moved after this event, namely,

$$\mathcal{P}(x, t) = \int_0^t P(x, t')W(t-t')dt', \quad (17)$$

where $W(t) = 1 - \int_0^t w(t')dt'$ denotes the probability of no jump during the time interval $(0, t)$. Performing the Fourier transform $\bar{p}(k) = \hat{\mathcal{F}}P(x)$ and the Laplace transform $\bar{w}(s) = \hat{\mathcal{L}}w(t)$, we obtain the Montroll-Weiss equation [16],

$$\bar{\mathcal{P}}(k, s) = \hat{\mathcal{F}}\hat{\mathcal{L}}\mathcal{P} = \frac{1 - \bar{w}(s)}{s} \cdot \frac{\bar{\mathcal{P}}_0(k)}{1 - \bar{p}(k)\bar{w}(s)}. \quad (18)$$

Equation (18) can be simplified for the long time $s \ll 1$ and the large scale $k \ll 1$ asymptotics that corresponds to the diffusion limit $(k, s) \rightarrow (0, 0)$. Taking into account the Fourier $\bar{p}(k)$ and the Laplace $\bar{w}(s)$ images in Eq. (18),

$$\bar{p}(k) = \frac{1}{1 + R^2k^2} \approx 1 - R^2k^2, \\ \bar{w}(s) = \frac{1}{1 + (s\tau)^\alpha} \approx 1 - (s\tau)^\alpha, \quad (19)$$

we obtain for the PDF in the Fourier-Laplace domain (see also [18])

$$\bar{\mathcal{P}}(k, s) = \frac{\bar{\mathcal{P}}_0(k)/s}{1 + D_\alpha s^{-\alpha}k^2}, \quad (20)$$

where $D_\alpha = R^2/\tau^\alpha$ is a generalized diffusion coefficient. Using the Laplace transform of the fractional integration

$$\hat{\mathcal{L}}[\partial_t^{-\nu}f(t)] = \hat{\mathcal{L}}\left[\frac{1}{\Gamma(\nu)}\int_0^t \frac{f(\tau)d\tau}{(t-\tau)^{1-\nu}}\right] = s^{-\nu}f(s), \quad \nu > 0,$$

one obtains the fractional integral equation

$$\mathcal{P}(x, t) - \mathcal{P}_0(x) = \partial_t^{-\alpha}D_\alpha \partial_x^2 \mathcal{P}(x, t). \quad (21)$$

Differentiating this equation with respect to time, one obtains that the CTRW is described by the FFPE [24]

$$\partial_t \mathcal{P}(x, t) - D_\alpha \partial_t^{1-\alpha} \partial_x^2 \mathcal{P}(x, t) = 0, \quad (22)$$

where ∂_t^ν is a designation of the Riemann-Liouville fractional derivative

$$\partial_t^\nu f(t) = \frac{d}{dt} \partial_t^{\nu-1} f(t) = \frac{1}{\Gamma(1-\nu)} \frac{d}{dt} \int_0^t \frac{f(\tau)d\tau}{(t-\tau)^\nu},$$

where $0 < \nu < 1$. From Eq. (22) one obtains for the second moment $\langle x^2(t) \rangle = \int_{-\infty}^\infty x^2 \mathcal{P}(x, t) dx$ the differential equation

$$\frac{d}{dt} \langle x^2(t) \rangle = \frac{2D_\alpha t^{\alpha-1}}{\Gamma(\alpha)}.$$

Here $\Gamma(z)$ is the gamma function, $x(t=0) = 0$, and we use the following property of the fractional derivative $\partial_t^\nu 1 = t^{-\nu}/\Gamma(1-\nu)$. Therefore, Eq. (22) describes subdiffusion

$$\langle x^2(t) \rangle = \frac{2D_\alpha t^\alpha}{\Gamma(1+\alpha)}, \quad (23)$$

with the transport exponent $\alpha = 0.4$. In the recent numerical studies of the discrete NLSE [13,14] the exponent α was found in the range $0.3 \div 0.4$.

This consideration can be extended on the wave-packet spreading in the framework of the generalized nonlinear Schrödinger equation

$$i\partial_t \psi = \hat{\mathcal{H}}_0 \psi + \beta |\psi|^{2n} \psi, \quad (24)$$

where $n \geq 1$ and the Hamiltonian $\hat{\mathcal{H}}_0$ has the pure point spectrum with the localized eigenfunctions: $\hat{\mathcal{H}}_0 \Psi_k = \mathcal{E}_k \Psi_k$. For example, the Hamiltonian describes Wannier-Stark localization [25], and the discrete counterpart of Eq. (24) with $n=1$ corresponds to delocalization in a nonlinear Stark ladder [26,27]. Repeating probabilistic consideration of the CTRW based on the overlapping integrals $A(\mathbf{k})$ of $2n+2$ eigenfunctions $\Psi_k(x)$, one obtains that Eq. (24) describes subdiffusion with the transport exponent

$$\alpha = \frac{2}{3+2n}. \quad (25)$$

For $n=1$ this expression coincides with the numerical result of Ref. [26].

The nonlinear Schrödinger equation in the presence of disorder is considered, and the dynamics of an initially localized wave packet is studied. A subdiffusive spreading of the wave packet is explained in the framework of a continuous time random walk. It is shown that the subdiffusive spreading of the initially localized wave packet is due to the transitions between those AMs which are strongly overlapped. This overlapping leads to the clustering with an effective potential well and, correspondingly, to effective trapping of the wave packet inside each cluster by the potential. Therefore, the dynamics of the wave packet corresponds to the CTRW, where the basic mechanism of subdiffusion is an entrapping of the wave packet with delay, or waiting, times distributed by the power law $w(t) \sim 1/t^{1+\alpha}$, $0 < \alpha < 1$. The trapping mechanism also determines the transport exponent α , which is due to the number of AMs contributed to the overlapping integrals according to Eq. (25). One should rec-

ognize that the PDF of the CTRW in Eq. (17) is associated with the true quantum distribution of the NLSE by virtue of Eq. (9) with the formal solution of Eq. (11). These expressions are an important intermediate result which establishes a relation between the NLSE and the probabilistic description. Note, that the PDF $\mathcal{P}(x, t)$ in Eq. (9) is the exact distribution, and it corresponds to the CTRW in the long time and the large scale asymptotics of Eq. (19).

It is worth noting that the linear property of Liouville Eq. (9) and its formal solution in the form of Eq. (11) are important for the probabilistic approach. This linear property was used for the CTRW consideration. Therefore, in conclusion, let us establish a relation between the Montroll-Weiss equation (18) and formal solution (11). The Liouville operator is approximately a sum of two operators $\hat{L} = \hat{L}_0 + \hat{L}_1$, where \hat{L}_0 corresponds to the trapping due to the overlapping integrals of the order of 1, while \hat{L}_1 corresponds to jumps due to the exponentially small overlapping integrals. Thus one obtains $\hat{L}^n \approx \hat{L}_0^n + n\hat{L}_0^{n-1}\hat{L}_1$, where all terms of the order of $\mathcal{O}(\hat{L}_1)$ are neglected. Then using the identity $\sum_{m=0}^{n-1} 1 = n$ and a definition

of the beta function $\int_0^1 y^m (1-y)^{n-1-m} dy = \frac{m!(n-1-m)!}{n!}$, we have from Eq. (11) $\mathcal{P}(x, t) = e^{\hat{L}_0 t} \mathcal{P}_0(x) + \int_0^t dt' e^{(t-t')\hat{L}_0} \hat{L}_1 e^{t'\hat{L}_0} \mathcal{P}_0(x)$. The probabilistic interpretation of the last expression is the following. The first term corresponds to a particle that at the initial time is at the position x , and there are no jumps until time t , and therefore $e^{\hat{L}_0 t} \mathcal{P}_0(x) \rightarrow W(t) \mathcal{P}_0(x)$. The last term corresponds to arrival at the position x at time t due to all possible jumps from (x', t') with the transition probability $\mathcal{G}(x-x'; t-t')$. Therefore, Eq. (11) now reads as

$$\mathcal{P}(x, t) = W(t) \mathcal{P}_0(x) + \int_0^t dt' \int_{-\infty}^{\infty} dx' \mathcal{G}(x-x'; t-t') \mathcal{P}(x', t').$$

Carrying out the Laplace and the Fourier transforms one obtains Montroll-Weiss Eq. (18), where the transition probability is $\mathcal{G}(x-x'; t-t') = p(x-x') w(t-t')$.

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