



Quantum continuous time random walk in nonlinear Schrödinger equation with disorder



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ABSTRACT

A quantum nonlinear Schrödinger equation in the presence of disorder is considered. The dynamics of an initially localized wave packet is studied and subdiffusion of the wave packet is obtained with a transport exponent $1/2$. It is shown that this transport exponent has pure quantum nature. A probabilistic description of subdiffusion in the framework of a quantum continuous time random walk is suggested and a quantum master equation is obtained.

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1. Introduction

In modern optical experiments on a quantum wave propagation in nonlinear media a suitable description can be suggested in the framework of the fractional kinetics based on fractional integro-differentiation. This concept of differentiation of non-integer orders arises from works of Leibniz, Liouville, Riemann, Grunwald, and Letnikov, see e.g., [1–3]. Its application is related to random processes with power law distributions. This corresponds to the absence of characteristic average values for processes exhibiting many scales [4,5].

A typical example of fractional dynamics in optics is realized in a competition between localization and nonlinearity that leads to anomalous transport [6–12] (See also a recent review [13]). This dynamics is described in the framework of the nonlinear Schrödinger equation (NLSE) in the presence of an external field $V = V(x)$, $x \in (-\infty, +\infty)$. The wave spreading, described by the wave function, is governed by the nonlinear Schrödinger equation in the presence of disorder

$$i\partial_t \psi = -\partial_x^2 \psi + \beta |\psi|^2 \psi + V \psi, \quad (1.1)$$

where β is a nonlinearity parameter. The variables are chosen in dimensionless units and the Planck constant is $\hbar = 1$. The random potential $V = V(x)$, $x \in (-\infty, +\infty)$ leads to Anderson localization for the linear case ($\beta = 0$) [14,15]. The system is described by the exponentially localized Anderson modes (AM)s $\Psi_{\omega_k} \equiv \Psi_k(x)$, such

that $[-\partial_x^2 + V(x)]\Psi_k(x) = \omega_k \Psi_k(x)$, where $\Psi_{\omega_k}(x)$ are real functions and the eigenspectrum ω_k is discrete and dense [15]. The problem in question is an evolution of an initially localized wave function $\psi(t=0) = \psi_0(x)$. It can be also a stationary state of the NLSE, which is localized with the same Lyapunov exponent [16,17].

This problem is relevant to experiments in nonlinear optics, for example disordered photonic lattices [18,19], where Anderson localization was found in the presence of nonlinear effects, as well as to experiments on Bose–Einstein condensates in disordered optical lattices [20–23]. A discrete analog of Eq. (1.1) is extensively studied numerically [6–9,12], 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 to be $2/5$ [9] and $1/3$ [8]. This difference has been explained in [24], where it has been shown that the former result is for the Markovian subdiffusion due to the range-dependent diffusion coefficient, while the latter one corresponds to non-Markovian fractional diffusion in a regime of percolation. 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).

A subdiffusive spreading of the wave packet was also obtained analytically [10,24] in the limit of the large times asymptotic dynamics, where the transport exponent α has been found as well.

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 [25]. The mathematical apparatus of the fractional CTRW is well established for many applications in physics, see e.g., [4,5,26–28].

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In the present research we present the physical mechanism of subdiffusion of a quantum wave packet spreading and propose a quantum master equation based on the CTRW consideration, related to the quantum properties of the nonlinear interaction term in Eq. (1.1). To this end we consider a quantum counterpart of the NLSE (1.1) (quantum NLSE), when the wave functions $\psi(x)$ are considered as operators $\hat{\psi}(x)$ satisfying to the commutation rule $[\hat{\psi}(x), \hat{\psi}^\dagger(x')] = \delta(x - x')$. The paper consists of two parts. The first one is a quantum analysis which is based on mapping of the quantum system on the basis of the coherent states, and in the framework of the obtained equations we study four-mode decays to understand quantum continuous time walks and construct a generalized master equation as a quantum counterpart of the Liouville equation. The second part is a classical analysis of the c -number Liouville equation for the mean probability amplitude $\langle |\hat{\psi}(x, t)|^2 \rangle$, where the transition elements in the Liouville operator are overlapping integrals of the AMs. Therefore, the further analysis is an application of the CTRW approach to the corresponding Liouville equation [29]. We also show that subdiffusion of the quantum wave packet with a transport exponent $\alpha = 1/2$ has a quantum nature.

2. Quantum NLSE

We concern with a quantum counterpart of the NLSE (1.1). In this case, an initial wave spreading is governed by the quantum nonlinear Schrödinger equation

$$i\hbar \partial_t \hat{\psi} = \hat{H}_0 \hat{\psi} + \beta |\hat{\psi}|^2 \hat{\psi}, \quad (2.1)$$

where $[\hat{\psi}(x), \hat{\psi}^\dagger(x')] = \delta(x - x')$. The Hamiltonian $\hat{H}_0$ corresponds to the Anderson localization problem $\hat{H}_0 \Psi_{\omega_k}(x) = \omega_k \Psi_{\omega_k}(x)$, where $\Psi_{\omega_k}(x)$ are the AMs, presented in Introduction. One should recognize that the classical NLSE (1.1) is independent of the Planck constant. Therefore, for the quantum analysis, an effective dimensionless Planck constant $\hbar$ is introduced explicitly. Projecting Eq. (2.1) on the basis of the AMs

$$\hat{\psi}(x, t) = \sum_{\omega_k} \hat{C}_{\omega_k}(t) \Psi_{\omega_k}(x) \equiv \sum_k \hat{C}_k(t) \Psi_k(x), \quad (2.2)$$

we obtain a system of equations for the operators of the expansion $\hat{C}_k$, where $[\hat{C}_k, \hat{C}_l^\dagger] = \delta_{k,l}$. This system of the Heisenberg equations $i\hbar \dot{\hat{C}}_k = [\hat{C}_k, \hat{H}]$ is governed by the quantum Hamiltonian

$$\hat{H} = \sum_k \hbar \omega_k \hat{C}_k^\dagger \hat{C}_k + \frac{\hbar^2 \beta}{2} \sum_{\mathbf{k}} A_{\mathbf{k}} \hat{C}_{k_1}^\dagger \hat{C}_{k_2}^\dagger \hat{C}_{k_3} \hat{C}_{k_4}, \quad (2.3)$$

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

$$A_{k_2, k_3}^{k, k_1} = \int \Psi_k(x) \Psi_{k_1}(x) \Psi_{k_2}(x) \Psi_{k_3}(x) dx. \quad (2.4)$$

For $\hbar = 0$, Eq. (2.3) reduces to the classical NLSE (1.1). The linear frequency is shifted by the nonlinear term due to the commutation $\omega_k \rightarrow \omega_k + \hbar \beta A_0$, where $A_0 = A_{kk}^{kk}$ is the diagonal overlapping integral in Eq. (2.4).

2.1. Phase space dynamics and the Liouville operator

For the quantum mechanical analysis we use a technique of mapping the Heisenberg equation of motion on a basis of the coherent states [30–32]. At the initial moment $t = 0$, one introduces the coherent states vector $|\mathbf{a}\rangle = \prod_q |a_q\rangle$ as the product of eigenfunctions of annihilation operators $\hat{a}_q = \hat{C}_q(t = 0)$, such that $\hat{a}_q |a_q\rangle = a_q |a_q\rangle$ and correspondingly $\hat{a}_q |\mathbf{a}\rangle = a_q |\mathbf{a}\rangle$, where also the coherent state is constructed from a vacuum state $|0\rangle$

$$|a_q\rangle = \exp[a_q \hat{a}_q^\dagger - a_q^* \hat{a}_q] |0\rangle, \quad \hat{a}_q |0\rangle = 0. \quad (2.5)$$

Introducing c -functions

$$C_q(t) = \langle \mathbf{a} | \hat{C}_q(t) | \mathbf{a} \rangle = C_q(t | \mathbf{a}^*, \mathbf{a}), \quad (2.6)$$

one maps the Heisenberg equation of motion on the basis $|\mathbf{a}\rangle$ as follows

$$i\hbar \dot{C}_q(t) = \langle \mathbf{a} | [\hat{C}_q(t) \hat{H} - \hat{H} \hat{C}_q(t)] | \mathbf{a} \rangle. \quad (2.7)$$

Accounting Eqs. (2.5) and (2.6), one obtains the mapping rules

$$\begin{aligned} \langle \mathbf{a} | \hat{C}_q(t) \hat{a}_q^\dagger | \mathbf{a} \rangle &= e^{-|a_q|^2} \frac{\partial}{\partial a_q} e^{|a_q|^2} C_q(t), \\ \langle \mathbf{a} | \hat{a}_q \hat{C}_q(t) | \mathbf{a} \rangle &= e^{-|a_q|^2} \frac{\partial}{\partial a_q^*} e^{|a_q|^2} C_q(t). \end{aligned} \quad (2.8)$$

The Hamiltonian is the integral of motion $\hat{H}(\{\hat{C}_q^\dagger, \hat{C}_q\}) = \hat{H}(\{\hat{a}_q^\dagger, \hat{a}_q\})$, therefore the mapping rules (2.8) yield equation of motion (2.7) for $C_q(t)$ in the closed form

$$i\dot{C}_q(t) = \hat{K}C(t), \quad (2.9)$$

where

$$\begin{aligned} \hat{K} &= \frac{1}{\hbar} e^{-\sum_k |a_k|^2} \left[\hat{H} \left(\left\{ \frac{\partial}{\partial a_q}, a_q \right\} \right) - \hat{H} \left(\left\{ a_q^*, \frac{\partial}{\partial a_q^*} \right\} \right) \right] e^{\sum_k |a_k|^2} \\ &= \sum_q \left[\omega_q a_q \frac{\partial}{\partial a_q} - c.c \right] \\ &\quad + \frac{\hbar \beta}{2} \sum_{\mathbf{q}} A_{\mathbf{q}} \left[2a_{q_1} a_{q_2} a_{q_3}^* \frac{\partial}{\partial a_{q_4}} + a_{q_1} a_{q_2} \frac{\partial}{\partial a_{q_3}} \frac{\partial}{\partial a_{q_4}} - c.c \right]. \end{aligned} \quad (2.10)$$

In the limit $\hbar \rightarrow 0$, the second derivative terms vanish, $\hbar a_{q_1} a_{q_2} \frac{\partial}{\partial a_{q_3}} \frac{\partial}{\partial a_{q_4}} \rightarrow 0$, and the operator (2.10) reduces to the classical Liouville operator [10].

2.2. Liouville equation

To construct a quantum kinetic equation, or master equation, we consider the density operator $\hat{\rho} = |\hat{\psi}|^2$ and map it on the basis of the coherent states $|\mathbf{a}\rangle$ in Eq. (2.5), such that

$$\mathcal{P}(t) \equiv \mathcal{P}(\mathbf{a}^*, \mathbf{a}, t) = \langle \mathbf{a} | \hat{\rho}(t) | \mathbf{a} \rangle. \quad (2.11)$$

Therefore, from the mapping rules one obtains the Liouville equation for the mean probability density

$$\partial_t \mathcal{P}(t) = \hat{L} \mathcal{P}(t). \quad (2.12)$$

Here the quantum “Liouville” operator is determined in Eq. (2.10)

$$\hat{L} = -i\hat{K}. \quad (2.13)$$

The initial condition is constructed as a superposition

$$\mathcal{P}(x, t = 0) = \mathcal{P}_0(x) = \sum_{k, k'} F_{k, k'}^{(0)} \Psi_k(x) \Psi_{k'}^*(x), \quad (2.14)$$

where $F_{k, k'}^{(0)} = a_k a_{k'}^*$. Eventually, we obtain that the quantum NLSE (2.1) is replaced by the Liouville Eq. (2.12), which is the linear equation with a formal solution in the exponential form

$$\mathcal{P}(x, t) = e^{\hat{L}t} \mathcal{P}_0(x) = \sum_{k, k'} \Psi_k(x) \Psi_{k'}^*(x) = \sum_{n=0}^{\infty} \left[\frac{t^n}{n!} \hat{L}^n \right] F_{k, k'}^{(0)}. \quad (2.15)$$

The Liouville operator can be considered as a sum of two operators $\hat{L} = \hat{L}_0 + \hat{L}_1$, where $\hat{L}_0$ corresponds to the dynamics inside a cluster, determined by the overlapping integrals of the order of 1, while $\hat{L}_1$ corresponds to jumps between these clusters due to the exponentially small overlapping integrals. Thus considering this dynamics in the “interaction picture”, where $\hat{L}_1(t) = e^{-\hat{L}_0 t} \hat{L}_1 e^{\hat{L}_0 t}$, one obtains

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