

# Dynamics of wave packets for the nonlinear Schrödinger equation with a random potential

Alexander Iomin

Department of Physics, Technion, Haifa 32000, Israel

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The dynamics of an initially localized Anderson mode is studied in the framework of the nonlinear Schrödinger equation in the presence of disorder. It is shown that the dynamics can be described in the framework of the Liouville operator. An analytical expression for a wave function of the initial time dynamics is found by a perturbation approach. As follows from a perturbative solution the initially localized wave function remains localized. At asymptotically large times the dynamics can be described qualitatively in the framework of a phenomenological probabilistic approach by means of a probability distribution function. It is shown that the probability distribution function may be governed by the fractional Fokker-Planck equation and corresponds to subdiffusion.

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In this work the dynamics of an initially localized Anderson mode is considered. It is described by the nonlinear Schrödinger equation (NLSE) in the presence of disorder [1–3]. In the linear one-dimensional case, eigenfunctions are localized [4,5]. This problem is relevant to experiments in nonlinear optics, for example, disordered photonic lattices [6,7], where Anderson localization was found in the presence of nonlinear effects, as well as to experiments on Bose-Einstein condensates in disordered optical lattices [8–12]. It was shown that the presence of nonlinearity leads to an essential complication of a mechanism of localization [1–3,13], and the interplay between disorder and nonlinear effects leads to interesting physics [9,10,14–21]. In particular, the problem of the spreading of wave packets and transmission are not simply related [22,23] in contrast with the linear case. In spite of the extensive research, many fundamental problems are still open. In particular, the spreading of an initially localized wave packet in nonlinear finite chains was challenged in numerical studies with realizations of subdiffusion [16–18] and discrete breathers [15,19–21,24]. The absence of the wave-packet diffusion was observed as well, and this behavior of initially localized wave packets was explained by quasiperiodic solutions in the long-time limit dynamics [24].

The system under consideration is the NLSE

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

where  $\beta$  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, 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  $\omega_k$  is discrete and dense [25].

Therefore, the problem in question is an evolution of an initially localized wave function  $\psi(t=0) = \Psi_{l_0}(x)$ . Projecting Eq. (1) on the basis of the Anderson modes

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

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

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

where  $A(\mathbf{k})$  is an overlapping integral

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

The initial conditions for the system of Eqs. (3) are

$$C_k(t=0) = a_{\omega_k} \equiv a_k = \delta_{k, l_0}. \quad (5)$$

Equations (3) correspond to a system of interacting nonlinear oscillators with the Hamiltonian

$$H = \sum_k \omega_k C_k^* C_k + \beta \sum_{\mathbf{k}} A(\mathbf{k}) C_{k_1}^* C_{k_2}^* C_{k_3} C_{k_4}. \quad (6)$$

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

$$\hat{L} = \frac{1}{i} \{H, \dots\}_{PB} = \frac{1}{i} \left( \frac{\partial H}{\partial C_k^*} \cdot \frac{\partial}{\partial C_k} - \frac{\partial H}{\partial C_k} \cdot \frac{\partial}{\partial C_k^*} \right) (\dots). \quad (7)$$

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

$$\hat{L} = \frac{1}{i} \left[ \frac{\partial H(\mathbf{a}_k, \mathbf{a}_k^*)}{\partial \mathbf{a}_k^*} \cdot \frac{\partial}{\partial \mathbf{a}_k} - \frac{\partial H(\mathbf{a}_k, \mathbf{a}_k^*)}{\partial \mathbf{a}_k} \cdot \frac{\partial}{\partial \mathbf{a}_k^*} \right] \quad (8)$$

and corresponds to the linear equation  $\partial_t \mathbf{C} = \hat{L} \mathbf{C}$ . Thus, the Liouville operator is the following combination:

$$\hat{L} = -i(\hat{L}_0 + \beta \hat{L}_1), \quad (9)$$

where  $\hat{L}_0 = \sum_k \omega_k (a_k \frac{\partial}{\partial a_k} - \text{c.c.})$  and

$$\hat{L}_1 = \sum_{\mathbf{k}} A(\mathbf{k}) \left[ a_{k_1}^* a_{k_2} a_{k_3} \frac{\partial}{\partial a_{k_4}} - \text{c.c.} \right].$$

Here c.c. denotes a complex conjugation. Finally, we obtain that the system of *nonlinear* ordinary differential Eqs. (3) is replaced by a system of *linear* partial differential equations:

$$\partial_t C_k(t) = \hat{L} C_k(t), \quad k = 1, 2, \dots \quad (10)$$

A formal solution of Eq. (14) is the expansion

$$\bar{C}_k(t) = \sum_{n=0}^{\infty} \left[ \frac{t^n}{n!} \hat{L}_1^n a_k \right]_{a_k = \delta_{k,l_0}}. \quad (11)$$

The nonzero contribution to the first power over  $t$  of expansion (11) is due to the term

$$\hat{L}_1^{(0)} = \sum_k A(l_0, l_0, l_0, k) |a_{l_0}|^2 \left( a_{l_0} \frac{\partial}{\partial a_k} - \text{c.c.} \right), \quad (12)$$

while  $(\hat{L}_1 - \hat{L}_1^{(0)})a_k \equiv 0$  is due to initial condition (5). Moreover, the contribution of  $\hat{L}_1 - \hat{L}_1^{(0)}$  without  $\hat{L}_1^{(0)}$  is zero in all powers of expansion (11). For example, the  $n$ th power term for  $k \neq l_0$  is

$$\left[ \sum_{l \neq l_0} A(l_0, l_0, l, l) |a_{l_0}|^2 \partial_{\phi_l} \right]^n a_k = i^n A^n(l_0, l_0, k, k) \delta_{k,l_0}.$$

It has a nonzero contribution only in the power of the  $n+1$  order after the action of the  $\hat{L}_1^{(0)}$  term [26]. Therefore, keeping only the  $\hat{L}_1^{(0)}$  term in Eq. (14) means neglecting  $O(\beta^2 t^2)$  terms in expansion (11). This solution is valid up to a time scale  $t < t_\beta = 1/\beta$ .

To obtain a solution in the framework of this approximation, first we eliminate the linear term  $\hat{L}_0$  from Eq. (10) by substitution

$$\bar{C}_k(t) = \exp(-i\hat{L}_0 t) C_k(t). \quad (13)$$

After this substitution, Eq. (10) reads

$$\partial_t \bar{C}_k = -i\beta \hat{L}_1(t) \bar{C}_k, \quad \hat{L}_1(t) = e^{-i\hat{L}_0 t} \hat{L}_1 e^{i\hat{L}_0 t}. \quad (14)$$

Taking into account that

$$\exp[-i\hat{L}_0 t] = \exp \left[ - \sum_k \omega_k t \frac{\partial}{\partial \phi_k} \right]$$

is the phase shift operator for the complex values  $a_k = |a_k| e^{i\phi_k}$ , we obtain

$$\hat{L}_1(t) = \sum_{\mathbf{k}} A(\mathbf{k}) \left[ \exp(i\Delta\omega t) a_{k_1}^* a_{k_2} a_{k_3} \frac{\partial}{\partial a_{k_4}} - \text{c.c.} \right], \quad (15)$$

where  $\Delta\omega = \omega_{k_1} + \omega_{k_4} - \omega_{k_2} - \omega_{k_3}$ .

Solutions of Eq. (14) for  $k \neq l_0$  are functions which are zero at  $t=0$ . These are

$$\bar{C}_k(t) = a_k + \frac{\beta A_1 |a_{l_0}|^2 a_{l_0}}{\Delta\omega + \beta A_0 |a_{l_0}|^2} (e^{-i\beta A_0 |a_{l_0}|^2 t} - e^{i\Delta\omega t}). \quad (16)$$

Here  $A_0 = A(l_0, l_0, l_0, l_0)$  and  $A_1 \equiv A_1(k) = A(l_0, l_0, l_0, k)$ ,  $k \neq l_0$ , while  $\Delta\omega$  now is  $\Delta\omega = \omega_k - \omega_{l_0}$ . The complex conjugation of Eq. (16) is a solution as well. A solution for  $k=l_0$  is a function of  $\phi_{l_0} - \beta A_0 |a_{l_0}|^2 t$ , which corresponds to the initial conditions Eq. (5):

$$\bar{C}_{l_0}(t) = a_{l_0} \exp(-i\beta A_0 |a_{l_0}|^2 t). \quad (17)$$

Using these analytical solutions for the coefficients  $\bar{C}_k(t)$  and Eq. (13), one obtains the solution of the NLSE (1) in the first order approximation over  $1/\beta$  as a sum

$$\begin{aligned} \psi(t) = & a_{l_0} \exp(-i\omega_{l_0} t) \Psi_{l_0}(x) - 4\beta |a_{l_0}|^2 a_{l_0} \\ & \times \sum_k' A_1(k) \frac{\sin \left[ \frac{\omega_k - \omega_{l_2}}{2} t \right]}{\omega_k - \omega_{l_2}} \sin \left[ \frac{\omega_k + \omega_{l_2}}{2} t \right] \Psi_k(x), \end{aligned} \quad (18)$$

where  $\omega_{l_1} = \omega_{l_0} + \beta A_0 |a|^2$  and  $\omega_{l_2} = \omega_{l_0} - \beta A_0 |a|^2$ , while prime means that  $k \neq l_0$ . When  $\beta \rightarrow 0$ , we have at the asymptotically large times  $t_\beta \rightarrow \infty$  that  $\omega_{l_1} = \omega_{l_2} = \omega_{l_0}$ , and the sinc function is

$$\lim_{t \rightarrow \infty} \frac{2 \sin \left[ \frac{\omega_k - \omega_{l_2}}{2} t \right]}{\omega_k - \omega_{l_2}} = 2\pi \delta(\omega_k - \omega_{l_2}).$$

The sum in Eq. (18) equals zero. Therefore, for  $\beta=0$ , one obtains  $\psi(t) = e^{-i\omega_{l_0} t} \Psi_{l_0}(x)$  that corresponds to a solution of the linear problem.

For nonzero values  $\beta$  and  $t < t_\beta$  the sinc function can be approximated by  $t_\beta$  for  $\omega_k \approx \omega_{l_2}$ . Then summation in Eq. (18) can be estimated by adding and subtracting the term with  $k=l_0$ . Using the definition of the overlapping integrals  $A_1(k)$  and  $\sum_k \Psi_k(x) \Psi_k(y) = \delta(y-x)$ , one obtains an approximation for Eq. (18)

$$\psi(t) \sim \Psi_{l_0}(x) e^{-i\omega_{l_0} t} - 4\beta t [\Psi_{l_0}^3(x) - A_0 \Psi_{l_0}(x)] \sin(\omega_{l_2} t). \quad (19)$$

It means that at  $t < t_\beta$  the wave function is localized and its evolution corresponds to the periodic oscillations with the frequencies  $\omega_{l_1}$  and  $\omega_{l_2}$ . It is worth mentioning that Eq. (18) is valid for both finite and infinite systems (either discrete or continuous).

Consideration of the dynamics beyond  $t > t_\beta$  relates to the calculation of nonzero contributions of operators  $[\hat{L}_1 - \hat{L}_1^{(0)}]^q$  and  $[\hat{L}_1^{(0)}]^p$ , acting on the initial conditions. This combinatorics leads to essential difficulties for analytical treatment. To overcome this obstacle the dynamics of the initially localized states can be considered qualitatively in the framework of a phenomenological probabilistic approach. To explain how the probabilistic approach works, let us demonstrate it first for the localized solution of Eq. (19). One obtains from expansion (11)

$$\sum_{n=1}^{\infty} \frac{(\beta t)^n}{n!} \left[ A_0 \frac{\partial}{\partial \phi_{l_0}} \right]^{n-1} [\hat{L}_1^{(0)}]. \quad (20)$$

The operator  $\hat{L}_1^{(0)}$  corresponds to the population of all states  $\Psi_k$  by transitions from the state  $\Psi_{l_0}$ . Since all the states are localized at certain coordinates  $X_k$ , these transitions correspond to ‘‘jumps’’ of a particle in the  $x$  coordinate space from the position  $X_{l_0}$  to positions  $X_k$ . Therefore the operator  $\hat{L}_1^{(0)}$

corresponds to an instant jump with the jump lengths distribution due to the exponential law in accordance with the overlapping integrals  $A_1(X_k)$ . Another operator  $A_0(\partial/\partial\phi_{l_0})$  changes only the phase of the complex amplitude  $C_k$ . Time duration of the action of this operator is  $t_\beta/n$ , which is different for different powers  $n$ . Now we introduce a probability distribution function (pdf)  $\mathcal{P}(X,t)=|C_k(t)|^2$  to be a particle at position  $X$  at time  $t$ . Since the dynamics of the pdf  $|C_k(t)|^2$  is determined by the same Liouville operator as in Eq. (8), namely,

$$\partial_t |C_k(t)|^2 = \hat{L} |C_k(t)|^2, \quad k = 1, 2, \dots, \quad (21)$$

we obtain that the pdf corresponds to the exponentially localized solution [27]  $\mathcal{P}(X,t) \sim A_1^2(X) \sin^2(\beta A_0 t/2)$  which is relevant to Eq. (19) for  $t < t_\beta$ .

For  $t \gg t_\beta$  Eq. (21) we present in the integral form

$$\mathcal{P}(X,t) = \int_0^t \hat{L} |C_k(t')|^2 dt'. \quad (22)$$

Since, in this terminology, summation over indexes  $\mathbf{k}$  corresponds to integration in space, the right-hand side of Eq. (22) can be rewritten in the form of the integral operator

$$\int_0^t \hat{L} |C_k(t')|^2 dt' \rightarrow \int_0^t dt' \int_{-\infty}^{\infty} dX' \mathcal{P}(X,t;X't') \mathcal{P}(X',t').$$

In this case all combinations of the overlapping integrals  $A(\mathbf{k})$  with corresponding differentiating over  $a_k$  play the role of the kernel or transition probability  $\mathcal{P}(X,t;X't')$  of this transformation. Therefore one has to consider a variety of combinations of the operators

$$\left[ A_0 \frac{\partial}{\partial \phi_l} \right]^{p_1} [\hat{L}_1^{(0)}]^{q_1} [\hat{L}_1 - \hat{L}_1^{(0)}]^{q_2} \left[ A_0 \frac{\partial}{\partial \phi_k} \right]^{p_2} [\hat{L}_1^{(0)}]^{q_3} \dots,$$

where  $p_1 + q_2 + \dots + q_1 + p_2 + \dots = P + Q = n$ . This corresponds to different realizations of instant jumps and waiting times between any two successive jumps. Note that  $[A_0(\partial/\partial\phi_l)]^{p_1}$  corresponds to waiting time of duration  $p_1 t/P$ . To proceed, we follow ideas of so-called continuous time random walk [28,29]. Therefore, the transition probability consists of the pdf of jump lengths  $f(X-X')$  and the pdf of waiting times  $w(t-t')$ . For simplicity, we suppose that  $\mathcal{P}(X,t;X't') = f(X-X')w(t-t')$ .

From the exponential decay of the overlapping integrals on the large scale one obtains that all jump lengths have finite expectation values and variances. Note that  $[\hat{L}_1^{(0)}]^{q_1} [\hat{L}_1 - \hat{L}_1^{(0)}]^{q_2}$  corresponds to a jump which is a composition of random walks (e.g., the simplest realization is presented in [26]). For large  $q_i$  the displacement  $\sum_{l=1}^{q_i} \Delta_l$  has Gaussian distribution due to the central limit theorem. Here  $\Delta_l = X_l - X'_l$  are transition lengths due to operator either  $\hat{L}_1^{(0)}$  or  $\hat{L}_1 - \hat{L}_1^{(0)}$ . Therefore, we can believe that these lengths also are approximately distributed by the Gaussian law  $f(X-X') = \exp(-\Delta^2/2\sigma^2)/\sqrt{2\pi\sigma^2}$  and  $\sigma^2 = \langle \Delta^2 \rangle$ . It is worth stressing that the overlapping integrals do not specify the pdf of waiting times. Therefore,  $w(\tau)$  can be defined from the average value of the waiting times  $\langle \tau \rangle = \int_0^\infty \tau w(\tau) d\tau$ . This value also

can be calculated from the following arguments. For asymptotically large  $t$ , waiting times are  $\tau = pt/P$ , where  $p \in [1, P]$  and  $P \in [1, n]$ . Therefore, one obtains for the average waiting time

$$\langle \tau \rangle = \lim_{n \rightarrow \infty} \frac{1}{n} \sum_{p=1}^n \frac{1}{P} \sum_{p=1}^P \frac{pt}{P} = t.$$

This value diverges with  $t \rightarrow \infty$ , and it means that there are infinitely many realizations of waiting times of the order of  $t$  [30]. To fulfill this condition, the waiting times are distributed by power law  $w(\tau) = \alpha t_\beta^\alpha / \tau^{1+\alpha}$  where  $0 < \alpha < 1$ , such that (see [30])

$$\int_{t_\beta}^\infty \frac{\alpha t_\beta^\alpha}{\tau^{1+\alpha}} d\tau = 1 \quad \text{and} \quad \int_{t_\beta}^\infty \frac{\alpha t_\beta^\alpha}{\tau^{1+\alpha}} \tau d\tau = \infty. \quad (23)$$

It is reasonable to suppose that random jumps and waiting times are independent and identically distributed processes. Therefore this random qualitative description of Markov operator  $\hat{L}$  in Eqs. (11) and (22), respectively, corresponds to the continuous time random walk (see, e.g., Refs. [31–33]) which is described by the fractional Fokker-Planck equation

$$\partial_t \mathcal{P}(X,t) - D_\alpha \partial_t^{1-\alpha} \partial_X^2 \mathcal{P}(X,t) = 0, \quad (24)$$

where  $D_\alpha = \sigma^2/t_\beta^\alpha$  is a generalized diffusion coefficient and  $\partial_t^\nu$  is a designation of the Riemann-Liouville fractional derivative

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

In this case only nonzero initial conditions can be taken into consideration. Without restriction of the generality one can consider  $\mathcal{P}(X,t=0) = \delta(X-X_0)$ . Equation (24) describes subdiffusion [31–33] since  $\alpha < 1$ . From Eq. (24) one obtains for the second moment

$$\langle X^2(t) \rangle = \int_{-\infty}^\infty X^2 \mathcal{P}(X,t) dX = D_\alpha t^\alpha. \quad (25)$$

The transport exponent  $\alpha$  cannot be specified here from the developed probabilistic arguments. In the recent numerical studies of the discrete NLSE [18,34] the exponent  $\alpha$  was found in the range 0.3–0.4.

In conclusion, the dynamics of the initially localized wave packet  $\psi(x,t)$  was studied in the framework of the NLSE in the presence of a random potential. It is shown that the dynamics may possibly be described in the framework the Liouville operator. The interplay between disorder and nonlinearity  $\beta$  leads to the complicated dynamics of the initially localized state  $\psi(x,t=0) = \Psi_{\omega_0}(x)$ . So, the influence of the nonlinearity on the initial time dynamics is weak, and a perturbation theory in  $\beta$  can be developed. An analytical expression for a wave function of the initial time dynamics is found by the perturbation approach. As follows from a perturbative solution, at the initial times  $t < 1/\beta$  the nonlinearity affects mainly the phase of the wave function, while the shape of the wave packet corresponds to the exponential localization due to the overlapping integrals described by Eq. (19).

At asymptotically large times  $t \gg 1/\beta$  the nonlinear effects become important. To evaluate the influence of the nonlinearity on the rate of spreading of the initial wave packet, one can consider the large times asymptotic dynamics of the tails of the packet. In this case, the dynamics can be described qualitatively in the framework of a phenomenological probabilistic approach by means of a probability distribution function  $\mathcal{P}(X,t)=|C_k(t)|^2$ . The last may be governed by the fractional Fokker-Planck Eq. (24) which describes the

asymptotic behavior of the tails of the wave packet; its solution corresponds to subdiffusive spread of the initially localized wave packet.

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