Universal spreading of wavepackets in disordered nonlinear systems

S. Flach, D. O. Kramer, and Ch. Skokos

1Max Planck Institute for the Physics of Complex Systems,
Nöthnitzer Str. 38, D-01187 Dresden, Germany

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In the absence of nonlinearity all eigenmodes of a chain with disorder are spatially localized (Anderson localization). The width of the eigenvalue spectrum, and the average eigenvalue spacing inside the localization volume, set two frequency scales. An initially localized wavepacket spreads in the presence of nonlinearity. Nonlinearity introduces frequency shifts, which define three different evolution outcomes: i) localization as a transient, with subsequent subdiffusion; ii) the absence of the transient, and immediate subdiffusion; iii) selftrapping of a part of the packet, and subdiffusion of the remainder. The subdiffusive spreading is due to a finite number of packet modes being resonant. This number does not change on average, and depends only on the disorder strength. Spreading is due to corresponding weak chaos inside the packet, which slowly heats the cold exterior. The second moment of the packet is increasing as $t^{\alpha}$. We find $\alpha = 1/3$.

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The normal modes (NM) of a one-dimensional linear system with uncorrelated random potential are spatially localized (Anderson localization). Therefore any wavepacket, which is initially localized, remains localized for all time \( |1\). When nonlinearities are added, NMs interact with each other \( 2\). Recently, experiments were performed on light propagation in spatially random nonlinear optical media \( 3\) and on Bose-Einstein condensate expansions in random optical potentials \( 4\).

Numerical studies of wavepacket propagation in several models showed that the second moment of the norm/energy distribution grows subdiffusively in time as $t^\alpha$ \( 3, 4\), with $\alpha \approx 1/3$. Reports on partial localization were published as well \( 5, 6\). Further numerical conductivity studies report Ohmic behaviour at finite energy densities \( 2\).

The aim of the present work is to clarify the mechanisms of wavepacket spreading and localization. We study two models. The Hamiltonian of the disordered discrete nonlinear Schrödinger equation (DNLS)

$$
H_D = \sum_l \epsilon_l |\psi_l|^2 + \frac{\beta}{2} |\psi_l|^4 - (\psi_{l+1} \psi_l^* + \text{c.c.).}
$$

with complex variables $\psi_l$. The random on-site energies $\epsilon_l$ are chosen uniformly from the interval $[-W/2, W/2]$. The equations of motion are generated by $\dot{\psi}_l = \partial H_D/\partial (i\psi_l^*)$.

The Hamiltonian of the quartic Klein-Gordon chain (KG) of coupled anharmonic oscillators with coordinates $u_l$ and momenta $p_l$

$$
H_K = \sum_l \frac{p_l^2}{2} + \frac{\epsilon_l}{2} u_l^2 + \frac{1}{4} u_l^4 + \frac{1}{2W} (u_{l+1} - u_l)^2.
$$

The equations of motion are $\dot{u}_l = -\partial H_K/\partial u_l$, and $\dot{\epsilon}_l$ are chosen uniformly from the interval $[\frac{1}{2}, 3/2]$.

We consider a wavepacket at $t = 0$ which is given by a single site excitation $\Psi_l = \delta_l l_0$ with $\epsilon_{l_0} = 0$ for DNLS, and $x_l = X \delta_l l_0$ with $p_l = 0$ and $\dot{\epsilon}_l = 1$ for KG. The value of $X$ controls the energy $E$ in the latter case.

We will use the DNLS for theoretical considerations, and present numerical results for both models \( 10\). For $\beta = 0$ the problem is reduced to the linear eigenvalue problem $\lambda l_l = \epsilon_l A_l - (A_{l+1} + A_{l-1})$. The eigenvectors $A_{l,l}$ are the NMs, and the eigenvalues $\lambda_l$ are the frequencies of the NMs.

We choose uniformly from the interval $[\frac{1}{2}, 3/2]$.

The equations of motion of (11) in normal mode space read

$$
i \dot{\phi}_\nu = \lambda_l \phi_\nu + \beta \sum_{\nu,\nu_1,\nu_2} I_{\nu,\nu_1,\nu_2,\nu_3} \phi_{\nu_1} \phi_{\nu_2}^* \phi_{\nu_3}
$$

with the overlap integral

$$I_{\nu,\nu_1,\nu_2,\nu_3} = \sum_l A_{\nu,l} A_{\nu_1,l} A_{\nu_2,l} A_{\nu_3,l}.
$$

The variables $\phi_{\nu}$ determine the complex time-dependent amplitudes of the NMs.

The nonlinear frequency shift at site $l_0$ is $\delta \lambda \approx \beta$. Then we expect three qualitatively different regimes of spreading: i) $\beta < \Delta \lambda$; ii) $\Delta \lambda < \beta < \Delta$; iii) $\Delta < \beta$. In case i) the local frequency shift is less than the average spacing between excited modes, therefore no initial resonance overlap of them is expected, and the dynamics may - at least for long times - evolve as the one for $\beta = 0$. In case ii) resonance overlap may happen immediately, and the packet should evolve differently. For iii) the frequency shift exceeds the spectrum width, therefore some renormalized frequencies of NMs (or sites) may be tuned out.

The equations of motion are $\dot{u}_l = -\partial H_K/\partial u_l$, and $\dot{\epsilon}_l$ are chosen uniformly from the interval $[\frac{1}{2}, 3/2]$.
follow norm density distributions \( \nu \) for the DNLS case.

FIG. 1: (color online) \( m_2 \) and \( P \) versus time in log-log plots. Left plots: DNLS with \( W = 4, \beta = 0.1, 1, 4.5 \) ((b)lue, (g)reen, (r)ed). Right plots: KG with \( W = 4 \) and initial energy \( E = 0.05, 0.4, 1.5 \) ((b)lue, (g)reen, (r)ed). The disorder realization is kept unchanged for each of the models. Dashed straight lines guide the eye for exponents 1/3 (\( m_2 \)) and 1/6 (\( P \)) respectively.

The above scenario was observed very clearly. Examples are shown in Fig.1. Regime iii) yields selftrapping (see also Figs.1,3 in [7]), therefore \( P \) does not grow significantly, while the second moment \( m_2 \sim t^\alpha \) with \( \alpha \approx 1/3 \) (red curves). Thus a part of the excitation stays highly localized [8], while another part delocalizes. Note that for large \( \beta \gg \Delta \) (or similar energy for the KG model) almost all the excitation is selftrapped. Regime ii) yields subdiffusive spreading with \( m_2 \sim t^\alpha \) and \( P \sim t^{\alpha/2} \) [8] (green curves). Regime i) shows Anderson localization up to some time scale \( \tau \) which increases with decreasing \( \beta \). For \( t < \tau \) both \( m_2 \) and \( P \) are not changing. However for \( t > \tau \) a detrapping takes place, and the packet starts to grow with characteristics as in ii) (blue curves). Therefore regime i) is a transient, which ends at some time \( \tau \), and after that regime ii) takes over.

FIG. 2: (color online) \( m_2 \) (in arbitrary units) versus time in log-log plots in regime ii) and different disorder strength. Lower set of curves: plain integration (without dephasing); upper set of curves: integration with dephasing of NMs, see text. Dashed straight lines with exponents 1/3 (no dephasing) and 1/2 (dephasing) guide the eye. Left panel: DNLS, \( W = 4, \beta = 3 \) (blue); \( W = 7, \beta = 4 \) (green); \( W = 10, \beta = 6 \) (red). Right panel: KG, \( W = 10, E = 0.25 \) (blue), \( W = 7, E = 0.3 \) (red), \( W = 4, E = 0.4 \) (green). The curves are shifted vertically in order to give maximum overlap within each group.

of resonance with the NM spectrum, leading to selftrapping. The above definitions are highly qualitative, since localized initial conditions are subject to strong fluctuations. Yet, regime iii) is also captured by a theorem presented in [7], which proves, that for \( \beta > \Delta \) the single site excitation can not uniformly spread over the entire (infinite) lattice for the DNLS case.

We order the NMs in space by increasing value of the center-of-norm coordinate \( X_\nu = \sum_l |A^{\nu}_l|^2 \). We analyze normalized distributions \( z_\nu \geq 0 \) using the second moment \( m_2 = \sum_\nu (\nu - \bar{\nu})^2 z_\nu \) and the participation number \( P = 1/\sum_\nu z_\nu \), which measures the number of the strongest excited sites in \( z_\nu \). Here \( \bar{\nu} = \sum_\nu \nu z_\nu \). For DNLS we follow norm density distributions \( z_\nu = |\phi_\nu|^2/\sum_\nu |\phi_\nu|^2 \).

For KG we follow normalized energy density distributions \( z_\nu = h_\nu/\sum_\nu h_\nu \) with \( h_\nu = a_\nu^2/2 + \omega_\nu^2 a_\nu^2/2 \), where \( a_\nu \) is the amplitude of the \( \nu \)th NM and \( \omega_\nu^2 = 1 + (\lambda_\nu + 2)/W \).

We systematically studied the evolution of wavepackets for [11] and [12]. The above scenario was observed very clearly. Examples are shown in Fig.1. Regime iii) yields selftrapping (see also Figs.1,3 in [7]), therefore \( P \) does not grow significantly, while the second moment \( m_2 \sim t^\alpha \) with \( \alpha \approx 1/3 \) (red curves). Thus a part of the excitation stays highly localized [8], while another part delocalizes. Note that for large \( \beta \gg \Delta \) (or similar energy for the KG model) almost all the excitation is selftrapped. Regime ii) yields subdiffusive spreading with \( m_2 \sim t^\alpha \) and \( P \sim t^{\alpha/2} \) [8] (green curves). Regime i) shows Anderson localization up to some time scale \( \tau \) which increases with decreasing \( \beta \). For \( t < \tau \) both \( m_2 \) and \( P \) are not changing. However for \( t > \tau \) a detrapping takes place, and the packet starts to grow with characteristics as in ii) (blue curves). Therefore regime i) is a transient, which ends at some time \( \tau \), and after that regime ii) takes over.

Partial nonlinear localization in regime iii) is explained by selftrapping [11]. It is due to tuning frequencies of excitations out of resonance with the NM spectrum, takes place irrespective of the presence of disorder and is related to the presence of exact \( t \)-periodic spatially localized states (also coined discrete breathers) for ordered [14] and disordered systems [15] (in the latter case also \( t \)-quasiperiodic states exist). These exact solutions act as trapping centers.

Anderson localization on finite times in regime i) is observed on potentially large time scales \( \tau \), and as in iii), regular states act as trapping centers [15]. For \( t > \tau \), the wavepacket trajectory finally departs away from the vicinity of regular orbits, and deterministic chaos sets in inside the localization volume, with subsequent spreading.

The subdiffusive spreading takes place in regime i) for \( t > \tau \), in regime ii), and for a part of the wavepacket also in regime iii). The exponent \( \alpha \) does not appear to depend on \( \beta \). In Fig.2 we show results for \( m_2(t) \) in the respective regime ii) for different disorder strength. Again we find no visible dependence of the exponent \( \alpha \) on \( W \). Therefore the subdiffusive spreading is rather universal.

Let each NM in the packet after some spreading to have norm \( |\phi_\nu|^2 \sim n \ll 1 \). The packet size is then \( 1/n \gg P_{\nu} \), and the second moment \( m_2 \sim 1/n^2 \). We can think of two possible mechanisms of wavepacket spreading. A NM with index \( \mu \) in a layer of width \( P_{\nu} \) in the cold exterior,
which borders the packet, is either heated by the packet, or resonantly excited by some particular NM from a layer with width $P_D$ inside the packet. Heating here implies a (sub)diffusive spreading of energy. Note that the numerical results yield subdiffusion, supporting the nonballistic diffusive heating mechanism.

For heating to work, the packet modes should have a continuous frequency part in their temporal spectrum (similar to a white noise), at variance to a pure point spectrum. Therefore at least some NMs of the packet should evolve chaotically in time. Ref. [6] assumed that all NMs in the packet are chaotic, and their phases can be assumed to be random. With [6] the heating of the exterior mode should evolve as $i\tilde{\delta}_\mu \approx \lambda_\mu \phi_\mu + \beta n^{3/2} f(t)$ where $\langle f(t)f(t') \rangle = \delta(t-t')$ ensures that $f(t)$ has a continuous frequency spectrum. Then the exterior NM is increasing its norm according to $|\phi_\mu|^2 \sim \beta^2 n^4 t$. The momentary diffusion rate of the packet is given by the inverse time it needs to heat the exterior mode up to the momentary diffusion rate of the packet is given by the numerical analysis. For a given NM $\nu$ min $\sim$ to at best a partial outcome. Not all NMs in the packet are chaotic, and dephasing is resonantly excited heated which borders the packet, is either

The perturbation approach breaks down, and resonances in the packet is constant, proportional to $\lambda_{\nu}$, and their fraction within the packet is $\sim \beta n$. Since packet mode amplitudes fluctuate in general, averaging is meant both over the packet, and over suitable long time windows (yet short compared to the momentary inverse packet growth rate). We conclude, that the continuous frequency part of the dynamics of a packet mode is scaled down by $\beta n$, compared to the case when all NMs would be chaotic. Then the exterior NM is heated according to $i\tilde{\delta}_\mu \approx \lambda_\mu \phi_\mu + \beta^2 n^{3/2} f(t)$. It follows $|\phi_\mu|^2 \sim \beta^2 n^{5/2}$, and the rate $D = 1/T \sim \beta^4 n^4$. The diffusion equation $m_2 \sim Dt$ yields

\[ m_2 \sim \beta^{4/3} t^\alpha, \quad \alpha = 1/3 . \]

The predicted exponent is close to the numerically observed one.

In order to clarify the nature of resonant mode pairs, we studied statistical properties of resonant pairs for $W = 4$ with $R_{\nu,\mu} < x_c$. Here $x_c \sim \beta n$ is a cutoff value, which decreases the more the packet spreads (in our simulations we reach values $x_c \sim 0.01$). The corresponding distributions of the overlap integral $|I_{\nu,\nu,\nu,\mu}|$ appear to be invariant, with an average value $\overline{T} \approx 0.05$. At the same time, the distributions of the frequency spacing $\delta = |\lambda_\nu - \lambda_{\mu}|$ favour smaller values the smaller $x_c$ is, with an average spacing $\overline{\delta} = 0.0026$ $(x_c = 0.1)$ and $\overline{\delta} = 0.00026$ $(x_c = 0.01)$. Both NMs from a resonant pair with small $R_{\nu,\mu}$ have a multipeak, or hybrid, structure (inset in Fig.3 right plot). We evaluated the probability density $P(d)$ of the peak distance $d$, estimated with twice the square root of the second moment of the distribution $z_l = A^2_{\nu,\nu} A^2_{\mu,\nu}$ (Fig.3 right plot). Its average increases from $d = 24.8$ for $x_c = 0.1$ to $d = 32.3$ for $x_c = 0.01$. With the help of semiclassical tunneling rate estimates [18] the level splitting of such a hybrid pair can be estimated to be $\delta \sim A^2_{\nu,\nu} l_0$ where $l_0$ marks the midpoint between the peaks. This leads to a splitting of the order of $\delta \sim e^{-d/\xi}$. Therefore, an increase of the packet size goes along with a much weaker increase of the distance $d$, in accord with our explanation from above.

Finally we consider the process of resonant excitation of an exterior mode by a mode from the packet. The number of packet modes in a layer of the width of the localization volume at the edge, which are resonant with a cold exterior mode, will be proportional to $\beta n$. After long enough spreading $\beta n \ll 1$. On average there will be no mode inside the packet, which could efficiently resonate with an exterior mode. Therefore, resonant growth
can be excluded.

The subdiffusive spreading is universal, i.e. the exponent \( \alpha \) is independent of \( \beta \) and \( W \), which are only affecting the prefactor in (6). Excluding selftrapping, any nonzero nonlinearity strength \( \beta \) will completely delocalize the wavepacket and destroy Anderson localization. The exponent \( \alpha \) is determined solely by the degree of nonlinearity, which defines the type of overlap integral to be considered in (6), and by the stiffness of the spectrum \( \{ \lambda_n \} \). We performed fittings by analyzing 20 runs in regime ii) with different disorder realizations. For each realization we fitted the exponent \( \alpha \), and then averaged over all computational measurements. We find \( \alpha = 0.33 \pm 0.02 \) for DNLS, and \( \alpha = 0.33 \pm 0.05 \) for KG. Therefore, the predicted universal exponent \( \alpha = 1/3 \) explains all available data.

Using the above approach, we estimate the growth of the second moment of a wavepacket which is excited on a spectrum \( 0: \) Let us generalize our results to \( d \)-dimensional lattices with nonlinearity order \( \sigma > 0 \). Assuming the wavepacket having norm density \( (n + n_0)^\sigma \) we find the rate \( D \sim \beta^4 (n + n_0)^\sigma \) and therefore the second moment of the wavepacket \( m_2 \sim 1/n^2 \sim \beta^4 (n + n_0)^4 t \). It follows that as long as \( n \gg n_0 \) holds, the wavepacket spreads subdiffusively \( m_2 \sim \beta^3 t^{4/3} \). But once the wavepacket decays such that \( n \sim n_0 \), normal diffusion \( m_2 \sim \beta^3 n_0^2 t \) sets in, in accord with (3). The crossover time scales to infinity as \( n_0 \) is approaching zero.

Let us generalize our results to \( d \)-dimensional lattices with nonlinearity order \( \sigma > 0 \):

\[
\dot{\psi}_t = \xi \psi_t + \beta |\psi_t|^\sigma \psi_t - \sum_{m \in D(l)} \psi_m , \tag{7}
\]

Here \( l \) denotes a \( d \)-dimensional lattice vector with integer components, and \( m \in D(l) \) defines its set of nearest neighbour lattice sites. We assume that (a) all NMs are spatially localized (which can be obtained for strong enough disorder \( W \)), and (b) the property \( W(x \rightarrow 0) \rightarrow \text{const} \neq 0 \) holds. A wavepacket with average norm \( n \) per excited mode has a second moment \( m_2 \sim 1/n^{2/\sigma} \).

Here, \( W \) is independent of \( \sigma \) and \( \beta \). It follows (19)

\[
m_2 \sim (\beta^4 t)^\alpha , \quad \alpha = \frac{1}{1 + d\sigma} , \tag{8}
\]

The exponent \( \alpha \) is bounded from above by \( \alpha_{\text{max}} = 1 \), which is obtained for \( \sigma = 0 \). For the above studied two-body interaction \( \sigma = 2 \) we predict \( \alpha(d = 2) = 1/5 \) and \( \alpha(d = 3) = 1/7 \).

It is a challenging task to determine the bounds of the domains of validity of (8). They will be reached when \( W(x \rightarrow 0) \rightarrow 0 \). Is further growth prohibited then? We think not, because trapping an excitation in a finite volume must generically lead to equipartition on finite times due to nonintegrability. That induces a finite (whatever weak) chaotic component in the dynamics, which will heat the cold exterior. Extending the above resonance scenario, higher order resonances are expected to persist and to yield further (though slower) spreading.

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Dephasing of NMs yields $\tilde{\alpha} = 2/(2 + d\sigma)$. 

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