Absence of Wave Packet Diffusion in Disordered Nonlinear Systems

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We study the spreading of an initially localized wave packet in two nonlinear chains (discrete nonlinear Schrödinger and quartic Klein-Gordon) with disorder. Previous studies suggest that there are many initial conditions such that the second moment of the norm and energy density distributions diverges with time. We find that the participation number of a wave packet does not diverge simultaneously. We prove this result analytically for norm-conserving models and strong enough nonlinearity. After long times we find a distribution of nondecaying yet interacting normal modes. The Fourier spectrum shows quasiperiodic dynamics. Assuming this result holds for any initially localized wave packet, we rule out the possibility of slow energy diffusion. The dynamical state could approach a quasiperiodic solution (Kolmogorov-Arnold-Moser torus) in the long time limit.

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It is well known that Anderson localization occurs for a one-dimensional linear system with uncorrelated random potential. Since all the linear eigenmodes—Anderson modes (AMs)—are localized, any wave packet which is initially localized remains localized for all time. Therefore, there is no energy diffusion [1]. When nonlinearities are added to such models, AMs interact with each other, giving rise to more complex situations [2]. Recently, experiments were performed on light propagation in spatially random nonlinear optical media [3] and on the expansion of a Bose-Einstein condensate in a random optical potential [4,5] (see also related theoterical studies [6,7]).

Numerical studies of wave packet propagation in several models showed that the second moment of the norm or energy distribution grows subdiffusively in time as t^{α} [8– 10], with α in the range 0.3–0.4, though not being accurately determined. The conclusion was that the initial excitation will completely delocalize for infinite times. A corresponding situation has been studied in the simpler case of spatially periodic nonlinear systems. The latter support discrete breathers (DBs), which are spatially localized time-periodic solutions [11] with frequencies outside the frequency spectrum of the linear system. The temporal evolution of a localized wave packet leads to the formation of a DB, while a part of the energy of the wave packet is radiated ballistically to infinity (in the form of weakly nonlinear plane waves) [12]. In that case, the second moment of the energy density distribution diverges as t^2 , falsely suggesting complete delocalization. The participation number P of the norm or energy distribution (or similar quantities) is a well-known measure of the degree of localization [13]. In the case of a periodic nonlinear lattice, P will saturate at a finite value, correctly indicating the formation of a DB.

For nonlinear random systems it was proven rigorously that AMs survive in the presence of nonlinearities as spatially localized and time-periodic solutions [14] with

frequencies which depend on the amplitude of the mode. The allowed frequencies form a fat Cantor set (with finite measure) whose density becomes unity for weak nonlinearity. They are located inside the frequency spectrum of the linear system. Numerical techniques for obtaining these (dynamically stable) intraband DB solutions at computer accuracy were developed [15]. When they are chosen as an initial wave packet, they persist for infinite time and there is no diffusion at all.

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Here we analyze carefully the evolution of the participation number of wave packets as a function of time, in situations where subdiffusion is claimed to exist [8–10]. We study two models. The Hamiltonian of the disordered discrete nonlinear Schrödinger equation (DNLS)

$$\mathcal{H}_{D} = \sum_{n} [\epsilon_{n} |\psi_{n}|^{2} - \frac{1}{2}\beta |\psi_{n}|^{4} - V(\psi_{n+1}\psi_{n}^{*} + \psi_{n+1}^{*}\psi_{n})]$$
(1)

with complex variables ψ_n . The random on-site energies ϵ_n are chosen uniformly from the interval $[-\frac{W}{2}, \frac{W}{2}]$. The equations of motion are generated by $\dot{\psi}_n = \partial \mathcal{H}_D/\partial (i\psi_n^*)$. We choose $\beta = 1$ and V = -1 here and note that varying the norm of the initial wave packet is strictly equivalent to varying β .

The Hamiltonian of the quartic Klein-Gordon chain (KG) is

$$\mathcal{H}_{K} = \sum_{n} \frac{p_{n}^{2}}{2} + \frac{\tilde{\epsilon}_{n}}{2} u_{n}^{2} + \frac{1}{4} g u_{n}^{4} + \frac{V}{2} (u_{n+1} - u_{n})^{2}.$$
 (2)

The equations of motion are $\ddot{u}_n = -\partial \mathcal{H}_K/\partial u_n$, $\tilde{\epsilon}_n = 1 + \epsilon_n(W=1)$, and g=1.

For $\beta=g=0$ both models are reduced to the linear eigenvalue problem $\lambda A_n=\epsilon_n A_n-V(A_{n+1}+A_{n-1})$. The eigenvectors A_n^{ν} are the AMs, and the eigenvalues λ_{ν} are the frequencies of the AMs for the DNLS, while the KG modes have frequencies $\omega_{\nu}=\sqrt{\lambda_{\nu}+1+2V}$.

Hamiltonian (1) [unlike (2)], in addition to conserving the energy, also conserves the total norm $S \equiv \sum_n |\psi_n|^2 = \langle \psi | \psi \rangle$. We use this norm conservation for proving rigorously that initially localized wave packets with a large enough amplitude cannot spread to arbitrarily small amplitudes. The consequence is that a part of the initial energy must remain well focused at all times.

This proof is inspired by [16]. We split the total energy $\mathcal{H}_D = \langle \psi | \mathbf{L} | \psi \rangle + H_{\rm NL}$ into the sum of its quadratic term of order 2 and its nonlinear terms of order strictly higher than 2. Then, \mathbf{L} is a linear operator which is bounded from below (and above). In our specific example, we have $\langle \psi | \mathbf{L} | \psi \rangle \geq \omega_m \langle \psi | \psi \rangle = \omega_m S$, where $\omega_m \geq -2 - \frac{W}{2}$ is the lowest eigenvalue of \mathbf{L} . Otherwise, the higher order nonlinear terms have to be strictly negative.

If we assume that the wave packet amplitudes spread to zero at infinite time, we have $\lim_{t\to +\infty}(\sup_n |\psi_n|) = 0$. Then $\lim_{t\to +\infty}(\sum_n |\psi_n|^4) < \lim_{t\to +\infty}(\sup_n |\psi_n^2|) \times (\sum_n |\psi_n|^2) = 0$ since $S = \sum_n |\psi_n|^2$ is time invariant. Consequently , for $t\to +\infty$ we have $\mathcal{H}_{\rm NL}=0$ and $\mathcal{H}_D \ge \omega_m \sum_n |\psi_n|^2 = \omega_m S$. Since \mathcal{H}_D and S are both time invariant, this inequality should be fulfilled at all times. However, when the initial amplitude A of the wave packet is large enough, it cannot be initially fulfilled because the nonlinear energy diverges as $-A^4$ while the total norm diverges as A^2 only. For example, a wave packet initially at a site 0 ($\psi_n = 0$ for $n \ne 0$ and $\psi_0 = \sqrt{A}$) has energy $\mathcal{H}_D = \epsilon_0 A^2 - \frac{1}{2} A^4$. Consequently, the above inequality is not fulfilled when $A^2 > -2(\omega_m - \epsilon_0) > 0$. Thus such an initial wave packet cannot spread to zero amplitudes at infinite time.

This proof is valid for DNLS models with any W (including the periodic case) and any lattice dimension and can be easily extended to larger classes of DNLS models where the nonlinear terms are either strictly negative, or strictly positive. Note that the large amplitude regime, where we prove that complete energy diffusion is impossible in DNLS models, is precisely the one where subdiffusion is claimed to completely delocalize the wave packet [10]. Thus we disprove these claims.

We performed extensive numerical simulations and characterized the wave packet spreading both in real space for DNLS and normal mode space (Anderson space or AS) for KG. We used initial wave packets with all the energy localized on a single site n_0 , or single AM, or combinations, close to n_0 . Nonlinearity induces diffusion in Anderson space, where each AM is characterized by an amplitude a_{ν} and momentum \dot{a}_{ν} . We analyze distributions $z_l \ge 0$ using the second moment $m_2 = \sum_l (l - l_0)^2 z_l$ and the participation number $P = (\sum_l z_l)^2 / \sum_l z_l^2$, which measures the number of the strongest excited sites in z_l [13]. We order the AMs in space by increasing value of the center-of-norm coordinate $X_{\nu} = \sum_n nA_n^2$. In the results presented here, for the DNLS $z_n = |\psi_n|^2$ is the norm density in real space, and for the KG $z_{\nu} = \dot{a}_{\nu}^2/2 + \omega_{\nu}^2 a_{\nu}^2/2$ is the (harmonic) energy density in AS. The

system size was N = 1000 for KG, and N = 2000 for DNLS. Excitations did not reach the boundaries during the integration time, and results are unchanged when further increasing N.

We show in Fig. 1 the KG energy distribution in AS for a single site excitation with energy E=1, and V=0.25 at times $t=6\times10^7$, 1.2×10^8 . Two rather strongly excited modes are surviving almost unchanged on these time scales. The insets show their eigenvectors, which are well localized, and practically do not overlap.

The same distributions on a logarithmic scale (KG and DNLS) show a chapeau of weaker excited AMs, with exponential tails due to its finite width (Fig. 2). This chapeau is perhaps slowly growing. The subdiffusive growth of the second moment at these times (see Fig. 3) is mainly due to weak excitation of tail modes.

The participation number P(t) is plotted in Fig. 3 for the same runs. We observe no growth. P fluctuates around a value of 7–10, confirming the results in Fig. 1, that we observe a localized state, similar to a DB. Assume that the rest of the weakly excited modes continues to subdiffuse in the chapeau. We use a modified distribution z_{ν} for the KG run, where the 10 strongest mode contributions are zeroed (top panel, green curve). The weak mode participation number is now fluctuating around 70, but again does not grow. Therefore, the chapeau appears not to diffuse, and the observed growth of $m_2 \sim t^{0.3...0.4}$ is not related to a delocalization process. Instead, we find that the packet does not delocalize. Indeed, assuming that the chapeau homogeneously spreads in a subdiffusive way as claimed, it follows that $P(t) \sim t^{\alpha/2}$, which clearly contradicts our observations. We repeated these runs with various initial conditions and disorder realizations with similar results. However, the localization pattern (Fig. 1), and the observed averaged participation number P, fluctuate. Performing an averaging of the final distribution over several realizations [8–10] will therefore completely smear out the sharp localization patterns in the distributions. Closer inspection of

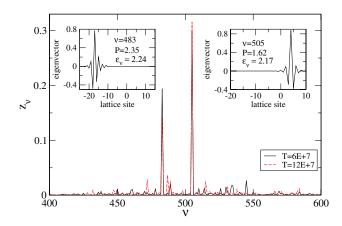


FIG. 1 (color online). KG: energy distribution at $t = 6 \times 10^7$ (black solid line) and $t = 1.2 \times 10^8$ (red dashed line) in AS. Initial single site excitation with energy E = 1, V = 0.25. Insets: profiles of the strongest excited AMs in real space.

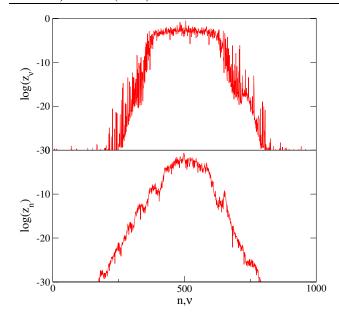


FIG. 2 (color online). Same as in Fig. 1 but on a logarithmic scale. Top panel: KG, $t = 1.2 \times 10^8$, AS. Bottom panel: DNLS, W = 4, $t = 1.2 \times 10^8$, real space.

the evolution of m_2 shows that the exponent α is strongly depending on the time intervals of study, and also on the given disorder realization. There are some indications suggesting that α might decay at long time and even that $m_2(t)$ may saturate, but further clarification may call for very extensive numerical investigations.

Finally we calculated the Fourier transform $I(\omega)$ of P(t) (after $t=2\times 10^7$, over an interval of $\Delta t=2000$), see Fig. 4. We find a quasiperiodic spectrum, which is close to periodic, with no hints of a chaos-induced continuous part. For the KG case the energy densities are quadratic

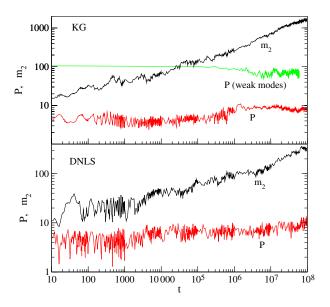


FIG. 3 (color online). P and m_2 vs time, on logarithmic scale. Parameters as in Fig. 2. Top panel: KG, AS. Bottom panel: DNLS, real space.

forms of the AM coordinates; thus the main peak position $\omega \approx 3$ corresponds to a frequency $\omega \approx 1.5$ for the AM coordinate dependence, which coincides with the frequencies of the strong excited Anderson modes in Fig. 1.

Our main result is that in both models (1) and (2), whatever the initial wave packet is (even if it is not fulfilling the conditions for our theorem), and irrespective of the model parameters and the disorder realization, the participation number does not diverge as a function of time as it should in case of subdiffusion (as $t^{\alpha/2}$) but instead fluctuates between finite upper and lower bounds.

Let us now propose an interpretation of our observations. First, it is useful to recall the wave packet behavior in the absence of disorder. When its amplitude is large enough for generating a DB, there is a transient dynamical state which is more or less chaotic, with a broad band time-Fourier spectrum overlapping the spectrum of the linear system. Because of that, a part of the energy of the wave packet is radiated to infinity. With that, the remaining DBlike excitation becomes quasiperiodic first, and finally, it approaches an equidistant spectrum of periodic motion, which completely stops further radiation. The energy which has been emitted spreads towards infinity. Therefore, there is a limit profile which is a localized time-periodic solution—an exact DB. This is the only possibility for the limit profile, in order to avoid radiation. This is an example where the initial wave packet selforganizes in order to stop radiation.

When the system is both random and nonlinear, radiation into the linear spectrum is impossible due to Anderson localization. Nevertheless, the same process starts as before, but the energy emitted by the initial wave packet cannot spread towards infinity since the participation number (full and partial) does not diverge. The following cascading scenario may be true. The core of the wave packet emits a part of its energy which remains within the linear localization length nearby the initial wave packet (due to the nonlinearity-induced coupling between the AMs). The same process should repeat for the emitted energy. A part of it remains localized while another part is reemitted a bit farther from the central site within the localization length and so on. This process of reemission repeats forever and generates a tail for the wave packet which will become much more extended than the localization length. The central amplitude of the wave packet does not tend to zero. The process of energy reemission slows down when the amplitude at the edge of the tail becomes small which explains the very slow numerical convergence. The final result is that at infinite time, the energy (or norm) distribution should converge to a nonvanishing limit profile which is summable since energy (or norm) is conserved. However, it may or may not have a finite second moment, which makes the question of the evolution of the second moment secondary. Unlike the standard DB case in spatially periodic systems, the limit profile is not a timeperiodic solution.

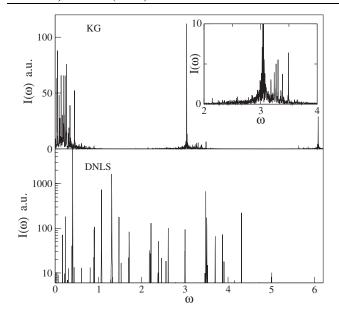


FIG. 4. $I(\omega)$ for KG and DNLS. Parameters as in Fig. 3. Inset: magnification of the main peak.

It was proven rigorously [17–19] that stable spatially localized quasiperiodic solutions with finite energy exist in similar nonlinear models with infinitely many degrees of freedom without or with degenerate linear spectrum. These Kolmogorov-Arnold-Moser (KAM) tori are quasiperiodic DBs which are combinations of Anderson modes surviving in the presence of nonlinearity. Indeed, we find that the Fourier spectrum of the wave packet dynamics becomes quasiperiodic, with narrow peaks and a small background as time grows, suggesting the motion tends to become quasiperiodic (Fig. 4).

If the limit profile becomes a KAM torus, we should also observe that the largest Lyapunov exponent tends to 0 as $t \to +\infty$. Indeed, we find that this Lyapunov exponent drops rapidly during the first expansion part of the wave packet, and slowly further decays, with characteristic values of 10^{-4} at the end of our simulations. The corresponding time scale is 10^4 and 4 orders of magnitude smaller than the simulation times. No chaotic dynamics is observable, and we think that the convergence to the final KAM torus is very slow because the surrounding KAM tori are expected to become dense. We should even expect to enter the regime of Arnol'd diffusion which is expected to be very slow and difficult to investigate both numerically and analytically.

Note that this convergence to a quasiperiodic limit profile can only occur in infinite systems because if the system is finite, the regularization process of the initially chaotic trajectories ends when the packet tails reach the edge of the box. Then, we should expect to get equipartition of the energy after a sufficiently large time and a trajectory which remains chaotic with a nonzero largest Lyapunov exponent.

In summary, we have proved by a rigorous analytical argument, and completed by numerical investigations of

the participation number, that a wave packet in a random nonlinear system does not spread ad infinitum. A limiting quasiperiodic profile is approached, and the slow increase of the second moment of the energy/norm distribution does not violate these findings. It is an open question whether the limiting profile will have a finite or infinite second moment. Thus, we observe absence of diffusion in nonlinear disordered systems. Note that this conclusion can be equally well applied to higher dimensional systems, provided all AMs are localized.

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