Double-humped states in the nonlinear Schrödinger equation with a random potential

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The role of double-humped states in spreading of wave packets for the nonlinear Schrödinger equation (NLSE) with a random potential is explored and the spreading mechanism is unraveled. Comparison to an NLSE with a double-well potential is made. There are two independent effects of the nonlinearity on the double-humped states for the NLSE: coupling to other states and destruction. The interplay between these effects is discussed.

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We consider the discrete nonlinear Schrödinger equation with a random potential in one dimension

$$i\frac{\partial \psi_n}{\partial t} = -\psi_{n+1} - \psi_{n-1} + \epsilon_n \psi_n + \beta|\psi_n|^2\psi_n, \tag{1}$$

where ϵ_n are random potentials chosen uniformly from the interval $[-2,2]$ and β is a positive constant. For $\beta=0$, this is the Anderson model whose eigenstates satisfy the eigenvalue equation

$$E_j u_{j,n} = u_{j,n+1} + u_{j,n-1} + \epsilon_n u_{j,n} \tag{2}$$

and are exponentially localized. Consequently, a wave packet that is initially localized will remain localized in the vicinity of its initial position. A question that is subject to extensive research is whether Anderson localization can survive the nonlinear term $\beta|\psi|^2\psi$ [1] and was recently generalized to a nonlinear form of the form $\beta|\psi|^p\psi$ [2,3]. Numerical simulations indicate that for Eq. (1), Anderson localization is destroyed and subdiffusion takes place [4–8]. Heuristic arguments were developed in order to explain these results [5,7,1], but the detailed mechanism of possible spreading is not clear. Additionally, perturbation results in β indicate that there is some time for which nothing spreads [9,10]. A natural way to study the nonlinear Schrödinger equation (NLSE) (1) is in the basis of the eigenstates of Eq. (2), expanding the wave function in the form

$$\psi_n(t) = \sum_j c_j(t)\exp(-iE_j t)u_{j,n}. \tag{3}$$

For the Anderson model (2), the c_j are constants while for the NLSE (1) they vary according to

$$i\partial_t c_n = \beta \sum_{m_1,m_2,m_3} V_n^{m_1 m_2 m_3} c_{m_1}^* c_{m_2} c_{m_3} \times \exp[i(E_n + E_{m_1} - E_{m_2} - E_{m_3})t], \tag{4}$$

where

$$V_n^{m_1 m_2 m_3} = \sum_k u_{n,k} u_{m_1,k} u_{m_2,k} u_{m_3,k}. \tag{5}$$

Resonances between eigenstates of the linear model (2) provide a reasonable mechanism for spreading in the dynamics generated by Eqs. (1) and (4) and it is the subject of the present paper. A method to find these states is outlined in the third paragraph.

Double-humped states φ_+, φ_- are two eigenstates of Eq. (2) which are localized over the same two sites that are far in real space while their energies are very close. An example for such states appears in Fig. 1. According to Rabi's formula, for the Anderson model (2), if one places (at time $t=0$) a wave packet on the site of one hump and the states are exactly symmetric or antisymmetric with respect to the interchange of the humps, one finds the packet on the other site in time t with the probability

$$P_{12}(t) = \sin^2\left(\Delta E \frac{t}{2\hbar}\right), \tag{6}$$

where ΔE is the difference between the energies of the two double-humped states and the time period is $T_{\text{Rabi}} = \frac{2\pi\hbar}{\Delta E}$. The period is preserved also for the case when the symmetry of the hump interchange is broken, as in the case of the random potential. This mechanism of jumping between sites has proved to be the main mechanism for low-frequency ac conductivity in disordered media [11]. It is expected that its behavior may be strongly affected by the nonlinear term. For a double-well potential, the low-energy states are symmetric and antisymmetric double-humped states, with the humps in the centers of the wells. In the absence of nonlinearity, Eq. (6) holds. But, for sufficiently strong nonlinearity, the wave packet will be confined to the initial well [12,13]. In the present work, we would like to explore if double-humped states contribute to a mechanism of resonant spreading in the NLSE.

In our study, we would like to distinguish between resonant spreading (caused by the double-humped states) and diffusive spreading from one state to its neighbors. For this purpose, we had to find realizations where the humped states

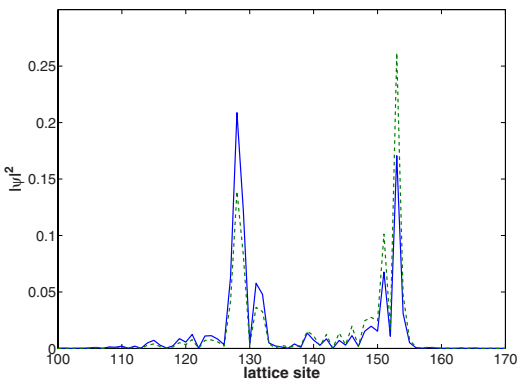

FIG. 1. (Color online) A pair of double-humped states for the linear system (2). The states are marked with blue solid line and green dashed line.

are located far from each other (in comparison to the localization length, in our case $\xi \approx 6$). The probability to find double-humped states with humps located at a distance L is proportional to $\exp(-L/\xi)$ [11] and therefore realizations which couple states located far from each other are very rare (as we are looking for them in a finite region in real space). In order to overcome this problem and create a pool of realizations with double-humped states in some region in real space, we have developed a strategy for "double humps hunting." We choose some random potential having localized eigenstates in the linear case (Anderson localization). We focus on two sites so that we will have double-humped states which are localized on these two sites. These sites will be denoted by O and P in what follows. The Hamiltonian of this realization is diagonalized, which results in a diagonal matrix with eigenenergies on the diagonal. Now, we vary the site energy of the original model on one site (say P) of the two sites mentioned above. According to Feynman-Hellman theorem, when we increase monotonically the potential of a site, its energy is monotonically increasing and we can easily find a point where the two diagonal terms are approximately equal. Since we change the realization, the Hamiltonian is not diagonal anymore and the sites are coupled by matrix elements of the order of $\exp(-L/\xi)$. Taking the potential realization which creates almost identical energies in the diagonal of the Hamiltonian (written in the initial eigenstates basis), we can usually construct double-humped states for this realization. In this way, we found a set of realizations having double-humped states with distance of 25 sites (about four localization lengths in our case) between the humped sites.

After choosing appropriate realizations, we had to know which values of β should be chosen in order to see the influence of the double humps. If we choose very small values of β, the system will behave similarly to the linear case and a wave packet initially localized on one-humped site will oscillate between the humped sites for very long times. However, for large values of β, the linear eigenstates become irrelevant very quickly (compared to the period of the oscillations) and the correlation between the double-humped states is broken before they have a chance to affect the dynamics. Moreover, high values of β suppress the oscillations between the humped states even in the double-well case [13] where there is no mixing with other states. So, we have to choose the β values very carefully. For this purpose, we use a double-well model [14] to set the scale of the effect of β. In particular, we find numerically for each disorder realization a value of $\beta_{1/4}$ for which only $\frac{1}{4}$ of the wave function oscillates between the humped sites O and P when the double-humped states are detached in the computation from all other states. When we run the dynamics of Eq. (1) for double-humped realizations with $\beta=\beta_{1/4}$, we can see clearly the influence of the resonance and we are still able to observe spreading for reasonable times.

In other words, the nonlinearity has two effects: destroying the double-humped states and populating other states of the linear model. In order to distinguish the two effects, we compare to the double-well model with a nonlinear term, where the two lowest-energy states can be assumed isolated from the other states.

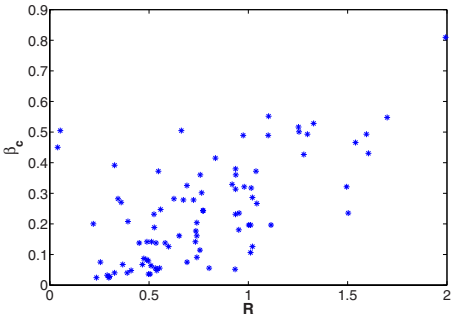

FIG. 2. (Color online) Correlation between R and β_c (blue asterisks).

The difference between the double-well model and Eqs. (1) and (4) is that in the double-well model, only two states participate in the dynamics (see the Appendix) and only these were taken into account for this model. Therefore, numerical calculations for the double-well model are much faster and allow us to estimate the behavior of Eqs. (1) and (4) without performing time consuming (split-step) calculations. In addition, the dynamics in the double-well problem is periodic and gives us the time scale of the oscillations. Deviations of Eq. (1) from the double-well model appear when additional states become involved in the dynamics. This happens, naturally, when we increase β. So, first we should calculate β_c, the largest β for which the double-well model dynamics is still similar to Eq. (1), and make sure that $\beta_c > \beta_{1/4}$ (otherwise, our results for $\beta_{1/4}$ will have no clear meaning for the NLSE). We have located an initial wave packet $u_{0,n}$ around one of the humps (as a superposition of the two double-humped states) at site O. We have followed the population difference between the double-humped states in the double-well model and in the NLSE during one time period T which is numerically calculated for each realization based on the nonlinear double-well model (see Appendix). β_c was defined as the highest β value for which $\frac{1}{T}\int_0^T (w_{\text{double-well}} - w_{\text{NLSE}})^2 dt < 0.001$, where w denotes the population difference. β_c is expected to be high when the overlap between the double-humped states and other states in the system is small and we can see a correlation between β_c and the parameter

$$R^{-1} = \sum_i{}' \left| \frac{V_i^{OOO}}{E_O - E_i} \right|. \tag{7}$$

The index i in the sum runs over all the eigenstates on the lattice except for the two double-humped states. E_O is the energy of the initial wave localized at site O and E_i are the eigenvalues of the system. The numerator is given by Eq. (5). The reasoning for the importance of Eq. (7) is explained in [4,7,8] (where R is defined in a slightly different way) and the correlation to β_c is shown in Fig. 2. The correlation deteriorates when V_i^{OOO} is replaced by other quartic combinations of components of $u_{m_i,n}$ and $u_{0,n}$ [see Eq. (5)].

In order to see the influence of the double-humped states in specific realizations, we should compare them to realizations where such states are broken that will be named "broken realizations." The broken realizations are the same set of

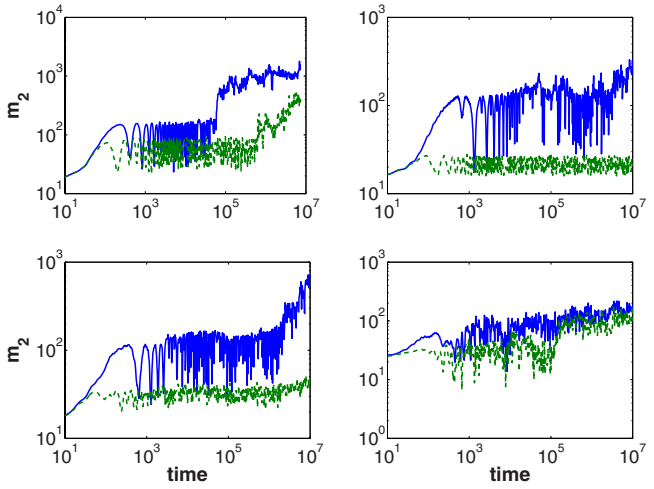

FIG. 3. (Color online) The second moment as function of time for a representative double-humped (solid blue) and broken (dashed green) realizations for wave packets started in the vicinity of O.

realizations as the realizations where double-humped states are found except for one fundamental difference—we have changed the disorder potential in one of the humped sites to be zero, namely, $\epsilon_P=0$, and by this broke the coupling and destroyed the double-humped states without causing qualitative changes to the other eigenstates of the system. For each pair of double-humped and "broken" realizations, we have chosen an initial wave function $\{u_{0,n}\}$ located around O as a superposition of the two double-humped states and followed the evolution of the wave function. The evolution of the wave packet in time was calculated according to Eqs. (1) and (4) with $\beta=\beta_{1/4}$ using the split step method [7]. A quantity which interests us when we measure the spreading of a wave function is the second moment, defined as

$$m_2 = \sum_n (n-\bar{n})^2 |\psi_n|^2, \tag{8}$$

where $\bar{n}=\Sigma_n n|\psi_n|^2$ is the averaged location of the wave function. When we compare the growth in the second moment for double-humped realizations and the broken realizations, we see that the second moment of the double-humped realizations grows faster; when the realizations are selected as was outlined above and in both cases, the initial wave packet is localized at O. Some examples are presented in Fig. 3. We examined 25 realizations of this form and the behavior presented in Fig. 3 is representative of all of them. This indicates that double-humped states do substantially contribute to the spreading process of a wave function more than typical states.

In conclusion, we see that in the presence of nonlinearity that is not too strong, the spreading of a wave packet prepared initially near some site O is substantially stronger if there is a double-humped state with one of its humps near O than if the states peaked near O are single humped. We found that there is a regime of values where β is sufficiently small so that the double-humped structure is preserved but the packet is not only oscillating between the humps but also leaks to other states, leading to spreading. In order to find this nonlinearity regime, we have used the double-well model to isolate the two double-humped states from the other eigenstates of Eq. (2). We found that if β is small enough so that the oscillations between the two states are not suppressed in the double-well model, then the double-humped states will contribute to the spreading for the NLSE. Since double-humped states are suppressed and do not contribute to the spreading for high nonlinearities, we cannot conclude that they dominate the spreading of the NLSE. Exploring what is the dominant mechanism for this problem is left for future a research.

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APPENDIX: DOUBLE-WELL MODEL

In order to predict the response of the double-humped states to variations of β, we first investigate a model where only two states exist: the double-well model. In this way, we avoid the influence of the other states of the NLSE. For this model, the NLSE is

$$i\frac{\partial\Psi(r,t)}{\partial t} = -\nabla^2\Psi(r,t) + [\epsilon(r) + \beta|\Psi(r,t)|^2]\Psi(r,t), \tag{A1}$$

where $\epsilon(r)$ is the double-well potential. It is convenient to write the wave function in the form [15]

$$\Psi(r,t) = \psi_1(t)\phi_1(r) + \psi_2(t)\phi_2(r), \tag{A2}$$

where $\phi_1(r)$ and $\phi_2(r)$ are symmetric and antisymmetric combinations of the double-humped eigenstates (and therefore they are orthogonal) while $\psi_1(t)$, $\psi_2(t)$ are the amplitudes of $\phi_1(r)$, $\phi_2(r)$ at time t. Equation (A1) takes the form

$$i\left[\phi_1\frac{d\psi_1}{dt} + \phi_2\frac{d\psi_2}{dt}\right] = -[\psi_1\nabla^2\phi_1 + \psi_2\nabla^2\phi_2] + [\epsilon(r) + \beta|\Psi(r,t)|^2]\Psi(r,t). \tag{A3}$$

After multiplying both sides by $\phi_1(r)$ (ϕ_1 and ϕ_2 are localized and therefore they can be chosen to be real) and integrating over r, Eq. (A3) becomes

$$\begin{aligned} i\frac{d\psi_1}{dt} = &-\int [\psi_1\phi_1\nabla^2\phi_1 + \psi_2\phi_1\nabla^2\phi_2]dr \\ &+ \int \epsilon[\phi_1^2\psi_1 + \phi_2\phi_1\psi_2]dr \\ &+ \beta\int dr[\psi_1^2\psi_1^*\phi_1^4 + (\psi_1^2\psi_2^* + 2|\psi_1|^2\psi_2)\phi_1^3\phi_2 \\ &+ (2|\psi_2|^2\psi_1 + \psi_2^2\psi_1^*)\phi_1^2\phi_2^2 + |\psi_2|^2\psi_2\phi_2^3\phi_1]. \end{aligned} \tag{A4}$$

Following [14], it is convenient to write Eq. (A4) as

$$\frac{d\psi_1}{dt} = -i(\omega_1 + \Omega_1|\psi_1|^2)\psi_1 - iK\psi_2 - i(2A_1\psi_2 + A_1\psi_1^2\psi_2^* + B\psi_2^2\psi_1^* + A_2|\psi_2|^2\psi_2 - 2A_1|\psi_2|^2\psi_2), \tag{A5}$$

where

$$\omega_1 = -\int (|\nabla\phi_1|^2 + \epsilon\phi_1^2 + 2\beta\phi_1^2\phi_2^2)dr,$$

$$\Omega_1 = -\beta\int (\phi_1^4 - 2\phi_1^2\phi_2^2)dr,$$

$$K = -\int (\nabla\phi_1\nabla\phi_2 + \epsilon\phi_1\phi_2),$$

$$A_1 = -\beta\int \phi_1^3\phi_2 dr, \quad A_2 = -\beta\int \phi_2^3\phi_1 dr,$$

$$B = -\beta\int \phi_1^2\phi_2^2 dr, \tag{A6}$$

and we have used the relation $|\psi_1|^2+|\psi_2|^2=1$. In a similar way,

$$\frac{d\psi_2}{dt} = -i(\omega_2 + \Omega_2|\psi_2|^2)\psi_2 - iK\psi_1 - i(2A_2\psi_1 + A_2\psi_2^2\psi_1^* + B\psi_1^2\psi_2^* + A_1|\psi_1|^2\psi_1 - 2A_2|\psi_1|^2\psi_1), \tag{A7}$$

where

$$\omega_2 = -\int (|\nabla\phi_2|^2 + \epsilon\phi_2^2 + 2\beta\phi_1^2\phi_2^2)dr \tag{A8}$$

and $\Omega_2=-\beta\int(\phi_2^4-2\phi_1^2\phi_2^2)dr$. In order to establish the connection with the double-humped states of Eq. (1), the coefficients of Eqs. (A6) and (A8) were taken from the Schrödinger Eq. (1). First we have expressed these coefficients for the linear case $\beta=0$ where only ω_1, ω_2, and K do not vanish. For this purpose, we find φ_+ and φ_-, the double-humped eigenstates of Eq. (1) for $\beta=0$. The amplitudes $\psi_1(t)$ and $\psi_2(t)$ of the symmetric and antisymmetric combinations

$$\phi_1(r) = \frac{1}{\sqrt{2}}(\varphi_+ + \varphi_-), \tag{A9}$$

$$\phi_2(r) = \frac{1}{\sqrt{2}}(\varphi_+ - \varphi_-) \tag{A10}$$

satisfy the Schrödinger Eqs. (A5) and (A7). Therefore, when we write the Hamiltonian (1) in a basis composed from ϕ_1 and ϕ_2 in addition to all the single-humped eigenstates of Eq. (1), K will appear as an off-diagonal term which couples ϕ_1 and ϕ_2 while ω_1 and ω_2 will appear as diagonal terms. In the nonlinear case, K stays the same while $\omega_{1,2}=\omega_{1,2}^{linear} - 2\beta\int\phi_1^2\phi_2^2 dr$. In order to find the corrections to $\omega_{1,2}$ for the nonlinear Hamiltonian and to calculate all the other coefficients (A6) and (A8), we find numerically the vectors ϕ_1 and ϕ_2 with the help of Eqs. (A9) and (A10) from Eq. (1) as explained above.

It is convenient to follow the dynamics described by the variables $u=\psi_1\psi_2^*+\psi_2\psi_1^*$, $v=-i(\psi_1\psi_2^*-\psi_2\psi_1^*)$, and $w=|\psi_1|^2 - |\psi_2|^2$. After some simple procedures, we obtain a vector equation of the motion [14],

$$\frac{d\vec{\rho}}{dt} = \vec{\rho}\times\vec{T}, \tag{A11}$$

in which $\vec{\rho}=(u,v,w)$ is a vector characterizing the state of the coupled system on the unit sphere, i.e., $u^2+v^2+w^2=1$, and $\vec{T}=(T_1,T_2,T_3)$, where

$$T_1 = \omega_1 - \omega_2 + \frac{1}{2}\Omega_1(1+w) - \frac{1}{2}\Omega_2(1-w) + (A_1 - A_2)u, \tag{A12}$$

$$T_2 = -Bv, \tag{A13}$$

$$T_3 = 2K + 2(A_1 + A_2) + Bu - A_1(1-w) - A_2(1+w). \tag{A14}$$

It is easy to find (numerically) $w(t)$ which gives us the time period and the amplitude of the double-well oscillations. For small nonlinearities, these results are good estimations of the NLSE behavior on a lattice. In this work, we have used Eq. (A11) to find $\beta_{1/4}$ values. For this purpose, we have chosen an initial value for w which represents a wave packet localized around site O. Following the dynamics of $w(t)$ for different values of nonlinearity β, we have found the maximal β for which at least $\frac{1}{4}$ of the wave packet is oscillating between sites O and P. This β is $\beta_{1/4}$.

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