Analytic Conditions for Targeted Energy Transfer between Nonlinear Oscillators or Discrete Breathers

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Abstract

It is well known that any amount of energy injected in a harmonic oscillator which is resonant and weakly coupled with a second harmonic oscillator, tunnels back and forth between these two oscillators. When the two oscillators are anharmonic, the amplitude dependence of their frequencies breaks, in general, any eventual initial resonance so that no substantial energy transfer occurs unless, exceptionally, an almost perfect resonance persists. This paper considers this interesting situation more generally between two discrete breathers belonging to two weakly coupled nonlinear systems, finite or infinite. A specific amount of energy injected as a discrete breather in a nonlinear system (donor) which is weakly coupled to another nonlinear system (acceptor) sustaining another discrete breather, might be totally transferred and oscillate back and forth between these donor and acceptor breathers. The condition is that a certain well defined detuning function is bounded from above and below by two coupling functions. This targeted energy transfer is selective, i.e., it only occurs for an initial energy close to a specific value. The explicit calculation of these functions in complex models with numerical techniques developed earlier for discrete breathers, allows one to detect the existence of possible targeted energy transfer, between which breathers, and at which energy. It should also help for designing models having desired targeted energy transfer properties at will. We also show how extra linear resonances could make the energy transfer incomplete and irreversible. Future developments of the theory will be able to describe more spectacular effects, such as targeted energy transfer cascades and avalanches, and energy funnels. Besides rather short term applications for artificially built devices, this theory might provide an essential clue for understanding puzzling problems of energy kinetics in real materials, chemistry, and bioenergetics.
1 Introduction: a brief review of discrete breather theory

It is a great pleasure to contribute to the volume dedicated to Professor E. N. Economou with work that attempts to bridge the gap between localization and propagation in complex discrete systems. In the long-standing contributions of Prof. Economou, localization is induced via quenched disorder while propagation is a result of either higher dimensions or nonlinearity. In our present work, coherent energy transfer occurs as a result of judicious interlocking of disorder with nonlinearity and an appropriate exploitation of the concept of nonlinear resonance. Resonance is the basic principle for energy propagation in spatially periodic linear systems. The simplest example in textbooks is obtained for two coupled identical harmonic oscillators. In this case, it is well known that any amount of energy deposited on one of the two oscillators tunnels back and forth between these two oscillators with a frequency proportional to the coupling. On the other side, in order to keep the energy localized in a given harmonic oscillator, the resonance between this oscillator and the other harmonic oscillators must be broken. This situation can be reached in a harmonic infinite system for an impurity mode or, more generally, by breaking translational invariance, for instance through strong enough disorder or by quasiperiodic modulations. Roughly speaking, finding a harmonic oscillator that is well resonant within the frequency interval $\delta \omega$ with another oscillator generally requires to go far from the initial one, typically at a distance $\delta \omega^{-1/D}$ in a model at dimension $D$. But since the effective coupling between these two almost resonant oscillators drops exponentially as a function of their distance, the resonance is generally not sufficient for allowing a substantial energy transfer. This effect blocks energy propagation and causes the Anderson localization of the eigenmodes [1,2].

When the system becomes nonlinear, this picture is drastically changed because the frequency of an anharmonic oscillator depends on its amplitude. Concerning the time-periodic solutions, we have shown that nonlinearity plays a “double game” [3–5]. First, by adjusting appropriately the amplitude of the nonlinear oscillators, nonlinearity could restore resonances between anharmonic oscillators which were lost in the linearized system. Indeed, small nonlinearity is sufficient to generate exact extended solutions in random systems while the whole linear spectrum is localized. Although these solutions appear spatially intermittent, they can propagate some nonvanishing amount of energy (much smaller though than standard uniform plane waves). Their existence demonstrates that random systems with a small nonlinearity can propagate energy while the same systems without nonlinearity cannot. Second, with different amplitudes for the nonlinear oscillators, nonlinearity can also maintain (or magnify) the lack of resonance of a localized vibration with the other modes. Thus, the same system can also sustain exact localized nonlinear modes. Moreover, the existence of these modes may not require random-
ness. Mode localization can also be achieved in a nonlinear spatially periodic system provided the frequency and its harmonics are nonresonant with the extended linear modes (i.e., they do not belong to the linear phonon band). These modes are called discrete breathers [6,7].

Discrete Breathers (DBs), also called Intrinsic Localized Modes, are spatially localized time-periodic solutions of discrete classical nonlinear dynamical systems which could be finite or infinite in arbitrary dimension, spatially periodic or random, etc. Many early works predated their discovery. For example, polarons are nonlinear objects belonging to the family of DBs introduced long ago by Landau [8]. The concept of local modes was independently introduced in chemistry also long ago [9–11] for small molecules. In that case, discreteness was implicitly necessary. Incidentally, these solutions are recognized to be important for understanding the quantization of molecular vibrations [12].

Renewed interest on these nonlinear concepts but within the framework of integrable models which have exceptional (but sometimes physically misleading) properties started during the 1970’s. The self-trapping equation introduced later in the mid-1980’s already revealed some features characteristic of DBs but only in special cases (see a recent interesting review by A. Scott [13]). Many interesting physical ideas of applications in physics were proposed, but were limited by flaws of the underlying theories. They could be reconsidered and amended using the more universal concept of DB.

It was only in 1988 that Sievers and Takeno [6] claimed the existence of DBs as long lifetime solutions in general models, finite or infinite, on the basis of approximate analytical and numerical calculations (see review [14]). Actually, their claims were definitely confirmed later by a rigorous proof of their existence as exact solutions in Klein-Gordon systems under rather general conditions of nonresonance [15]. Moreover, DBs were proven to be linearly stable and robust to model perturbations (i.e., not restricted to specific models). Subsequently, the scope of validity of this proof has been extended to more general models with optical or acoustic phonons and with arbitrary complexity in any dimension [16–20]. This general theory also brought new methods for systematic and accurate numerical investigations [21].

The existence of DBs essentially requires discreteness and nonlinearity (randomness is not necessary despite the fact that DBs could persist in its presence). Thus, these conditions fully take into account two essential characteristics of real matter. It is discrete, because it is made of atoms, and nonlinear, because the interatomic potentials are nonlinear. DBs may exist generically as exact solutions when the frequency of a local mode and all of its harmonic frequencies either belong to phonon gaps or are above the whole phonon spectrum. Otherwise, these local modes would radiate away their energy by the fundamental frequency or some harmonics and thus survive only over a finite
time. However, if the radiation occurs by high order harmonics, the lifetime of this local mode at 0 K may be long but nevertheless finite. Thus, it is clear that DB existence as exact solution crucially depends on the gap structure of the phonon spectrum. An exact DB solution at a given frequency (or action) may exist in one model but may disappear in another very similar model just because some high order harmonic becomes resonant with phonons. Another essential property is that DBs come as one parameter family which can be parametrized by their frequency (or, better, their action which can be used for semiclassical quantization) [1].

DBs may have a lot of other amazing properties not fully explored yet but which depend on the considered models. They scatter elastically linear phonons (without energy exchange) like static impurities. They may filter phonon noise coloring the spectrum [22]. Inelastic interactions with small amplitude phonons (generally) occur at higher order. Then, DBs may slowly decay while in other situations unexpectedly they may grow [23] by pumping energy from the background. They are generally pinned to the lattice but may become highly mobile in some special situations [24] and then they contribute to energy propagation instead of trapping it. They can also react by fission or fusion [25].

Because they are exact solutions at 0 K, and the interaction between DBs drops very fast as a function of their distance, at low temperature the only physical way for a quasi-isolated DB to decay is by the small interaction with its own phonon background. Actually, the real spectrum of this phonon background is essential for determining the true DB lifetime. Phenomenological interactions modeled for example by a white Langevin noise and damping (or, equivalently, a coupling with a large collection of harmonic oscillators with a uniform structureless spectrum), systematically destroy the DB as an exact solution simply because the phonon spectrum extends to infinity without gaps. Thus, the lifetime obtained by such approaches widely used in physics, is nothing but the result of the assumptions that are made and might be physically misleading.

Consequently, when the temperature is sufficiently low (compared to the DB energy) and the DBs sufficiently far apart, energy trapping by DBs may be substantial and persist over extremely long time in apparent violation of the standard Fourier law. Therefore, the most important feature characterizing (pinned) DBs (and distinguishing them from ordinary phonons and local modes), is that in appropriate conditions where they can be created (by

1 The DBs we discuss here are extraband DBs, to be distinguished from intraband DBs defined in Refs.[3–5]. Intraband DBs may only exist when the phonon modes are spatially localized in quasicontinuation of the Anderson modes. The essential difference is that the frequencies (or harmonics) of intraband DBs lie inside the phonon spectrum but then these frequencies are restricted to fat Cantor sets. As a consequence, the intraband DBs do not form continuous families versus frequency.
external excitations or by other processes breaking initially the thermal equilibrium), they may spontaneously appear and persist as spatially localized dynamical structures with unusually long lifetime.

Numerical simulations clearly demonstrate that in systems where linearly stable DBs exist, they show up spontaneously under thermal shocks [26,27] or when starting from initial states far from thermodynamic equilibrium [28]. They trap energy over very long time and generate unusual energy relaxation (stretched exponentials). This long lifetime of DBs should be relevant for understanding many anomalous energy relaxations especially in disordered matter (glasses, polymers, biopolymers) which up to day do not have yet truly satisfactory interpretations.

Up to now, experimentalists did not pay much attention to this new paradigm in physics. One of the reasons might have been that DBs could be easily confused with early concepts inherited from the theory of integrable systems such as (nondiscrete) breathers and solitons (perhaps because of the terminology). Otherwise, the localization or the anomalous relaxation of energy observed in real experiments, are usually interpreted by randomness, metastable states etc.

In spite of the general belief, some experimentalists recently observed DBs with different techniques and in different systems, for example in coupled nonlinear optical wave guides [29,30], in coupled arrays of Josephson junctions [31,32], in some nonlinear materials [33], in magnetic systems [34] and even possibly in myoglobin [35].

After this brief review we now come to the main aim of this paper which is to present a novel property termed targeted DB energy transfer that enables possible perfect transfer of energy between two DBs. This idea was already briefly suggested in [36] and considered in term of phase dynamics in [37]. We give here a precise analytic treatment of this effect through a generalized dimer model. We should point out that our results do not agree with the scenario imagined in [37]. Although, this phenomenon can only exist in appropriate models and for appropriate DBs, it could become the key for understanding puzzling phenomena of well-focused energy transfer in physics and especially in biomolecules.

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2 They only exist in very special integrable models and, moreover, their properties are fragile to perturbations in contrast with the highly robust DBs.
2 Generalized Dimer Model for the Energy Transfer between two
Discrete Breathers

The energy tunneling between two resonant harmonic oscillators is described
through the linear superposition of the symmetric and antisymmetric modes.
This is of course not possible when the oscillators are (strongly) anharmonic.
We show in this section that we can model the energy transfer in this case
by an integrable generalized dimer model. We shall study more generally the
energy transfer between two DBs so that the energy transfer between two
oscillators becomes a particular case.

We consider an arbitrary anharmonic system (D) (finite or infinite) called
donor molecule described by some set of variables and conjugate variables
\{p^D_i, q^D_i\} and a Hamiltonian \(H_D(\{p^D_i, q^D_i\})\). We assume that this molecule can
sustain DBs and select one of them called donor DB.

As we know, DBs come as continuous family parametrized for example through
their action (which is \(I_D = \int \sum_i p_i d q_i / 2\pi\) integrated on the loop representing
the DB in the phase space). Then, DB’s energy \(H_D(I_D)\) becomes a function
of action and its frequency is \(\omega_b = dH_D/dI_D\). We also assume that this DB
family is gapless, i.e., \(H_D(I_D) \to 0\) for \(I_D \to 0\) when the DB is vanishing at
zero energy\(^3\).

We consider a second arbitrary anharmonic system (A) (finite or infinite)
called acceptor molecule with properties similar to the donor molecule. We
select on the acceptor molecule a family of acceptor DB with action \(I_A\) and
energy \(H_A(I_A)\). As with the donor system, we assume that acceptor DB is also
gapless.

Subsequently, we introduce a weak coupling between the donor molecule and
the acceptor molecule. These two systems could physically represent two in-
dependent molecules or two linked parts of the same macromolecule relatively
far from one another. The weak coupling interaction could either come from
contact (hydrogen bonds, van der Waals forces), from (screened) Coulomb
interactions, could be mediated by the solvent, or come directly from the in-
termediate link of the macromolecule if any, etc.

We would like to find the conditions for complete transfer of the energy of
a DB from donor molecule with action \(I_T\), after some time, to a DB on the
acceptor molecule. Since the coupling is weak, this transfer will be slow. Then,
at any intermediate time \(t\), the dynamics of the system will be well described

\(^3\) Note that DBs in space-periodic systems in more than one dimension cannot be
gapless \[38\] but we essentially consider here systems where the space periodicity is
broken by the presence of the donor or acceptor sites.
over a time scale long compared to the period by two DBs with action $I_D$ on the donor and $I_A$ on the acceptor. This solution is well represented in terms of loop dynamics [25] as an almost invariant closed loop in the phase space which projects like DBs on the isolated molecules in the complementary donor and the acceptor subspace. Thus, the action of this loop is nothing but the sum of the actions of these two isolated DBs. Because of the weak coupling between donor and acceptor systems, this loop evolves slowly in the phase space. Liouville theorem states that the action of a loop evolving in the phase space is time-constant. Thus, we have

$$I_T = I_D + I_A. \quad (1)$$

Another necessary condition is the conservation of the total energy $E_T = H_D(I_D) + H_A(I_A)$ yielding

$$H_D(I_D) + H_A(I_T - I_D) = E_T \quad (2)$$

which is a function independent of $I_D$ for $0 \leq I_D \leq I_T$. Differentiating (2) with respect to $I_D$ readily yields that the frequencies $\omega_D = dH_D/dI_D$ of the donor DB and $\omega_A = dH_A/dI_A$ remain identical during the energy transfer, i.e., the two DBs remain resonant.

Actually, this condition (2) does not need to be perfectly fulfilled (since the coupling energy should also be involved in the energy conservation) but we shall assume that it is almost fulfilled. We wish to describe the coupled donor-acceptor system through an effective Hamiltonian expressing the energy transfer only as a function of the variables $I_D$ and $I_A$ and their conjugate variables $\theta_D$ and $\theta_A$.

However, the restriction to two pairs of variables will be valid only if condition (2) is not fulfilled precisely or even approximately by any other DB of the acceptor molecule for the same total action $I_T$ and the same total energy $E_T$. In other words, we assume that the acceptor DB is unique. We shall assume also, but only for simplicity, that the donor DB is unique. This condition is imposed for avoiding more complex situations with bifurcating transfer of energy to two or more acceptor DB. It is in principle fulfilled for molecules without any special symmetry.

A priori, the small coupling energy, $C(I_D, I_A, \theta_D, \theta_A)$ depends on $I_D \equiv I_0 + I$ and $I_A \equiv I_0 - I$, on the angle difference $\theta = \theta_D - \theta_A$ (conjugate to $I$) supposed to vary slowly because of the above assumptions (weak coupling and almost resonance), and on the total angle $\theta_0 = \theta_D + \theta_A$ (conjugate to $I_0$) which on

4 Otherwise we should have to involve other donor DBs in the return transfer. This problem, which is also interesting and related to energy funnelling, will be treated elsewhere.
the opposite varies fast at the scale of the DB periods. It is then justified to average the coupling over the fast variable \( \theta_0 \) (which varies practically linearly over relatively long time) and drop the \( \theta_0 \) dependence. Next, it is convenient to split the coupling energy as a sum

\[
C(I_0, I, \theta) = C_0(I_0, I) + C_1'(I_0, I, \theta),
\]

where \( C_0(I_0, I) \) is the average of \( C(I_0, I, \theta) \) over \( \theta \), while the average of \( C_1'(I_0, I, \theta) \) over \( \theta \) is zero.

Then, the effective Hamiltonian regarding the two DBs of the coupled molecules can be written in the form

\[
\mathcal{H}(I_0, I, \theta) = H_0(I_0, I) + V(I_0, I, \theta)
\]

where \( H_0(I_0, I) = H_D(I_0 + I) + H_A(I_0 - I) + C_0(I_0 + I, I_0 - I) \) and \( V(I_0, I, \theta) = C_1'(I_0 + I, I_0 - I, \theta) \) which has zero average with respect to \( \theta \). Moreover, for \( I = \pm I_0 \), either the acceptor DB or the donor DB vanishes which removes any \( \theta \) dependence. Then, \( V(I_0, \pm I_0, \theta) = 0 \).

Since this Hamiltonian does not depend on \( \theta_0 \), \( \dot{I}_0 = -\partial\mathcal{H}/\partial\theta_0 = 0 \), which implies that the total action \( I_D + I_A = 2I_0 \) is conserved. Because of the averaging over the fast variable \( \theta_0 \), \( \theta \) essentially represents the difference between the DB phases on the donor and acceptor molecules. Effective Hamiltonian (3) with \( I_0 \) a constant parameter is nothing but the Hamiltonian for the DB phase (see ref. [37] for a formal theory of phase dynamics).

For donor and acceptor molecules with explicitly given Hamiltonians and coupling, it is possible to calculate numerically this effective Hamiltonian and thus to predict the possibility of complete targeted transfer. This Hamiltonian can be formally written as a generalized Discrete Nonlinear Schrödinger (DNLS) dimer model when defining the complex variables

\[
\psi_D = \sqrt{I_0 + I} \ e^{-i(\theta_0 + \theta)/2}
\]

at the donor site \( D \) and

\[
\psi_A = \sqrt{I_0 - I} \ e^{-i(\theta_0 - \theta)/2}
\]

at the acceptor site \( A \). Then, the conservation of the total action \( I_0 \) is equivalent to the conservation of the total norm \( |\psi_D|^2 + |\psi_A|^2 \). This approach could be easily modified when the frequency of one of the two DBs is resonant with a harmonic of the other one. We could then analyze more accurately for DBs the problem of Fermi resonance usually considered for quasilinear modes. This approach can be also extended when there are more than two weakly coupled nonlinear oscillators. We then obtain a generalized DNLS model on a lattice. It is also extendable for quantum anharmonic oscillators. We then obtain a quantum generalized DNLS model which is nothing but a boson model on a lattice. In this case, the assumption of conservation of the classical action becomes conservation of the number of bosons and nonlinearity becomes many-body interactions. On this basis we can generalize early calculations based on rotating wave approximations, which were initially restricted to specific models (e.g. theory of the Davydov soliton, see [13]). Expanding the obtained effective Hamiltonians at the lowest significant order simply yields standard quartic DNLS models. However, we also learn from our approach that these approximations are only
valid in the weak coupling limit, i.e., close to an anticontinuous limit, which was not clearly stated in the early approaches. It is thus inconsistent to describe later these DNLS models from their continuous limit where they are integrable. These extended problems will be discussed later in further publications.

3 Targeted energy transfer solutions in the generalized dimer model

We search for solutions of the dynamical system defined by Hamiltonian (3), which correspond to a total energy transfer. These solutions are such that if at the initial time all the energy is on the donor molecule, i.e., \( I_D(0) = 2I_0 \neq 0 \) and \( I_A(0) = 0 \), it will be completely transferred at a later time \( t_T \) on the acceptor molecules, i.e., \( I_D(t_T) = 0 \) and \( I_A(t_T) = I_D(0) \). Then, \( I(0) = I_0 \) and \( I(t_T) = -I_0 \). We say by definition that when this situation occurs, we have targeted energy transfer.

Since for \( I = I_0 \), as well as for \( I = -I_0 \), the angle \( \theta \) is undetermined, the topology of the phase space defined by the conjugate variables \((I, \theta)\) is the one of a 2D sphere represented in cylindrical coordinates \( \theta \). Any point \( P \) of this sphere can be represented by the two coordinates which are the angular coordinate \( \theta \) (longitude) of its projection in the \((x, y)\) plane and \( I \) is its \( z \) coordinate (latitude). The poles of the sphere are the points where \( I = \pm I_0 \).

There are two time invariants for this Hamiltonian which are \( I_0 \) and the total energy \( E \). Then,

\[
V(I_0, I, \theta) + H_0(I_0, I) = E
\]

defines contour lines on the sphere \((I, \theta)\) which represent the orbits of the dynamical systems in the 2D phase space.

Since these contour lines are closed loops, \( I(t) \) is time-periodic. Actually, the solution in the original system consisting of the coupled donor and acceptor molecules, is a two site DB the period of which varies periodically with the same period as \( I(t) \). Thus, the global solution is quasiperiodic.

The dynamical solutions of the system can be classified in two types. Type 1 corresponds to the orbits on the sphere which are homotopic to zero, i.e., that can be continuously shrunk to zero without crossing a pole. For these trajectories, \( \theta \) oscillates between two bounds. The limit case where \( \theta \) does not

\[\text{The topology of this sphere was also considered in [37] for two weakly coupled pendula.}\]
oscillate, corresponds to exact DBs. They correspond to extrema of the energy (4) on the sphere at fixed $I_0$.

Type 2 corresponds to the orbits which turn around the axis connecting the two poles. Then, $\theta$ rotates by $2\pi$ around the sphere at each period of $I(t)$.

A trajectory corresponding to a targeted energy transfer between the donor DB and the acceptor DB is such that along the orbit, $I(t)$ varies between $I_0$ and $-I_0$. Thus, it is an orbit connecting directly the two poles of the sphere $(I, \theta)$. It is straightforward to see that a necessary and sufficient condition for having a targeted transfer solution at action $I_0$, is that the system only accepts type 1 solutions at this total action.

Let us explicit more carefully, this condition. Since the two poles must be at the same energy, we have

$$H_0(I_0, I_0) = H_0(I_0, -I_0) = E.$$  \hspace{1cm} (5)

At the uncoupled limit $V(I_0, I, \theta) \equiv 0$, this condition is fulfilled when (2) is fulfilled. If $H_0(I_0, I)$ is not constant, the contour lines are just circles at constant $I$ and are of type 2 and thus, we do not have targeted energy transfer.

When the coupling is turned on, targeted energy transfer requires that there exists an action $I_T$ associated with an energy $E_T$ such that Eq.(5) is fulfilled for $I_0 = I_T/2$ and $E = E_T$. Then, for $E = E_T$, this closed orbit on the sphere is defined by implicit equation

$$V(I_T/2, I, \theta) = H_0(I_T/2, \pm I_T/2) - H_0(I_T/2, I) = \epsilon_T(I).$$ \hspace{1cm} (6)

Function $\epsilon_T(I)$ vanishes at the poles for $I = \pm I_T/2$ and characterizes the detuning between the donor and acceptor DBs during the energy transfer. We term it detuning energy function. In some sense, $-\epsilon_T(I)$ extends the concept of Peierls-Nabarro energy barrier, which concerns only static excitations, to DBs, which are dynamical nontopological excitations. However, note now that the barrier in energy might be positive or negative. With no restrictions on the choice of the coupling functions $V(I_T/2, I, \theta)$, it is rather easy to find sophisticated dependence on $\theta$ (but a bit unrealistic), such that there cannot exist any contour line connecting the two poles. Thus, it is convenient to require some properties for the $\theta$ dependence which also make the coupling physically reasonable especially if this coupling is small. We shall assume that it is sine-like and that it has only one maximum and one minimum per period for $-I_T/2 < I < I_T/2$. This coupling function $V(I_T/2, I, \theta)$ has two (and only two) zeros per period with respect to $\theta$ since its average is zero. More

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6 In the case of a nonresistive and noninductive Josephson junction (JJ), which can be described by a dimer model, type I and class II characterizes the two possible states of the JJ without DC current and with DC current, respectively [39].
generally, Eq. (6) determines either two values modulo $2\pi$ for $\theta$ or no values. A necessary and sufficient condition for having two solutions $\theta_+(I)$ and $\theta_-(I)$ which are continuous functions of $I$ on the sphere $(I, \theta)$ is simply

$$V_-(I) = \min_{\theta} V(I_T/2, I, \theta) < \epsilon_I(I) < \max_{\theta} V(I_T/2, I, \theta) = V_+(I)$$ (7)

Functions $\theta_+(I)$ and $\theta_-(I)$ determine the two segments of the closed contour line which connects the two poles of the sphere $(I, \theta)$. The corresponding trajectory is a trajectory which realizes a targeted energy transfer. We note that during the time $t_T$, the phase difference between the donor and acceptor DBs $\theta_\pm(I)$ does not rotate over the trigonometric circle but varies in some interval.

We have just demonstrated (for a physically reasonable sine-like dependence of the coupling on the phase difference) that targeted energy transfer solutions do persist when the detuning energy function is not strictly zero provided the detuning energy function is bounded by the max and the min of the coupling function. When the detuning function is small, this coupling may be also small.

The targeted energy transfer solution at $I = I_T/2$ may be lost when varying the model parameters. It suffices that condition (7) is no more fulfilled. At the threshold, there is a certain value $I_b$ of $I$ where $V(I_T/2, I, \theta) = V_+(I)$. Then, $\theta = \theta_b = \theta_+(I_b) = \theta_-(I_b)$. Consequently, point $(I_b, \theta_b)$ is an extremum of the energy (4) on the sphere so that $I(t) = I_b, \theta(t) = \theta_b$ is time-independent, which in the initial system is time-periodic. They correspond to exact DB solutions of the coupled system made of the donor and acceptor molecules.

Thus, the threshold where targeted transfer disappears, can be precisely associated with the appearance of a new DB solution of the whole system. When approaching this threshold, the targeted transfer solution becomes cnoidal, i.e., the time of transfer diverges because the energy transfer slows down in the vicinity of $I_b$ where the new DB solution will appear.

4 Explicit solutions in the general quartic dimer model

We now investigate explicitly the targeted energy transfer solutions in exactly solvable dimer models which describe quite well the general behavior in the weak coupling limit. DNLS Dimer models were studied in many early works [40–42] but only in special cases with no special attention to the detuning function. Energy transfer solutions were already found but for relatively large coupling in cases where the detuning function (6) was not small. It is thus instructive to reconsider a more general quartic DNLS dimer model as an
illustration of our general theory. We consider a dimer with Hamiltonian

\[ \mathcal{H} = \left( \frac{1}{2} \chi_1 |\psi_1|^4 + \omega_1 |\psi_1|^2 \right) + \left( \frac{1}{2} \chi_2 |\psi_2|^4 + \omega_2 |\psi_2|^2 \right) - \lambda (\psi_1 \psi_2^* + \psi_2 \psi_1^*) \quad (8) \]

where \( \chi_1, \chi_2, \omega_1 \) and \( \omega_2 \) are parameters. \( \lambda \) is the inter-site coupling chosen positive for convenience. (\( \psi_1^*, i\psi_1 \)) and (\( \psi_2^*, i\psi_2 \)) are pairs of conjugate variables. Defining first the new pair of conjugate variables (\( I_1, \theta_1 \)) and (\( I_2, \theta_2 \)) by \( \psi_1 = \sqrt{I_1} e^{-i\theta_1} \) and \( \psi_2 = \sqrt{I_2} e^{-i\theta_2} \) and next the pair of conjugate variables (\( I_0 = (I_1 + I_2)/2, \theta_0 = \theta_1 + \theta_2 \)) and (\( I = (I_1 - I_2)/2, \theta = \theta_1 - \theta_2 \)), an equivalent form of Hamiltonian (8) is

\[ \mathcal{H}(I, \theta, I_0, \theta_0) = H_0(I_0, I) + V(I_0, I, \theta) \quad (9) \]

with

\[ H_0(I_0, I) = \frac{1}{2} \chi_0 (I_0^2 + I^2) + \chi I_0 I + \omega_0 I_0 + \omega I \quad (10) \]
\[ V(I_0, I, \theta) = -2\lambda \sqrt{I_0^2 - I^2} \cos \theta \quad (11) \]

and the new model parameters

\[ \chi_0 = \chi_1 + \chi_2, \quad \chi = \chi_1 - \chi_2, \quad \omega_0 = \omega_1 + \omega_2, \quad \omega = \omega_1 - \omega_2 \quad (12) \]

Complete targeted energy transfer is obtained for

\[ I_T = -\frac{2\omega}{\chi}, \quad E_T = \frac{\omega}{\chi} \left( \frac{\omega \chi_0}{\chi} - \omega_0 \right) \quad (13) \]

The detuning function (6) and the coupling functions \( V_+(I) \) and \( V_-(I) \) in Eq.(7) are

\[ \epsilon_T(I) = \frac{1}{8} \chi_0 (I_T^2 - 4I^2) \quad \text{and} \quad V_+(I) = -V_-(I) = \lambda \sqrt{I_T^2 - 4I^2} \quad (14) \]

so that inequality (7) is fulfilled for all \( I \) when

\[ \lambda > \left| \frac{\omega \chi_0}{4\chi} \right| \quad (15) \]

Targeted energy transfer is obtained for any nonzero coupling when \( \chi_0 = 0 \), i.e., when the nonlinear coefficients on the two sites are opposite. On the contrary, it is never obtained when \( \chi = 0 \), i.e., when the nonlinear coefficients on both sites are equal, except when \( \omega = 0 \). The case \( \chi = 0, \omega = 0 \), which was treated in Ref.[40], is special because \( I_T \) is undetermined. Then, there are exact energy transfer solutions for any \( I_0 \) when the coupling is large enough, i.e., \( \lambda > \chi_0 I_0/4 \). Exceptionally, energy transfer is not selective in this case.
Fig. 1. Cylindrical projections of the contour lines on the sphere \((I, \theta)\) of Hamiltonian (9) for \(I_0 = 0.5\) (a), \(I_0 = 1.0\) (b) (ideal targeted transfer), \(I_0 = 2.0\) (c). Model parameters are \(\chi_0 = 0, \chi = 1, \omega_0 = 0, \omega = -1, \lambda = 1/2\).

Eq.(4) for Hamiltonian (9) yields the model trajectories which appear as contour lines on the sphere \((I, \theta)\) defined by
\[
E = \frac{1}{2} \chi_0 (I_0^2 + I^2) + \chi I_0 I + \omega_0 I_0 + \omega I - 2\lambda \sqrt{I_0^2 - I^2} \cos \theta \tag{16}
\]

They are shown for several values of the total action \(I_0\) and for a choice of the model parameters such that targeted energy transfer occurs for a certain initial action \(I_0\) and energy \(E\) (cf. Fig.1). An example is also shown when targeted energy transfer never occurs at any action \(I_0\) and energy \(E\) (cf. Fig.2).

Eliminating \(\theta\) between Eq.(16) and the Hamilton equation
\[
\dot{I} = - \frac{\partial \mathcal{H}}{\partial \theta} = -2\lambda \sqrt{I_0^2 - I^2} \sin \theta \tag{17}
\]
yields
\[
\frac{1}{2} \dot{I}^2 + \mathcal{P}(I) = 0 \tag{18}
\]
Fig. 2. Same as fig.1 for \( I_0 = 0.5 \) (a) and \( I_0 = 2.0 \) (b) but with parameters \( \chi_0 = 5, \chi = 1, \omega_0 = 0, \omega = -1, \lambda = 1/2 \).

where

\[
P(I) = \frac{1}{2} \left( \frac{1}{2} \chi_0 I^2 + (\chi I_0 + \omega) I + \frac{1}{2} \chi_0 I_0^2 + \omega_0 I_0 - E \right)^2 - 2\lambda^2 (I_0^2 - I^2)
\]

Eq.(18) describes a single nonlinear oscillator at zero energy with unit mass in a potential \( P(I) \). The solutions of eq.(18) oscillate in an interval determined by two consecutive zeros of \( P(I) \) and where \( P(I) \) is negative. They are determined (apart from a time shift) from the knowledge of the two invariants \( E \) and \( I_0 \) and the interval of zeros.

Since in our case \( P(I) \) is a fourth degree polynomial, the number of real zeros is even. Note also that all the real zeros \( I_\alpha \) of \( P(I) \) \( (P(I_\alpha) = 0) \), necessarily belong to the interval \( -I_0 \leq I_\alpha \leq I_0 \) since outside this interval \( P(I) \) is the sum of two positive terms in Eq.(19) and thus cannot vanish.

The situation where \( P(I) \) has no zeros never occurs, whatever the initial conditions are, because \( \dot{I}^2 \) has to be positive at time 0. When \( P(I) \) has one pair of real zeros, there is a unique solution (apart from a time shift) for \( I(t) \) (and \( \theta(t) \)) which is time-periodic. It corresponds to a quasiperiodic solution of the initial DNLS equation since

\[
\dot{\theta}_0 = \frac{\partial H}{\partial I_0} = \frac{-2\lambda}{\sqrt{I_0^2 - I^2}} I_0 \cos \theta + \chi_0 I_0 + \chi I_0 + \omega_0.
\]

Note that we have to discard the fake time-constant solutions \( I(t) = I_\alpha \), where \( I_\alpha \) is some zero of \( P(I) \), which are not solutions of the real dynamical system. The reason is that the time conservation of \( H \) is trivial for time-constant solutions but it is not sufficient to insure they fulfill the dynamical equations.
When $P(I)$ has two pairs of real zeros, there are two time-periodic solutions $I(t)$ that, again, correspond to quasiperiodic solutions of the initial DNLS equation.

Time-periodic solutions (corresponding to DBs) are obtained when $I(t)$ becomes time-constant (the interval of oscillation shrinks to zero), i.e., when $P(I)$ gets a degenerate pair of zeros.

For solutions corresponding to a targeted transfer of energy between site 1 and 2, $I(t)$ should oscillate between $+I_0$ and $-I_0$ which requires that $\pm I_0$ are zeros of $P(I)$. This condition yields $I_0 = I_T/2$ and $E = E_T$ defined by Eqs.(13). Otherwise, $P(I)$ must not have any other zeros, yielding for this parameter value

$$P(I) = \frac{1}{8} \chi_0^2 \left( I^2 - \frac{\omega^2}{\chi^2} + \frac{16 \lambda^2}{\chi^2} \right) \left( I^2 - \frac{\omega^2}{\chi^2} \right)$$

which implies

$$k = \left| \frac{\omega \chi_0}{4 \lambda \chi} \right| < 1$$

equivalent to condition (15). Then, the solution of Eq.(18) for $P(I)$ given by eq.(21) is a Jacobi elliptic cosine with modulus $0 \leq k < 1$

$$I(t) = -\frac{\omega}{\chi} \text{cn}(\lambda \sqrt{2t}; k)$$

which describes explicitly the targeted energy transfer between the two sites. Then, the frequency of the targeted transfer is

$$\omega_T = \frac{\pi \lambda}{\sqrt{2K(k)}}$$

where $K(k)$ is the first kind complete elliptic integral.

$\omega_T$ is minimum and proportional to the coupling $\lambda$ when $\chi_0 = 0$, i.e., when the “nonlinear tuning” between the two sites is optimal. Then the oscillation of the difference of action $I(t)$ between the two oscillators becomes a pure cosine. In this case, the explicit solution describing the optimal targeted transfer from the donor to the acceptor obtained for $E = E_T = -\omega \omega_0/\chi$ and $I_0 = I_T/2 = -\omega/\chi$ is rather simple

$$\psi_1(t) = \sqrt{-\frac{\omega}{\chi}} \cos \lambda t \exp -i\left( \frac{1}{4 \lambda} \sin 2\lambda t + \frac{\omega_0 t}{2} \right)$$
$$\psi_2(t) = i \sqrt{-\frac{\omega}{\chi}} \sin \lambda t \exp -i\left( \frac{1}{4 \lambda} \sin 2\lambda t + \frac{\omega_0 t}{2} \right)$$
Fig. 3. 3D plot of the rate $A$ of transfer for the action between the two sites of the dimer versus $E$ and $I_0$ for Hamiltonian (9) at $\chi_0 = 0, \chi = 2, \omega_0 = 0, \omega = -1$. Coupling $\lambda = 0.01$ is weak. 100% transfer occurs at the top of the peak while away from the peak, action transfer becomes negligible.

Fig.3 shows the 3D plot of the rate of action transfer $A = (\max_t I(t) - \min_t I(t))/(2I_0)$ between the two sites as a function of the energy $E$ and the total action $I_0$ of the solution.

The targeted energy transfer solution disappears when its frequency reaches zero, i.e., $k$ becomes equal to 1. Then, polynomial $\mathcal{P}(I)$ gets a degenerate zero at $I = 0$ which means that a time-periodic solution at $I = 0$ appears. It corresponds to a new DB solution which suddenly blocks the targeted transfer. At the limit $k = 1$, the elliptic cosine becomes a sech function [40] and close to this limit, the transfer of energy becomes intermittent.

The time-periodic solutions (DBs and multibreathers) are characterized by $\dot{I} = 0$ in Eq.(17) and $\dot{I} = \partial H/\partial I = 0$ yields $\theta = 0$ or $\pi$ and

$$4\lambda^2 I_b^2 - (\chi_0 I_b + \chi I_0 + \omega)^2(I_0^2 - I_b^2) = 0.$$ (27)
Fig. 4. Transfer rate in action versus $I_0$ for $\chi = 2$, $\omega = -1$, $\lambda = 0.01$ and several values of $\chi_0 = -0.8$ (thick dashed), $-0.5$ (thin dashed-dotted), $0$ (thick full line), $0.25$ (thick dashed), $0.5$ (thin dashed-dotted), $5$ (thin full).

This is a fourth degree equation which may have 2 or 4 real zeros, functions of $I_0$. The energy of these solutions $E_b(I_0)$ determines the boundaries of the domain in the plane of initial conditions $E,I_0$ that can be realized.

We can also analyze partial energy transfer by considering the set of initial conditions where all the energy is at site 1. These conditions are characterized by $I(0) = I_0$ and $E = (\chi_0 + \chi)I_0^2 + (\omega + \omega_0)I_0$. Then, polynomial (19) becomes

$$P(I) = \frac{1}{2}(I - I_0) \left( (I - I_0) \left( \frac{1}{2} \chi_0(I + I_0) + \chi I_0 + \omega \right)^2 + 4\lambda^2(I_0 + I) \right).$$

(28)

Then, $I(t)$ oscillates between $I_0$ and the largest zero $I_m$ of this polynomial. Fig.4 shows the rate of transfer in action $(I_0 - I_m)/(2I_0)$ versus $I_0$ for a given set of parameters $\chi,\omega,\lambda$ and for several values of $\chi_0$. 100\% transfer is obtained at $I_0 = I_T/2 = 1/2$ when condition (15) is fulfilled, i.e., $|\chi_0| < 4|\lambda\chi|/|\omega| = 0.08$. There are discontinuities on these curves where the oscillation regime of $I(t)$ becomes cnoidal which are due to the appearance of new time-periodic solutions blocking the energy transfer.
5 Detecting targeted energy transfer in complex models

This theory of targeted transfer can be used in practice in complex systems to detect targeted transfer because the functions involved in the effective dimer Hamiltonian (3) can be explicitly calculated. For that purpose, the initial system has to be separated into two coupled subsystems. The first one will sustain the donor DB and the second one the acceptor DB. The coupling between the two systems is not necessarily weak if the considered DBs are far from each other but the effective coupling has to be weak.

Using the numerical techniques developed earlier for the calculations of DBs in arbitrarily complex systems [3–5], one chooses a DB solution in the isolated donor system and calculate its dynamical configuration \( \{ p_D^i(\omega_1 t), q_D^i(\omega_1 t) \} \), its energy, and its action. Then, varying the frequency, one obtains function \( H_D(I) \). The same can be done for a DB in the acceptor system. For a complete targeted transfer, we require that both DBs be gapless, i.e., \( H_D(I) \) and \( H_A(I) \) can be continued to \( I = 0 \) where \( H_D(0) = H_A(0) = 0 \).

Since the effective coupling between the two DBs is supposed to be small, \( I_T \) can be determined approximately by the equality \( H_D(I_T) = H_A(I_T) \), which requires that the two curves intersect at \( I \neq 0 \). For having targeted transfer at reasonably small coupling, function \( \epsilon(I) = H_D(I_T/2 + I) + H_A(I_T/2 - I) \) should be small. Once these conditions are fulfilled, we have to check that our dimer assumption is valid, i.e., that there is no other DB either on the donor system or the acceptor system with almost the energy functions \( H_D(I) \) or \( H_A(I) \) in the interval \([0, I_T]\).

Next, the coupling energy between the two systems is considered. It is originally a function of the global system configuration \( \{ p_D^i, q_D^i \} \) and \( \{ p_A^i, q_A^i \} \) It yields the effective coupling in the dimer model by averaging this energy over the fast variable \( \theta_0 \) for the system configuration \( \{ p_D^i((\theta_0 + \theta)/2), q_D^i((\theta_0 + \theta)/2) \} \) and \( \{ p_A^i((\theta_0 - \theta)/2), q_A^i((\theta_0 - \theta)/2) \} \). It is thus only a function of \( I_0, I \) and \( \theta \) which has to be small.

Comparing the precise detuning function and the coupling functions as in Eq.(7), we can predict rather accurately the possible existence of targeted transfer solutions between these donor and acceptor DBs. In the cases we tested up to now, where these conditions are correctly fulfilled, molecular dynamics confirmed the existence of targeted transfer where almost 100% of the energy oscillates for a very long time between the donor and the acceptor DB. As expected also, this energy transfer is blocked as soon as the initial amount of energy is not optimal or the coupling too weak [43].
6 Irreversibility in the energy targeted transfer

DBs are out of equilibrium excitations. In real systems, which are not strictly at 0 K, they interact with the phonon modes and other excitations which should make their lifetime finite. Thermalization should be in principle a consequence of intrinsic nonlinearities of the system. However, standard approaches usually simulate thermalization and relaxation by a white Langevin noise and an extra damping. This is known to be equivalent to a coupling of the initial system with a fictitious extra system consisting of an infinite set of harmonic oscillators with a uniform distribution of frequencies [44]. This is clearly a bias which makes the DBs to systematically radiate energy in this bath and artificially washes out their existence as very long lifetime solutions. Actually, the long lifetime of DBs is precisely due to the fact that they have no resonance with the linear phonon spectrum which implies that either their frequencies are above the phonon spectrum or there are gaps in this phonon spectrum. It is the nonuniform and specific phonon spectrum of the model itself which should be considered for studying DB lifetime as we started to do in some recent works [23,28]. In other words, real systems exhibit a selective damping depending on the frequencies of their modes which should be explicitly taken into account to be physically correct. Thus, the thermal bath assumption with a uniform phonon spectrum is not physically founded and, worst, induces the denaturation of the model.

We discussed above the ideal case for targeted energy transfer at 0 K. For obtaining an ideal transfer, besides the adiabaticity hypothesis, the donor and acceptor DBs must be gapless. This condition requires that there exist no linear modes in the donor (or the acceptor) system with frequency in the range of variation of the DBs frequency. Indeed, it has been shown in [3–5] that before the frequency of a DB collides with a linear mode frequency, it systematically bifurcates with another one. In this case, the DB is not strictly continuatable to zero amplitude. There is a frequency discontinuity corresponding to the region where the resonance with the linear mode destroys the DB. Strictly speaking, when there is a linear mode in the range of variation of frequency of a DB on the donor (or acceptor) system, this DB exhibits a nonvanishing energy gap which in principle invalidates our assumptions for describing the coupled system as a generalized dimer model (3). As a consequence, the frequency of the ideal targeted transfer solution precisely oscillates in between the edges of a gap of the linear phonon spectrum.

We would like to briefly discuss here what can happen to targeted energy transfer if there is just a single resonant linear mode in the phonon gap, first in the case of strong coupling, i.e., this linear mode is spatially located close to the donor (or the acceptor) DBs. As we just said, the DB of the donor (or the acceptor) will exhibit an energy gap, so that the detuning function cannot
be defined for the whole interval of variation of $I$. The energy transfer will become incomplete and irreversible. As the frequency of the targeted energy transfer solution approaches the linear resonance, a substantial fraction of the energy will be suddenly transferred to this linear mode instead of the acceptor DB. Consequently, the frequency of the donor DB will change independently of the acceptor DB. The loss of resonance between donor and acceptor DB stops immediately the energy transfer. If one assumes that the energy captured by the linear resonant mode does not return significantly to the donor DB, the part of the energy left on the donor system and of the linear mode, could be dissipated into phonons through chaotic processes and finally heat. Then, only a well-defined fraction of the initial energy on the donor has been transferred and the excess of energy has been dissipated into heat. We obtained only an incomplete but irreversible targeted transfer.

The effect should be much less sharp when the linear mode which is resonant with the donor DB is weaker, i.e., the resonant linear mode is physically located far away from the donor and acceptor DBs, say, in order to fix the ideas, on the donor system. Then, there is only a small discontinuity gap in frequency to jump for the donor DBs where function $H_D(I_D)$ is undefined. We think that despite a small energy loss when crossing the resonance, targeted energy transfer could be continued beyond this resonance and be almost completed. If there are many such weak resonances they could be described as a frequency dependent damping depending on the distribution and coupling with resonant linear modes. Resonances with bands of extended phonons should have a similar effect.

Actually, in realistic systems there are likely some linear modes in the phonon gap causing some energy dissipation and making energy transfer irreversible. On the opposite, at finite temperature, thermal activation of the linear modes could also help targeted energy transfer by stochastic resonance effects. These problems will be investigated in the future.

7 Concluding remarks and new perspectives

We have demonstrated here that the essential difference between linear and nonlinear resonance (allowing the targeted energy transfer) is that nonlinear resonance is selective in energy (or action), unlike linear resonance, which is not. Targeted energy transfer occurs because the frequencies of the donor oscillator or DB and acceptor oscillator or DB, although they both vary during the transfer, remain almost equal. This condition can be achieved at weak coupling, only for a certain initial energy $E_T$ and when a certain detuning function is small enough compared to the coupling energy. In the ideal case, an amount of energy $E_T$ deposited on the donor DB oscillates slowly and periodically
back and forth between donor and acceptor. It is totally transferred between
the donor and the acceptor DB at periodic times. Otherwise, although there
is some energy oscillation, the energy transfer becomes negligible.

We do not believe that the obtained targeted energy transfer solutions corre-
spond to strictly exact solutions of the initial model because of the hypothesis
of adiabaticity which cannot be perfectly fulfilled. However, situations close
to the ideal case could exist where the number of energy oscillations between
donor and acceptor DBs is very large. The high sensitivity to the initial energy
makes that this energy transfer can be easily stopped by intermediate linear
resonance which can be viewed as a kind of transistor effect. This effect could
be used in practical devices (e.g., with optical fibers).

Within the perspectives opened up by this approach, we would like to suggest
a series of new physical problems to be investigated in the near future.

We may consider situations where, instead of one, there are several DBs on
the donor system with almost identical functions $H_D(I)$ and one acceptor
DB on the acceptor system. Then, if we are in the condition of targeted
energy transfer for a single donor DB, any donor DBs excited at the energy
$E_T$ will transfer their energy to the acceptor DB. However, the transfer has
good chances to be irreversible because when the transfer is completed, the
acceptor energy could return simultaneously to all donor DBs but then the
resonance between the donor DBs and the acceptor DB will be broken and
the transfer will be blocked. This situation is interesting for realizing energy
funneling analogous to what is observed in chlorophyll [45].

We may also consider situations such that for an energy $E_T' < E_T$, the accep-
tor DB (A) is tuned to another acceptor DB ($A'$). Then, before the transfer
from the initial donor (D) to the acceptor (A) is completed, this acceptor (A)
transfer its energy to the next acceptor ($A'$) with some energy loss (note that
the DB $A'$ acts initially like an intragap linear resonance) but instead of dis-
sipating energy, it may collect most of the acceptor energy. By this way,
recurrent transfer could be built along a certain well determined sequence of
acceptor DBs. We could then realize irreversible cascades of energy transfer
(with some energy losses however). It is also important to realize now that
DBs in molecules may have piezoactive effects, i.e., they might generate de-
formation of the molecules as emphasized in [20].

This effect could be important for example for understanding the energy con-
version of ATP into mechanical energy (molecular motors). The energy depo-
sition from ATP could occur first as a DB located at a certain receptive site of
the moving biomolecule (e.g., kinesin adsorbed on a microtubule). Then, this
DB could cascade by targeted energy transfer through a series of DBs located
at specific sites of the biomolecule generating a well determined sequence of de-
formations which lead to a well determined motion of the biomolecule (step) along the oriented microtubule after the time necessary for this cascade process. Beyond this time, the DB energy is finally relaxed into heat. Thus, excitations by ATP randomly repeated at time intervals longer than this characteristic time should produce systematically a directive walk of this biomolecule along the microtubule (this motion should become randomly intermittent in time if the ATP concentration is low). In the future, we plan to use and to develop our tools for calculating DBs in nonlinear systems for controlling precisely their targeted energy transfer, funnelling, cascades, piezoelectricity of DBs and thus for designing artificial models with desired properties mimicking those of biosystems.

Let us also note that instead of being atomic vibrations, these DBs could be electronic vibrations (excitons), polarons, or atomic vibrations combined with an electronic charge (polarobreathers) [17]. Thus, there are many possible variations of the targeted transfer principle depending on the considered physical problem (transfer of energy, charge, spin, etc) and its scale of energy. This theory of targeted transfer could be useful, for example, for revisiting the standard theories of fluorescence ([46]), chemical reactions, catalysis, etc.

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