The fractional nonlinear $\mathcal{PT}$ dimer

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We study a fractional Discrete Nonlinear Schrodinger dimer, where the usual first derivative in the time evolution is replaced by a non-integer order, *à* la Caputo. The dimer is nonlinear (Kerr) and $\mathcal{PT}$ symmetric, and we examine the excitation exchange dynamics between both sites. By means of a Laplace transformation technique, the linear $\mathcal{PT}$ dimer is solved in closed form in terms of Mittag-Leffler functions, while for the nonlinear regime, we resort to numerical computations using the direct explicit Grunwald algorithm. The main effect of the fractional derivative is to decrease the amplitude of the exchange oscillations towards zero. It also affects the standard selftrapping transition by decreasing the trapped fraction as the nonlinearity is increased past threshold.

I. INTRODUCTION

The topic of fractional calculus has experienced a rekindled interest in recent times. Essentially, it extends the notion of a derivative or an integral of integer order, to one of a fractional order, $(d^n/dx^n) \rightarrow (d^\alpha/dx^\alpha)$ for real α. The subject has a long history, dating back to letters exchanged between Leibnitz and L'Hopital, and later contributions by Euler, Laplace, Riemann, Liouville, and Caputo to name some[1–5]. The starting point was the computation of $d^\alpha x^k/dx^\alpha$, where α is a non-integer number:

$$\frac{d^n x^k}{dx^n} = \frac{\Gamma(k+1)}{\Gamma(k-n+1)} x^{k-n} \rightarrow \frac{d^\alpha x^k}{dx^\alpha} = \frac{\Gamma(k+1)}{\Gamma(k-\alpha+1)} x^{k-\alpha}. \tag{1}$$

For instance $(d^{1/2}/dx^{1/2})x = (2/\sqrt{\pi})\sqrt{x}$, and $dx/dx = (d^{1/2}/dx^{1/2})(d^{1/2}/dx^{1/2})x = (2\sqrt{\pi})(\Gamma(3)/\Gamma(1))x^0 = 1$, as expected. From Eq.(1) the fractional derivative of an analytic function $f(x) = \sum_k a_k x^k$ can be computed by deriving term by term. This basic procedure is not exempt from ambiguities. For instance, $(d^\alpha/dx^\alpha)\ 1 = (d^\alpha x^0/dx^\alpha) = (1/\Gamma(1-\alpha))x^{-\alpha} \neq 0$, according to Eq.(1). However, one could also take $(d^{\alpha-1}/dx^{\alpha-1})(d/dx)\ 1 = 0$. For the case of a fractional integral, a more rigorous starting point is Cauchy's formula for the integral of a function. From the definition

$$I_x^1 f(x) = \int_0^x f(s) ds, \tag{2}$$

we apply the Laplace transform $\mathcal{L}$ to both sides of Eq.(2)

$$\mathcal{L}\ \{I_x^1\ f(x)\} = (1/s)\ \mathcal{L}\{f(x)\} \tag{3}$$

After n integrations, one obtains

$$\mathcal{L}\ \{I_x^n\ f(x)\} = (1/s^n)\ \mathcal{L}\{f(x)\} \tag{4}$$

Extension to fractional α is direct:

$$\mathcal{L}\ \{I_x^\alpha\ f(x)\} = (1/s^\alpha)\ \mathcal{L}\{f(x)\} \tag{5}$$

After noting that the RHS of Eq.(5) is the product of two Laplace transforms we have, after using the convolution theorem

$$I_x^\alpha\ f(x) = \frac{1}{\Gamma(\alpha)} \int_0^x \frac{f(s)}{(x-s)^{1-\alpha}}\ ds \tag{6}$$

From this definition, it is possible to define the fractional derivative of a function $f(x)$ as

$$\frac{d^\alpha f(x)}{dx^\alpha} = \left(\frac{d^m}{dx^m}\right)\ I_x^{m-\alpha}\ f(x) = \\ = \frac{d^m}{dx^m}\left[\frac{1}{\Gamma(m-\alpha)} \int_0^x (x-s)^{m-\alpha-1} f(s)\ ds\ \right], \tag{7}$$

where, $m-1 < \alpha < m$. Eq.(7) is known as the Riemann-Liouville form. An alternative, closely related form, is the Caputo formula[5]:

$$\frac{d^\alpha f(x)}{dx^\alpha} = I_x^{m-\alpha}\left(\frac{d^m}{dx^m}\right) f(x) = \\ = \frac{1}{\Gamma(m-\alpha)} \int_0^x (x-s)^{m-\alpha-1} f^{(m)}(s) ds, \tag{8}$$

which has some advantages for differential equations with initial values. The various technical matters that arise in fractional calculus have prompted a whole line of research that has extended to current times. Long regarded as a mathematical curiosity, it has now regained interest due to its potential applications to complex problems in several fields: fluid mechanics[6, 7], fractional kinetics and anomalous diffusion[8–10], strange kinetics[11], fractional quantum mechanics[12, 13], Levy processes in quantum mechanics[14], plasmas[15], electrical propagation in cardiac tissue[16] and biological invasions[17]. In general, fractional calculus constitutes a natural formalism for the description of memory and non-locality effects found in various complex systems.

On the other hand, when dealing with effectively discrete, interacting units, as one encounters in atomic physics (interacting atoms), or in optics (coupled optical fibers), it is common to deal with discrete versions of the continuum Schrödinger equation, or the paraxial wave equation. The effective discreteness comes from expanding the solution sought in terms of (continuous) modes that can be labelled unambiguously. The simplest of such examples is the bonding, anti-bonding electronic mode that one finds for a two-sites (dimer) molecule after diagonalizing the two-site Schrödinger equation in the tight-binding approach. Something similar happens in optics, where the paraxial equation is formally equivalent

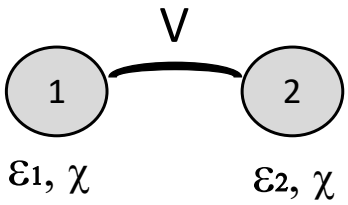

Figure 1. Nonlinear anisotropic fractional dimer where the excitation is on site 1 initially ($t = 0$). In the $\mathcal{PT}$ case, $\epsilon_1 = -\epsilon_2 = i\gamma$

to the Schrödnger equation. In that case, for two optical waveguides, the total electric field is expanded in terms of the electromagnetic modes in each guide which interact through the evanescent field between the two guides giving rise to a transversal dynamics for the optical power. The procedure can be extended to N interacting units, either atoms or waveguides, where the relevant dynamics is given by a discretized version of the Schrödinger equation for N units[18, 19]. Of course, at the end one has to collect all the discrete amplitudes and multiply them by the corresponding continuous mode profiles and superpose them, to obtain the final field. The simplest case $N = 2$ is termed a dimer and oftentimes constitute a basic starting point when studying an interacting, discrete system. Ensembles of interacting dimers have been studied before in classical and quantum statistics[20–22], and more recently, they have been considered in model of correlated disorder[24] and in magnetic metamaterial modeling[23].

In this work we consider the discrete Schrödinger equation for a dimer system, where the standard time derivative is replaced by a fractional one. The dimer considered is rather general and contains asymmetry, $\mathcal{PT}$ symmetry and nonlinearity (Fig.1). Our main interest is in ascertaining the effect of the fractional derivative on the excitation exchange between the sites, its stability and selftrapping behavior, for several cases of interest.

II. THE FRACTIONAL DIMER

Let us consider the fractional evolution equations for a general nonlinear dimer

$$i\frac{d^\alpha C_1(t)}{dt^\alpha} + \epsilon_1 C_1(t) + V C_2(t) + \chi|C_1(t)|^2 C_1(t) = 0$$
$$i\frac{d^\alpha C_2(t)}{dt^\alpha} + \epsilon_2 C_2(t) + V C_1(t) + \chi|C_2(t)|^2 C_2(t) = 0 \quad (9)$$

where α is the fractional order of the (Caputo) derivatives with $0 < \alpha < 1$. Quantities $C_{1,2}$ are probability amplitudes in a quantum context, or electric field amplitudes, in an optical setting. Parameter V is the coupling term and χ is the nonlinearity parameter.

Let us first consider the case of a general linear ($\chi = 0$) dimer, and assume $C_1(0) = 1, C_2(0) = 0$. We will solve this case in closed form by the use of Laplace transforms: For $0 < \alpha < 1$, the Laplace transform of the Caputo fractional derivative of order α is given by

$$\mathcal{L}\{f(t)\} = s^\alpha \mathcal{L}\{f(t)\} - s^{\alpha-1} f(0^+). \quad (10)$$

After applying the Laplace transform $\mathcal{L}$ to both sides of Eq.(9) we have

$$i(s^\alpha \mathcal{L}(C_1) - s^{\alpha-1}) + \epsilon_1 \mathcal{L}(C_1) + V\mathcal{L}(C_2) = 0$$
$$i\ s^\alpha \mathcal{L}(C_2) + \epsilon_2 \mathcal{L}(C_2) + V\mathcal{L}(C_1) = 0. \quad (11)$$

Solving for $\mathcal{L}(C_1)$ and $\mathcal{L}(C_2)$ gives:

$$\mathcal{L}(C_1) = \frac{-i(\epsilon_2 + is^\alpha)s^{\alpha-1}}{s^{2\alpha} - i(\epsilon_1+\epsilon_2)s^\alpha + V^2 - \epsilon_1\epsilon_2} \quad (12)$$

and

$$\mathcal{L}(C_2) = \frac{i\ V s^{\alpha-1}}{s^{2\alpha} - i(\epsilon_1+\epsilon_2)s^\alpha + V^2 - \epsilon_1\epsilon_2}. \quad (13)$$

Using the inverse Laplace formula[25]

$$\mathcal{L}^{-1}\left\{\frac{s^{\rho-1}}{s^\alpha + as^\beta + b}\right\} =$$
$$t^{\alpha-\rho}\sum_{r=0}^{\infty}(-a)^r t^{(\alpha-\beta)r} E^{r+1}_{\alpha,\alpha+(\alpha-\beta)r-\rho+1}(-bt^\alpha), \quad (14)$$

we obtain:

$$C_1(t) = \sum_{r=0}^{\infty}(i(\epsilon_1+\epsilon_2))^r\ t^{\alpha r} E^{r+1}_{2\alpha,\alpha r+1}((\epsilon_1\epsilon_2 - V^2)t^{2\alpha})$$
$$-i\epsilon_2 t^\alpha \sum_{r=0}^{\infty}(i(\epsilon_1+\epsilon_2))^r t^{\alpha r} E^{r+1}_{2\alpha,\alpha(1+r)+1}((\epsilon_1\epsilon_2 - V^2)t^{2\alpha}) \quad (15)$$

$$C_2(t) = iVt^\alpha \sum_{r=0}^{\infty}(i(\epsilon_1+\epsilon_2))^r t^{\alpha r} E^{r+1}_{2\alpha,\alpha(1+r)+1}((\epsilon_1\epsilon_2 - V^2)t^{2\alpha}) \quad (16)$$

where $E^\gamma_{\alpha,\beta}(z)$ is defined as

$$E^\gamma_{\alpha,\beta}(z) = \sum_{k=0}^{\infty}\frac{(\gamma)_k\ z^k}{k!\ \Gamma(\alpha k + \beta)} \quad (17)$$

where $(\gamma)_n = \Gamma(\gamma+n)/\Gamma(\gamma)$, and $\alpha, \beta, \gamma \in \mathcal{C}$, $\mathrm{Re}(\alpha) > 0, \mathrm{Re}(\beta) > 0, z \in C$. Figure 2 shows examples of the time evolution of the square of the dimer amplitudes, for several site energy parameters, and fractional derivative orders. In general we observe that, as soon as α differs from unity, the dynamics is either bounded or unbounded, depending on the values of the site energy parameters. For the bounded cases, there is some oscillation initially, with a decreasing envelope towards zero.

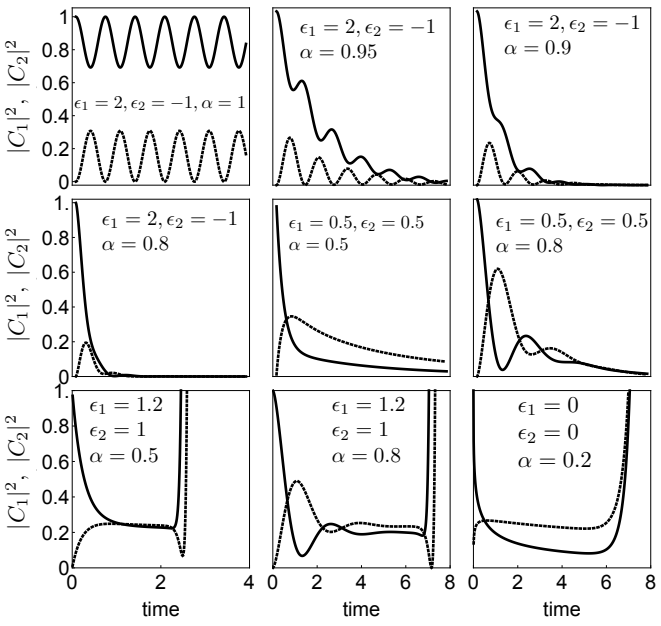

Figure 2. Dimer amplitudes for the linear case ($\chi = 0$) and several site energy parameters ϵ_1, ϵ_2 and different fractional derivative orders α. Solid(dashed) line denotes $|C_1|^2$ ($|C_2|^2$).

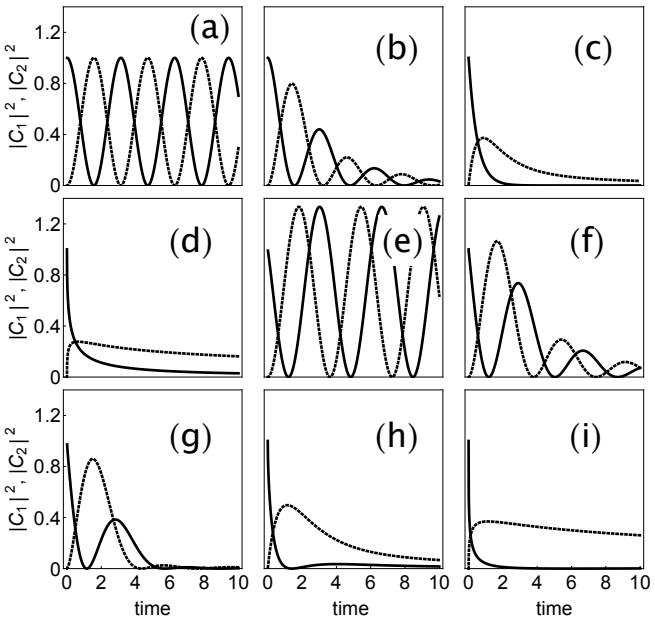

Figure 3. Dimer amplitudes $|C_1(t)|^2$ (continuous line) and $|C_2(t)|^2$ (dashed line) for the linear $\mathcal{PT}$ case ($\chi = 0, \epsilon \neq 0$) for several fractional derivative orders and various gain/loss parameters. (a) $\alpha = 1, \epsilon = 0$, (b) $\alpha = 0.9, \epsilon = 0$, (c) $\alpha = 0.5, \epsilon = 0$, (d) $\alpha = 0.25, \epsilon = 0$, (e) $\alpha = 1, \epsilon = 0.5$, (f) $\alpha = 0.9, \epsilon = 0.5$, (g) $\alpha = 0.8, \epsilon = 0.5$, (h) $\alpha = 0.5, \epsilon = 0.5$, (i) $\alpha = 0.25, \epsilon = 0.5$.

A. The linear $\mathcal{PT}$ dimer

A particularly interesting case of Eq.(9), is the fractional $\mathcal{PT}$-symmetric dimer. For systems that are invariant under the combined operations of parity ($\mathcal{P}$) and time reversal ($\mathcal{T}$), it was shown that they display a real eigenvalue spectrum, even though the underlying Hamiltonian is not hermitian[27, 28]. In these systems there is a balance between gain and loss, leading to a bounded dynamics. However, as the gain/loss parameter exceeds a certain value the system undergoes a spontaneous symmetry breaking, where two or more eigenvalues become complex. At that point, the system loses its balance and its dynamics becomes unbounded. According to the general theory, for our system to be $\mathcal{PT}$ symmetric, the real part of the site energies in Eq.(9) must be even in space while the imaginary part must be odd: $\mathrm{Re}(\epsilon_1) = \mathrm{Re}(\epsilon_2)$ and $\mathrm{Im}(\epsilon_1) = -\mathrm{Im}(\epsilon_2)$. For simplicity we take the real parts of ϵ_1, ϵ_2 as zero and thus, $\epsilon_1 = -\epsilon_2 \equiv i\,\epsilon$, where ϵ is the gain/loss parameter. This leave us with the equations:

$$
\begin{aligned}
i\frac{d^\alpha C_1(t)}{dt^\alpha} + i\epsilon C_1(t) + VC_2(t) = 0 \\
i\frac{d^\alpha C_2(t)}{dt^\alpha} - i\epsilon C_2(t) + VC_1(t) = 0
\end{aligned}
\tag{18}
$$

whose exact solutions can be extracted from the general solution, Eqs.(15),(16) as

$$
\begin{aligned}
C_1(t) &= -\epsilon t^\alpha E_{2\alpha,\alpha+1}((\epsilon^2 - V^2)t^{2\alpha}) + E_{2\alpha,1}((\epsilon^2 - V^2)t^{2\alpha}) \\
C_2(t) &= iVt^\alpha E_{2\alpha,\alpha+1}((\epsilon^2 - V^2)t^{2\alpha}),
\end{aligned}
\tag{19}
$$

where, $E_{\alpha,\beta}(z) = E^1_{\alpha,\beta}(z)$ is known as the generalized Mittag-Leffler function. The Mittag-Leffler function

$$
E_{\alpha,\beta}(z) = \sum_k \frac{z^k}{\Gamma(\alpha k + \beta)} \tag{20}
$$

is the natural extension of the exponential function and plays the same rol for fractional differential equations, as the exponential function does for the standard integer differential equations. Figure 3 shows examples of time evolutions for $|C_1|^2, |C_2|^2$ for several fractional orders and several gain/loss parameter values. As we can see, as α decreases from 1, both amplitudes decrease too, with oscillations that become monotonically decreasing, converging to zero at long times.

The asymptotic behavior of $C_1(t), C_2(t)$ depends on the behavior of the Mittag-Leffler functions $E_{\alpha,\beta}(z)$ at large values of $|z|$. After writing $z = |z|\exp(i\phi)$, we have[26]

$$
E_{\alpha,\beta}(z) \approx (1/\alpha)\; Q^{1-\beta}\exp(Q) \tag{21}
$$

where $Q = z^{1/\alpha} = \exp((1/\alpha)\log(|z|) + i\,\phi)$ and $|\phi/\alpha| \leq \pi$ ($\phi = \epsilon^2 - V^2$). This implies,

$$
\exp(Q) = \exp(|z|^{1/\alpha}\cos((1/\alpha)\phi)) \times \exp(i\,|z|^{1/\alpha}\sin((1/\alpha)\phi)) \tag{22}
$$

Thus, bounded behavior in time will occur for $(\pi/2) < |\phi/\alpha| < \pi$, while unbounded behavior occurs for $0 <$

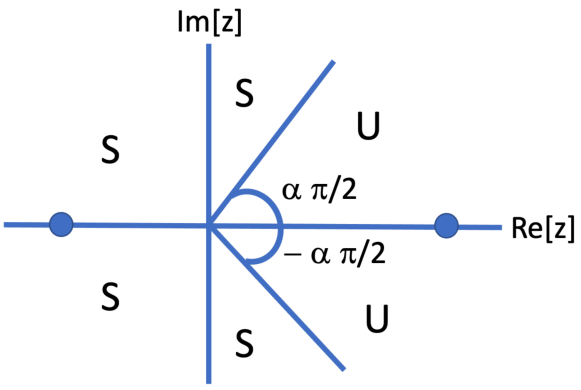

Figure 4. Asymptotic stability for the amplitudes $C_1(t), C_2(t)$ for the fractional $\mathcal{PT}$ dimer system (19). Here, U ≡ unbounded, S ≡ bounded, and $z = (\epsilon^2 - V^2)t^{2\alpha}$. The dots denote the position of our two phases, phase$(\epsilon^2 - V^2) = 0$ for $\epsilon^2 - V^2 > 0$, and phase$(\epsilon^2 - V^2) = \pi$ for $\epsilon^2 - V^2 < 0$.

$|\phi/\alpha| < \pi/2$. In our case, $\phi = \arg(\epsilon^2 - V^2) = 0, \pi$, implying that $C_1(t)$ and $C_2(t)$ will increase (decrease) asymptotically in time if $(\epsilon^2 - V^2)$ is positive (negative). This behavior is sketched in Fig.4.

B. The nonlinear $\mathcal{PT}$ dimer

We now explore a $\mathcal{PT}$ dimer in the presence of nonlinearity, and subject to fractional evolution equations

$$i\frac{d^\alpha C_1(t)}{dt^\alpha} + i\epsilon C_1(t) + VC_2(t) + \chi|C_1(t)|^2 C_1(t) = 0$$
$$i\frac{d^\alpha C_2(t)}{dt^\alpha} - i\epsilon C_2(t) + VC_1(t) + \chi|C_2(t)|^2 C_2(t) = 0 \quad (23)$$

In the absence of $\mathcal{PT}$ symmetry ($\epsilon = 0$), and for order $\alpha = 1$, eqs.(23) have been explored before in the literature[29–31]. For initial conditions $C_1(0) = 1, C_2(0) = 0$, it was shown that they lead to the phenomenon of a seltrapping transition: The existence of a critical nonlinearity parameter $\chi_c/V = 4$ below which, the long-time average of the square of the amplitudes, is the same and equal to 1/2, $\langle|C_1|^2\rangle = \langle|C_2|^2\rangle = 1/2$. At nonlinearity values above χ_c/V, $\langle|C_1|^2\rangle$ increases past 1/2 and converges to 1 at large χ/V values. The behavior of $\langle|C_2|^2\rangle$ is the opposite, decreasing from 1/2 and approaching zero in the large nonlinearity limit. The trapped fraction at the initial site, $\langle|C_1|^2\rangle$, changes abruptly as the critical nonlinearity is crossed. Another interesting feature is the existence of a conserved quantity: $P = |C_1(t)|^2 + |C_2(t)|^2 =$ constant.

For a fractional order derivative ($0 < \alpha < 1$), where we take the Caputo version of the fractional derivative, and in the presence of $\mathcal{PT}$ symmetry, we resort to the Grunwald algorithm[32] to compute the time evolution of $C_1(t), C_2(t)$ for initial conditions $C_1(0) = 1, C_2(0) = 0$.

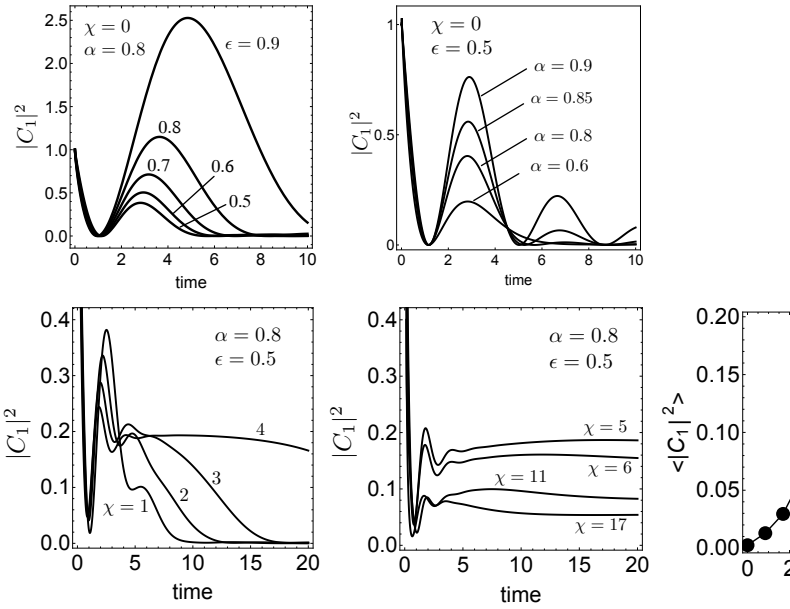

Figure 5. Dimer amplitude at initial site $|C_1(t)|^2$ for the nonlinear $\mathcal{PT}$ case for several fractional derivative orders, various gain/loss parameters and different nonlinearities.

This approach is based on finite differences, and in our case leads to the following difference equations:

$$X_{n+1} = \sum_{\nu=1}^{n+1} \Phi_\nu^\alpha X_{n+1-\nu} + ih(Y_n + i\epsilon X_n + \chi\,|X_n|^2 X_n) + r_{n+1}^\alpha X_0$$
$$Y_{n+1} = \sum_{\nu=1}^{n+1} \Phi_\nu^\alpha Y_{n+1-\nu} + ih(X_n - i\epsilon Y_n + \chi\,|Y_n|^2 Y_n) + r_{n+1}^\alpha Y_0 \quad (24)$$

where, $X \equiv C_1, Y \equiv C_2$, and

$$\Phi_\nu^\alpha = (-1)^{\nu-1}\binom{\alpha}{\nu} \qquad r_\nu^\alpha = \frac{\nu^{-\alpha}}{\Gamma(1-\alpha)}. \quad (25)$$

Numerical results are shown in Fig.5. In panel (a) we show the behavior of $|C_1(t)|^2$ in the linear limit ($\chi = 0$), for a fixed α and several different gain/loss parameter values. We see that the effect of increasing ϵ is to augment the amplitude and decrease the frequency of the oscillation. When ϵ approaches V, the amplitude grows unbounded and the oscillation stops. In panel (b) we take $\chi = 0$ as before, with a fixed gain/loss ϵ and for several order α values. As we noticed before, the presence of $0 < \alpha < 1$ induces a decreasing oscillation behavior in $|C_1(t)|^2$. If we reduce now the value of α, we see a further decrease of the oscillation amplitude, with little effect on the frequency. We now move to the nonlinear case. In panels (c, d) we show the behavior of $|C_1(t)|^2$ in time for fixed α, ϵ parameters and for several χ values. Roughly speaking, what we observe here is that for $\chi < 4V$ the

$|C_1(t)|^2$ curves decrease to zero at long times, while at χ values greater than $4V$, the curves approach a constant value. This looks just like a manifestation of the selftrapping effect observed in the standard case ($\alpha = 1$). But there is a significative difference: As χ is increased past $4V$ the selftrapped fraction decreases with χ instead of increasing, as in the standard case.

III. CONCLUSIONS

In spite of interesting differences with the standard integer derivative case, the very general features of the dimer remain more or less the same; (1) there is exchange between the sites, (2) in the presence of PT symmetry there are two clearly demarked regimes where the amplitudes decrease to zero or diverge to infinity.(3) there is still a selftraping transitions, whose details depend on the value of the fractional derivative order. The persistence of this general phenomenology in the face of a different rate of change, suggest that this phenomenology is robust against "mathematical perturbations". This kind of robustness has been also observed for the fractional DNLS equation, where the Laplacian is replaced by a fractional one[33, 34]. Thus , the concept of power exchange between sites, selftrapping transitions and existence of nonlinear excitations (discrete solitons) are concepts of wide validity.

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