Variational Approach to studying solitary waves in the nonlinear Schrödinger equation with Complex Potentials

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We discuss the behavior of solitary wave solutions of the nonlinear Schrödinger equation (NLSE) as they interact with complex potentials, using a four parameter variational approximation based on a dissipation functional formulation of the dynamics. We concentrate on spatially periodic potentials with the periods of the real and imaginary part being either the same or different. Our results for the time evolution of the collective coordinates of our variational ansatz are in good agreement with direct numerical simulation of the NLSE. We compare our method with a collective coordinate approach of Kominis and give examples where the two methods give qualitatively different answers. In our variational approach, we are able to give analytic results for the small oscillation frequency of the solitary wave oscillating parameters which agree with the numerical solution of the collective coordinate equations. We also verify that instabilities set in when the slope of $dp(t)/dv(t)$ becomes negative when plotted parametrically as a function of time, where $p(t)$ is the momentum of the solitary wave and $v(t)$ the velocity.

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I. INTRODUCTION

The behavior of solitary waves in the presence of complex potentials and in particular solitary wave solutions of the NLSE in the presence of complex potentials has been the subject of much recent investigation [1] [2] [3] [4]. Complex potentials in Quantum Mechanics with $\mathcal{PT}$ symmetry [5–7] possess special properties such as having real spectra. By further imposing other relations such as solvability as a result of supersymmetry one can restrict the behavior of solitary waves which occur when we add these potentials to the NLSE [3]. In a recent paper, some of us studied the behavior of the exact solitary wave solutions of the NLSE in the presence of a complex $\mathcal{PT}$ symmetric trapping potential [4]. Motivated to a considerable degree by the study of the specially balanced $\mathcal{PT}$-symmetric dynamical models [5–7], there has been, in the past 15 years, a large number of studies of open systems having both gain and loss.

The original proposal of Bender and collaborators to study such systems was made as an alternative to the postulate of hermiticity in quantum mechanics. Yet, in the next decade, proposals aimed at the experimental realization of such $\mathcal{PT}$-symmetric systems found a natural setting in the realm of optics [2, 9]. Within the latter, the above theoretical proposal (due to the formal similarity of the Maxwell equations in the paraxial approximation and the nonlinear Schrödinger equation) quickly led to a series of experiments [10]. As noted in [1] $\mathcal{PT}$ symmetric behavior should be observable in standard quantum well semiconductor lasers or semiconductor optical amplifiers [11]. The possibility of experimentally observing the effects of $\mathcal{PT}$ symmetry has motivated experiments in numerous other areas, which include the examination of $\mathcal{PT}$-symmetric electronic circuits [12, 13], mechanical systems [14] and whispering-gallery microcavities [15]. In all these systems solitary waves play an important role in the dynamics and the behavior of the solitary waves in these complex potentials can now be explored experimentally. Thus having a simple way of examining the dynamics of these solitary waves and their stability properties is quite important for future experiments.

Our paper is organized as follows. In section II we introduce a generalized variational method for obtaining the NLSE in the presence of complex potentials. This requires the introduction of a dissipation functional. In that section we also show how to introduce macroscopic collective variables, which depend only on time, based on the real density and current familiar from the Schrödinger equation. The dynamics of these macroscopic variables depend on integrals over the real and imaginary parts of the external potential. These results just depend on assuming the solitary wave wave-function ψ is a function of $x - q(t)$ and is a solution of the NLSE in the presence of an external complex potential. In section III, we make use of the variational formulation of the dynamics to introduce a reduced parameter space approximation to the dynamics, where the dynamics is obtained from the variational principle which includes a dissipation function. In this approach we parametrize the solitary wave function by collective variables representing the amplitude, width, position, and phase of the solitary wave. We have successfully used this four collective coordinate approach (4 CC) earlier [17] [18] [19] in studying the effect of external forces in the NLSE. There we found the stability criterion

$$\frac{dp}{dv} > 0, \tag{1}$$

where $p(t), v(t) = \dot{q}(t)$ are a parametric representation of the curve $p(v)$. Here $p(t) = P(t)/M(t)$, is the scaled momentum of the soliton, and $v(t) = \dot{q}(t)$ is the velocity of of the solitary wave. We will define these variables more precisely below. What we found in our previous studies [17] [18] [19], was that whenever Eq. (1) was violated anywhere on the curve $p(v)$ the soliton became unstable. i.e. $dp/dv < 0$ is a sufficient condition for instability. We will show in what follows that this instability either leads to the solitary wave then oscillating at another frequency, or blowing up or collapsing. The usefulness of this criterion for studying soliton stability in generalized NLSEs was investigated in detail in [20]. In section IV we discuss the simplification of the collective coordinate dynamics that occurs when the complex external potential is $\mathcal{PT}$ symmetric. In Section V we briefly describe our method of numerically solving the NLSE. In section VI we consider several examples of complex potentials previously considered by Kominis [3], in order to compare our approach to his and also to direct numerical simulations. In section VI we summarize our main conclusions.

II. DISSIPATION FUNCTIONAL FORMULATION OF THE NLSE WITH A COMPLEX POTENTIAL

We are interested in devising a variational principle for obtaining the equation for the wave function and its complex conjugate for the NLSE in a complex potential. The complexity of the potential makes the problem non-conservative and there are several approaches to dealing with this problem. Here we will use an extension of the Dissipation Functional method that we used previously [19] when the complex part of the potential was a constant.

The equations we are interested in studying are:

$$i\psi_t + \partial_x^2 \psi + g(\psi^*\psi)^\kappa \psi - (V + iW)\psi = 0 \tag{2}$$

as well as its complex conjugate equation:

$$-i\psi_t^\star + \partial_x^2 \psi^* + g(\psi^*\psi)^\kappa \psi^* - (V - iW)\psi^* = 0. \tag{3}$$

Let us define the usual conservative part of the action as

$$\Gamma = \int dt L_c, \tag{4}$$

where the conservative part of L_c depends only on the real part of the potential and is given by

$$L = \int \mathcal{L} dx = \frac{i}{2} \int dx (\psi^* \psi_t - \psi_t^\star \psi) - H_c. \tag{5}$$

For the NLSE with arbitrary nonlinearity parameter κ in d spatial dimensions we have

$$H_c = \int dx [\partial_x \psi^* \partial_x \psi - g \frac{(\psi^*\psi)^{\kappa+1}}{\kappa+1} + \psi^* V(x)\psi]. \tag{6}$$

We will introduce the Dissipation Functional F via

$$F = \int \mathcal{F} dx dt, \tag{7}$$

where

$$\mathcal{F} = iW(x)\left(\psi_t \psi^\star - \psi_t^\star \psi\right). \tag{8}$$

The equations for the wave function of the NLSE in the presence of a complex potential follow from the generalized Euler-Lagrange Equations:

$$\frac{\delta \Gamma}{\delta \psi^*} = -\frac{\delta F}{\delta \psi_t^\star} \tag{9}$$

and its complex conjugate equation. Equation (9) leads to

$$\partial_t \frac{\partial \mathcal{L}}{\partial \psi_t^\star} + \partial_x \frac{\partial \mathcal{L}}{\partial \psi_x^\star} - \frac{\partial \mathcal{L}}{\partial \psi^*} = \frac{\partial \mathcal{F}}{\partial \psi_t^\star}, \tag{10}$$

which yields Eq. (2). The complex conjugate of Eq. (9) leads to the complex conjugate of the NLSE equation, namely Eq. (3).

If we multiply Eq. (2) by ψ^* and add the complex conjugate, then W drops out from the resulting equation and we can obtain a Virial Theorem for the spatial average of the potential. Explicitly we find:

$$\frac{i}{2} \int dx (\psi^* \psi_t - \psi_t^\star \psi) - \int dx \left[\partial_x \psi^* \partial_x \psi - g \frac{(\psi^*\psi)^{\kappa+1}}{\kappa+1} \right] = \int dx \psi^* V(x)\psi]. \tag{11}$$

Another approach for handling complex potentials has been recently put forth by Rossi et al [8]. However, for the problem at hand the dissipation function is sufficient as it leads to results consistent with the equations for the single particle variables of the soliton, such as mass, position and momentum derived directly from the NLSE, as discussed in the next subsection. In what follows we will be interested in the particular case $\kappa = 1, g = 2$. (g of course can be scaled out of the NLSE by a rescaling of the fields).

A.   General Properties of the NLSE in complex potentials

A general approach for studying soliton dynamics has been discussed for real potentials in the work of Quintero, Mertens and Bishop [20] and also by Kominis [3] for complex potentials. Here we follow the approach of [20]. We are

interested in solitary wave solutions that approach zero exponentially at $\pm\infty$. For these solutions we define the mass density $\rho(x,t) = \psi^*\psi$, and the mass or norm $M(t)$ as

$$M(t) = \int dx\, \rho(x,t) = \int dx\, \psi^*(x,t)\psi(x,t). \tag{12}$$

We also define the current as:

$$j(x,t) = i(\psi\psi_x^\star - \psi^*\psi_x). \tag{13}$$

From the NLS equations we have

$$\frac{\partial\rho(x,t)}{\partial t} + \frac{\partial j(x,t)}{\partial x} = 2W(x)\rho(x,t). \tag{14}$$

Integrating over space, and assuming that $\rho(x,t) = \rho(x-q(t),t)$, where $q(t)$ is the position of the solitary wave, we find

$$\frac{dM(t)}{dt} = 2\int dx\, W(x)\,\rho(x-q(t),t) \tag{15}$$

$$= 2\int dy\, W[y+q(t)]\,\rho(y,t). \tag{16}$$

Here the explicit time dependence in $\rho(x-q(t),t)$ takes into account that the shape of the soliton may depend on time. We observe that M is conserved when $W(x) = 0$. From this we have that when $W(x) = -\alpha$, with α a positive constant, the mass dissipates to zero, since

$$\frac{dM(t)}{dt} = -2\alpha M(t) \rightarrow M(t) = M(0)e^{-2\alpha t}. \tag{17}$$

If $\rho(x,t)$ is symmetric about its midpoint, then $q(t)$ can be defined through:

$$M(t)q(t) = \int dx\, x\, \psi^*(x-q(t),t)\psi(x-q(t),t). \tag{18}$$

Multiplying the continuity equation Eq. (14) by x and integrating over all space we find:

$$\frac{d}{dt}\int dx\, x\,\rho(x,t) = 2P(t) + \int dx\,(2x\,W(x)\,\rho(x,t)), \tag{19}$$

where

$$P(t) = \frac{1}{2}\int dx\, j(x) = \int dx\,\left[\frac{i}{2}(\psi\psi_x^\star - \psi^*\psi_x)\right]. \tag{20}$$

Again assuming $\rho(x,t) = \rho(x-q(t),t)$, we can write this equation, using $y = x-q(t)$, as:

$$\frac{d}{dt}[M(t)\,q(t)] = 2\,P(t) + \int dy\, 2\,y\,W[y+q(t)]\,\rho(y,t) + 2\,q(t)\int dx\, W[x]\,\rho(x-q(t),t). \tag{21}$$

We recognize the last term as $q(t)dM(t)/dt$, so that we finally have:

$$M(t)\frac{dq(t)}{dt} = 2\,P(t) + \int dy\, 2\,y\,W[y+q(t)]\,\rho(y,t). \tag{22}$$

Letting $p(t) = P(t)/M(t)$, we obtain

$$\dot{q}(t) = 2p(t) + \frac{1}{M(t)}\int dy\, 2\,y\,W[y+q(t)]\,\rho(y,t). \tag{23}$$

Taking the time derivative of the momentum $P(t)$, using the equations of motion for ψ and ψ^* and integrating by parts, we find

$$\frac{dP}{dt} = -\int dx \; \rho(x,t) \frac{\partial V}{\partial x} + \int dx \; j(x,t) \, W(x). \tag{24}$$

Assuming as in quantum mechanics that

$$\frac{1}{i}\frac{\partial}{\partial x}\psi(x,t) = p(t)\,\psi(x,t), \tag{25}$$

or equivalently

$$\frac{1}{2}j(x,t) = p(t)\,\rho(x,t), \tag{26}$$

which is the local version of the integral relationship $P(t) = M(t)p(t)$, then the last term in Eq. (24) is $p\,dM/dt$, so that we find:

$$M(t)\frac{dp}{dt} = -\int dx \; \rho(x - q(t),t)\frac{\partial V}{\partial x}. \tag{27}$$

Again changing variable to $y = x - q(t)$, we find

$$M(t)\frac{dp}{dt} = -\frac{\partial}{\partial q(t)}\int dy\,\rho(y,t)\,[V(y+q(t)]. \tag{28}$$

By dividing Eq. (15) by Eq. (27), we find that

$$\frac{d\log M}{dp} = -2\frac{\int dx \; W(x)\,\rho(x - q(t),t)}{\int dx \; \rho(x - q(t),t)\frac{dV(x)}{dx}}. \tag{29}$$

Now suppose we have (as a result of some symmetry such as supersymmetry) that

$$W(x) = C_1\frac{dV(x)}{dx}. \tag{30}$$

Then

$$\frac{d\log M}{dp} = -2C_1. \tag{31}$$

Integrating we obtain a conservation law

$$\log M + 2C_1\,p = C_2. \tag{32}$$

This is quite similar to Eq. (10) of Kominis [3] , however he has v instead of $2p$ which is not correct when the potential has an imaginary part. In both approaches, the resulting conservation law reduces the space of these particle-like variables so it is confined to a two dimensional subspace. However the correct subspace is in the variables p, M and not $\dot{q}, M$. We can also introduce the (unnormalized) two-point correlation function, where again $y = x - q(t)$:

$$G_2(t) = \int dy \; y^2\,\rho(y,t). \tag{33}$$

Multiplying the continuity equation by x^2, integrating over all space and then changing variables to y one finds:

$$\frac{dG_2}{dt} = 2\int dy \; y \; j(y,t) + 2\int dy \; y \; \rho(y,t)\,W[y+q]. \tag{34}$$

III.   COLLECTIVE COORDINATE APPROACH TO SOLITARY WAVE BEHAVIOR IN COMPLEX POTENTIALS

We start with the exact solution [21] for the solitary wave in the NLSE when the potential is zero for the case $\kappa = 1, g = 2$, namely:

$$\psi(x,t) = \beta \operatorname{sech}[\beta(x - vt)]e^{i[p(x-vt)-\phi(t)]}, \tag{35}$$

where

$$p = \frac{v}{2}; \quad \phi(t) = -\left(\frac{v^2}{4} + \beta^2\right)t + \phi_0. \tag{36}$$

The mass M of the solitary wave is defined as

$$M = \int dx\, \psi^*\psi = \beta \int dy \operatorname{sech}^2 y = 2\beta, \tag{37}$$

and the momentum P is defined as

$$P(t) = \frac{1}{2} \int dx\, j(x) = M(t)p(t). \tag{38}$$

We next assume that we can parametrize the "approximate" solitary wave by the *same* parameters that the solitary wave has when the potential is zero, with the difference being that $\beta \to \beta(t)$, $vt \to q(t)$, $p \to p(t)$, and $\phi(t)$ now are unspecified functions of t [22]. That is, we will take as our trial wave function:

$$\psi(x,t) = \beta(t)\operatorname{sech}[\beta(t)(x - q(t))]e^{i[p(t)(x-q(t))-\phi(t)]}. \tag{39}$$

For the free part of the Lagrangian, we get the effective free action

$$S_0 = \int dt L_0 = \int dt M(t)\left[p\dot{q} + \dot{\phi} - p^2 - \frac{\beta^2}{3}\right], \tag{40}$$

where $M(t) = 2\beta(t)$. The self-interaction contributes

$$S_I = \int dt L_I = \int dt M(t)\left[\frac{2\beta^2}{3}\right]. \tag{41}$$

The real part of the potential contributes:

$$\begin{aligned}
S_v &= -\int dt \beta^2(t)\int dx\, V(x)\operatorname{sech}^2[\beta(x - q(t))] \\
&= -\int dt \beta(t)\int dz V\left(\frac{z}{\beta} + q\right)\operatorname{sech}^2 z \\
&\equiv -\int dt\, 2\beta(t)U_{eff}(\beta, q),
\end{aligned} \tag{42}$$

where

$$U_{eff}(\beta, q) = \frac{1}{2}\int dz V\left(\frac{z}{\beta} + q\right)\operatorname{sech}^2 z. \tag{43}$$

Thus

$$\Gamma = \int dt L_c = 2\int dt \beta(t)\left[p\dot{q} + \dot{\phi} - p^2 + \frac{\beta^2}{3} - U_{eff}(\beta, q)\right]. \tag{44}$$

For the dissipation function we obtain:

$$F = i \int dx\, dt W(x) \left(\psi_t \psi^\star - \psi_t^\star \psi \right)$$

$$= -2 \int dt \beta^2(t) dx\, W(x) \text{sech}^2 \beta(x - q(t)) \left[\dot{p}(x - q(t)) - p\dot{q} - \dot{\phi} \right]$$

$$= -2 \int dt \left(\beta(t) \int dz W \left(\frac{z}{\beta} + q \right) \text{sech}^2 z \left[\frac{z}{\beta}\dot{p} - p\dot{q} - \dot{\phi} \right] \right),$$

(45)

where we have set $z = \beta(x - q)$. When the imaginary part of the potential is a negative constant $W(x) \to -\alpha$, then we obtain

$$F = - \int dt \left[4\alpha\beta(t) \left(p\dot{q} + \dot{\phi} \right) \right].$$

(46)

The equation for β comes from:

$$\frac{d}{dt} \frac{\delta L}{\delta \dot{\phi}} = -\frac{\delta F}{\delta \dot{\phi}}.$$

(47)

For an arbitrary complex potential whose imaginary part is W we obtain:

$$2\dot{\beta} = 2\beta(t) \int dz W \left(\frac{z}{\beta} + q \right) \text{sech}^2 z,$$

(48)

which is just a restatement of Eq. (15).

Defining

$$W_{eff}[\beta, q] = \frac{1}{2} \int dz W \left(\frac{z}{\beta} + q \right) \text{sech}^2 z,$$

(49)

we can write this equation as

$$\dot{\beta} = 2\beta(t) W_{eff}[\beta, q].$$

(50)

In the special case $W(x) \to -\alpha$ we obtain

$$2\dot{\beta} = -4\alpha\beta.$$

(51)

Since $M(t) = 2\beta$ for our variational ansatz, this is exactly the collective coordinate version of the equation for the dissipation of $M(t)$ we discussed earlier [Eq. (17)].

In general the equations for the collective coordinates are

$$\frac{\delta\Gamma}{\delta Q_i} = -\frac{\delta F}{\delta \dot{Q}_i},$$

(52)

where $Q_i = q, p, \phi, \beta$.

Choosing $Q_i = p$, we obtain from

$$\frac{\delta\Gamma}{\delta p} = -\frac{\delta F}{\delta \dot{p}}$$

(53)

that

$$\dot{q} = 2p + \frac{1}{\beta} \int dz W[z/\beta + q] z\, \text{sech}^2 z,$$

(54)

which is the collective coordinate version of Eq. (23). Defining

$$Y_{eff}[q, \beta] = \int dz W[z/\beta + q] z\, \text{sech}^2 z,$$

(55)

we can write this equation as

$$\dot{q} = 2p + \frac{1}{\beta} Y_{eff}[q, \beta]. \tag{56}$$

From the Euler-Lagrange equations:

$$-\frac{d}{dt}\frac{\delta L}{\delta \dot{q}} + \frac{\delta L}{\delta q} = -\frac{\delta F}{\delta \dot{q}} \tag{57}$$

we obtain

$$-\frac{d}{dt}[2\beta p] - 2\beta\frac{\partial U_{eff}}{\partial q} = -2\beta p \int dz W[z/\beta + q]\text{sech}^2 z. \tag{58}$$

The last term we recognize as $-2\dot{\beta}p$, so we obtain the simple result:

$$\dot{p}(t) = -\frac{\partial U_{eff}}{\partial q}. \tag{59}$$

Finally the equation for ϕ is obtained by choosing $Q_i = \beta$:

$$-\frac{d}{dt}\frac{\delta L}{\delta \dot{\beta}} + \frac{\delta L}{\delta \beta} = -\frac{\delta F}{\delta \dot{\beta}} \rightarrow \frac{\delta L}{\delta \beta} = 0. \tag{60}$$

From this we obtain:

$$\dot{\phi} = p^2 - p\dot{q} - \beta^2 + \frac{\partial}{\partial \beta}\left[\beta U_{eff}(\beta, q)\right], \tag{61}$$

which reduces to the exact result of Eq. (36) when $V = 0$.

IV. $\mathcal{PT}$ SYMMETRIC POTENTIALS

Recently there has been much interest in $\mathcal{PT}$ symmetric potentials for the NLSE because they represent equal gain and loss in nonlinear optical devices. Under $\mathcal{P}$: $x \rightarrow -x$ and under $\mathcal{T}$: $t \rightarrow -t$ and $i \rightarrow -i$, the complex potential

$$V(x) + iW(x) \rightarrow V(-x) - iW(-x), \tag{62}$$

so that if $V(x)$ is even and $W(x)$ is odd one has that the complex potential is $\mathcal{PT}$ symmetric. Let us consider now a particular potential considered by Kominis [3]:

$$V(x) = V_0 \cos k_0 x, \quad W(x) = W_0 \sin l_0 x. \tag{63}$$

From this we can evaluate

$$U_{eff}(\beta, q) = \frac{V_0}{2} \int dz \cos[k_0 z/\beta + k_0 q]\text{sech}^2 z. \tag{64}$$

Expanding the $\cos(x)$ term and keeping only the even part we then have that the integral is

$$\cos k_0 q(t) \int dz \cos[k_0 z/\beta]\text{sech}^2 z = 2\cos(k_0 q) \, K_0 \, \text{csch}(K_0). \tag{65}$$

Thus

$$U_{eff}(\beta, q) = V_0 \cos(k_0 q) \, K_0 \text{csch} K_0, \tag{66}$$

where we have introduced the notation

$$K_0 = \frac{\pi k_0}{2\beta}, \quad L_0 = \frac{\pi l_0}{2\beta}. \tag{67}$$

To determine the dissipation function we need to evaluate

$$W_{eff}(\beta, q) = \frac{W_0}{2} \sin(l_0 q) \int dz \cos[l_0 z/\beta] \text{sech}^2 z = W_0 \sin(l_0 q) L_0 \text{csch}(L_0), \tag{68}$$

as well as

$$Y_{eff}(\beta, q) = \int dz z W[z/\beta + q] \text{sech}^2 z = W_0 \cos(l_0 q) \int dz z \sin[l_0 z/\beta] \text{sech}^2 z. \tag{69}$$

We have

$$\int dz\, z\, \sin[az] \text{sech}^2 z = \pi \text{csch}^2\left(\frac{\pi a}{2}\right) \left(\frac{\pi a}{2} \cosh\left(\frac{\pi a}{2}\right) - \sinh\left(\frac{\pi a}{2}\right)\right), \tag{70}$$

so that

$$Y_{eff}(\beta, q) = W_0 \cos(l_0 q) \left[\pi \text{csch}^2(L_0)(L_0 \cosh(L_0) - \sinh(L_0))\right]. \tag{71}$$

From our general formalism of the previous section we now have from Eq. (56)

$$\dot{q} = 2p + \frac{1}{\beta} W_0 \cos(l_0 q) \left[\pi \text{csch}^2(L_0)(L_0 \cosh(L_0) - \sinh(L_0))\right]. \tag{72}$$

From Eq. (59) we obtain

$$\dot{p} = k_0 V_0 \sin(k_0 q) K_0 \text{csch} K_0 \tag{73}$$

and from Eq. (50)

$$\dot{\beta} = 2\beta W_0 \sin(l_0 q) L_0 \text{csch} L_0. \tag{74}$$

Finally, once we obtain p, q, β we can obtain ϕ from Eq. (61):

$$\dot{\phi} = p^2 - p\dot{q} - \beta^2 + (K_0)^2 V_0 \coth(K_0) \text{csch}(K_0) \cos(k_0 q). \tag{75}$$

Note that if we make the restriction $k_0 = l_0$ then indeed we satisfy the condition Eq. (30), and we obtain from Eqs. (73) and (74) that

$$\frac{d \log 2\beta}{dp} = \frac{2W_0}{k_0 V_0} = D_1 \tag{76}$$

leading to the conservation law we derived in general [Eq. (32)]

$$\log 2\beta - D_1 p = \text{Constant}. \tag{77}$$

We can use this conservation law to simplify the analysis of the stability of the solitary wave. If we let $p \to p_0 + \delta p, \beta \to \beta_0 + \delta\beta$, and assume the variation is small, we obtain the relation:

$$\delta\beta = D_1 \beta_0 \delta p. \tag{78}$$

For the results shown in Fig. 1 we let $D_1 = 1$ so that $\beta_0 = 1/2$ and the amplitude of oscillations is small. For that case, the relation that $\delta\beta = \frac{1}{2}\delta p$ is borne out in the simulations, showing that the simulations preserve the conservation law Eq. (32).

We now use Eq. (77) and let $\beta = \beta_0 + D_1 \beta_0 \delta p$, $q = q_0 + \delta q$, $p = p_0 + \delta p$. Using these relations we can study the two coupled equations for $\delta\dot{p}$ and $\delta\dot{q}$, which can be written as a simple matrix equation:

$$Y = AX, \tag{79}$$

where Y is the column vector $(\delta\dot{q}, \delta\dot{p})$ and X is the column vector $(\delta q, \delta p)$. The eigenvalues of A determine the frequencies of oscillation for small oscillations of these variables.

V. NUMERICAL APPROACH FOR SOLVING THE NLSE IN THE PRESENCE OF COMPLEX POTENTIALS

We have numerically solved Eq. (2) with the initial condition (39) using the Crank-Nicolson scheme [23]. We have considered the evolution of solitary waves up to 10^3 time units with step size $\Delta t = 10^{-3}$. The complex solitary wave in the spatial domain was represented on a regular grid with mesh size $\Delta x = 10^{-3}$, and free boundary conditions were imposed. We found that during the time evolution, the shape of the mass density $\rho(x, t)$ was well parametrized by the form:

$$\rho(x, t) = \beta^2(t)\text{sech}^2[\beta(t)(x - q(t))], \tag{80}$$

with no sign of any phonon radiation in the cases that we studied.

VI. COMPARISON OF TWO DIFFERENT COLLECTIVE COORDINATE APPROACHES WITH NUMERICAL SIMUATIONS

Here we would like to present several cases that were also studied in a two collective coordinate (2 CC) approach by Kominis [3]. For comparison, we will give (in our notation) the equations used by Kominis in his approach. For the mass equation (in our notation $M = 2\beta$) one obtains the same first-order differential equation:

$$\dot{\beta} = 2\beta\, W_0 \sin(l_0 q)\,[(L_0\text{csch}(L_0)]\,. \tag{81}$$

However, Kominis (incorrectly) identifies $p = \dot{q}/2$ and as a result obtains a second-order equation for $q(t)$, namely:

$$\frac{1}{2}\ddot{q} = k_0 V_0 \sin(k_0 q)\ K_0\text{csch}K_0, \tag{82}$$

instead of our two coupled first order equations Eqs. (72) (73). He obtains a similar conservation law when $k_0 = l_0$ with our $p(t)$ replaced by $\dot{q}/2$.

We will see below in which situations Kominis' equations lead to worse agreement when compared with the numerical simulations of the NLSE. In all the following plots, when we plot $p(t)$ it is only for the 4 CC theory. For the 2 CC theory $p = \dot{q}/2$, and $dp/dv = 1/2$, so one can never use our stability criterion.

A. Trapped Solitary Waves

First we consider a case when the solitary wave is trapped at the origin and where our linear stability analysis is valid. This is achieved by taking as our parameters and initial conditions: $V_0 = -0.01; W_0 = V_0/2; k_0 = l_0 = 1; q_0 = 0.1; v_0 = 0; \beta_0 = 0.5; \phi_0 = 0$. The linear stability analysis discussed in the previous section, Eq. (79), yields a period $T = 85.6$, which agrees with the numerical results from the CC equations which yields $T = 85.1$ for the period of oscillation for all the CC parameters. For this trapped solitary wave, the 2 CC equations lead to almost the same result for the behavior of $\dot{q}$ and β as the 4 CC equations and both agree with the numerical simulations.

However, if we change the initial conditions and increase the ratio of the strength of the imaginary to real part to be one, i.e. $W_0 = V_0$ as well as change the initial position of the solitary wave to be one and give the solitary wave a small velocity, i.e. choose $V_0 = -0.01; W_0 = V_0; k_0 = l_0 = 1; q_0 = 1; v_0 = 0.1; \beta_0 = 0.5; \phi_0 = 0, p_0 = 0.0531649$, then the 4 CC approach we advocate here gives different results than the 2 CC approach of Kominis. In this case we are outside the range where the linear stability analysis is valid. A comparison of the two approximations can be seen in Fig. 1. We find that our results (solid black curves) agree with the numerical simulations (blue open circles) and disagree significantly from the 2 CC equations of Kominis (red dashed lines). In order to compare the phases, we have subtracted the linear dependence of the phase from the original data. For that reason we have defined a relative phase,

$$\phi_{\text{relative}}(t) = \phi(t) - (A\,t + B),$$

where the coefficients A and B follow from the linear-least-squares fitting of the original data.

Because of the conservation law, Eq. (77), only the p, q first order differential equations are needed. Performing the linear stability analysis discussed earlier, we obtain that the period of oscillation should be $T = 118.133$ which is little lower than that seen in the solution of the CC equations which yields $T = 142.857$. The agreement with the linear stability analysis can be made better by decreasing the initial velocity, but this would then mask the differences between the outcome of using 2 CC or 4 CC equations.
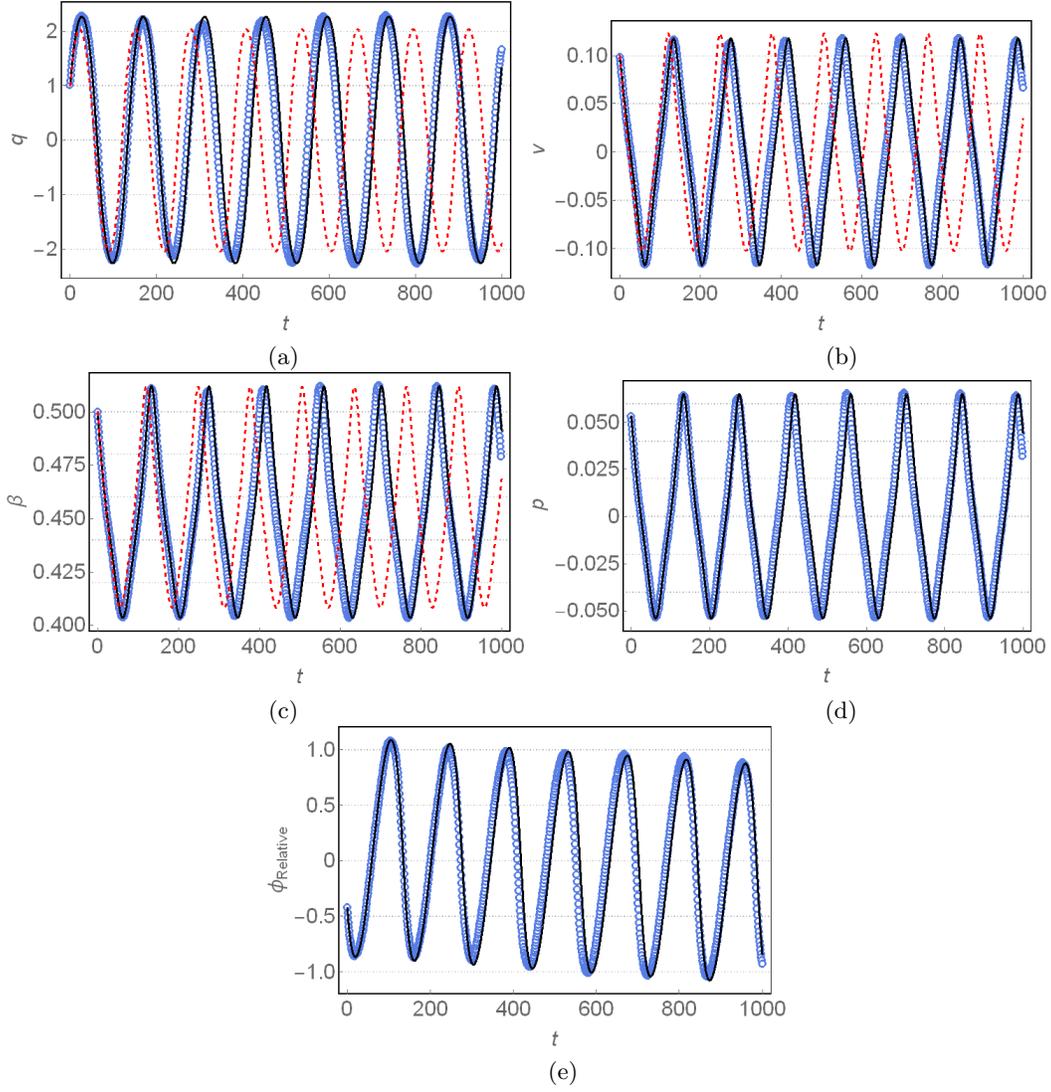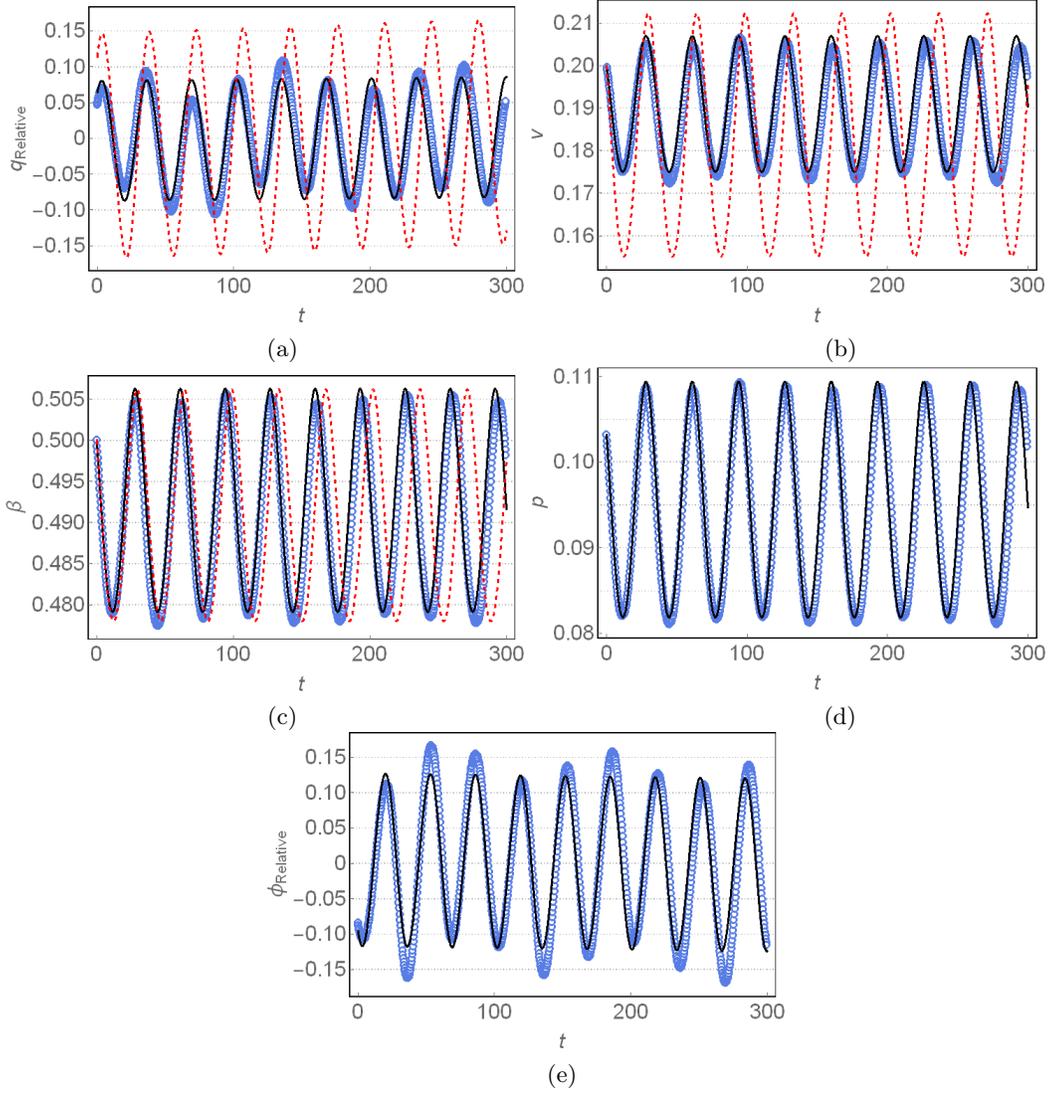
FIG. 1. Solitary wave in the trapped case. Comparison of the 4 CC theory (black solid lines) with the 2 CC theory (red dashed lines) and numerical simulation(blue open circles) (a) position $q(t)$; (b) velocity $v(t)$; (c) amplitude $\beta(t)$; (d) momentum $p(t)$; (e) relative phase $\phi_{\mathrm{relative}}(t)$. $l_0 = 1$, $k_0 = 1$, $V_0 = -0.01$, $W_0 = -0.01$, $\beta_0 = 0.5$, $q_0 = 1$, $v_0 = 0.1$, $p_0 = 0.0531649$, $\phi_0 = 0$.

B. Traveling Soliton

For the traveling soliton, one already sees instances where our 4 CC approach differs from the 2 CC approach of Kominis. Taking for our parameters and initial conditions:

$$V_0 = -0.01 = W_0; k_0 = 1 = l_0; q_0 = 1; v_0 = 0.2; \beta_0 = 0.5; \phi_0 = 0; p_0 = .0531649; \phi_0 = 0, \tag{83}$$

we are again in a situation where the conservation law Eq. (77) holds. We find in this case that our results (black solid lines) agree with the numerical simulations (blue open circles) and differ significantly from the 2 CC approach of Kominis (red dashed lines) as seen in Fig. 2.

As it was done with the phase, here we have subtracted the linear dependence of the position from the original data. Therefore, we have defined a relative position,

$$q_{\mathrm{relative}}(t) = q(t) - (A\,t + B),$$

where the coefficients A and B follow from the linear-least-squares fitting of the original data.

FIG. 2. Traveling solitary wave. Comparison of the 4 CC theory (black solid lines) with the 2 CC theory (red dashed lines) and numerical simulation(blue open circles) (a) relative position $q_{\text{relative}}(t)$, (b) velocity $v(t)$, (c) amplitude $\beta(t)$, (d) momentum $p(t)$, and (e) relative phase $\phi_{\text{relative}}(t)$. Here $l_0 = 1$, $k_0 = 1$, $V_0 = 0.01$, $W_0 = 0.01$, $\beta_0 = 0.5$, $q_0 = 1$, $v_0 = 0.2$, $p_0 = 0.103165$, $\phi_0 = 0$.

C.   Results with $k_0 \neq l_0$

When $k_0 \neq l_0$, then the simple relation between $\beta(t)$ and $p(t)$ no longer holds and the phase space is now three dimensional. In this case our 4 CC approach can differ significantly from the approach of Kominis and also we can understand when there is an instability. First let us consider a case where the solitary wave is quasi-periodic. For this case we choose for our initial conditions:

$$V_0 = -0.01, W_0 = V_0, k_0 = 1, l_0 = \sqrt{2}, q_0 = \pi, v_0 = 0.05; , \beta_0 = 0.5, \phi_0 = 0, p_0 = 0.0243222. \tag{84}$$

For this case our 4 CC approach again agrees quite well with the numerical simulation. The 2 CC approach generally agrees with the 4 CC approach in this case but does not give information about the phase ϕ. The quasiperiodicity is seen best in the soliton amplitude $\beta(t)$ and phase $\phi(t)$, see Figs. 3 (c), (e). In the other CCs the quasiperiodicity is less pronounced. This difference is also obvious in the Discrete Fourier Transforms (DFT) of $\beta(t)$ and $v(t)$ in Fig. 5.

Also in our approach $p \neq \dot{q}/2$ and we have a criterion for when the period is about to change–namely when $dp/dv = 0$, as shown in Fig. 4 which agrees with the numerical simulations.
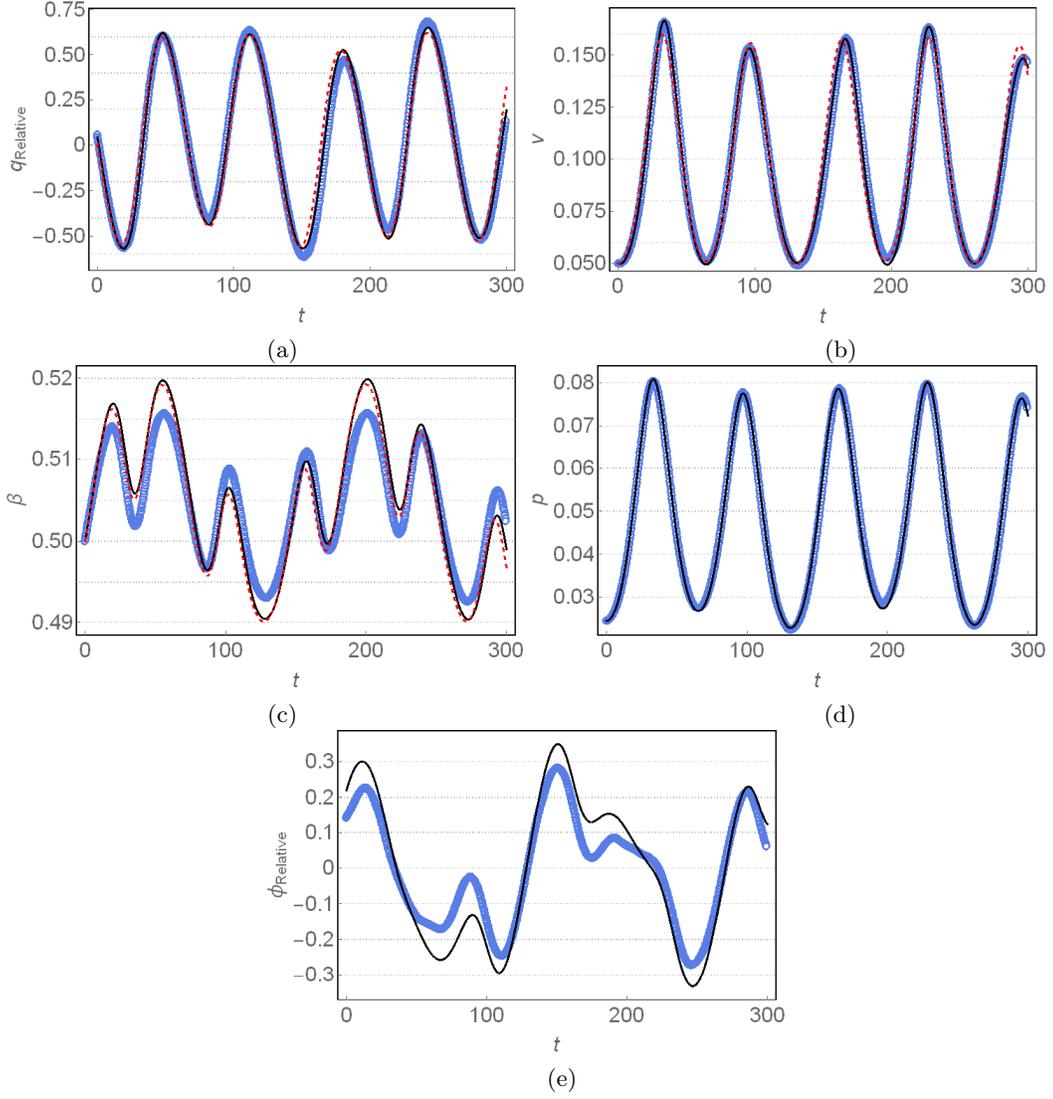
FIG. 3. Moving solitary wave in the quasiperiodic case, (a) relative position $q_{\text{relative}}(t)$, (b) velocity $v(t)$, (c) amplitude $\beta(t)$, (d) momentum $p(t)$, and (e) relative phase $\phi_{\text{relative}}(t)$. Here $l_0 = \sqrt{2}$, $k_0 = 1$, $V_0 = 0.01$, $W_0 = 0.01$, $\beta_0 = 0.5$, $q_0 = \pi$, $v_0 = 0.05$, $p_0 = 0.0243222$, $\phi_0 = 0$.

As was done previously, here we have subtracted the linear dependence of the position as well as the phase from the original data using a linear fit.

To explore a blowup case (amplitude increasing in time) we will choose as our parameters:

$$V_0 = -0.01, W_0 = V_0, k_0 = 1, l_0 = 1/3, q_0 = \pi, v_0 = -0.1, \beta_0 = 0.5, \phi_0 = 0. \tag{85}$$

The numerical results track the 4 CC approximation up to $t \approx 300$ when the instability sets in as seen in Fig. 6. Again the 2 CC approximation breaks down much earlier around $t = 100$.

We also want to relate the onset of the instabilities to the situation when $dp/dv < 0$. This quantity changes sign initially when $v = -0.2$ and next when $v = 0.2$ which correlates to two changes in the oscillation frequency of $v(t)$ and ultimately to the blowup of the amplitude β as seen in Fig. 6 (f).
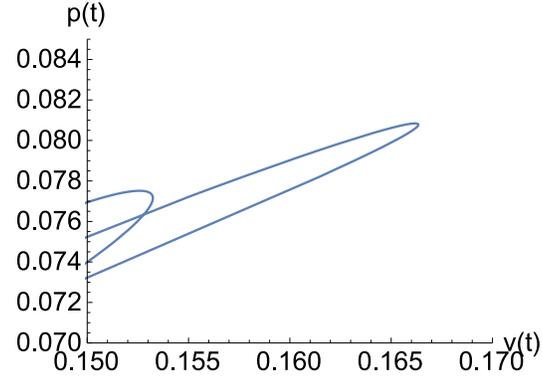
FIG. 4. Moving solitary wave in the quasiperiodic case when $k_0 = 1$, $l_0 = \sqrt{2}$. Magnification of the turnaround in the parametric plot of the momentum $p(t)$ vs. velocity $v(t)$. The slope dp/dv is negative for short pieces of the curve.
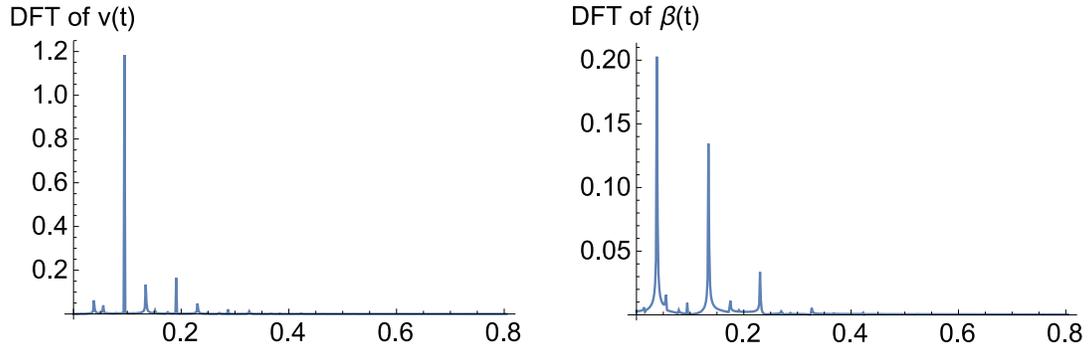

FIG. 5. Moving solitary wave in the quasiperiodic case. Left Panel: Discrete Fourier Transform of $v(t)$. Right Panel: DFT of $\beta(t)$.
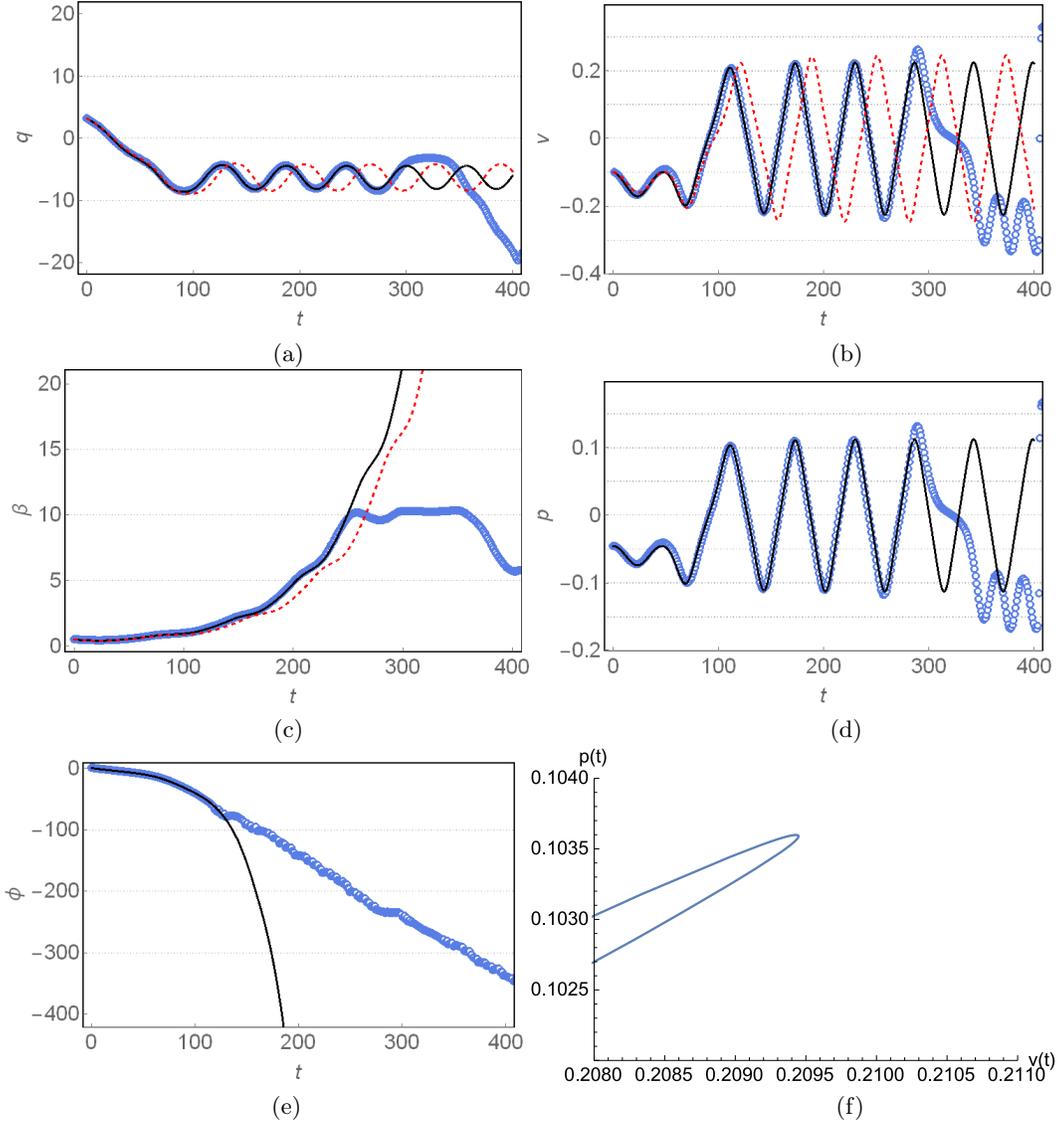
FIG. 6. Blowup (increasing amplitude) situation (a) position $q(t)$, (b) velocity $v(t)$, (c) amplitude $\beta(t)$, (d) momentum $p(t)$, (e) phase $\phi(t)$, and (f) magnification of the turnaround in the parametric plot of the momentum $p(t)$ vs. velocity $v(t)$. Parameters and initial conditions: $l_0 = 1/3$, $k_0 = 1$, $V_0 = -0.01$, $W_0 = -0.01$, $\beta_0 = 0.5$, $q_0 = \pi$, $v_0 = -0.1$, $p_0 = -0.0457085$, $\phi_0 = 0$.

D. Shifted Potential: $V(x) = V_0 \cos(k_0 x + \Delta)$, $W(x) = W_0 \sin l_0 x$

We next turn to two other situations discussed by Kominis to compare the 2 CC and 4 CC methods. Here we shift the real part of the potential $V(x)$ away from the origin, keeping $W(x)$ unshifted. This again breaks the conservation law. First we consider a case where the solitary wave is trapped but the amplitude is decreasing. Here we choose

$$V_0 = -0.01, W_0 = V_0/2, K_0 = 1, L_0 = 1, \Delta = -\pi/3, q_0 = 1.3\pi/3, v_0 = 0, \beta_0 = 0.5, \phi_0 = 0. \tag{86}$$

In this case, the oscillations of $q(t)$, $v(t)$, and $p(t)$ increase, but the amplitude (mass) $\beta(t)$ decreases. This is seen in Fig. 7. Here we find that the 4 CC result tracks well the numerics up to $t = 500$, whereas the 2 CC result begins failing around $t = 200$.

In the next case we look at initial conditions which lead to a moving soliton whose amplitude gradually increases in time. Interestingly, the frequency of the oscillations of $v(t)$ and $\beta(t)$ only increase gradually: this is seen in Fig. 9. The parameters and initial conditions we choose are

$$V_0 = -0.01, W_0 = V_0/2, K_0 = 1, L_0 = 1; , \Delta = -\pi/3, q_0 = 2.8\pi/3, v_0 = 0, \beta_0 = 0.5, \phi_0 = 0, p_0 = 0.000608946. \tag{87}$$
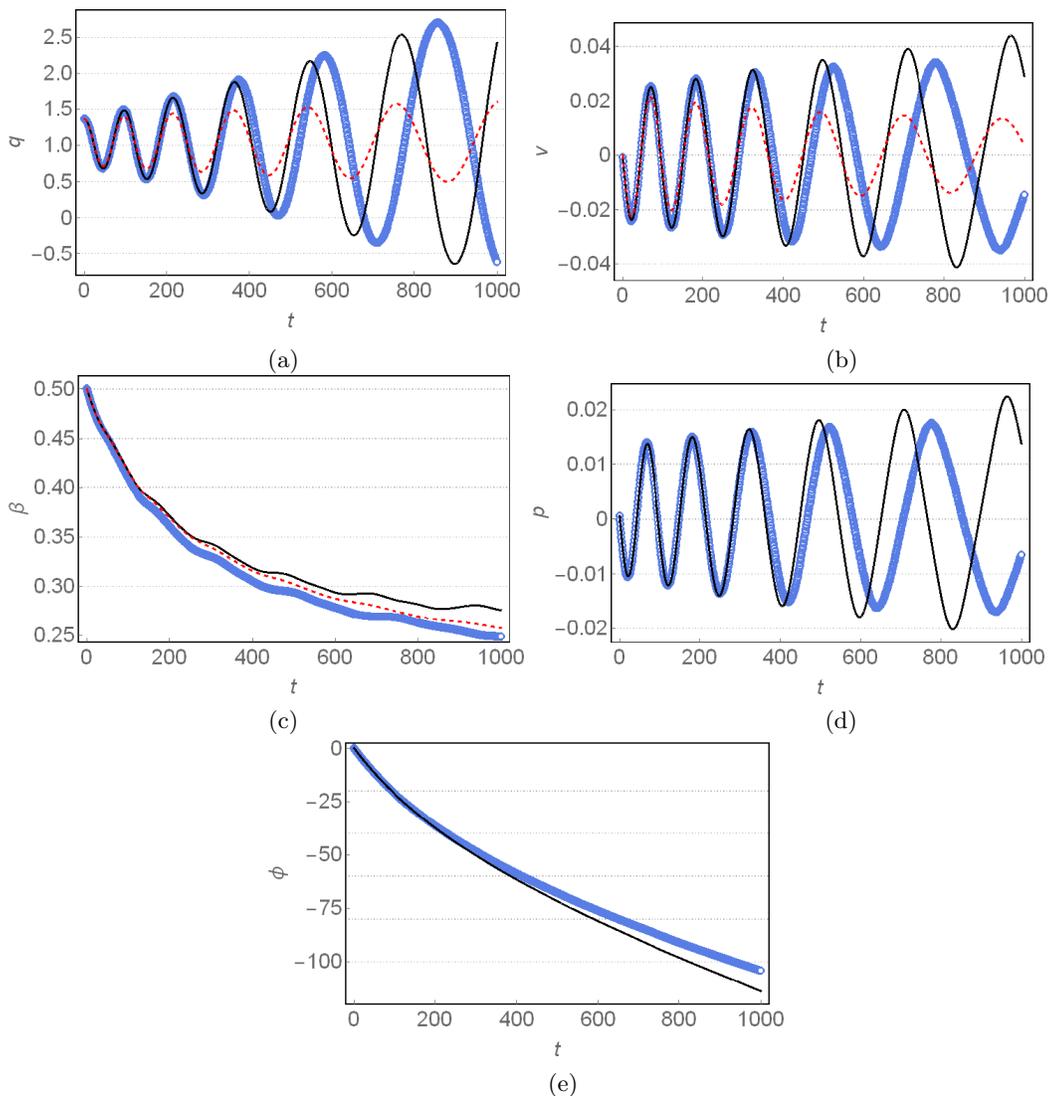
FIG. 7. Shifted potential-trapped case: (a) position $q(t)$, (b) velocity $v(t)$, (c) amplitude $\beta(t)$, (d) momentum $p(t)$, and (e) phase $\phi(t)$. Here $l_0 = 1$, $k_0 = 1$, $V_0 = -0.01$, $W_0 = -0.005$, $\beta_0 = 0.5$, $q_0 = 1.3\pi/3$, $v_0 = 0$, $p_0 = 0.000608946$, $\phi_0 = 0$, $\Delta = -\pi/3$.

Here we find that the 2 CC theory breaks down at around $t = 100$, whereas the 4 CC theory is qualitatively accurate for the entire time of simulation. This is seen in Fig. 9.

VII. CONCLUSIONS

We have studied the behavior of exact solitary wave solutions of the unforced NLSE in the presence of complex external potentials in a collective coordinate approximation which parametrizes the wave function with four time dependent parameters. This approximation gave excellent agreement with numerical simulations of the NLSE in most situations except the late time "blowup" situations. We demonstrated that our criterion for instabilities to occur, namely $dp/dv < 0$ was a good indicator for that to happen both in our variational approximation as well as for the full numerical simulation. We also showed that our approach was a great improvement over that of Kominis in many regimes of parameter space for various external complex potentials. We have also demonstrated that the use of the Dissipation Functional formalism combined with a judicious choice of parametrization of the solitary wave leads to a very simple way of understanding the response of solitary waves to external complex potentials.
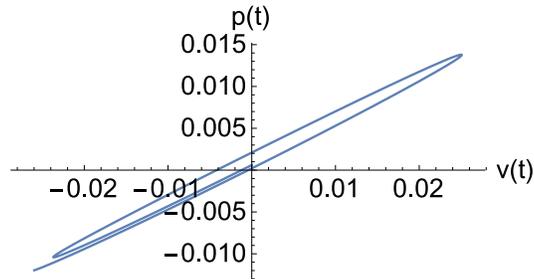
FIG. 8. Trapped solitary wave when $\Delta = -\pi/3, q_0 = 1.3\pi$. Parametric plot of $p(t)$ vs. $v(t)$ for $0 < t < 120$. Blue curve is our 4 CC approximation.

VIII.   ACKNOWLEDGMENTS

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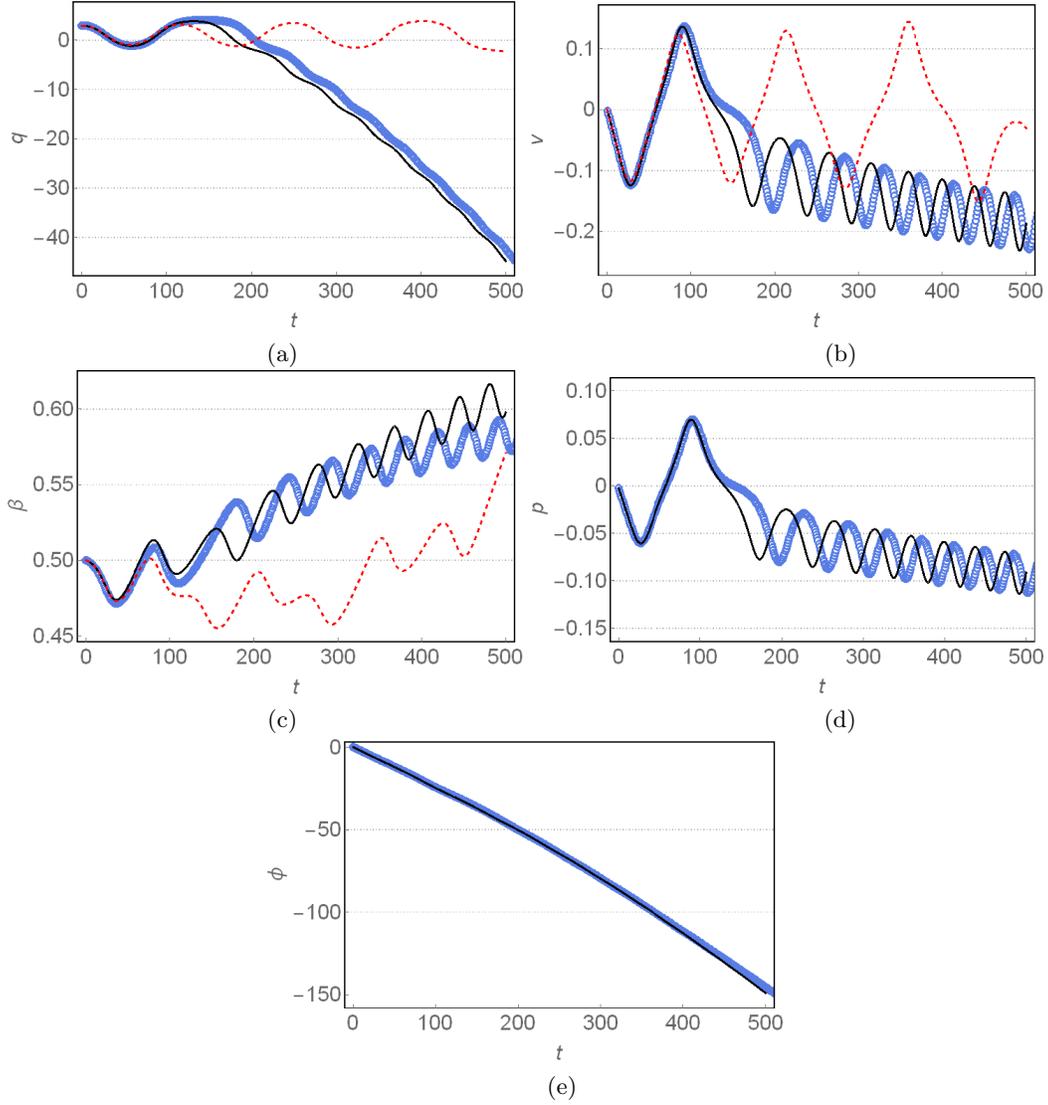
FIG. 9. Moving solitary wave in a shifted potential in a blowup situation: (a) position $q(t)$, (b) velocity $v(t)$, (c) amplitude $\beta(t)$, (d) momentum $p(t)$, and (e) phase $\phi(t)$. Here $l_0 = 1$, $k_0 = 1$, $V_0 = -0.01$, $W_0 = -0.005$, $\beta_0 = 0.5$, $q_0 = 2.8\pi/3$, $v_0 = 0$, $p_0 = 0.000608946$, $\phi_0 = 0$, $\Delta = -\pi/3$.

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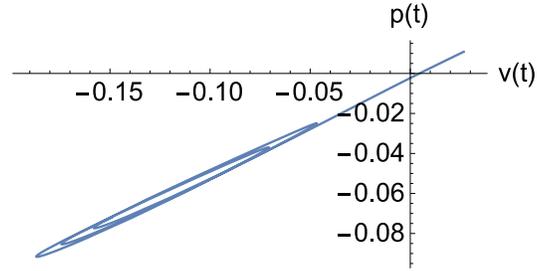
FIG. 10. Moving solitary wave when $\Delta = -\pi/3$, $q_0 = 2.8\pi/3$. Parametric plot of the momentum $p(t)$ vs. $v(t)$.