Singular instability of exact stationary solutions of the nonlocal Gross-Pitaevskii equation

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In this paper we show numerically that for nonlinear Schrödinger type systems the presence of nonlocal perturbations can lead to a beyond-all-orders instability of stable solutions of the local equation. For the specific case of the nonlocal one-dimensional Gross-Pitaevskii equation with an external standing light wave potential, we construct exact stationary solutions for an arbitrary interaction kernel. As the nonlocal and local equations approach each other (by letting an appropriate small parameter $\epsilon \to 0$), we compare the dynamics of the respective solutions. By considering the time of onset of instability, the singular nature of the inclusion of nonlocality is demonstrated, independent of the form of the interaction kernel.

In almost all applications where the nonlinear Schrödinger (NLS) equation is relevant, it arises as a simplified model of a nonlocal description. This is true in water waves, plasma physics, nonlinear optics, and Bose-Einstein condensates (BECs). For water waves [1] and plasmas [2], the nonlocality occurs due to a Fourier transformation of nonlinear equations. In nonlinear optics [3], the nonlocality is due to the spatial dependence of the susceptibility tensor. Locality in each of these cases is obtained as a quasi-monochromatic approximation of the nonlocal model. In plasma physics the nonlocal effect is known as Landau damping. The use of mean-field theory results in nonlocality for BECs [4–6], which reduces to the Gross-Pitaevskii (GP) equation (the NLS equation with external potential) when assuming a hard pairwise interaction potential. As such, the consideration of non-local perturbations of solutions of the NLS equation is important. Such perturbations result in the NLS equation with the cubic nonlinearity replaced by a nonlocal, nonlinear term. The nonlocal, nonlinear term is a convolution of the modulus squared of the solution with an interaction kernel, prescribed by the physical problem. In this paper our objective is to numerically examine the stability of solutions of this nonlocal NLS equation, and discuss how it differs from the local description.

To consider a specific nonlocal model, we examine mean-field theory of many-particle quantum mechanics with the particular application of BECs trapped in a standing light wave. The classical derivation given here is included to illustrate how the local and nonlocal models are related. The inherent complexity of the dynamics of N pairwise interacting particles in quantum mechanics often leads to the consideration of such simplified mean-field descriptions. These descriptions are a blend of symmetry restrictions on the particle wave function [4] and functional form assumptions on the interaction potential [4–6]. Here we do not impose any assumptions on the pairwise interaction potential.

The dynamics of N identical pairwise interacting quantum particles is governed by the time-dependent, N-body Schrödinger equation

$$i\hbar\frac{\partial\Psi}{\partial t}=-\frac{\hbar^2}{2m}\Delta^N\Psi+\sum_{i=1}^N W(\boldsymbol{x}_i-\boldsymbol{x}_j)\Psi+\sum_{i=1}^N V(\boldsymbol{x}_i)\Psi, \quad (1)$$

where $\boldsymbol{x}_i = (x_{i1}, x_{i2}, x_{i3})$, $\Psi = \Psi(\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3, ..., \boldsymbol{x}_N, t)$ is the wave function of the N-particle system, $\Delta^N = \left(\nabla^N\right)^2 = \sum_{i=1}^N \left(\partial_{x_{i1}}^2 + \partial_{x_{i2}}^2 + \partial_{x_{i3}}^2\right)$ is the kinetic energy or Laplacian operator for N-particles, $W(\boldsymbol{x}_i - \boldsymbol{x}_j)$ is the symmetric interaction potential between the i-th and j-th particle, and $V(\boldsymbol{x}_i)$ is an external potential acting on the i-th particle. Also, $\hbar$ is Planck's constant divided by 2π and m is the mass of the particles under consideration.

One way to arrive at a mean-field description is by using the Lagrangian reduction technique [7], which exploits the Hamiltonian structure of Eq. (1). The Lagrangian of Eq. (1) is given by [4]

$$L = \int_{-\infty}^{\infty} \left\{ i\frac{\hbar}{2}\left(\Psi\frac{\partial\Psi^*}{\partial t} - \Psi^*\frac{\partial\Psi}{\partial t}\right) + \frac{\hbar^2}{2m}\left|\nabla^N\Psi\right|^2 \right.$$
$$\left. - \sum_{i=1}^N \left(W(\boldsymbol{x}_i - \boldsymbol{x}_j) + V(\boldsymbol{x}_i)\right)|\Psi|^2 \right\} d\boldsymbol{x}_1 \cdots d\boldsymbol{x}_N \quad (2)$$

The Hartree-Fock approximation (as used in [4]) for bosonic particles uses the separated wave function ansatz

$$\Psi = \psi_1(\boldsymbol{x}_1, t)\psi_2(\boldsymbol{x}_2, t)\cdots\psi_N(\boldsymbol{x}_N, t) \quad (3)$$

where each one-particle wave function $\psi(\boldsymbol{x}_i)$ is assumed to be normalized so that $\langle\psi(\boldsymbol{x}_i)|\psi(\boldsymbol{x}_i)\rangle^2 = 1$. Since identical particles are being considered,

$$\psi_1 = \psi_2 = \ldots = \psi_N = \psi, \quad (4)$$

enforcing total symmetry of the wavefunction. Note that for the case of BECs, assumption (3) is only approximate if the temperature is not identically zero.

Integrating Eq. (2) using (3) and (4) and taking the variational derivative with respect to $\psi(\boldsymbol{x}_i)$ results in the Euler-Lagrange equation [7]

$$i\hbar\frac{\partial\psi(\boldsymbol{x},t)}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi(\boldsymbol{x},t) + V(\boldsymbol{x})\psi(\boldsymbol{x},t)$$
$$+ (N-1)\psi(\boldsymbol{x},t)\int_{-\infty}^{\infty} W(\boldsymbol{x}-\boldsymbol{y})|\psi(\boldsymbol{y},t)|^2 d\boldsymbol{y}. \quad (5)$$

Here, $\boldsymbol{x} = \boldsymbol{x}_i$, and Δ is the one-particle Laplacian in three dimensions. The Euler-Lagrange equation (5) is identical for all $\psi(\boldsymbol{x}_i,t)$. Equation (5) describes the non-linear, nonlocal, mean-field dynamics of the wave function $\psi(\boldsymbol{x},t)$ under the standard assumptions (3) and (4) of Hartree-Fock theory [4]. The coefficient of $\psi(x,t)$ in the last term in Eq. (5) represents the effective potential acting on $\psi(x,t)$ due to the presence of the other particles.

At this point, it is common to make an assumption on the functional form of the interaction potential $W(\boldsymbol{x}-\boldsymbol{y})$. This is done to render Eq. (5) analytically and numerically tractable. Although the qualitative features of this functional form may be available, for instance from experiment, its quantitative details are rarely known. One convenient assumption in the case of short-range potential interactions is $W(\boldsymbol{x} - \boldsymbol{y}) = \kappa\delta(\boldsymbol{x} - \boldsymbol{y})$ where δ is the Dirac delta function. This leads to the Gross-Pitaevskii [5,6] mean-field description:

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi + \beta|\psi|^2\psi + V(\boldsymbol{x})\psi, \quad (6)$$

where $\beta = (N-1)\kappa$ reflects whether the interaction is repulsive ($\beta > 0$) or attractive ($\beta < 0$). This assumption on the interaction potential $W(\boldsymbol{x}-\boldsymbol{y})$ is difficult to physically justify. Nevertheless, Lieb and Seiringer [8] show that Eq. (6) is the correct asymptotic description in the dilute-gas limit. In this limit, Eqs. (5) and (6) are asymptotically equivalent. Thus the nonlocal Eq. (6) can be interpreted as a perturbation to the local Eq. (5). Note that the results of [8] do not have implications for the asymptotic equivalence of the stability of solutions.

Since their first successful demonstrations in 1995 [9,10], continuous progress is being made in trapping, controlling, and manipulating Bose-Einstein condensates in a variety of experimental configurations [11]. Although many experiments rely solely on harmonic confinement to trap the condensate, we consider the situation of an external standing-light wave potential within a confining potential [12–14]. This standing-light wave pattern is generated by the interference of two quasi-monochromatic lasers in a quasi-one-dimensional configuration. The quasi-one-dimensional regime holds when the transverse dimensions of the condensate are on the order of its healing length and its longitudinal dimension is much longer than the transverse ones. The rescaled governing mean-field evolution (5) in the quasi-one-dimensional regime is given by

$$i\frac{\partial\psi}{\partial t} = -\frac{1}{2}\frac{\partial^2\psi}{\partial x^2} + \alpha\psi\int_{-\infty}^{\infty} R(x-y)|\psi(y,t)|^2 dy + V(x)\psi. \quad (7)$$

Here $\alpha = \pm 1$ is the sign of the interaction potential $W(x-y)$ at close range. Thus, α determines whether the close-range interaction is repulsive ($\alpha = 1$), or attractive ($\alpha = -1$). Hence, $\alpha = \text{sign}(a)$, where a is the s-wave scattering length of the atomic species. Depending on the species, a is either positive or negative, so that both signs of $\alpha = \text{sign}(a)$ are relevant for BEC applications. With these defintions, $R(x-y)$ is the rescaled interaction potential, which is positive at close range and is normalized to unity $\int_{-\infty}^{\infty} R(z)dz = 1$. This normalization condition is equivalent to a rescaling of variables.

The external potential which models the standing light wave is given by [11,14]

$$V(x) = V_0 \sin^2(kx) \quad (8)$$

where k is the wavelength of the periodic potential.

The nonlocal, nonlinear equation (7) with the periodic potential (8) admits a one-parameter family of exact solutions. These solutions are found using an amplitude-phase decomposition

$$\psi(x,t) = r(x)\exp\left[i\theta(x) - i\omega t\right]. \quad (9)$$

Then

$$r(x)^2 = A\sin^2(kx) + B \quad (10)$$

where B is a free parameter and

$$A(k) = \frac{-V_0}{\alpha\beta(k)}, \quad (11a)$$

$$\tan(\theta(x)) = \sqrt{1 - \frac{V_0}{\alpha B\beta(k)}} \ \tan(kx), \quad (11b)$$

$$\omega(k) = \frac{V_0 + k^2}{2} + \alpha B - \frac{V_0}{2\beta(k)}, \quad (11c)$$

$$\beta(k) = \int_{-\infty}^{\infty} R(z)\cos(2kz)\, dz = \hat{R}(2k), \quad (11d)$$

where $\hat{R}(2k)$ is the Fourier transform of $R(z)$ evaluated at $2k$. Equations (11) can be verified by direct substitution, using the addition formula for $\cos(2(y-x)+2x)$ and the fact that $R(x-y)$ is even. This is the only essential mathematical assumption made on the interaction potential $R(x-y)$ in obtaining this family of exact solutions, including the normalization condition. The solutions to GP theory (6) found in [14] are easily recovered by letting $R(z) = \delta(z)$, i.e., $\beta = 1$.

From Eq. (11d) and $\beta = V_0/\alpha A(k)$, it follows that measuring the amplitude $A(k)$ of the oscillations for varying external potential wavelengths k leads to the construction of the Fourier transform of the interaction potential $\hat{R}(2k)$. Thus by inversion

$$R(z) = \frac{V_0}{2\pi\alpha} \int_{-\infty}^{\infty} \frac{\cos(2kx)}{A(k)} dk. \qquad (12)$$

In principle, this gives a method to determine the pair-wise particle interaction potential experimentally.

Now, we investigate numerically the stability of solutions of both the local (6) and nonlocal (7) equations without applying any additional perturbations. The computational procedure used is a 4th order Runge-Kutta method in time and filtered pseudo-spectral method in space. Our objective is to explore the question of *asymptotic equivalence of stability* (AES): as the non-local equation (7) approaches the local equation (6) does the dynamics of the solution (9) of the nonlocal equation converge to the dynamics of the solution (9, with $\beta = 1$) of the local equation?

For a sufficiently high offset value B, the local solution is stable [13,14] as illustrated in Fig. 1. In this case, the time of onset of instability $t^* = \infty$, even under the influence of large perturbations [13,14].

To investigate the nonlocal behavior, a choice must be made for the interaction potential $R(z)$. A reasonable first choice is a Gaussian profile

$$R(z) = \frac{1}{\sqrt{2\pi}\epsilon} e^{-z^2/2\epsilon^2} \qquad (13)$$

where as $\epsilon \to 0$, $R(z) \to \delta(z)$ and the solution (9) approaches the local limit. Thus examining AES amounts to examining t^* as a function of ϵ. The unstable dynamics and its spectral evolution are illustrated in Fig. 2 for $\epsilon = 0.01$. For $\epsilon \in [0.0025, 0.16]$, numerically $t^* \approx 10.1$, independent of ϵ (see Fig. 4). This result contradicts the expectation that $t^* \to \infty$ as $\epsilon \to 0$ and suggests the presence of a beyond-all-orders phenomenon. The Fourier spectrum in Fig. 2 provides the primary diagnostic for studying the instability and its convergence. Not only does it provide the value of t^*, it also illustrates that the spectral bandwidth, which is the support of the unstable modes, is independent of ϵ for $\epsilon \in [0.0025, 0.16]$. Hence, AES is not obtained, even in a convergence-in-measure sense. These results raise the following questions: is lack of AES due to the choice of $R(z)$? Is AES a consequence of nonlocality or can it occur for local generalizations of NLS?

The choice of $R(z)$ is addressed by choosing different forms of the interaction potential, which are even and decaying at infinity. Three additional $R(z)$ choices were considered: $R(z) = \epsilon/(\pi(z^2 + \epsilon^2))$ with $t^* = 10.2$, $R(z) = 1/(2\epsilon)$ for $x \in [-\epsilon, \epsilon]$ and $R(z) = 0$ otherwise with $t^* = 10.1$, and $R(z) = 1/(2\epsilon)\exp(-|z|/\epsilon)$ with $t^* = 10.4$. Thus the lack of AES appears to be a universal feature that is independent of the interaction potential.
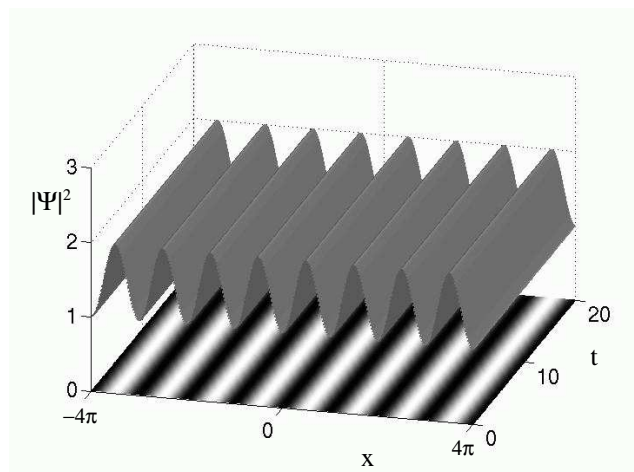

FIG. 1. Stable evolution of the stationary solution (9) with $\alpha = 1$ (repulsive), $\beta = 1$ (local), $k = 1$, $V_0 = -1$, and $B = 1$.
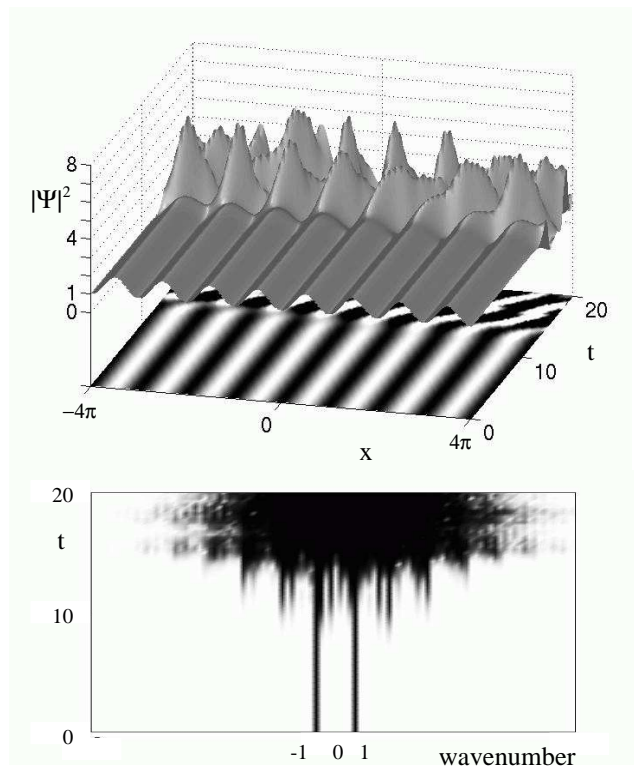

FIG. 2. Unstable evolution of the stationary solution 9 with $\alpha = 1$ (repulsive), $k = 1$, $V_0 = -1$, $B = 1$, and $\epsilon = 0.01$ in Eq. (13). The bottom figure is a density plot of the evolution of the Fourier modes.

A local generalization of the NLS equation (7) is

$$i\frac{\partial\psi}{\partial t} = -\frac{1}{2}\frac{\partial^2\psi}{\partial x^2} + \alpha\psi\left(|\psi|^2 + \epsilon\frac{\partial^2|\psi|^2}{\partial x^2}\right) + V(x)\psi. \qquad (14)$$

3

where $\epsilon = \int_{-\infty}^{\infty} z^2 R(z)dz$. This equation is derived by a change of variables $y = x - z$ followed by a Taylor expansion of $|\psi|^2$ about $z = 0$ in (7). Finally assuming $R(z) = \delta(z)$ results in (14). Such an equation has been considered in the multidimensional, attractive ($\alpha = -1$) case as a successful means to arrest collapse and blow-up of solutions [15,16]. The effect of this additional term on the stability of solutions was never addressed. A family of exact solutions for this case is given by (9) with $\beta = 1 - 4\epsilon k^2$. The dynamics is found to be unstable as illustrated in Fig. 3 for $\epsilon = 0.02$. More importantly, $\lim_{\epsilon \to 0} t^* = \infty$ as shown in Fig. 4. In contrast to the nonlocal Eq. (7), the presence of the local perturbation in Eq. (14) does not destroy AES. This suggests that non-locality is responsible for the beyond-all-orders failure of AES.

Nonlocality for NLS-type equations is a generic feature arising in physical systems. Although nonlocality has previously been used to prevent the non-physical features of collapse and blow-up, its effect on the stability of solutions appear detrimental. We have demonstrated this beyond-all-orders singularity arising from nonlocal perturbations. The specific model considered is the Gross-Pitaevskii equation with a standing-light wave potential for which an exact family of stationary solutions is constructed. *Asymptotic equivalence of stability* (AES) for the nonlocal equation (7) is not achieved since the nonlocal equation dynamics does not approach the local equation dynamics as $\epsilon \to 0$. This is a truly nonlocal and universal phenomenon as illustrated by the study of a local correction model and the consideration of different interaction kernels. The instability discussed is similar to a parametric instability. It differs from it in that it is driven by the change of a function, not one parameter. Further, the equations that are being compared are asymptotically equivalent, as are their solutions. There is a caveat to our conclusions: in a physical setting, many additional effects are present which are excluded by the NLS-type model. The success of such models can be accounted for by the presence of these effects which may counteract the instability mechanism found here.

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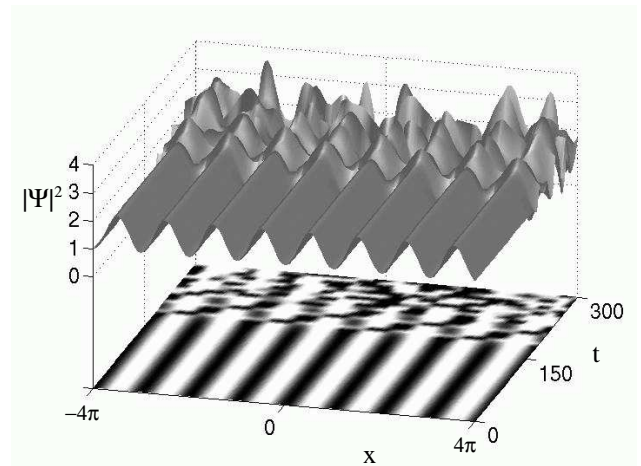[16] S. T. Turitsyn, Teor. Mat. Fiz. **64**, 226 (1985).

FIG. 3. Unstable evolution of the stationary solution 9 with $\alpha = 1$ (repulsive), $k = 1$, $V_0 = -1$, $B = 1$, and $\epsilon = 0.02$ in Eq. (14).
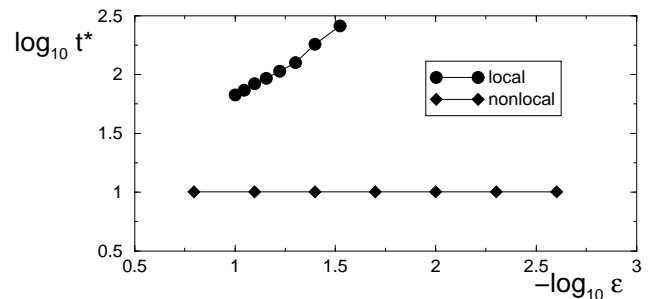

FIG. 4. Time of onset of instability t^* as a function of ϵ. Note that $-\log_{10} \epsilon$ gives the position of the most significant digit in ϵ.