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Solitary-wave solutions to nonlinear Schrödinger equations

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We examine the solitary-wave behavior of eigenstate solutions to various nonlinear Schrödinger equations (NLSE's) in an arbitrary number of dimensions and with a general potential. These eigenstate solutions are the only wave functions that can rigorously preserve their shape. We show that solitary-wave motion is only possible if the nonlinearity is decoupled from the absolute position of the wave packet and if the potential in the moving frame differs by at most a linear term from that for the eigenstate problem. If these conditions are satisfied then the motion is along the fully classical trajectory, although the nonlinear term may introduce an additional acceleration. We comment on the implications of these results to the study of the behavior of Bose-Einstein condensed atoms in harmonic trapping potentials, for which the relevant NLSE is the Gross-Pitaevskii equation. Numerical simulations are presented for harmonic and anharmonic potentials in one dimension to illustrate our results. [S1050-2947(97)05006-3]

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I. INTRODUCTION

The recent observations of Bose-Einstein condensation (BEC) in inhomogeneous dilute alkali gases with positive scattering lengths [1,2] have intensified theoretical efforts to predict the properties of this macroscopic quantum-mechanical system. The starting point for such predictions is usually the Gross-Pitaevskii (GP) equation with a harmonic trapping potential. This is a cubic nonlinear Schrödinger equation (CNLSE) and is presumed to be valid for a dilute gas ($na^3 \ll 1$, where n is the average density and a is the s-wave scattering length) at zero temperature where quantum and thermal fluctuations can be neglected [3]. For a discussion of the solutions to this equation see Refs. [4,5] and the citations therein. There is particular interest in applying the theory to the next generation of experiments, which will look for novel features of BEC (for example, properties that depend on the nonlinear term describing particle interactions), the response to external perturbations, and methods of manipulating the condensate. As part of this work we have been studying some of the features of condensate motion one would expect from the GP equation.

In this paper, however, we take a wider perspective and consider the motion of eigenstates of various nonlinear Schrödinger equations (NLSE's) with arbitrary potentials.[1] We are interested in finding solutions that propagate without change of shape, i.e., solitary waves. Some features of this problem have already been examined by a number of other authors. Chen and Liu, for example, considered the case of a linear [6] and quadratic [7] potential for the CNLSE for optical solitons propagating in inhomogeneous media. Nassar [8] used stochastic mechanics to solve the logarithmic nonlinear Schrödinger equation with a time-dependent forced harmonic-oscillator potential, while Hasse [9] considered NLSE's with a variety of nonlinearities and a linear potential. This work was extended by de Moura [10], who treated a general NLSE and concluded that the existence and shape of the solitons is not affected by an external potential, a result that conflicts with this work. In a more recent paper de Moura [11] extended his treatment by considering the possibility of "breathing modes" in which the width of the wave packet can change with time but the fundamental shape does not. Some results from this later work are also inconsistent with our analysis. The case of solitons of the CNLSE with time-dependent linear and harmonic potentials has been thoroughly dealt with by Nogami and Toyama [12].

All these treatments have been restricted to one dimension, however, and with the exception of Refs. [7,8,12], the propagating wave was an eigenstate of the NLSE in free space (i.e., all the potentials were external). We extend this work by considering rectilinear motion in an arbitrary number of dimensions for general potentials and by allowing a time-independent part of the potential to affect the shape of the solution. By considering the validity of our method we are able to show that only eigenstate solutions to the relevant NLSE can propagate as exact solitary waves and then only when the nonlinearity and potentials satisfy certain criteria. Although our primary interest is in the GP equation relevant to BEC, our analysis applies to a wide variety of NLSE's. We present numerical simulations in one dimension to illustrate and confirm the arguments presented. We do not consider the possibility that the wave might change its shape temporarily only to reform at a later stage of its evolution. An example of this for the case of a soliton incident on a potential step can be found in Ref. [13].

The shape of a wave is determined by its modulus, so our method involves decomposing the wave function into a modulus and phase and insisting that the modulus should only depend on time via a change in its mean position. This method is essentially the same as that of Refs. [6]–[12] and the work of Husimi [14] and Kerner [15], who both treated the linear case in some detail. Much of our work mirrors that of de Moura [11], although we do not consider the possibility of breathing modes and draw somewhat wider conclusions for solutions of fixed width.

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[1]For applications to BEC, an eigenstate represents a condensed assembly of trapped atoms.

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II. SOLITARY-WAVE SOLUTIONS

For simplicity we start with the one-dimensional NLSE in reduced units

$$i\frac{\partial\Psi}{\partial t}=-\frac{\partial^2\Psi}{\partial x^2}+V(x,t)\Psi+W\Psi . \qquad (1)$$

This equation describes a field of particles of mass m, where the unit of time is $1/\omega$ and that of length is $\sqrt{\hbar/2m\omega}$, with $\hbar\omega$ some convenient energy scale in the problem (e.g., the level spacing for a harmonic potential).[2] W is the nonlinear potential term and in applications to BEC is given by $W\propto|\Psi|^2$. This form for W gives the GP equation mentioned above.

We decompose $V(x,t)$ into two parts, writing it as $V(x)+P(x,t)$, and in what follows we shall refer to $V(x)$ as the "fixed potential" and to $P(x,t)$ as the "external potential." This procedure is convenient but arbitary since only $V(x,t)$ is well defined. However, all decompositions lead to the same physics and we can transform between them very simply as shown in the Appendix. The purpose of the decomposition is to allow for the possibility that the shape of a solitary wave may be affected by the presence of a time-independent potential and it will usually be obvious from the physical situation which decomposition is most appropriate.

We assume that an eigenstate solution $\Psi(x,t)=\phi(x)e^{-i\epsilon t}$ to the fixed potential problem has already been found so that $\phi(x)$ satisfies

$$\epsilon\phi(x)=-\frac{d^2\phi(x)}{dx^2}+V(x)\phi(x)+W\phi(x), \qquad (2)$$

where ϵ is the energy in units of $\hbar\omega$. This equation determines the shape of our solitary waves. The question arises as to whether further solitary waves exist whose shape is not determined by an equation of this form, but we show in the Appendix that the structure of all solitary waves is determined by Eq. (2) for some choice of $V(x)$. We now look for a solution to the full potential of the form

$$\Psi_{\mathrm{new}}(x,t)=\Psi_{\mathrm{old}}(x-x_0(t),t)e^{iS(x,t)}$$
$$=\phi(x-x_0(t))e^{-i\epsilon t}e^{iS(x,t)}, \qquad (3)$$

where $x_0(t)$ is the time-dependent shift in the position of the wave function, i.e., $x_0(t)=\mu(t)-\mu_0$, where $\mu(t)$ is $\langle x\rangle_{\mathrm{new}}$ and μ_0 is the mean of the solution to Eq. (2), i.e., $\mu_0=\int x|\phi|^2dx$. This new wave function corresponds to propagation of the original solution without change of shape if and only if $S(x,t)$ is real. We shall see that requiring $S(x,t)$ to be real leads to a consistency condition which simultaneously determines the time dependence of $x_0(t)$ and restricts the potentials $V(x)$ and $P(x,t)$ and the nonlinearity W that allow such solutions.

Although the theory we will develop applies to any solution of Eq. (2), in applications to BEC the ground state will be of most interest since this is usually the state formed in an evaporative cooling experiment. It is perhaps worth mentioning that excited-state solutions can look like dark solitary waves on a finite background [16] since at each node there is a kink in the density profile (for example, consider the first excited state for a harmonic potential and cubic nonlinearity, which vanishes at the origin by virtue of its odd parity). These solitary waves correspond to a synchronous motion of the kink and the finite background. Our method cannot deal with possible solitary waves that consist of the motion of a kink relative to a finite background as in this case the overall shape is not exactly preserved. The motion of a kink relative to an infinite background is included in our analysis, however, since this motion is indistinguishable from the synchronous motion described by Eq. (3).

We substitute the expression for $\Psi_{\mathrm{new}}(x,t)$ into Eq. (1) and change variables from $\{x,t\}$ to $\{q,t\}$, where $q=x-x_0(t)$ and is the coordinate that determines the internal structure of the solitary wave. This gives

$$\begin{aligned}i\frac{\partial\phi(q)}{\partial t}-\frac{\partial S}{\partial t}\phi(q)\\
&=\left\{-\frac{d^2\phi(q)}{dq^2}+V(q)\phi(q)+W\phi(q)-\epsilon\phi(q)\right\}\\
&\quad-\left[2i\frac{\partial S}{\partial q}\frac{d\phi(q)}{dq}+i\frac{\partial^2S}{\partial q^2}\phi(q)-\left(\frac{\partial S}{\partial q}\right)^2\phi(q)\right]\\
&\quad+\Delta V(q+x_0,x_0)\phi(q)+P(q+x_0,t)\phi(q), \qquad (4)\end{aligned}$$

where $\Delta V(q+x_0,x_0)=\Delta V(x,x_0)\equiv V(x)-V(q)$, the q derivatives are evaluated at constant t and the t derivatives at constant x. We have assumed that W has exactly the same functional form in the q variable as in the x variable, i.e. that it depends only on the internal coordinate of the wave function. In fact, this represents the requirement on the nonlinearity for solitary wave motion to be possible and is discussed in more detail in Sec. III. We note at this stage, however, that the GP equation describing BEC is indeed of this form.

The term in curly brackets in Eq. (4) vanishes as a result of Eq. (2). We now write $\phi=\rho e^{i\Omega}$, where ρ and Ω are real functions of q, and separate Eq. (4) into real and imaginary parts, which (for $\rho\neq 0$) are, respectively,

$$\begin{aligned}-\frac{\partial S}{\partial t}+\frac{dx_0}{dt}\frac{d\Omega}{dq}&=2\frac{\partial S}{\partial q}\frac{d\Omega}{dq}+\left(\frac{\partial S}{\partial q}\right)^2+\Delta V(q+x_0,x_0)\\
&\quad+P(q+x_0,t), \qquad (5)\end{aligned}$$

$$\rho\frac{dx_0}{dt}\frac{d\rho}{dq}=2\rho\frac{d\rho}{dq}\frac{\partial S}{\partial q}+\rho^2\frac{\partial^2S}{\partial q^2}$$

The imaginary part can be integrated immediately to give

$$\frac{\partial S}{\partial q}=\frac{1}{2}\frac{dx_0}{dt}+A(t)/\rho^2. \qquad (7)$$

[2]Note the factor of 2 in the scale of length, which occasionally makes results appear unfamiliar at an intermediate stage of the calculation.

For localized solutions we must set $A(t)=0$ to give a finite energy and particle current [17]. Thus Eq. (7) becomes

$$\frac{\partial S}{\partial q}=\frac{\partial S}{\partial x}=\frac{1}{2}\frac{dx_0}{dt}. \tag{8}$$

Integrating again gives

$$S(x,t)=\frac{1}{2}\frac{dx_0}{dt}x+B(t), \tag{9}$$

where $B(t)$ is an (as yet undetermined) function of time.

If we now substitute Eq. (8) into the real part [Eq. (5)] and convert back to the x coordinate description we obtain

$$\frac{\partial S}{\partial t}=-\frac{1}{4}\left(\frac{dx_0}{dt}\right)^2-\Delta V(x,x_0)-P(x,t). \tag{10}$$

This is an energy equation, the terms on the right-hand side being, respectively, the additional kinetic energy due to the center-of-mass motion and the change in the potential energy due to both the displacement in the fixed potential and the applied external potential. Integration of Eq. (10) gives

$$S(x,t)=-\int\frac{1}{4}\left(\frac{dx_0}{dt}\right)^2dt-\int[\Delta V(x,x_0)+P(x,t)]dt+C(x), \tag{11}$$

where $C(x)$ is a time-independent ''constant'' of integration.

We now have two expressions for $S(x,t)$ in the form of Eqs. (9) and (11), which must be consistent with each other if solitary wave motion is to be possible. The condition this imposes is most simply obtained by taking the partial derivative of Eq. (8) with respect to t (noting that x_0 depends only on t) and the partial derivative of Eq. (10) with respect to x and equating the results. This gives the equation of motion

$$\frac{1}{2}\frac{d^2x_0}{dt^2}=\frac{1}{2}\frac{d^2\mu}{dt^2}=-\frac{\partial}{\partial x}[\Delta V(x,x_0)+P(x,t)], \tag{12}$$

where μ is the mean of the solitary wave [see beneath Eq. (3)]. Since the left-hand side (LHS) depends only on t then, if the wave function is to propagate without change of shape, the right-hand side (RHS) must also depend only on t. Hence the quantity $[\Delta V(x,x_0)+P(x,t)]$ must be at most a linear function of x.[3] This is the condition on the potentials for solitary wave motion to exist and is the central result of this paper. The physical content of this restriction is discussed in Sec. III.[4]

[3]If $[\Delta V(x,x_0)+P(x,t)]$ does not depend on x, then a comparison of Eqs. (9) and (11) shows that $C(x)=\frac{1}{2}(dx_0/dt)x$. This leads to a possible motion since in this case $\frac{1}{2}(dx_0/dt)$ is independent of time.

[4]This restriction on the potentials is in contradiction to the result of Ref. [10] since in that paper the author does not consider the consistency of his equations. It is also in contradiction to the statement in Ref. [11] that no solitary wave exists in a harmonic potential. In that case the reason is that no allowance is made for the possibility that the shape of the wave may be affected by the potential.

The classical equation of motion, in these units, for a particle (considered to be localized at the mean of the wave function) in the given fixed and external potentials is

$$\frac{1}{2}\frac{d^2\mu}{dt^2}=-\left(\frac{\partial}{\partial x}[V(x)+P(x,t)]\right)_{x=\mu}, \tag{13}$$

where the factor of 1/2 is an artifact of our scaling of the original Schrödinger equation. In order to compare the classical equation of motion with Eq. (12) we note that

$$\Delta V(x,x_0)=V(x)-V(x-x_0(t)) \tag{14}$$

and therefore that

$$\left(\frac{\partial}{\partial x}\Delta V(x,x_0)\right)_{x=\mu}=\left(\frac{d}{dx}V(x)\right)_{x=\mu}-\left(\frac{d}{dq}V(q)\right)_{q=\mu(0)}. \tag{15}$$

Thus Eq. (12) can be identified as the classical equation of motion, provided that the final term of Eq. (15) is zero, which will be the case as long as a Taylor expansion of $V(x)$ about the mean position of the fixed eigenstate contains no linear contribution. Classically, this term would have to be zero for a stationary solution, but this is not the case in quantum mechanics (consider, for example, a particle in an infinite potential well with a tilted base). The effect of this term is to add an acceleration to the motion and although this will usually be of little importance in the application of the theory to atoms trapped near a potential minimum, it can be introduced by certain nonlinearities as discussed in Sec. III.

We should also confirm that Eq. (12) is consistent with Ehrenfest's theorem, which gives the usual quantum equation of motion for the mean of a localized wave packet. If W is a function (rather than an operator) then we obtain the following equation of motion for the mean of a wave packet:

$$\frac{1}{2}\frac{d^2\mu}{dt^2}=-\left\langle\frac{\partial[V(x)+P(x,t)]}{\partial x}\right\rangle-\left\langle\frac{\partial W}{\partial x}\right\rangle, \tag{16}$$

which is valid for any localized wave packet regardless of whether or not it maintains its shape (see Ref. [18] for a general derivation or Ref. [9] for a discussion relevant to NLSE's). In general the nonlinear term does contribute to the equation of motion, although it vanishes for solutions with good parity (as is the case in the study of BEC). For an eigenstate of the fixed potential NLSE, however, the solution is stationary so that we must have $-\langle\partial V(x)/\partial x\rangle=\langle\partial W/\partial x\rangle$. If the wave function then propagates as a solitary wave, the nonlinear contribution is unchanged so that the equation of motion is

$$\frac{1}{2}\frac{d^2\mu}{dt^2}=-\left\langle\frac{\partial[\Delta V(x,x_0)+P(x,t)]}{\partial x}\right\rangle, \tag{17}$$

with $\Delta V(x,x_0)$ defined as before. This result is identical to Eq. (12) since for the solitary wave motion to be possible $[\Delta V(x,x_0)+P(x,t)]$ must be at most a linear function of x. If the final term in Eq. (15) is zero, then the motion of the mean is identical to the classical motion whereas Ehrenfest's theorem usually results in a pseudoclassical motion since $\langle\partial V/\partial x\rangle\neq(\partial V/\partial x)_{\langle x\rangle}$ in general. We illustrate the distinction between these two motions numerically later in the paper for a solution that does not maintain its shape.

III. GENERAL NONLINEARITIES AND PHYSICAL INTERPRETATION

In Eq. (4) we assumed that W has exactly the same functional form in the q variable as in the x variable, which means that it depends only on the internal coordinate of the wave function. This will be true for any function of ϕ and $\partial/\partial x$ since $\partial/\partial x=\partial/\partial q$ and ϕ takes the new argument q when the wave function is shifted. W may even be an operator as in the derivative nonlinear Schrödinger equation for which $W\propto(\hat{p}|\phi|^2+|\phi|^2\hat{p})$, where $\hat{p}$ is the momentum operator [19]. However, nonlinearities that depend explicitly on the variable x (i.e., other than through ϕ) have to be excluded since there is then a coupling between the external and internal motions. An example of such a nonlinearity is $W\propto x^2|\phi|^2$. If nonlinearities of this form are present (and assuming they are real), then they will lead to an additional ϕ-dependent term in Eq. (5). This certainly will not be a linear function of x and hence (given a sensible external potential) it will be impossible for Eqs. (5) and (6) to be consistent. Thus the only nonlinearities that allow solitary wave motion are those that are independent of the absolute position of the wave packet.

A further effect of the nonlinearity in some cases is to produce a constant acceleration term which is absent from the classical equation of motion [this is the final term in Eq. (15)]. An example of this may be found if we consider a harmonic fixed potential and a nonlinearity of the form $W\propto|\Psi|^2+(\partial/\partial x)|\Psi|^2$. This nonlinearity does not have good parity and as a result the mean μ_0 of an eigenstate is not at the minimum of the harmonic potential. The final term in Eq. (15) is thus nonzero and the solitary wave solution oscillates at the trap frequency about μ_0 rather than about the trap minimum. We see, therefore, that although the nonlinear term does not appear explicitly in the equation of motion, it may have an implicit effect on the evolution of the solitary wave.

The restrictions on the potentials and the form of the nonlinearity have a simple physical interpretation. An eigenstate solution is the result of a precise balance between the kinetic, potential and nonlinear terms in the Schrödinger equation. If the nonlinear term depends only on internal coordinates, then its contribution is entirely unaffected by a displacement of the eigenstate. The change in the potential experienced by the wave packet is then exactly the term $[\Delta V(x,x_0)+P(x,t)]$, which appears in the equation of motion. If this is linear in x it corresponds to a spatially uniform force which accelerates all parts of the wave packet in the same way and hence does not cause any deformation. If the wave packet represents a condensate so that $|\phi|^2$ is proportional to the particle density, then a linear potential corresponds to a uniform acceleration of these particles. Hence it does not affect their separation and so their interactions (represented by the nonlinear term) are unchanged and we would expect the wave function to maintain its shape. We see, therefore, that nonlinear terms that depend only on the internal coordinate of the wave function play no role in determining whether or not solitary wave motion is possible, although they will of course affect how the shape changes with time should such motion not be possible. As a consequence of this, we see that for a harmonic trapping potential[5] a more drastic perturbation than shaking (i.e., randomly displacing the minimum) is required to give a good indication of the presence or absence of a condensate (for example, one could try ''squeezing'' the condensate by rapidly varying the trap frequency, thereby setting up excitations [20]).

We should stress that we have assumed the existence of eigenstate solutions to the fixed potential problem in our analysis. Our results are only valid, therefore, if the combination of nonlinearity and fixed potential allows such solutions. An example of the restriction this imposes can be found in the case of no fixed potential (free space), where the nonlinearity must be negative (representing attractive interactions) if the energy functional is to have local minima.

IV. EXTENSION TO HIGHER DIMENSIONS

The above physical argument suggests that our results are not restricted to one dimension provided that motion along one axis does not affect the dependence of the potential on the other coordinates. To examine this we consider rectilinear motion in a space of arbitrary dimension and single out the x axis as the axis of interest, denoting the other coordinates by $\{y_i\}$. We write the potential as $V(x)+V_y(\{y_i\})+U(x,\{y_i\})+P(x,\{y_i\},t)$. Here V_y is any function of the $\{y_i\}$ only and the U potential contains all cross terms involving x. P is again the time-dependent external potential. Equations (5) and (6) are respectively modified to

$$
\begin{aligned}
-\frac{\partial S}{\partial t}+\frac{dx_0}{dt}\frac{\partial\Omega}{\partial q}={}&2\frac{\partial S}{\partial q}\frac{\partial\Omega}{\partial q}+\left(\frac{\partial S}{\partial q}\right)^2\\
&+\sum_i\left[2\frac{\partial S}{\partial y_i}\frac{\partial\Omega}{\partial y_i}+\left(\frac{\partial S}{\partial y_i}\right)^2\right]\\
&+\Delta V(q,x_0)+\Delta U(q+x_0,x_0,\{y_i\})\\
&+P(q+x_0,\{y_i\},t),
\end{aligned}
\tag{18}
$$

$$
\frac{1}{2}\frac{dx_0}{dt}\frac{\partial\rho^2}{\partial q}=\frac{\partial\left(\rho^2\frac{\partial S}{\partial q}\right)}{\partial q}+\sum_i\frac{\partial\left(\rho^2\frac{\partial S}{\partial y_i}\right)}{\partial y_i}. \tag{19}
$$

The quantity ΔU in Eq. (18) has a similar definition to ΔV. Notice that $V_y(\{y_i\})$ does not appear in these equations and it may thus be any function of the coordinates including an anharmonic one. Integration of Eq. (18) will give S at least the phase dependence on $\{y_i\}$ that appears in ΔU (unless P is chosen to cancel this). It seems unlikely, therefore, that the solution can be consistent with Eq. (19). In the special case that $U=0$ and P is independent of $\{y_i\}$, however, we can take S to be dependent only on x and t. In this case the full potential contains no cross terms involving x (although there may be cross terms in the $\{y_i\}$ in V_y) and the

[5] $\Delta V(x,x_0)$ is linear in x for a harmonic potential (see later discussion).

problem reduces to that considered in the one-dimensional case. This confirms what we would expect physically, but at first sight may appear a little strange since we may create cross terms in the potential by rotating our coordinates. It should be remembered, however, that we chose to look along the x axis for propagation without change of shape. It appears, therefore, that solitary wave motion can only exist along specific axes for which the potential is decoupled from the other coordinates. A particular case of interest relevant to the experiments in Refs. [1,2] is $V\sim\omega_\perp(x^2+y^2)+\omega_z z^2$, i.e., the anisotropic harmonic potential in three dimensions.[6] For such a potential we see that there is solitary wave behavior in the x-y plane and along the z axis but not in other directions.

V. APPLICATION TO SIMPLE POTENTIALS

We now illustrate the above discussion by considering some particular fixed potentials.

A. Constant potential

In this case ΔV is zero and there is only a solitary-wave solution for $P(x,t)=f(t)x$, i.e., if there is a constant external force across the wave packet. This contradicts the result of Ref. [10]. The existence of an eigenstate solution requires that the nonlinear term be negative, as mentioned above. The equation of motion is

$$\frac{d^2x_0}{dt^2}=-2f(t). \tag{20}$$

If $f(t)=0$ the solution has a constant velocity and the term $C(x)$ in Eq. (11) must be nonzero.

B. Quadratic potential

This is a case of particular importance for the study of BEC in dilute gases. Eigenstate solutions exist for both positive and negative nonlinearities. If we take the energy scale as the level spacing of the harmonic oscillator, then $V(x)=\frac{1}{4}x^2$ and $\Delta V(x,x_0)=\frac{1}{4}(2x-x_0)x_0$. Since ΔV is linear in x we now have solutions with $P(x,t)$ either linear or zero. The case of zero external potential allows for solutions in which the wave packet oscillates freely in the harmonic potential (for example, the initial state might be displaced from the minimum), although in practice this would be achieved by displacing the trap using a linear external potential. The equation of motion for $P(x,t)=f(t)x$ is

$$\frac{d^2x_0}{dt^2}+x_0=-2f(t), \tag{21}$$

which is the usual forced harmonic-oscillator equation.

C. Anharmonic potentials

In this case ΔV contains higher powers of x than linear ones and for $P(x,t)=0$ there are no solitary-wave solutions. It is possible, however, to choose the external potential judiciously so that $\Delta V+P(x,t)$ is linear and so obtain solutions that propagate without change of shape. This will only be the case, however, for very particular choices of $P(x,t)$, tailored to given initial conditions, and is unlikely to be realizable experimentally unless one can control the strength of various different polynomial potentials independently and rapidly.

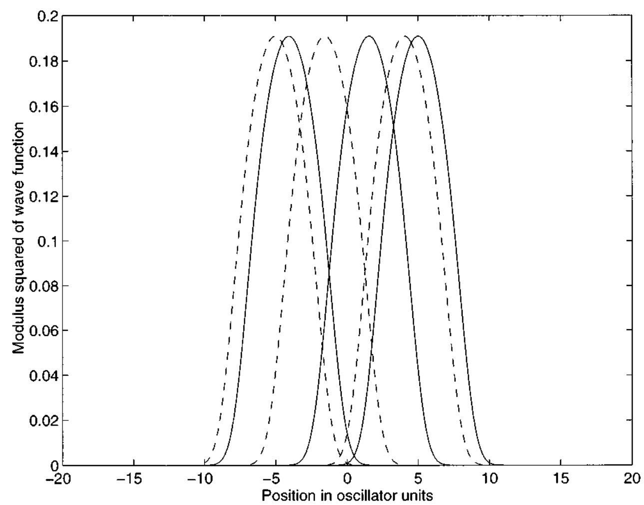

FIG. 1. Plot of $|\Psi|^2$ for the propagation of the ground state with $C_{\rm nl}=20$ in a harmonic fixed potential. The profiles are shown at intervals of $\pi/5$ with the far right profile at $t=0$ and the far left one at $t=\pi$.

VI. NUMERICAL RESULTS

We present numerical results for harmonic and anharmonic fixed potentials in one dimension for a nonlinear term of the form $W=C_{\rm nl}|\Psi|^2$, which gives the GP equation relevant to the study of BEC.

A. Harmonic potential

1. $P(x,t)=0$

In this case the solution to Eq. (21) is $\mu(t)=\mu_0\cos(t+\theta)$. We consider the case that $\theta=0$, which corresponds to a stationary initial state displaced in the fixed potential. Equation (11) gives a phase factor of

$$S(x,t)=-\frac{1}{2}\mu_0 x\sin(t)+\frac{1}{8}\mu_0^2\sin(2t), \tag{22}$$

which is the expression derived for the ground state in the linear case in Ref. [18]. The predicted motion has been observed for the ground and first excited states with $C_{\rm nl}=20$, and for the second excited state with $C_{\rm nl}=8$ and the ground state with $C_{\rm nl}=-5$. The phase dependence was that predicted in Eq. (22) to within 10^{-3} rad for the first pair and to within 10^{-2} rad for the second pair. Figure 1 shows a plot of the ground state propagation with $\mu(t=0)\approx 5$.

2. $P(x,t)=-\cos(2t)x$

The solution to Eq. (21) for a wave packet initially at rest and centered on the origin is $\mu(t)=\frac{2}{3}[\cos(t)-\cos(2t)]$. The phase dependence from Eq. (11) is

[6] The work reported in [2] used a modified potential, but we believe that more recent work involves a potential of this form.

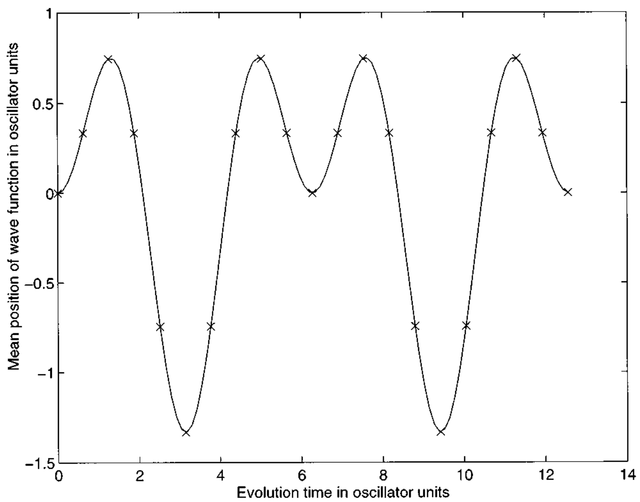

FIG. 2. Plot of the mean position of the ground state with $C_{\mathrm{nl}}=20$ in a harmonic fixed potential, subject to an external potential $P(x,t)=-\cos(2t)x$. The crosses are numerical points and the full line is the classical prediction.

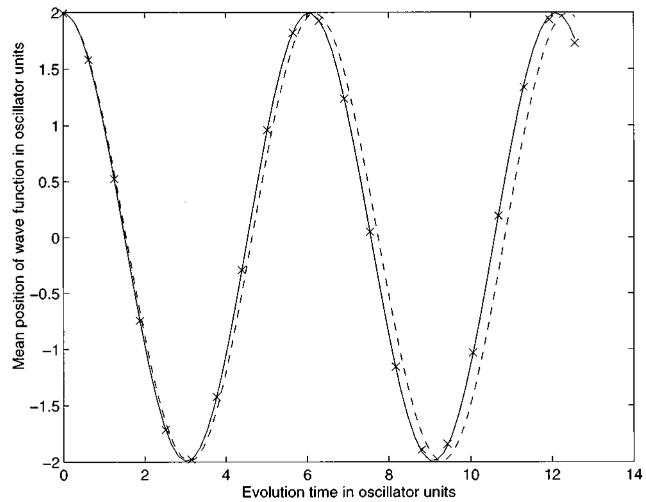

FIG. 3. Plot of the mean position of the displaced ground state of the anharmonic potential in the text and nonlinearity $C_{\mathrm{nl}}=5$. The crosses are numerical points, the dotted line is the fully classical prediction, and the full line is the prediction of Ehrenfest's theorem.

$$S(x,t)=-\frac{3}{18}t+\frac{1}{3}x[2\sin(2t)-\sin(t)]+\frac{1}{9}\left[\sin(t)+\frac{1}{2}\sin(2t)-\sin(3t)+\frac{5}{8}\sin(4t)\right]. \tag{23}$$

The profile used in the simulation was a ground state with $C_{\mathrm{nl}}=20$. Figure 2 is a plot of its mean position and that of the classical prediction. It is clear that the motion is along the classical trajectory, as expected. The shape is well preserved and the phase prediction of Eq. (23) is satisfied to an accuracy of order 10^{-3} rad.

B. Anharmonic potential

We consider an anharmonic fixed potential of the form $V(x)=A(\frac{1}{4}x^4)+\frac{1}{4}x^2$, with $A=\frac{1}{200}$ and two different external potentials.

1. $P(x,t)=0$

The initial wave function was the ground state of the above anharmonic potential with $C_{\mathrm{nl}}=5$, displaced in the potential to $\mu(t=0)\approx 2$. In this case the wave function does not maintain its shape as it evolves, although the changes are not dramatic (occurring at the 10% level) owing to the small anharmonicity. Figure 3 shows a plot of the mean position of the wave packet as a function of time together with the fully classical prediction and the Ehrenfest prediction. It is clear that the motion is governed by Ehrenfest's equation and is not exactly classical.

2. Forced motion

For the above potential we have that

$$\Delta V=A\mu x^3-\tfrac{3}{2}A\mu^2x^2+\left(A\mu^3+\tfrac{1}{2}\mu\right)x-\tfrac{1}{4}\mu^2(1+A\mu^2). \tag{24}$$

Thus, if we choose $P(x,t)=-A\mu x^3+\frac{3}{2}A\mu^2x^2-A\mu^3x$, then Eq. (12) leads to $d^2\mu/dt^2+\mu=0$, which gives $\mu\sim\cos(t)$ for an initially stationary wave packet. We took $\mu(t=0)\approx 2$, as for the simulation above. Equation (10) for $\partial S/\partial t$ is the same as for the case of a harmonic potential with $P(x,t)=0$, except for an additional contribution of $\frac{1}{4}A\mu^4$ on the RHS. The phase prediction is therefore the same as in Eq. (22) with an additional term of $\frac{1}{16}A\mu_0^4[\frac{3}{2}t+\sin(2t)+\frac{1}{8}\sin(4t)]$. The wave function does maintain its shape, as expected, and the phase satisfies the theoretical prediction to within 0.03 rad. Unfortunately, this accuracy is insufficient to test the additional phase term given above, except for the linear contribution which is significant near the end of the simulation $(t=4\pi)$. Figure 4 shows a plot of the mean position of the wave packet, proving that it does indeed follow the fully classical trajectory.

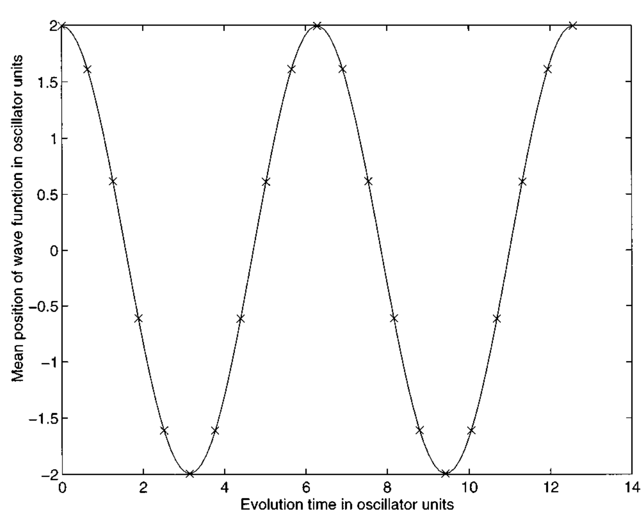

FIG. 4. Plot of the mean position of the ground state of an anharmonic potential and nonlinearity $C_{\mathrm{nl}}=5$ subject to an external force. The crosses are numerical points and the bold line is the fully classical prediction.

VII. CONCLUSION

We have shown that the shapes of exact solitary waves of the time-dependent NLSE are given by the eigenstate solutions of a time-independent NLSE for some fixed potential. These eigenstate solutions can only propagate as solitary waves provided the nonlinearity does not depend explicitly on the absolute position of the wave packet and if the change in the potential experienced by the wave packet as it moves is a linear function of position. If solitary waves do exist then their motion is generally exactly classical, although there may be an additional acceleration for certain nonlinearities. We have shown that for free space or for a harmonic fixed potential, any eigenstate behaves as a solitary wave when subject either to no external force or to one that is independent of position. Such motion is not possible for more general fixed potentials without carefully chosen external forces.

In applications of the theory to BEC, it is the form of the potentials that determines the existence of solitary-wave solutions rather than the nonlinearity. This indicates that shaking a harmonic trap containing a condensate is not a good method of confirming the existence of a nonlinear interaction term and other perturbations (such as squeezing perhaps) will be required. The analysis also shows that a condensate in a harmonic trap will be stable with respect to fluctuations in the position of the minimum, as these are equivalent to imposing a temporally fluctuating external linear potential. Finally, it is clear that one can manipulate such a condensate without affecting its internal properties, by applying a linear potential.

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APPENDIX: POSSIBLE SHAPES OF SOLITARY WAVES

In this appendix we address the problem of what determines the shape of a solitary wave and in particular we consider whether there exist solitary-wave solutions to NLSE's whose shapes are not determined by Eq. (2). As in the main text, we start with the time-dependent NLSE in reduced units

$$i\frac{\partial\Psi}{\partial t}=-\frac{\partial^2\Psi}{\partial x^2}+V(x,t)\Psi+W\Psi\ . \tag{A1}$$

We will consider the case that the nonlinear potential W is a function rather than an operator and furthermore that it is real (which is required for the Hamiltonian to be Hermitian) and time independent (other than through its dependence on Ψ). A solution to this equation that rigorously preserves its shape must have a modulus that depends on time only via a translation. We can therefore write a prospective solitary wave as

$$\Psi(x,t)=\rho(x-x_0(t))e^{i\Omega}, \tag{A2}$$

where ρ and Ω are real functions and substitute this directly into Eq. (A1). We proceed as in the main text by separating the result into real and imaginary parts, decomposing the potential as $V(x,t)=V(x)+P(x,t)$, and introducing the center-of-mass coordinate $q=x-x_0$. As before, this leads to two equations for Ω for which the consistency condition is

$$\frac{1}{2}\frac{d^2x_0}{dt^2}=-\frac{d}{dq}\left\{-\frac{1}{\rho}\frac{d^2\rho}{dq^2}+V(q)+W\right\}-\frac{\partial}{\partial x}[\Delta V(x,x_0)+P(x,t)]. \tag{A3}$$

Here $\Delta V(x,x_0)$ is defined as in the main text by $V(x)=V(q)+\Delta V(x,x_0)$ and we have assumed that W is translationally invariant as required for a solitary wave.[7] The limitation on the possible solitary waves is provided by the fact that the LHS of this equation is a function of time only and so the same must be true of the RHS if we are to satisfy the NLSE. Equation (A3) therefore determines both the motion and the shapes of any possible solitary wave.

Now the term in curly brackets in Eq. (A3) depends only on e and q, so it may be written as $F(\rho,q)$. However, for a solitary wave ρ itself depends only on q so that F is really a function of q alone. If we write it as $F(\rho,q)=\epsilon-G(q)$ we obtain the equations

$$\epsilon\rho=-\frac{d^2\rho}{dq^2}+[V(q)+G(q)]\rho+W\rho, \tag{A4}$$

$$\frac{1}{2}\frac{d^2x_0}{dt^2}=-\frac{\partial}{\partial x}[\Delta V(x,x_0)+\Delta G(x,x_0)+P(x,t)-G(x)], \tag{A5}$$

where $\Delta G(x,x_0)$ is defined analogously to $\Delta V(x,x_0)$. The first of these equations determines the shape of the solitary wave and the second gives its equation of motion and the validity condition since the LHS again depends on t only. The eigenstate solutions discussed in the main text correspond to the case $G=0$. If G is nontrivial, then we can define new potentials $V_{\mathrm{new}}(x)=V(x)+G(x)$ and $P_{\mathrm{new}}(x,t)=P(x,t)-G(x)$, whose sum is still $V(x,t)$. Using these new potentials, Eqs. (A4) and (A5) become

$$\epsilon\rho=-\frac{d^2\rho}{dq^2}+[V_{\mathrm{new}}(q)]\rho+W\rho, \tag{A6}$$

$$\frac{1}{2}\frac{d^2x_0}{dt^2}=-\frac{\partial}{\partial x}[\Delta V_{\mathrm{new}}(x,x_0)+P_{\mathrm{new}}(x,t)], \tag{A7}$$

where $\Delta V_{\mathrm{new}}(x,x_0)=\Delta V(x,x_0)+\Delta G(x,x_0)$. Equation (A6) shows that for any solitary wave, ρ is a solution to the eigenstate problem of Eq. (2) for the particular decomposition where $V(x)=V_{\mathrm{new}}(x)$. Thus a solution with $G\neq 0$ can be mapped to one with $G=0$.

The above mapping shows that any decomposition $V(x,t)=V(x)+P(x,t)$ will lead to the same physics. Of

[7]If we do not make this assumption then Eq. (A5) will contain an extra term of the form ΔW on the RHS. Since this depends on Ψ it will not be a linear function of position and cannot be canceled by physically reasonable forms of the potentials (see the comment in Sec. III).

course, in a given physical situation some decompositions will be more appropriate than others; for example, if one is describing an inhomogeneous condensate, then $V(x)$ should clearly be the trap potential. The simplest decomposition will usually correspond to $G=0$ since if we have a description in which G is nontrivial then we can see from Eq. (A5) that it must be canceled by a time-independent contribution to $P(x,t)$ if we are to have a solitary wave. The same physics would be described more simply by redefining the potentials such that $G=0$. In this description the fixed potential contains all the time-independent part of $V(x,t)$[8] (except possibly a linear contribution) and the shape of the solution corresponds to an eigenstate of the NLSE in that fixed potential. Thus we see that the only allowed rigorous solitary-wave solutions to Eq. (A1) are eigenstates of some ''fixed'' potential NLSE and thus our method in the main text is quite general.

[8]This follows from Eq. (A7) and the fact that $\Delta V_{\mathrm{new}}(x,x_0)$ will depend on time.

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[17] This does not entirely restrict our method to localized solutions, however, as it applies to any wave function with $A(t)=0$. An example of a nonlocalized wave function with $A(t)=0$ is the well-known kink solution to the homogeneous CNLSE $[V(x,t)=0,\ W\propto|\Psi|^2]$:

$$\Psi(x,t)=2\eta\sqrt{\frac{2}{Cnl}}\tanh[2\eta(x-x_c+a\mu t)]$$
$$\times\exp[-2\imath\mu x-4\imath(\mu^2+2\eta^2)t]$$

(see for example, F. Abdullaev, *Theory of Solitons in Inhomogeneous Media* (Wiley, Chichester, 1994), or Ref. [16]). We note that there may exist approximate solutions to the NLSE that do not have $A(t)=0$ as given, for example, by the WKB approximation.

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