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Bound and resonance states of the nonlinear Schrödinger equation in simple model systems

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Received 28 September 2004, in final form 9 November 2004

Published 9 February 2005

Online at stacks.iop.org/JPhysA/38/1777

Abstract

We study the stationary nonlinear Schrödinger equation, or Gross–Pitaevskii equation, for a single delta potential and a delta-shell potential. These model systems allow analytical solutions, and thus provide useful insight into the features of stationary bound, scattering and resonance states of the nonlinear Schrödinger equation. For the single delta potential, the influence of the potential strength and the nonlinearity is studied as well as the transition from bound to scattering states. Furthermore, the properties of resonance states in a repulsive delta-shell potential are discussed.

PACS numbers: 03.65.Ge, 03.65.Nk, 03.75–b, 05.45.Yv

1. Introduction

In the case of low temperatures, the dynamics of a Bose–Einstein condensate can be described in a mean-field approach by the nonlinear Schrödinger equation or Gross–Pitaevskii equation [1]. We will focus on the one-dimensional case, which can be achieved experimentally by a tight confinement in the two other spatial directions (see, for example, [2] and references therein). The nonlinear Schrödinger equation for the macroscopic wavefunction is then given by

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) + g|\psi(x,t)|^2\right)\psi(x,t) = i\hbar\frac{\partial\psi(x,t)}{\partial t}, \quad (1)$$

where $g = 4\pi\hbar^2 a N/m$ is the nonlinear ‘interaction strength’ and N is the number of particles in the condensate. The wavefunction is normalized to $\|\psi\| = 1$. In this ansatz, one only takes elastic s -wave scattering into account, characterized by the s -wave scattering length a . The scattering length a and thus the nonlinearity g are negative for an attractive nonlinear interaction and positive for a repulsive one. Another important application of the nonlinear Schrödinger equation is the propagation of electromagnetic waves in nonlinear media (see, e.g., [3], chapter 8).

Here we study the nonlinear Schrödinger equation for two simple potentials: a single delta potential

$$V(x) = \lambda\delta(x), \quad (2)$$

modelling a short range interaction, and the delta-shell potential

$$V(x) = \begin{cases} +\infty & \text{for } x < 0 \\ \lambda\delta(x-a) & \text{for } x \geq 0 \end{cases} \quad (3)$$

with $a > 0$. The delta shell is a popular model system for the study of resonances and decay. We confine ourselves to the stationary case, where the time dependence is given by the factor $e^{-i\mu t/\hbar}$. Using units with $\hbar = 1$ and $m = 1$, the stationary nonlinear Schrödinger equation reads

$$\left(-\frac{1}{2} \frac{d^2}{dx^2} + V(x) + g|\psi(x)|^2\right) \psi(x) = \mu\psi(x). \quad (4)$$

The solutions of equation (4) for the delta potential and the delta-shell potential are essentially those of the free nonlinear Schrödinger equation. The wavefunction itself is continuous, but due to the delta potential, its first derivative is discontinuous at $x = 0$, resp. $x = a$:

$$\lim_{\epsilon \rightarrow 0^+} (\psi'(a+\epsilon) - \psi'(a-\epsilon)) = 2\lambda\psi(a). \quad (5)$$

One can easily show that this behaviour, well known for the Schrödinger equation, is not changed by the nonlinearity. Furthermore, in the case of the delta-shell potential, the boundary condition $\psi(0) = 0$ has to be obeyed.

The motivation for a detailed discussion of these simple model systems is twofold. Firstly, analytic solutions of the nonlinear Schrödinger equation for a non-vanishing potential $V(x)$ are very rare. By an analysis of such simple potentials we can show analytically that nonlinear bound and resonance states exhibit new fundamental qualities in comparison to linear systems.

Secondly, these new features of nonlinear bound and resonance states are important in the context of nonlinear transport past obstacles, e.g. in atom chip experiments (see [4] and references therein). For example, the flow past a single short-range obstacle, that can be approximated by a delta potential, is studied in [5, 6].

Another important application is the transport through a double barrier, that crucially depends on the resonances of the potential, as studied in [4]. It can be argued that the transport phenomena do not depend sensitively on the specific shape of the potentials [4] and an analysis of the resonances in a delta-shell potential, or equivalently the anti-symmetric resonances of a double-delta potential, will be quite useful. For example the shift of the resonance positions and widths due to the nonlinearity calculated numerically in [7] for a Gaussian-shaped double-barrier can be deduced analytically up to first order in the nonlinearity for the delta-shell potential.

2. Single delta potential

The single delta potential (2) is the easiest model for the study of the existence and the properties of bound and scattering states. It has been studied rather briefly in the context of a nonlinear flow [5, 6].

In the linear case, $g = 0$, equation (4) with $\lambda < 0$ supports a single bound state with energy $E_0 = -\lambda^2/2$ and a continuous spectrum for $E > 0$, however, without embedded resonances. The normalized bound state wavefunction is

$$\psi_0(x) = \sqrt{|\lambda|} e^{\lambda|x|}. \quad (6)$$

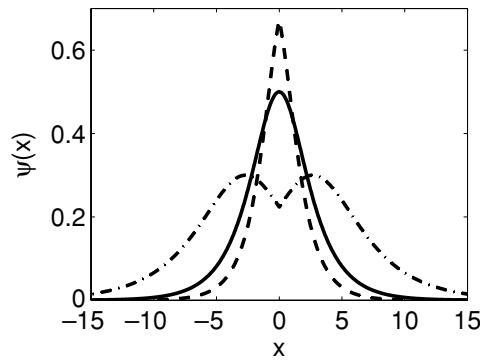


Figure 1. Wavefunctions $\psi(x)$ of bound states of the nonlinear Schrödinger equation (attractive nonlinearity, $g = -1$) for a delta potential $V(x) = \lambda\delta(x)$ with $\lambda = -0.2$ (---), $\lambda = 0$ (—) and $\lambda = +0.2$ (-·-).

In the following, we will study the modifications of this linear case due to an attractive resp. repulsive nonlinearity. By means of the scaling $x = x'/|g|$, $\psi = \psi'\sqrt{|g|}$, $\lambda = \lambda'|g|$ and $\mu = \mu'g^2$ (which conserves the normalization), the parameter g in (4) can be removed up to a sign. Therefore, we will fix the nonlinearity to $g = \pm 1$ (with the exception of section 2.3).

2.1. Attractive nonlinearity

In the case of an attractive nonlinearity, $g = -1$, the nonlinear Schrödinger equation (4) has the well-known bright soliton solution for $\lambda = 0$ and $\mu < 0$ [8, 9],

$$\psi(x) = k \operatorname{sech}(k(x - x_0)) \quad \text{with} \quad k = \sqrt{-2\mu}. \tag{7}$$

In order to find nonlinear bound states, i.e. normalizable solutions of equation (4), bright soliton solutions of form (7) for $x > 0$ and $x < 0$ are matched at $x = 0$ by means of condition (5). Obviously, the wavefunction $\psi(x)$ has to be symmetric with respect to $x = 0$ and is therefore given by expression (7) for $x \geq 0$ and $\psi(x) = \psi(-x)$ otherwise. Inserting this ansatz into equation (5) leads to the condition

$$\tanh(kx_0) = \lambda/k. \tag{8}$$

Combined with the normalization of the wavefunction,

$$\begin{aligned} 1 &= \int_{-\infty}^{+\infty} |\psi(x)|^2 dx = 2k^2 \int_0^{+\infty} \operatorname{sech}^2(k(x - x_0)) dx \\ &= 2k(1 + \tanh(kx_0)), \end{aligned} \tag{9}$$

this yields

$$k = \frac{1}{2} - \lambda, \quad \text{i.e.} \quad \mu = -\frac{1}{8}(2\lambda - 1)^2. \tag{10}$$

Because of $|\tanh(kx_0)| < 1$, one finds a condition for the existence of a bound state:

$$\lambda < \lambda_c = \frac{1}{4}. \tag{11}$$

A bound state exists for any attractive delta potential but also for a repulsive one, provided that its strength is not too large. This effect is due to the attractive self-interaction $-|\psi(x)|^2$ which can compensate a limited external repulsion.

Figure 1 shows the wavefunctions for such bound states for three different values of the potential strength λ . Quite generally, for an attractive delta potential with a negative value of x_0 , the wavefunction tends to concentrate at the delta potential with decreasing λ . A repulsive

delta potential repels the wavefunction, x_0 is positive, and one observes two peaks of $\psi(x)$ at $x = \pm x_0$ that are pushed further away as λ is increased toward λ_c . For $\lambda \rightarrow \lambda_c$ the wavefunction evolves into two infinitely separated bright soliton solutions.

Remarkably, the bound state ceases to exist at a finite negative value of the chemical potential

$$\mu_c = -\frac{1}{8}(2\lambda_c - 1)^2 = -\frac{1}{32}. \quad (12)$$

This difference to the linear equation or the case of repulsive nonlinearity (see below) corresponds to the fact that the wavefunction is no longer bound by an external potential but by the internal self-interaction.

For $\lambda > \lambda_c$, there is no longer a bound state solution, but one can actually find periodic stationary solutions in terms of Jacobi elliptic functions [8, 9]

$$\psi(x) = \frac{4\sqrt{p}K(p)}{L} \operatorname{cn}\left(4K(p)\frac{x-x_0}{L} \middle| p\right). \quad (13)$$

Here L is the period, $p \in [0, 1]$ the elliptic parameter of the Jacobi elliptic function cn and $K(p)$ denotes the complete elliptic integral of the first kind. The chemical potential is related to these parameters by

$$\mu = 8(1-2p)K^2(p)/L^2. \quad (14)$$

These solutions are of course no longer normalizable, and will be denoted as scattering states in the following. Such a periodic solution, characterized by three parameters, the chemical potential μ , the period L and the shift x_0 , has to fulfil only condition (5). Thus, for a fixed value of the potential strength λ , there exists a variety of solutions, whereby the chemical potential μ and the period L can be chosen more or less independently. The value of x_0 is then fixed to satisfy condition (5).

In the following, we discuss a particular class of solutions that merge continuously into the bound state solution when λ is decreased below its critical value λ_c . Therefore we make the ansatz that μ and $\psi(x=0)$ depend continuously on the strength λ of the delta potential at λ_c . In fact, we assume the functional relation to be the same for $\lambda > \lambda_c$ and $\lambda < \lambda_c$, i.e. given by equation (10), and

$$\psi(0) = k \operatorname{sech}(\operatorname{arctanh}(\lambda/k)), \quad (15)$$

respectively. For a given value of λ , we construct solutions (13) that fulfil condition (5) and yield the desired values of μ and $\psi(0)$. Such solutions can indeed be found and figure 2 illustrates such a wavefunction for $\lambda = 0.26$, just above the critical value $\lambda_c = 0.25$, in comparison to a bound state solution for $\lambda = 0.24$.

In the vicinity of the delta potential at $x = 0$, both wavefunctions look rather similar and thus the transition from a bound to a scattering state seems to be continuous. The observed difference between the bound state and the periodic solution for $|x| > L$ disappears in the limit $\lambda \searrow \lambda_c$ because the period L of the Jacobi elliptic solution moves toward infinity.

To explore this transition in some detail, we consider the position x_0 of the first maximum of $|\psi(x)|^2$, as a function of λ , given by

$$x_0(\lambda) = \frac{1}{1/2 - \lambda} \operatorname{arctanh}\left(\frac{\lambda}{1/2 - \lambda}\right) \quad (16)$$

for $\lambda < \lambda_c$ and by the solution of the complex equations

$$\begin{aligned} \psi(0) &= k \sqrt{\frac{p}{2p-1}} \operatorname{cn}\left(\frac{kx_0(\lambda)}{\sqrt{2p-1}} \middle| p\right) \quad \text{and} \\ \lambda\psi(0) &= k^2 \frac{\sqrt{p}}{2p-1} \operatorname{sn}\left(\frac{kx_0(\lambda)}{\sqrt{2p-1}} \middle| p\right) \operatorname{dn}\left(\frac{kx_0(\lambda)}{\sqrt{2p-1}} \middle| p\right) \end{aligned} \quad (17)$$

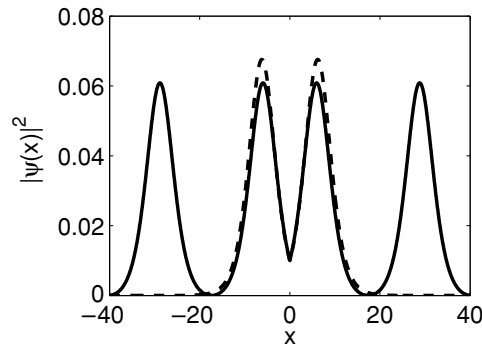


Figure 2. Wavefunctions of a bound state (—, $\lambda = 0.24$) and a scattering state (---, $\lambda = 0.26$) for a repulsive delta potential $V(x) = \lambda\delta(x)$ for an attractive nonlinearity close to the transition at $\lambda_c = 0.25$.

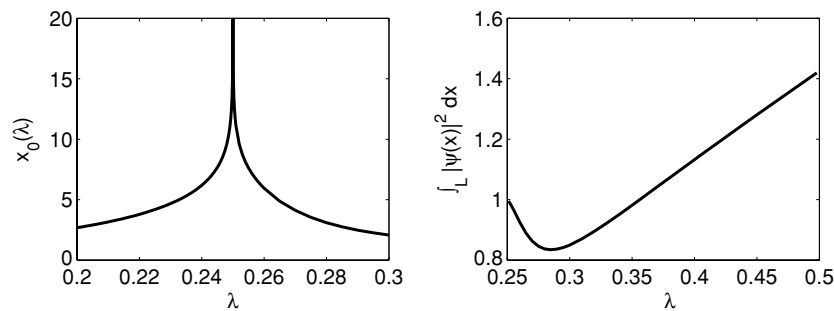


Figure 3. Transition from a bound to a scattering state. Left: position $x_0(\lambda)$ of the first maximum of the wavefunction. Right: norm per period L . Note that $L \rightarrow \infty$ as $\lambda \searrow \lambda_c$.

for $\lambda > \lambda_c$, where k and $\psi(0)$ are fixed by equations (10) and (15) as discussed above. At λ_c , the function $x_0(\lambda)$ shown in figure 3 on the left has a logarithmic singularity.

On the right of figure 3, the norm per period $\int_{-L/2}^{L/2} |\psi(x)|^2 dx$ is displayed, which tends to unity at the critical point λ_c , i.e. it approaches the bound state normalization. Hence the norm is also continuous.

2.2. Repulsive nonlinearity

In the case of a repulsive nonlinearity, $g = +1$, the nonlinear Schrödinger equation has the well-known dark soliton solutions for $\lambda = 0$ [9, 10]:

$$\psi = \sqrt{\mu} \tanh(\sqrt{\mu}(x - x_0)). \quad (18)$$

Making such an ansatz separately for $x > 0$ and $x < 0$ and matching at $x = 0$ with respect to condition (5) yields $x_0 = 0$ regardless of the value of λ . Remarkably, the wavefunction has a zero at $x = 0$ even for an attractive delta potential. But solutions of this kind are of course not normalizable. Another possible solution is

$$\psi(x) = k \operatorname{cosech}(k(x - x_0)), \quad \text{with } k = \sqrt{-2\mu}, \quad (19)$$

which is usually discarded because of its unphysical singularity at $x = x_0$. In the case of a delta potential, however, this ansatz reveals proper stationary bound states. Assuming (19) for $x > 0$, a short calculation shows that the wavefunction has to be symmetric, $\psi(-x) = \psi(x)$.

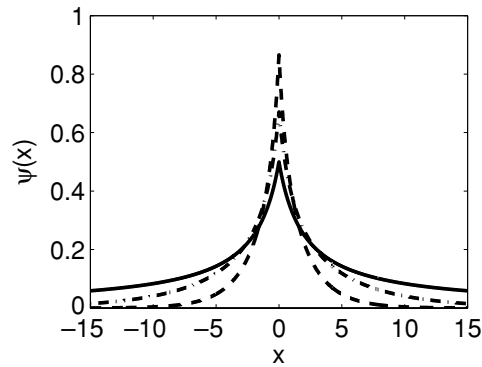


Figure 4. Wavefunctions $\psi(x)$ of bound states of the nonlinear Schrödinger equation (repulsive nonlinearity, $g = +1$) for a delta potential $V(x) = \lambda\delta(x)$ for three values of the potential strength $\lambda = -1$ (- · - ·), $\lambda = -0.7$ (- · -) and for the critical case $\lambda = -0.5$ (—).

In addition, x_0 must be negative because otherwise the wavefunction would become singular at $x = x_0$. Condition (5) yields

$$\tanh(kx_0) = k/\lambda \quad (20)$$

and the normalization of the wavefunction requires

$$\begin{aligned} 1 &= \int_{-\infty}^{+\infty} |\psi(x)|^2 dx = 2k^2 \int_0^{+\infty} \operatorname{cosech}^2(k(x - x_0)) dx \\ &= -2k(1 + \coth(kx_0)). \end{aligned} \quad (21)$$

This leads to

$$k = -\frac{1}{2} - \lambda \quad (22)$$

which must be positive, yielding the condition

$$\lambda < \lambda_c = -\frac{1}{2}, \quad (23)$$

i.e. the delta potential must be sufficiently attractive to overcome the repulsive self-interaction in order to support a bound state.

In figure 4, such bound states are displayed for different values of the potential strength λ . For decreasing values of λ , the wavefunction concentrates at the position of the delta potential. In the opposite limit, $\lambda \nearrow \lambda_c$, we see by series expansion of the tanh and the sinh functions, that

$$x_0 \rightarrow x_c = 1/\lambda_c \quad \text{and} \quad \mu \rightarrow \mu_c = 0 \quad (24)$$

and that the wavefunction converges to the limiting function

$$\psi_c(x) = \frac{1}{|x| - x_c} = \frac{1}{|x| + 2} \quad (25)$$

also shown in figure 4. This is in contrast to the case of an attractive nonlinearity where the bright soliton peaks move to $\pm\infty$ at the critical value λ_c .

For $\lambda > \lambda_c$, one again finds periodic solutions in terms of Jacobi elliptic functions [9, 10]

$$\psi(x) = \frac{4\sqrt{p}K(p)}{L} \operatorname{sn}\left(4K(p)\frac{x - x_0}{L} \middle| p\right), \quad (26)$$

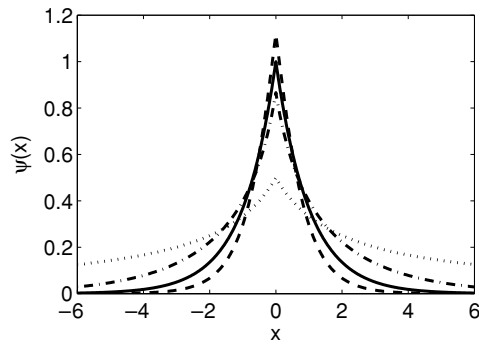


Figure 5. Bound state wavefunctions $\psi(x)$ of the nonlinear Schrödinger equation for an attractive delta potential $V(x) = -\delta(x)$ for different values of the nonlinearity: $g = -1$ (—), $g = 0$ (---), $g = +1$ (- · -) and $g = g_c = 2$ (· · ·).

where L is the periodicity, $p \in [0, 1]$ the elliptic parameter of the Jacobi elliptic function and $K(p)$ denotes the complete elliptic integral of the first kind. The chemical potential is given by

$$\mu = 8(p + 1)K(p)^2/L^2. \tag{27}$$

For a fixed value of the potential strength λ , one again finds a variety of solutions, whereby the chemical potential μ and the period L can be chosen more or less independently. Note that such periodic solutions can only be found for $\mu > 0$.

Nevertheless, one can find a lower bound for the period L . From equation (27) it follows that

$$L = \sqrt{\frac{8(p + 1)}{\mu}} K(p) \geq \frac{2\pi}{\sqrt{2\mu}}. \tag{28}$$

For $\lambda \searrow \lambda_c$ and $\mu \searrow 0$ the period of the wavefunction L tends to infinity and the wavefunction is not periodic any more in this limit. But in this case one cannot find a continuous transition to the bound state wavefunction (19). For $\lambda \nearrow \lambda_c$ one finds the bound state (25) with $\psi(0) = 1/2$ and $\mu = 0$. In contrast, we have $\psi(0) \rightarrow 0$ for $\mu \searrow 0$ for the periodic solution (26) because of equation (27). In fact, the elliptic function sn evolves continuously into the \tanh when the elliptic parameter p tends to unity [11].

Actually, there exist Jacobi elliptic functions that merge continuously into the cosech as the elliptic modulus p tends to one. These solutions are given in terms of the Jacobi elliptic functions ds and cs [11]. But these functions have poles at the zeros of the sn and thus are not physical.

2.3. Variation of the nonlinearity

In this section, we will briefly discuss the influence of the mean-field interaction strength, i.e. the nonlinearity g , on the solutions of the nonlinear Schrödinger equation for an attractive delta potential. We therefore reintroduce the parameter g .

The bound state solutions have already been deduced in the previous sections. In figure 5, the wavefunction of such a bound state is displayed for three different values of the nonlinearity $g = -1, 0, +1$ and a fixed potential strength $\lambda = -1$. With increasing nonlinearity g , the wavefunction is pushed outward.

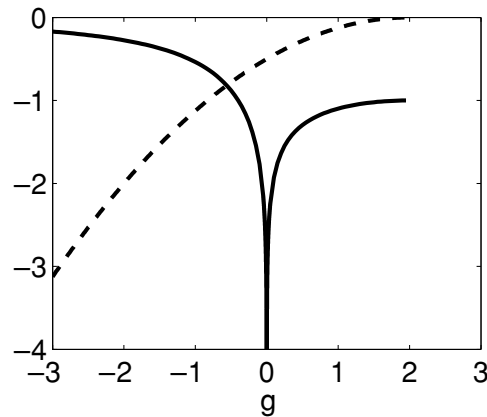


Figure 6. Dependence of the chemical potential μ (---) and the parameter x_0 (—) on the nonlinearity $g \leq g_c = 2$ for the bound state of the nonlinear Schrödinger equation for an attractive delta potential $V(x) = -\delta(x)$.

In both cases of attractive and repulsive nonlinearity, the chemical potential is given by

$$\mu = -\frac{1}{8}(2\lambda + g)^2, \quad (29)$$

which follows directly from the matching condition (5) and the normalization of the wavefunction. At a critical value of g , the chemical potential μ becomes zero and the bound state ceases to exist. The condition for the existence of a bound state is the same as discussed in section 2.2. Reformulated in terms of the nonlinearity parameter g , it reads

$$g < g_c = -2\lambda. \quad (30)$$

When g approaches the critical value g_c , the situation is similar to the case of a fixed repulsive nonlinearity g and $\lambda \nearrow \lambda_c$ as discussed in the previous section. The wavefunction at the critical value of g is

$$\psi_c(x) = \frac{\sqrt{-\lambda}}{|x| - 2\lambda}. \quad (31)$$

The dependence of x_0 and μ on the nonlinearity g is illustrated in figure 6. The position x_0 is given by equation (8) for $g < 0$ and (20) for $g > 0$, however with $k = -\lambda - g/2$.

For $g = 0$, one finds the well-known value $\mu = -\lambda^2/2$, whereas the function $x_0(g)$ has a logarithmic singularity. Nevertheless, the bound state wavefunction $\psi(x)$ evolves smoothly into the well-known bound state (6) of the linear problem for an attractive as well as a repulsive nonlinearity.

For $g \rightarrow g_c = -2\lambda$, the chemical potential μ tends to zero and x_0 tends to the finite value $1/\lambda$. The disappearance of the bound state if g is increased above g_c is similar to the effect observed by Moiseyev *et al* [12] for a smooth potential $V(x)$ where a bound state is transformed into a resonance-like state at a critical nonlinear interaction.

3. Delta-shell potential

In this section we discuss another simple and very popular model system: the delta-shell potential. A detailed discussion of the linear three-dimensional delta-shell potential can be found in [13]. Here we restrict ourselves to the one-dimensional case

$$V(x) = \begin{cases} +\infty & \text{for } x < 0 \\ \lambda\delta(x - a) & \text{for } x \geq 0 \end{cases} \quad (32)$$

with $a > 0$. First we briefly resume the basic features of the delta-shell potential in the linear case ($g = 0$), in particular the existence of bound states in an attractive potential and resonances in a repulsive one. As we have already discussed the properties of bound states in a single delta potential in some detail, we now concentrate on the case of a repulsive potential ($\lambda > 0$). We set $\hbar = 1$ and $m = 1$ as above.

3.1. The linear case

In the linear case $g = 0$, the wavefunction in a delta-shell potential is given by

$$\psi_k(x) = \begin{cases} \sin(kx) & \text{for } x < a \\ \sin(kx) + \frac{2\lambda}{k} \sin(ka) \sin(k(x-a)) & \text{for } x > a. \end{cases} \quad (33)$$

The phase shift $\delta(k)$ between incoming and outgoing waves for $x > a$ is easily calculated and yields

$$\tan \delta(k) = \frac{\cos(2ka) - 1}{\sin(2ka) + k/\lambda}. \quad (34)$$

The S -matrix $S(k)$ is defined in terms of the phase shift $\delta(k)$ by [14]

$$S(k) = \frac{1 + i \tan \delta(k)}{1 - i \tan \delta(k)}. \quad (35)$$

Bound states correspond to poles of the S -matrix $S(k)$ on the positive imaginary axis. Calculating these poles one arrives at

$$e^{2ika} = 1 - \frac{ik}{\lambda}. \quad (36)$$

This equation has a solution on the positive imaginary axis if the condition

$$\lambda a > -\frac{1}{2} \quad (37)$$

is fulfilled. This implies that the delta-shell potential has to be sufficiently attractive to support a bound state. If the distance a is reduced or λ is increased, so that condition (37) is not fulfilled any longer, the bound state is lost and one finds a virtual state instead. A virtual state corresponds to a pole of the S -matrix $S(k)$ on the negative imaginary axis [14]. The wavefunction of such a state diverges exponentially. For $a \rightarrow \infty$ the delta-shell potential is equivalent to a single delta potential and the energy is $E \rightarrow -\lambda^2/2$.

Naturally there exist no bound states in a repulsive delta-shell potential, but one can find resonance states. A resonance is defined by a pole of the S -matrix $S(k)$ in the lower half plane [14]. The energy of the n th resonance is also complex

$$\mathcal{E}_n = k_n^2/2 = E_n - i\Gamma_n/2, \quad (38)$$

where the imaginary part Γ_n is interpreted as a decay rate. In the vicinity of a resonance, the phase shift $\delta(k)$ rapidly changes by an amount of π .

The amplitude of a resonance wavefunction is enhanced for $x < a$. This is illustrated in figure 7 for a delta-shell potential of strength $\lambda = 10$ at $a = 1$. The ratio of the amplitudes on the left-hand side ($x < a$) and on the right-hand side ($x > a$) of the delta-shell potential, denoted as A_l resp. A_r , is plotted for real values of the energy. The peaks of the amplitude ratio A_l/A_r close to the resonances are clearly visible. The squared modulus of the wavefunction of the most stable resonance at $\mathcal{E}_1 = 4.488 - 0.063i$ is displayed on the right. Nevertheless one has to keep in mind that the wavefunction finally diverges exponentially for complex energies \mathcal{E} , whereas it is periodic for real energies.

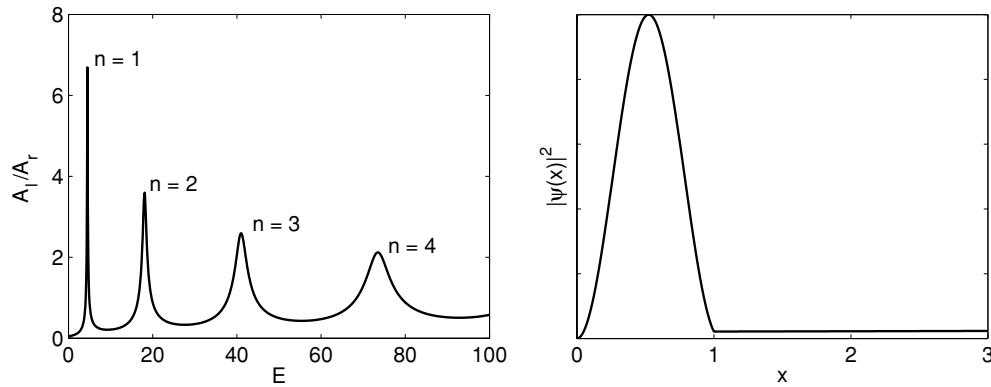


Figure 7. Left: amplitude ratio A_l/A_r for a delta-shell potential with $a = 1$ and $\lambda = 10$ in the linear case. Right: squared modulus of the wavefunction of the most stable resonance at $\mathcal{E}_1 = 4.488 - 0.063i$.

3.2. Resonances in the nonlinear case

Now we come back to the nonlinear Schrödinger equation

$$\left(-\frac{1}{2} \frac{d^2}{dx^2} + \lambda \delta(x-a) + g|\psi(x)|^2 \right) \psi(x) = \mu \psi(x) \quad \text{for } x \geq 0. \quad (39)$$

In the following we will only discuss the case of a repulsive delta-shell potential ($\lambda > 0$). By means of a scaling $x = x'/s$, $\psi = \psi' \sqrt{s}$, $\lambda = \lambda' s$ and $\mu = \mu' s^2$ for $s > 0$ (which conserves the normalization), the number of independent parameters is reduced to two. As we are mainly interested in the effects of a varying nonlinearity, the potential is fixed by $a = 1$ and $\lambda = 10$ in the following examples. In the linear case we find resonances for this potential. Now we want to identify and characterize resonances in the nonlinear case as well.

But the definition of a resonance becomes somewhat ambitious in the nonlinear case. A decomposition into incoming and outgoing waves and thus a definition of the S -matrix $S(k)$ is not possible. One method widely used to compute resonances in the linear case is exterior complex scaling (see, e.g., [15]). This technique has also been successfully applied to the nonlinear Schrödinger equation [7, 12].

We will not adopt this approach but rather look for solutions that can be expressed analytically. We have already learned that the real solutions of the free nonlinear Schrödinger equation are given in terms of Jacobi elliptic functions. These solutions are matched at $x = a$ to obtain solutions for the delta-shell potential. The chemical potential μ of such a solution is real. Thus we can define a resonance neither by a complex eigenenergy nor via the S -matrix. In the following we will rather call a state a resonance, when its amplitude is resonantly enhanced in the vicinity of the potential, i.e. for $x < a$.

Let us briefly discuss the time evolution of nonlinear resonances. Note that the states

$$\psi(x, t) = \exp(-i\mu t) \psi(x) \quad (40)$$

with a complex chemical potential $\mu = \mu_r - i\Gamma/2$ do *not* fulfil the time-dependent nonlinear Schrödinger equation, because the norm of these states is not constant. One can circumvent this problem by introducing an additional source term or one considers states (40) just as an adiabatic approximation [7]. In contrast states (40) with a real chemical potential μ discussed in this paper fulfil the time-dependent nonlinear Schrödinger equation but do *not* decay.

Furthermore we have to be cautious about the nonlinear parameter g . A meaningful definition of the nonlinearity requires that the norm or the amplitude of a solution must be fixed in some way, e.g. by $\|\psi\| = 1$ in section 2. This is not applicable any longer since resonance states are not normalizable. As a global measure of the nonlinear interaction we thus define the mean-field potential $g|\psi(x)|^2$, integrated over the ‘interaction-region’ $0 < x < a$ of the external potential:

$$g_{\text{eff}} = g \int_0^a |\psi(x)|^2 dx. \quad (41)$$

3.3. Attractive nonlinearity

First we discuss the nonlinear Schrödinger equation with a negative nonlinearity g , corresponding to an attractive mean-field interaction. As stated above, the real-valued periodic solutions of the free nonlinear Schrödinger equation with a negative nonlinearity can be expressed in terms of the Jacobi elliptic function cn [8, 9]. Thus, in order to find solutions for the delta-shell potential we make an ansatz of the form (26) separately for $x < a$ and $x > a$:

$$\psi(x) = \begin{cases} \psi_l(x) = A_l \text{cn}\left(4K(p_l)\left(\frac{x}{L_l} + \frac{1}{4}\right) \middle| p_l\right) & \text{for } x < a \\ \psi_r(x) = A_r \text{cn}\left(4K(p_r)\frac{x+x_0}{L_r} \middle| p_r\right) & \text{for } x > a. \end{cases} \quad (42)$$

The amplitudes $A_{l,r}$ and the periods $L_{l,r}$ are given by

$$A_{l,r} = \frac{4\sqrt{p_{l,r}}K(p_{l,r})}{\sqrt{|g|L_{l,r}}} \quad \text{and} \quad \mu = \frac{8(1-2p_{l,r})K(p_{l,r})^2}{L_{l,r}^2}, \quad (43)$$

where $p_{l,r}$ are the elliptic parameters of the solution on the left-hand ($x < a$) and on the right-hand ($x > a$) side of the delta shell. Clearly one has only one value for the chemical potential, whereas the amplitude A , the parameter p and the period L generally differ for $x < a$ and $x > a$. This is different from the linear case, where the period L is fixed with the energy. The chemical potential is positive, $\mu \geq 0$, if the elliptic parameter is restricted to $p_{l,r} \in [0, 1/2]$.

The boundary condition $\psi(0) = 0$ is automatically fulfilled by this ansatz. Furthermore the wavefunction must be continuous at $x = a$, whereas its derivative is discontinuous according to equation (5), leading to the conditions:

$$\begin{aligned} \text{(I.)} \quad & A_l \text{cn}(u_l|p_l) = A_r \text{cn}(u_r|p_r) \\ \text{(II.)} \quad & 2\lambda A_l \text{cn}(u_l|p_l) = -\frac{4A_r K_r}{L_r} \text{sn}(u_r|p_r) \text{dn}(u_r|p_r) + \frac{4A_l K_l}{L_l} \text{sn}(u_l|p_l) \text{dn}(u_l|p_l), \end{aligned} \quad (44)$$

where the abbreviations $u_l = K(p_l)(4a/L_l + 1)$ and $u_r = 4K(p_r)(a+x_0)/L_r$ have been used. The first condition can be fulfilled by an appropriate choice of x_0 , as long as $|A_l \text{cn}(u_l|p_l)| \leq |A_r|$. Then one can insert the first condition into the second one and arrive at

$$\begin{aligned} & \frac{2\lambda^2}{\mu} \frac{p_l}{1-2p_l} \text{cn}(u_l|p_l)^2 - \frac{4\lambda}{\sqrt{2\mu}} \frac{p_l}{(1-2p_l)^{3/2}} \text{cn}(u_l|p_l) \text{dn}(u_l|p_l) \text{sn}(u_l|p_l) \\ & = \frac{(1-p_r)p_r}{(1-2p_r)^2} - \frac{(1-p_l)p_l}{(1-2p_l)^2}. \end{aligned} \quad (45)$$

As argued above we are looking for solutions whose amplitudes are resonantly enhanced for $x < a$, i.e. for solutions with a maximum amplitude ratio A_l/A_r . This ratio is given

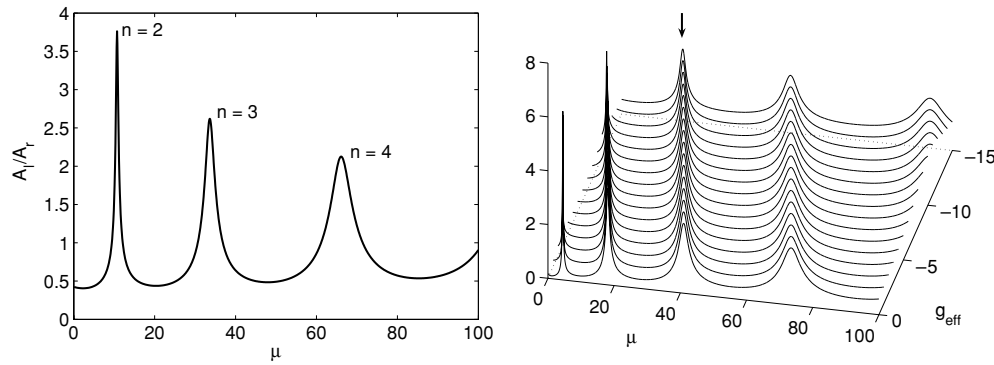


Figure 8. Amplitude ratio A_l/A_r as a function of the chemical potential μ for an effective nonlinearity $g_{\text{eff}} = -5$ (left) and for different effective nonlinearities g_{eff} (right). The shift of the resonance marked by an arrow is displayed as a function of g_{eff} in figure 9.

directly by the elliptic parameters $p_{l,r}$:

$$\frac{A_l}{A_r} = \left[\frac{p_l(1 - 2p_r)}{(1 - 2p_l)p_r} \right]^{1/2}. \quad (46)$$

A resonant enhancement of the amplitude ratio demands that $p_l \gg p_r$.

In order to identify and analyse resonances of the nonlinear Schrödinger equation we now calculate the amplitude ratio A_l/A_r as a function of the chemical potential for different values of the effective nonlinearity g_{eff} . The left-hand side of figure 8 shows the amplitude ratio as a function of μ for an effective nonlinearity $g_{\text{eff}} = -5$. As in the linear case, illustrated in figure 7, resonances can be clearly identified as maxima of the amplitude ratio A_l/A_r . The resonances are, however, shifted to smaller values of μ , whereas the width of the resonances remains similar.

On the right-hand side of figure 8 the amplitude ratio $A_l/A_r(\mu)$ is plotted for different values of the effective nonlinearity g_{eff} . Resonances are clearly identified for all values of g_{eff} , but the shift of the resonance positions is clearly visible in this illustration. We note that the resonance heights barely change with g_{eff} .

The observed shift of the resonances will be explained in the following. For convenience we rather calculate the chemical potential where $A_l = A_r$ at the sides of each resonance, in dependence of g_{eff} . These values of the chemical potential will be denoted $\mu_n^<$ and $\mu_n^>$ in the following. They are easier to calculate than the resonance positions μ_n because $p_l = p_r$ holds at these values, furthermore this calculation will also reveal the influence of g_{eff} on the resonance width. We note that the wavefunction on the interval $x \in [0, 2a]$ is symmetric (antisymmetric) around $x = a$ for $\mu = \mu_n^<$ ($\mu = \mu_n^>$).

Using both equations (43), the chemical potential can be written as

$$\mu = gA^2 \left(1 - \frac{1}{2p} \right). \quad (47)$$

The elliptic parameter p can be calculated from the relation

$$pK(p)^2 = \frac{|g|A^2L^2}{16}. \quad (48)$$

Solving this relation for p leads to

$$p = \frac{|g|A^2L^2}{4\pi^2} - \frac{1}{2} \left(\frac{|g|A^2L^2}{4\pi^2} \right)^2 + \mathcal{O}(g^3A^6), \quad (49)$$

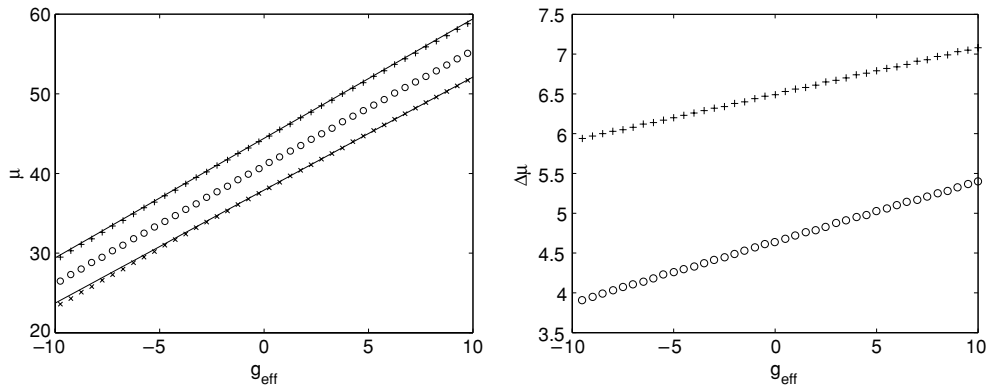


Figure 9. Left: dependence of the resonance position μ_n (o) and $\mu_n^>$ (+) and $\mu_n^<$ (x) on the effective nonlinearity g_{eff} for $n = 3$. The solid lines are the approximations (51) and (55). Right: width of the resonance, defined as $\Delta\mu = \mu_3^> - \mu_3^<$ (+) and as FWHM (o).

and inserting this into equation (47), we find the desired dependence of the chemical potential on the nonlinear interaction

$$\mu = \frac{2\pi^2}{L^2} \left(1 + \frac{3gA^2L^2}{8\pi^2} + \mathcal{O}(g^2A^4) \right). \tag{50}$$

Formula (50) is valid for both $\mu_n^>$ and $\mu_n^<$. Now we insert the specific values of the period L and replace gA^2 by the effective nonlinearity g_{eff} . At $\mu_n^>$ the period of the wavefunction is $L_n^> = 2a/n$, i.e. $\psi(a) = 0$. Equation (41) for the effective nonlinearity can be easily evaluated in lowest order in p , since then the elliptic function cn equals a cosine, which yields $g_{\text{eff}} \approx gA^2a/2$. This finally leads to

$$\mu_n^> \approx \frac{n^2\pi^2}{2a^2} + \frac{3g_{\text{eff}}}{2a}. \tag{51}$$

Similarly one obtains an expression for $\mu_n^<$. In the linear case the period $L_n^<$ is given by the solution of the implicit equation

$$\tan\left(\frac{2\pi a}{L_n^<}\right) = -\frac{2\pi}{\lambda L_n^<}. \tag{52}$$

For the example illustrated in figure 9 ($a = 1, \lambda = 10$ and $n = 3$) one has $L_3^< = 0.7215$. The change of $L_n^<$ with g_{eff} is negligible. Again equation (41) for the effective nonlinearity is readily evaluated in lowest order in p and yields

$$g_{\text{eff}} \approx \frac{gaA^2}{2} \left(1 - \frac{\sin(4\pi a/L_n^<)}{4\pi a/L_n^<} \right) \tag{53}$$

$$= \frac{gaA^2}{2} \left(1 + \frac{1}{\lambda a(1 + (2\pi)^2/(\lambda L_n^<)^2)} \right). \tag{54}$$

Inserting into equation (50), one finally arrives at

$$\mu_n^< \approx \frac{2\pi^2}{(L_n^<)^2} + \frac{3g_{\text{eff}}}{2a} \left(1 - \frac{\sin(4\pi a/L_n^<)}{4\pi a/L_n^<} \right)^{-1}. \tag{55}$$

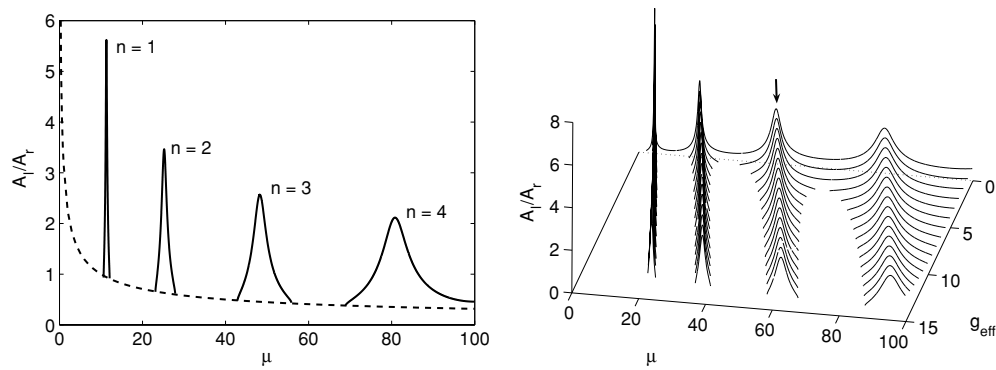


Figure 10. Left: amplitude ratio as a function of the chemical potential μ for an effective nonlinearity $g_{\text{eff}} = 5$. Condition (62) for the amplitude ratio is plotted as a dashed line. Right: amplitude ratio as a function of the chemical potential μ for different effective nonlinearities. The shift of the resonance marked with an arrow is displayed as a function of g_{eff} in figure 9.

The same results are obtained in the case of a repulsive interaction ($g > 0$, see below). Thus we compare the approximations (51) and (55) to the numerically exact results for $g < 0$ and $g > 0$ together in figure 9. We considered the resonance with $n = 3$, that is marked with an arrow in figures 8 and 10. We observe a good agreement. Furthermore the positions $\mu_{n=3}$ of the resonances are displayed.

From the different scaling of $\mu_n^>$ and $\mu_n^<$ we conclude that the resonance width also changes with the effective nonlinearity. In fact, the width increases almost linearly with g_{eff} and the resonances become slightly asymmetric. The dependence of the width $\Delta\mu = \mu_3^> - \mu_3^<$ on the effective nonlinearity g_{eff} is illustrated in figure 9 on the right.

It should not be concealed that also bound states can exist in a repulsive delta-shell potential due to the attractive self-interaction, falling off as $\text{sech}(\sqrt{-2\mu}(x - x_0))$ for $x > a$. However, we will not consider these states here as we already discussed a similar phenomenon for the single delta potential.

3.4. Repulsive nonlinearity

As stated above, the real non-singular solutions of the free nonlinear Schrödinger equation with a repulsive nonlinearity can be expressed in terms of the Jacobi elliptic function sn [9, 10]. Thus we make the ansatz:

$$\psi(x) = \begin{cases} \psi_l(x) = A_l \text{sn}\left(4K(p_l)\frac{x}{L_l} \middle| p_l\right) & \text{for } x < a \\ \psi_r(x) = A_r \text{sn}\left(4K(p_r)\frac{x+x_0}{L_r} \middle| p_r\right) & \text{for } x > a. \end{cases} \quad (56)$$

The amplitudes $A_{l,r}$ and the periods $L_{l,r}$ are now given by

$$A_{l,r} = \frac{4\sqrt{p_{l,r}}K(p_{l,r})}{\sqrt{|g|}L_{l,r}} \quad \text{and} \quad \mu = \frac{8(p_{l,r} + 1)K(p_{l,r})^2}{L_{l,r}^2}, \quad (57)$$

where $p_{l,r} \in [0, 1]$ are the elliptic parameters of the solution on the left ($x < a$) and on the right ($x > a$) of the delta shell.

The boundary condition $\psi(0) = 0$ is automatically fulfilled by ansatz (56). The remaining conditions for the wavefunction and its derivative at $x = a$ (cf equation (5)) read

$$\begin{aligned} \text{I. } & A_l \text{sn}(u_l|p_l) = A_r \text{sn}(u_r|p_r) \\ \text{II. } & 2\lambda A_l \text{sn}(u_l|p_l) = \frac{4A_r K_r}{L_r} \text{cn}(u_r|p_r) \text{dn}(u_r|p_r) - \frac{4A_l K_l}{L_l} \text{cn}(u_l|p_l) \text{dn}(u_l|p_l), \end{aligned} \quad (58)$$

where the abbreviations $u_l = 4K(p_l)a/L_l$ and $u_r = 4K(p_r)(a + x_0)/L_r$ have been used.

If $|A_l \text{sn}(u_l|p_l)| \leq |A_r|$ the first condition can always be fulfilled by an appropriate choice of the 'phase shift' x_0 . Inserting the first condition into the second one and using the addition theorems of the Jacobi elliptic functions one arrives at

$$\begin{aligned} \frac{2\lambda^2}{\mu} \frac{p_l}{p_l + 1} \text{sn}^2(u_l|p_l) + \frac{p_l}{(p_l + 1)^{3/2}} \frac{4\lambda}{\sqrt{2\mu}} \text{cn}(u_l|p_l) \text{dn}(u_l|p_l) \text{sn}(u_l|p_l) \\ = \frac{p_r}{(p_r + 1)^2} - \frac{p_l}{(p_l + 1)^2}. \end{aligned} \quad (59)$$

The amplitude ratio A_l/A_r is given by

$$\frac{A_l}{A_r} = \left[\frac{p_l(p_r + 1)}{(p_l + 1)p_r} \right]^{1/2} \quad (60)$$

in terms of the elliptic parameters. A resonant enhancement of the amplitude ratio demands that $p_l \gg p_r$.

Again we calculated the amplitude ratio A_l/A_r as a function of the chemical potential μ for different values of the effective nonlinearity g_{eff} . The results are illustrated in figure 10. The left-hand side shows the amplitude ratio A_l/A_r for an effective nonlinearity $g_{\text{eff}} = 5$, which should be compared to figures 7 and 8. The first observation is that one cannot find solutions for all values of μ . In fact there exist no solutions with an amplitude ratio below a certain threshold. Resonances are still clearly identified as maxima of the amplitude ratio. Again the resonance positions are shifted in comparison to the linear case.

On the right-hand side the amplitude ratio is plotted for different values of g_{eff} . One observes that the solutions cease to exist with an increasing effective nonlinearity, whereas the resonances survive longest. The resonances are shifted similarly to the case of an attractive interaction.

We noted that solutions with a small amplitude ratio A_l/A_r cease to exist when g_{eff} is increased. In fact the second condition in (58) cannot be fulfilled any longer if the amplitude ratio A_l/A_r drops below a certain threshold. A condition for the existence of a solution can be derived from equations (60) and (57) and yields

$$\left(\frac{A_l}{A_r} \right)^2 \geq \frac{2p_l}{p_l + 1} = \frac{gA_l^2}{\mu}. \quad (61)$$

Inserting $g_{\text{eff}} \approx gA_l^2/2$ on the right-hand side, one is led to the approximation

$$\frac{A_l}{A_r} \gtrsim \left(\frac{2g_{\text{eff}}}{a\mu} \right)^{1/2}. \quad (62)$$

As a consequence solutions apart from the resonances with small amplitude ratios cease to exist when g_{eff} is increased. This approximate condition is well confirmed by the numerical exact results displayed in figure 10.

The shift of the resonances is understood in the same way as in the case of an attractive interaction. The chemical potential is now given by

$$\mu = gA^2 \left(\frac{1}{2} + \frac{1}{2p} \right), \quad (63)$$

while equation (49) still holds. Inserting into equation (63) and expanding up to the linear term in gA^2 again leads to equation (50). Thus one arrives at the same results as in the case of an repulsive interaction, in particular at equation (51) for $\mu_n^>$ and equation (55) for $\mu_n^<$. The results for $n = 3$ are displayed in figure 9. The approximations agree well with the numerical exact results. From the different scaling of $\mu_n^>$ and $\mu_n^<$ with g_{eff} we conclude that a repulsive nonlinearity increases the resonance width.

4. Conclusion

In this paper we analysed the properties of bound, scattering and resonance states of the nonlinear Schrödinger equation using two simple model systems.

Bound, i.e. normalizable, states were calculated and analysed for a single delta potential. New features occur in the case of an attractive nonlinearity, as states are no longer bound by an external potential but by the internal interaction. In this case bound states can exist despite a repulsive external potential, and they cease to exist at a negative value of the chemical potential. In addition we investigated the transition from bound to scattering states.

Furthermore we discussed a repulsive delta-shell potential as a simple model showing resonances. Resonances can still be identified in the nonlinear case, though the definition of a resonance becomes somewhat ambitious. Two major effects of the nonlinearity were analysed in detail: firstly, the resonance positions are shifted proportionally to the effective nonlinearity and the resonance width increases with g_{eff} . Secondly, scattering states cease to exist with an increasing repulsive nonlinearity, whereas resonances survive longest.

Acknowledgments

Support from the Deutsche Forschungsgemeinschaft via the Graduiertenkolleg ‘Nichtlineare Optik und Ultrakurzzeitphysik’ is gratefully acknowledged. We thank N Moiseyev and P Schlagheck for stimulating discussions.

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