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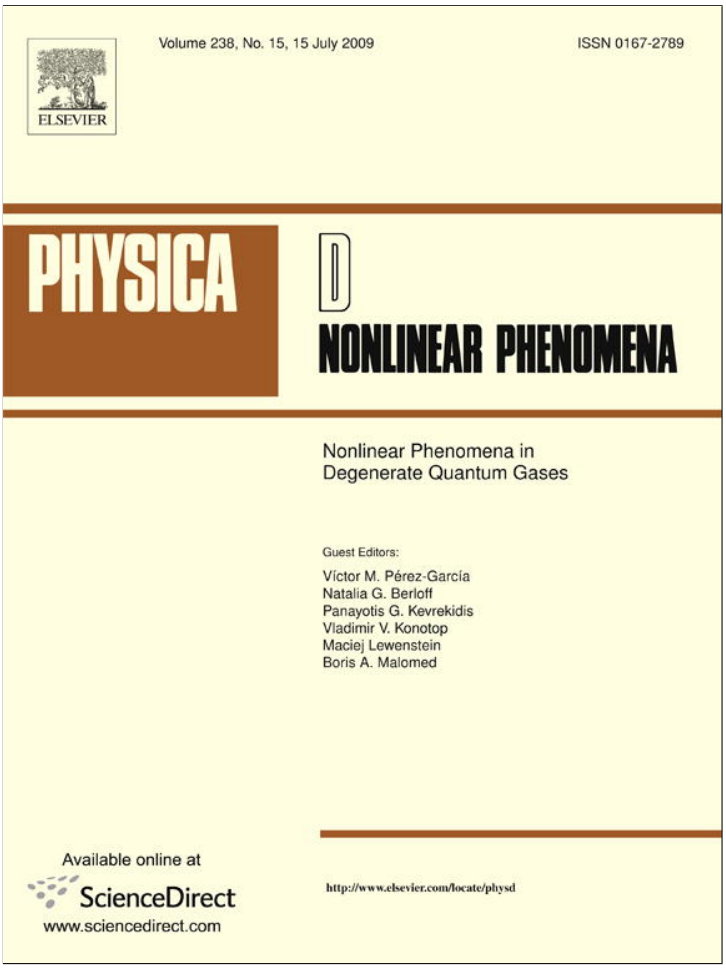

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Localization phenomena in nonlinear Schrödinger equations with spatially inhomogeneous nonlinearities: Theory and applications to Bose–Einstein condensates

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ABSTRACT

We study the properties of the ground state of nonlinear Schrödinger equations with spatially inhomogeneous interactions and show that it experiences a strong localization on the spatial region where the interactions vanish. At the same time, tunneling to regions with positive values of the interactions is strongly suppressed by the nonlinear interactions and as the number of particles is increased it saturates in the region of finite interaction values. The chemical potential has a cutoff value in these systems and thus takes values on a finite interval. The applicability of the phenomenon to Bose–Einstein condensates is discussed in detail.

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1. Introduction

The experimental generation of Bose–Einstein condensates (BEC) with ultracold dilute atomic vapors [1] has turned out to be of exceptional importance for physics. The formation of a condensate occurs when the temperature is low enough and most of the atoms occupy the ground state of the system. This process is visible both in momentum and in real space due to the spatial inhomogeneities exhibited by the order parameter on a macroscopic scale because of the trapping potentials.

The properties of the ground state of trapped BECs are well known. In the mean field limit simple analytical expressions are available in the Thomas–Fermi approximation [2] and beyond [3,4]. These approximations and direct numerical simulations describe accurately the properties of the experimentally found ground states [5,6].

Nonlinear interactions between atoms in a Bose–Einstein condensate are dominated by the two-body collisions that can be controlled by the so-called Feschbach resonance (FR) management [7]. The control in time of the scattering length has been used to generate bright solitons [8–10] and induce collapse [11] and has been the basis for theoretical proposals to obtain different types of nonlinear waves [12–18]. Moreover, interactions can be made spatially dependent by acting on either the spatial dependence of the magnetic field or the laser intensity (in the case of optical control of FRs [19]) which acts on the Feschbach resonances. This possibility has motivated many theoretical studies on the behavior of solitons in Bose–Einstein condensates (BECs) with spatially inhomogeneous interactions [20–36].

In this paper we describe a novel nonlinear phenomenon related to the ground state of a BEC in the mean field limit when the interactions are spatially inhomogeneous. We will show that when the scattering length is non-negative and vanishes on a certain spatial region, a striking localization phenomenon of the atom density occurs at the regions where the interactions vanish. By tuning appropriately the control (magnetic or optical) fields this phenomenon can be used to design regions with large particle densities and prescribed geometries. Another interesting phenomenon to be studied in this article is the nonlinear limitation of tunneling of atoms to the regions in which the interactions are stronger and the fact that the chemical potential exhibits a cutoff value.

Although it is reasonable to think that a BEC will avoid regions of large repulsive interactions and prefer to remain in regions with smaller interactions, the localization phenomenon to be described in this paper here goes beyond what one would naively expect.

Related phenomena have been described in the mathematical analysis of logistic equations [38] for vanishing g in bounded

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domains, see [39–41]. However to consider situations of real physical interest we must move to unbounded domains where the analysis goes beyond previous theoretical studies.

2. The problem and its mathematical modelling

2.1. Physical system to be studied

In this paper we will consider physical systems ruled by the nonlinear Schrödinger equation (NLS)

$$\mathrm{i}\frac{\partial\psi}{\partial t} = -\frac{1}{2}\Delta\psi + V(x)\psi + g(x)|\psi|^p\psi, \tag{1}$$

in $\mathbb{R}^d$, where $p > 1$ is a real parameter and g, $V \geq 0$ are continuous non-negative real functions. V describes an external localized potential acting on the system satisfying,

$$V(x) \to \infty, \quad \text{as } |x| \to \infty, \tag{2}$$

and g is a spatially dependent nonlinear coefficient. Stationary solutions of Eq. (1) are defined through

$$\psi(x,t) = \phi(x)\exp(\mathrm{i}\lambda t) \tag{3}$$

which leads to

$$\lambda\phi = -\frac{1}{2}\Delta\phi + V(x)\phi + g(x)|\phi|^p\phi. \tag{4}$$

Of all the possible solutions of Eq. (4) we will be interested on the so-called ground state, which is the the real, stationary positive solution of the Gross–Pitaevskii equation (4) which minimizes the energy functional

$$E(\phi) = \int_{\mathbb{R}^3}\left[\frac{1}{2}|\nabla\phi|^2 + V(x)|\phi|^2 + \frac{1}{2}g(x)|\phi|^{p+2}\right], \tag{5}$$

under the constraint of a fixed $\int_{\mathbb{R}^3}|\phi|^2\mathrm{d}x$.

For our purposes the only relevant property is the positivity. Thus we will consider positive solutions of

$$-\frac{1}{2}\Delta u + V(x)u = \lambda u - g(x)u^p, \qquad x \in \mathbb{R}^d \tag{6}$$

where V satisfies (2).

From the physical point of view Eq. (6) is a model of different physical systems. However, as stated in the introduction, in this paper we will focus mainly on its applicability to the description of the ground state of a trapped Bose–Einstein condensate with spatially inhomogeneous interactions in the mean field limit where physically it is both possible to control the interactions and achieve large values for the coefficient $g(x)$. Although Eq. (4) is written in non-dimensional units it is easy to connect this problem with the realistic quantum problem for three spatial dimensions (see e.g. [1]), considering that the coordinates x and time t are measured in units of $a_0 = \sqrt{\hbar/mw}$ and $1/w$, respectively, while the energies and frequencies are measured in units of $\hbar w$ and w respectively, w being a characteristic frequency of the potential. Finally, in three spatial dimensions $g(x) = 4\pi a_s(x)/a_0$ is proportional to the local value of the s-wave scattering length $a_s(x)$ and the parameter $p = 2$. Another relevant physical quantity, the number of particles, is directly related to the L^2-norm of the solution through

$$N = \|u\|_2^2 = \int_{\mathbb{R}^d} u^2\mathrm{d}x. \tag{7}$$

In this paper we will study properties of the positive solution of Eq. (6) (ground state) when the interactions g vanish on a certain set of points. Set $\omega := \{x \in \mathbb{R}^d : g(x) > 0\}$, let us denote by $\overline{\omega}$ the adherence of ω. Let us finally define $\Omega_0 := \mathbb{R}^d \setminus \overline{\omega}$, Ω_0, which represents the interior of the region where g vanishes, i.e.

$$\Omega_0 := \mathrm{int}\{x \in \mathbb{R}^d : g(x) = 0\}. \tag{8}$$

Through this paper we will assume that Ω_0 which essentially describes the region in which the interactions vanish, is composed by a finite number of connected components Ω_j, $1 \leq j \leq J$, which are disjoint $\overline{\Omega_i} \cap \overline{\Omega_j} = \emptyset$ if $i \neq j$ and it is assumed that each component Ω_j is regular enough.

The solution will blow up in every point of a certain subset of the vanishing set. This results will be precisely stated in Theorem 5.6.

2.2. The Thomas–Fermi limit

The Thomas–Fermi approximation is used extensively in the field of Bose–Einstein condensation to describe the solutions in the situation in which the nonlinear term is "large" and proceeds by neglecting the kinetic energy or equivalently the term proportional to $\Delta\phi$ in Eq. (4) which leads to

$$\phi_{TF}(x) \simeq \sqrt{\frac{\lambda - V(x)}{g(x)}}. \tag{9}$$

Thus, the TF approximation provides the profile of the stationary positive solution (i.e. the ground state). In the case of spatially homogeneous interactions $g(x) = g_0$ the so-called classical turning points for which $\lambda = V(x)$ delimit the regions in which the approximation breaks, since near those points the amplitude is small and thus the kinetic energy cannot be neglected anymore.

It is remarkable that, when the interactions are spatially inhomogeneous a new feature appears, which is that the amplitude of the Thomas–Fermi solution diverges on the set Ω_0. Although it is obvious, that in the vicinity of Ω_0 the Thomas–Fermi approximation is not correct, this divergence is the first indication of an interesting nonlinear phenomenon with relevant physical implications whose study is the purpose of this paper: *the tendency of positive solutions of* Eq. (6)*, or in physical terms the ground state of Bose–Einstein condensates with spatially inhomogeneous interactions, to localize strongly on the regions where the scattering length is close to zero provided the system is sufficiently nonlinear.*

3. Localization phenomena: A "toy" example

Let us first consider the exactly solvable one-dimensional "toy" model on the interval $x \in [-L, L]$, given by

$$\lambda u = -u'' + g(x)u^3, \tag{10a}$$

$$u(L) = u(-L) = 0, \tag{10b}$$

which can be understood as a version of Eq. (6) with a potential of the form

$$V(x) = \begin{cases} 0 & |x| < L, \\ \infty & |x| > L. \end{cases} \tag{11}$$

We will take the interactions as given by the equation

$$g(x) = \begin{cases} g_0 & |x| < a, \\ 0 & |x| > a. \end{cases} \tag{12}$$

This is a model for an ideal quasi-one-dimensional BEC in a box.

In this simple case, the positive, stationary solution, can be obtained analytically and is given by

$$u(x) = C\sin\left[\sqrt{2\lambda}\,(x - L)\right], \quad a < |x| < L, \tag{13a}$$

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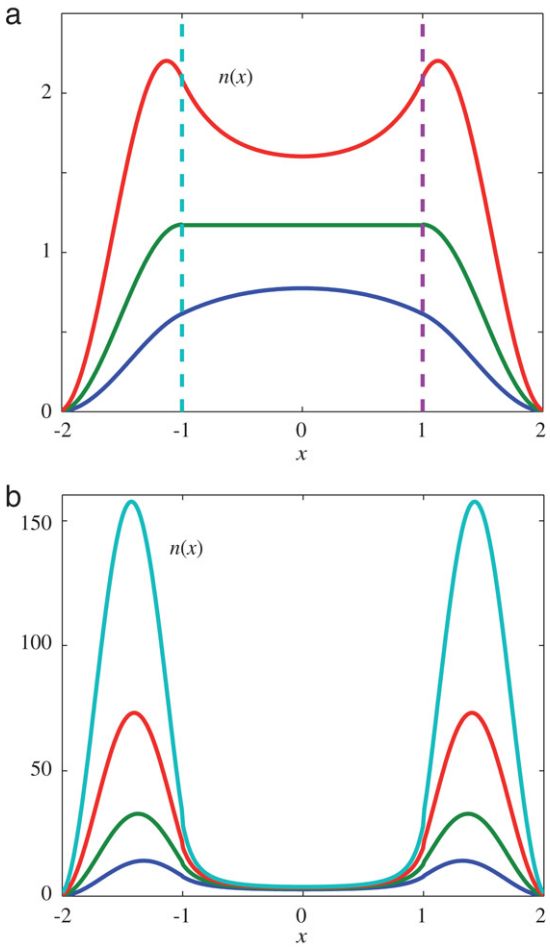

Fig. 1. [Color online] Spatial distribution of $n(x) = u^2(x)$ for the ground state solutions given by Eqs. (13a) and (13b) with $L = 2, a = 1$ and different values of λ corresponding to different values of N (a) From the lower to the upper curve $g_0N = 2, 3.55$ (corresponding to λ_*) and $g_0N = 6$. (b) From the lower to the upper curve $g_0N = 25, 50, 100, 200$.

while for $|x| < a$ the solutions are given by

$$u(x) = \begin{cases} \sqrt{\dfrac{\alpha\lambda}{g_0}}\ \mathrm{sn}\left(x\sqrt{\lambda\alpha} + \delta; k^2\right), & \lambda < \lambda_* \\ \pi / \left(2\sqrt{2g_0}|a - L|\right), & \lambda = \lambda_*, \\ \sqrt{\dfrac{\alpha\lambda}{g_0}}\ \mathrm{dc}\left(x\sqrt{\lambda\alpha}; k^2\right), & \lambda > \lambda_* \end{cases} \tag{13b}$$

where $\alpha(k) = 2/(1 + k^2)$, sn and dc are two of the standard Jacobi elliptic functions and k is the elliptic modulus. Both the elliptic modulus and amplitude C can be obtained from the matching conditions for $\phi(a)$ and $\phi'(a)$. These conditions also give $\lambda_* = \pi^2/\left[8(a - L)^2\right]$.

It is interesting to point out that there is a cutoff value for the eigenvalue, λ_c beyond which stationary solutions do not exist. Its explicit value can be obtained from the condition of maximum slope at $x = a$ which leads to $\lambda_c = \pi^2/[2(a - L)^2]$. In that limit the L^2-norm (number of particles in the condensate) diverges, since the amplitude in the outer region $C \to \infty$.

The spatial profiles of the ground state density for different values of g_0N shown in Fig. 1 support our conjecture based on the Thomas–Fermi solution, i.e. the existence of a strong localization of the solution in the region where the interactions vanish.

Physically it is also remarkable that the atom density in the inner part of the domain, i.e. the region where there are

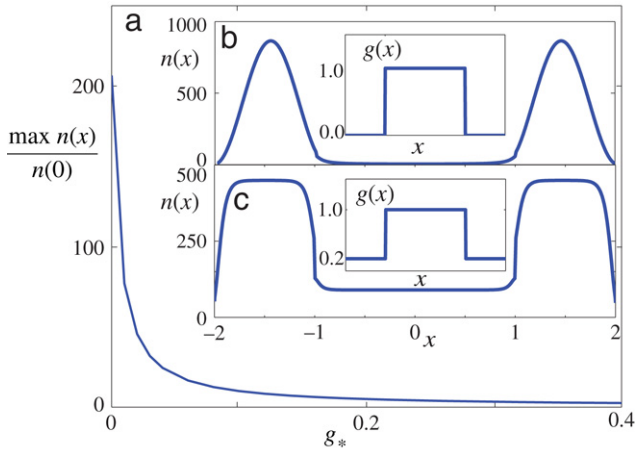

Fig. 2. [Color online] (a) Ratio between the maximum atom density and the atom density at $x = 0$ as a function of the scaled scattering length g_* on the spatial region $|x| > a$ (for $g_0 = 1$). (b and c) Scaled atom density profiles for (b) $g_* = 0$ and (c) $g_* = 0.2$ in both cases for a total scaled number of particles $N = 1000$. The insets show the profile of $g(x)$.

nonlinear interactions, remains almost constant independently of the number of particles in the condensate once a certain critical density is achieved. This region is a nonlinear analogue of the classically forbidden region in ordinary potentials and is energetically less favorable due to the extra repulsive energy provided by the nonlinear interactions. However, the tunneling of atoms in this region is essentially limited to a constant value, *independently of the number of atoms*, which differs essentially from ordinary tunneling.

The suppression of tunneling strongly depends on the value of the scattering length in the outer region, that we will take to be nonzero in what follows. If instead we set $g(x) = g_*$ when $|x| > a$ and study the dependence of the ratio between the maximum atom density and the atom density at $x = 0$ (which is a measure of the amplitude of the tunneling), we find a strong dependence on this parameter as is shown in Fig. 2(a).

This effect is also seen in the atom density profiles when comparing the cases with $g_* = 0$ [Fig. 2(b)] and $g_* = 0.2$ [Fig. 2(c)] for $N = 1000$. Larger values of N lead to a stronger effect.

Thus we have shown a simple example which already presents the main features of the nonlinear phenomena to be studied with more detail in this paper: the localization of the ground state in the regions where the interactions vanish, the suppression of tunneling induced by the presence of inhomogeneous interactions and the limited range of variation for the eigenvalue λ (chemical potential).

4. Numerical results

4.1. Introduction

In this section we will consider more realistic situations corresponding to problems posed on unbounded domains and strongly confining potentials satisfying condition (2). In the examples to be presented in this section we will use harmonic potentials $V(x) \propto x^2$ which arise naturally in the modelling of magnetic trapping potentials for ultracold atoms.

To study the localization phenomenon we have computed numerically the ground state solutions of equations of the form (1) using a standard steepest descent algorithm on the energy functional complemented with a projection over the set of solutions of given L^2-norm [42].

We will consider nonlinear coefficients $g(x)$ also of realistic forms which vanish or are very small on certain sets. In this section

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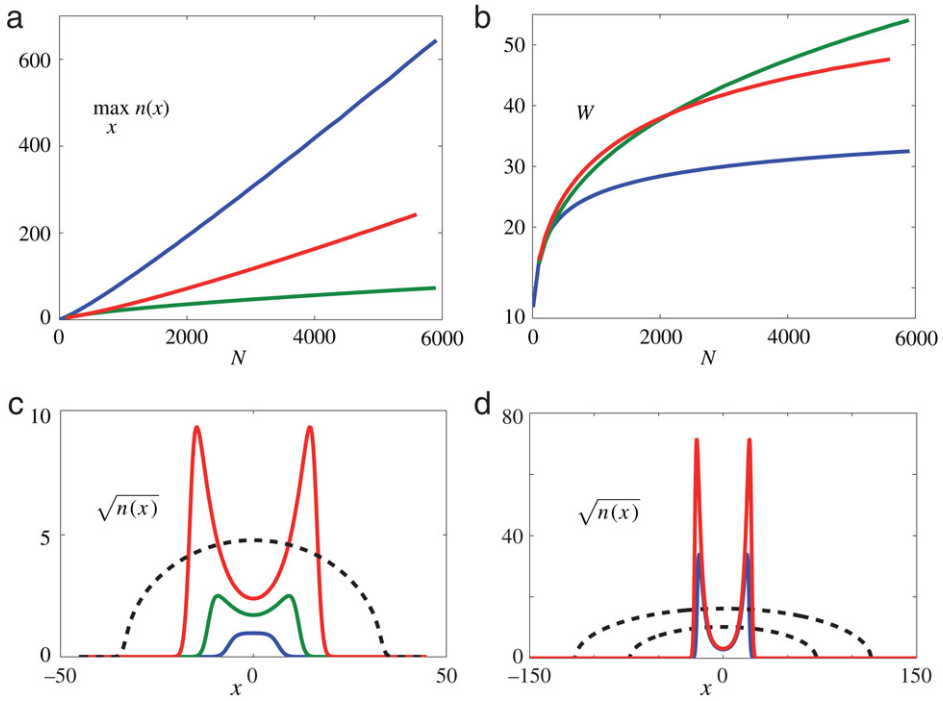

Fig. 3. [Color online] Ground states of Eq. (4) for $V(x) = 0.02x^2$ and $g_0(x) = 1$, $g_1(x) = \exp(-x^2/200)$, and $g_2(x) = \exp(-x^2/50)$, for different values of the scaled number of particles N. (a) Maximum particle density $\max_x n(x)$ and (b) width $W^2 = \int x^2 n(x)dx/N$ for g_0 (green), $g_1(x)$ (red) and $g_2(x)$ (blue). (c) Spatial profiles of $\sqrt{n(x)}$ for $N = 10$ (blue), $N = 100$ (green), $N = 1000$ (red) for $g(x) = g_1(x)$. The dashed black line is the ground state with homogeneous interactions and $N = 1000$. (d) Same as (c) but for $N = 10\,000$ (blue), and $N = 40\,000$ (green), in comparison with the case of spatially homogeneous interactions (dashed black lines).

we will use a more physical language thinking on the applications of our results to BEC systems.

4.2. One-dimensional systems

Let us consider Eq. (4) in one-dimensional scenarios ($d = 1$), and take the potential to be of the form $V(x) = 0.02x^2$. This corresponds to a typical BEC in a trap with a ratio $w_z/w_\perp = 0.14$ which is already in the quasi-one-dimensional regime and easy to obtain experimentally. Due to the possibilities for optical control of nonlinearities which are possible in BEC systems we will choose the nonlinear coefficient to be of the form

$$g_a(x) = \exp\left(-x^2/2a^2\right), \tag{14}$$

for different values of $a \leq +\infty$. These choices will allow us to study different degrees of localization of the interactions starting from the case of no localization.

Our results are summarized in Fig. 3. First, in Fig. 3(a) we observe how the maximum density ($n(x) = u^2(x)$) increases drastically for spatially decaying nonlinearities (blue and red curves) as a function of the effective number of particles in the quasi-one-dimensional condensate N. This amplitude growth is due to a strong localization effect near the region where $g(x)$ vanishes as is seen in Fig. 3(c, d). In contrast, the condensate density for spatially homogeneous interactions grows slowly according to the Thomas–Fermi prediction $\max n(x) \propto N^{2/3}$. When the number of particles is small, the size of the atomic cloud is smaller than the localization region of $g(x)$. For larger values of N the ground state extends beyond the localization region of $g(x)$ and the atom density becomes more and more localized near its edge. This effect is more clear for larger N and is accompanied by a saturation in the amplitude growth in the region where $g(x)$ is far from zero [Fig. 3(d)].

In the case of spatially homogeneous interactions the width grows according to the law $W \propto N^{1/3}$ [Fig. 3(b)]. When interactions are spatially dependent and due to the localization of the amplitude close to the zero of $g(x)$ the width growth saturates for large values of N to a value depending on the size of $g(x)$.

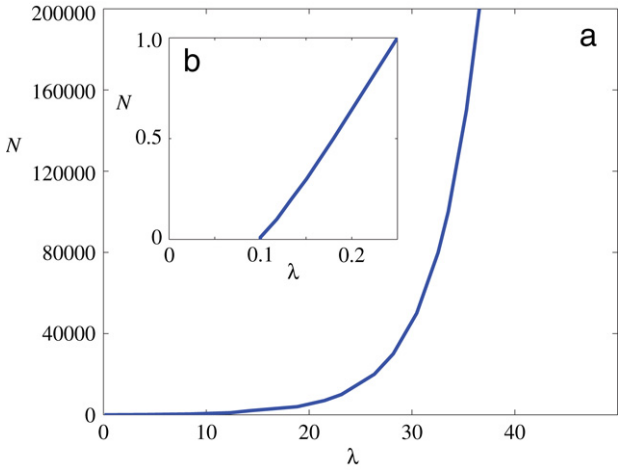

Fig. 4. [Color online] (a-b) Dependence of the number of particles in the ground state N on the eigenvalue (chemical potential) λ for $g(x) = \exp(-x^2/200)$, and $V(x) = 0.02x^2$. Subplot (b) shows the behavior in for small N where the eigenvalue approaches the linear limit.

It is interesting to point out that although the nonlinearity does not vanish strictly anywhere there is an effect similar to the existence of the cutoff discussed in the previous example, the number of particles increasing enormously for increasing values of λ, as is shown in Fig. 4

These effects are even more clear when the nonlinearity decays to zero faster and is exactly zero on a certain region. For instance, taking a nonlinear coefficient given by $g_4(x) = (1 - 0.001x^2)_+$ (i.e. an inverted parabola with maximum amplitude $g = 1$ at $x = 0$ and zero values for $|x| > 31.6$) as shown in Fig. 5, we see that the

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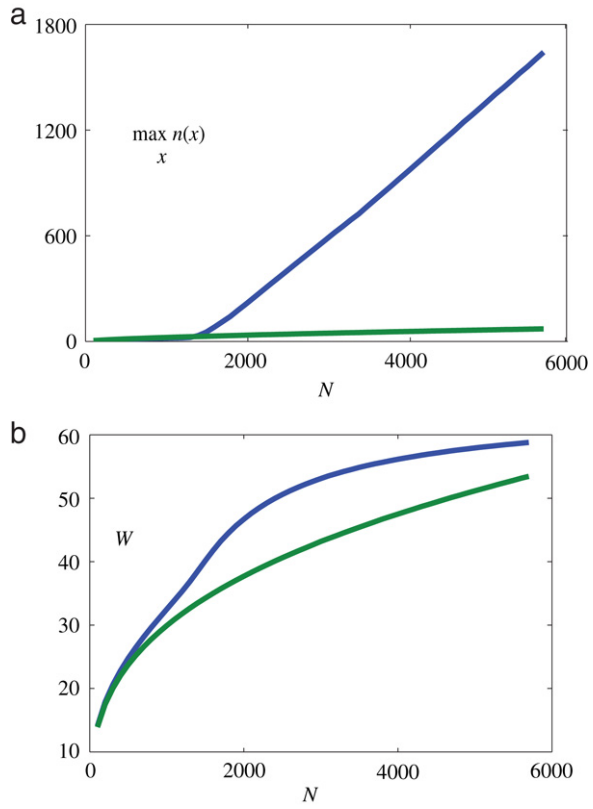

Fig. 5. [Color online] Ground state maximum particle density (a) and width $W = \int x^2 n(x)\mathrm{d}x/N$ (b) for $V(x) = 0.02x^2$ and $g_0(x) = 1$ (red lines) and $g_4(x) = (1 - 0.001x^2)_+$ (blue lines).

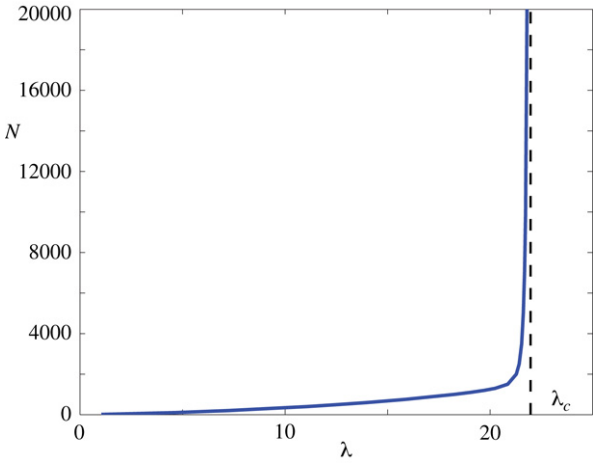

Fig. 6. [Color online] Dependence of the number of particles in the ground state N on the eigenvalue (chemical potential) λ for $g_4(x) = (1 - 0.001x^2)_+$, and $V(x) = 0.02x^2$.

maximum densities are even higher than those for $g_1(x), g_2(x)$. In this case, in comparison with our first simple example, we can see an even stronger localization since the existence of the potential makes energetically more favorable the localization close to the point where the interactions vanish.

In this case we also observe the existence of a cutoff in the values of the eigenvalue λ (chemical potential) close to a certain value λ_c. An example is shown in Fig. 6.

As a final example, in Fig. 7 we show again the localization phenomenon but now near $x = 0$ for localized interactions given by $g(x) = 1 - \exp(-x^2/50)$ and $V(x) = 0.02x^2$. In this case

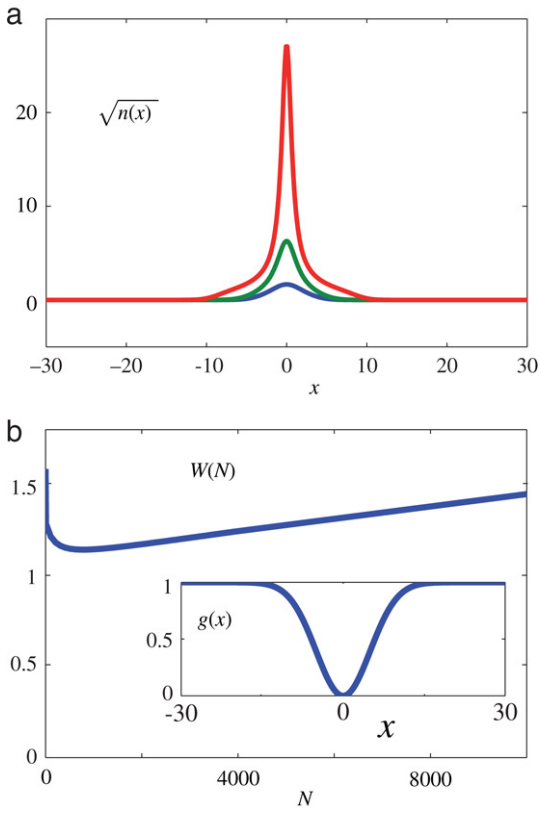

Fig. 7. [Color online] Ground states for $V(x) = 0.02x^2$ and $g(x) = 1 - \exp(-x^2/50)$ (shown in panel (c)). (a) $\sqrt{n(x)}$ for $N = 10$ (blue line), $N = 100$ (green line) and $N = 1000$ (red line). (b) Condensate width as a function of N.

interactions vanish in a single point $x = 0$ being very small in its vicinity. It is interesting to see how localized the density becomes to "avoid" penetrating into the regions with appreciable values of the scattering length.

The product of gN considered in this section are all realistic. Typically in quasi-one-dimensional scenarios $g_{1D}N = 2a_sN/a_0$ [37]. Typical transverse trap sizes are of the order of a micron and scattering lengths range from a few to a hundred nanometers for different atomic species. Since typical atom numbers are between 10^5 and 10^6 atoms we get that the product $g_{1D}N$ can range from very small values corresponding to low atom numbers to up to $g_{1D}N \simeq 10^5$ in the most favorable cases. All of our numbers lie in this experimentally accessible region of parameters.

4.3. A three-dimensional example

The same localization phenomenon is also present in three-dimensional geometries.

As a simple example we will take a set of parameters of applicability to BECs describing a ^{87}Rb condensate where the nonlinear interactions gN are typically in the range 10^3–10^5 for typical numbers of atoms and trap sizes. As to the potential and nonlinearity we will take them to be of the form

$$V(x, y, z) = \frac{1}{2}\left(x^2 + y^2 + z^2\right), \tag{15a}$$

$$g(x, y, z) = g_0\left[1 - \exp\left(-\frac{x^2 + y^2 + z^2}{2w^2}\right)\right], \tag{15b}$$

with $w = 0.5$ (i.e. half the trap width). Our results are summarized in Fig. 8 where again the same localization phenomenon, here inside the "hole" of the nonlinear coefficient, is seen. For larger number of atoms the localization phenomenon can be even enhanced as in the previous one-dimensional examples.

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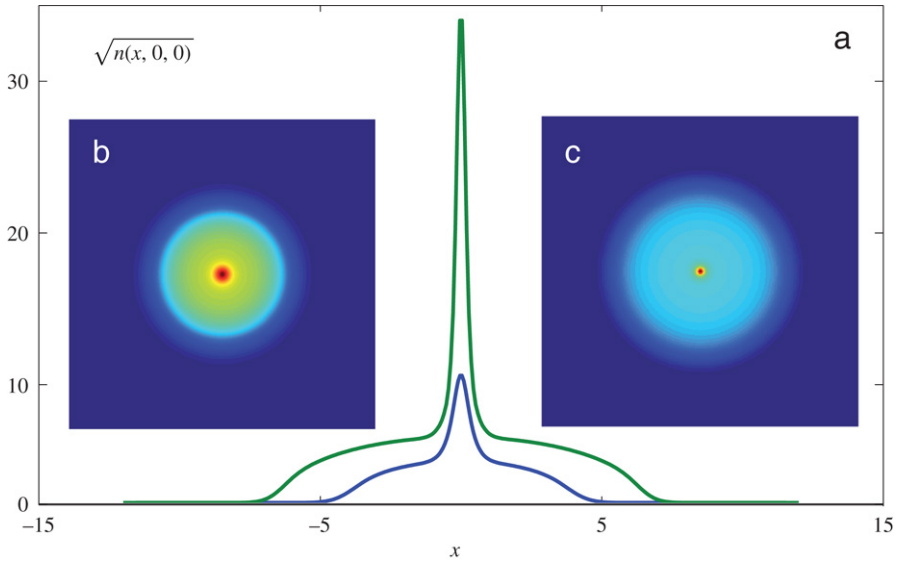

Fig. 8. [Color online] (a) Comparison of the profile of $\sqrt{n(x,0,0)}$ for $g_0N = 10^3$ (blue line) and $g_0N = 10^4$ (red line) showing the localization of the atom density. (b, c) Pseudocolor plot of $\sqrt{n(x,y,0)}$ for (b) $g_0N = 10^3$ on the spatial region $(x,y) \in [-10,10] \times [-10,10]$ and (c) $g_0N = 10^4$ on the spatial region $(x,y) \in [-15,15] \times [-15,15]$.

5. Theory

5.1. Introduction

In Sections 3 and 4 we have presented an analytic simple example and several numerical simulations showing a striking localization of the solutions of Eq. (6) close to the zeros of the nonlinear coefficient $g(x)$. Here, we will provide a rigorous support for two of the observed phenomena: (i) the existence of a finite range of values of the chemical potential (i.e. the existence of a cutoff) and (ii) the divergence of the amplitude of the solution close to that point.

In this section we will use a more formal and precise language and provide some mathematically rigorous results which will support our results in general scenarios.

5.2. Preliminaries and notation

We shall fix the potential V satisfying hypothesis (2). Following [43], let $\Omega \subset \mathbb{R}^d$ be an open nonempty set, possibly unbounded, with boundary regular enough, let us denote

$$H(\Omega, V) := \left\{ u \in H_0^1(\Omega) : \int_\Omega V u^2 < +\infty \right\}, \tag{16}$$

$H(\Omega, V)$ is the completion of $C_0^\infty(\Omega)$ in the metric derived from the norm

$$\|u\| := \left(\int_\Omega |\nabla u|^2 + V u^2 \right)^{1/2}, \tag{17}$$

and $H(\Omega, V)$ is a Hilbert space with the scalar product

$$\langle u, v \rangle := \int_\Omega \nabla u \nabla v + V uv. \tag{18}$$

Let us consider the operator L defined by

$$Lu := -\Delta u + V u, \quad \text{for } u \in D(L, \Omega) \tag{19}$$

where

$$D(L, \Omega) := \{ u \in H(\Omega, V) : -\Delta u + Vu \in L^2(\Omega) \}. \tag{20}$$

Let us first write the following lemma.

Lemma 5.1. *Let $\Omega \subset \mathbb{R}^d$ be an open nonempty set, possibly unbounded, with boundary regular enough. If V satisfies hypothesis (2), then the following assertions are true.*

(i) *$H(\Omega, V) \hookrightarrow L^2(\Omega)$ with compact embedding.*
(ii) *The operator L defined by Eq. (19), has a discrete spectrum, denoted by $\sigma(L, \Omega)$, i.e. $\sigma(L, \Omega)$ consists of an infinite sequence of isolated eigenvalues $\{\sigma_n(\Omega)\} \uparrow \infty$ with finite multiplicities.*
(iii) *Moreover, the Rayleigh sup-inf characterization for the eigenvalues holds, and in particular the first eigenvalue, denoted by $\sigma_1(\Omega)$, satisfies*

$$\sigma_1(\Omega) = \inf_{\psi \in H(\Omega, V)} \frac{\int_\Omega |\nabla \psi|^2 + V \psi^2}{\int_\Omega \psi^2}. \tag{21}$$

(iv) *The first eigenvalue is positive, simple with a positive eigenfunction, $\phi_1(\Omega) > 0$, and there is no other eigenvalue with a positive eigenfunction.*

This lemma consists of known results. For $d = 1, 2$ they are well known. In higher dimensions, parts (i)–(iii) are contained in [43] for $d > 2$, more precisely, see [43, Theorem 1.2] and the beginning of its proof for parts (i) and (ii) respectively, see [43, Lemma 2.1] for part (iii). With respect to part (iv), it is also well known that the elliptic operator L as defined in (19) admits a unique principal eigenvalue in Ω. This principal eigenvalue is the bottom of the spectrum of L in the functional space $H(\Omega, V)$, and it admits an associated positive principal eigenfunction, denoted by $\phi_1 > 0$. This result follows from the Krein–Rutman theory and from compactness arguments (cf. [44,45]).

In general, the domain of the operator, the eigenvalues and the eigenfunctions depend not only on the domain Ω but also on the potential V i.e. $D(L, \Omega) = D(L, \Omega, V)$, $\sigma_n(\Omega) = \sigma_n(\Omega, V)$, $\phi_n(\Omega) = \phi_n(\Omega, V)$ and so on. We will consider a fixed V and in what follows we will skip the dependence on V to clarify the notation, except for the ambiguous cases.

The following lemma is the Lax–Milgram lemma, see [46, Lemma V.8]. Let $[H(\Omega, V)]^*$ denote the dual space of all linear and continuous functionals defined on $H(\Omega, V)$,

Lemma 5.2. *For any $f \in [H(\Omega, V)]^*$ there exists a unique $u \in H(\Omega, V)$ such that*

$$\int_\Omega \nabla u \nabla \psi + Vu\psi = \int_\Omega f\psi, \ \forall \psi \in H(\Omega, V). \tag{22}$$

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Remark 5.3. The above lemma can be understood in the following way, the inverse operator $L^{-1} : [H(\Omega, V)]^* \to H(\Omega, V)$ is well defined. Thanks to the compact embedding in Lemma 5.1(i), we can consider the inverse operator L^{-1} restricted to $L^2(\Omega)$ as a compact operator from $L^2(\Omega)$ into itself.

Next, we will compare the eigenvalues defined on Ω with the eigenvalues defined in the whole $\mathbb{R}^d$. We will denote by $H, D(L), \sigma_n, \phi_n, \ldots$ the space, the domain of the operator, the eigenvalues and the eigenfunctions and so on whenever the operator L is defined on the whole $\mathbb{R}^d$. More precisely, let us define the Hilbert space

$$H := \left\{ u \in H^1(\mathbb{R}^d) : \int_{\mathbb{R}^d} V u^2 < +\infty \right\}, \tag{23}$$

and consider the operator L defined by

$$Lu := -\Delta u + V u, \quad \text{for } u \in D(L) \tag{24}$$

where now

$$D(L) := \left\{ u \in H : -\Delta u + Vu \in L^2(\mathbb{R}^d) \right\}. \tag{25}$$

Observe that the above Lemmas 5.1 and 5.2 still hold, in particular $H \hookrightarrow L^2(\mathbb{R}^d)$, with compact embedding whenever $d > 2$ and V satisfies hypothesis (2). The elliptic operator L as defined in (24) admits a unique principal eigenvalue in $\mathbb{R}^d$ denoted by σ_1. This principal eigenvalue is the bottom of the spectrum of L in the function space H, and it admits an associated positive principal eigenfunction.

In the following lemma we collect the monotonicity properties of the eigenvalues with respect to the domain, see [43, Theorem 2.3] for a proof. As a consequence, we can compare the eigenvalues defined on $\Omega \subsetneq \mathbb{R}^d$ with the eigenvalues defined in the whole $\mathbb{R}^d$.

Lemma 5.4. *Let $\sigma_1(\Omega) \le \sigma_2(\Omega) \le \cdots$ be the eigenvalues of L, with corresponding eigenfunctions $\phi_1(\Omega)$, $\phi_2(\Omega) \cdots$ defined on $H(\Omega)$. For a subdomain $\Omega^* \subset \Omega$ with boundary regular enough, let $\sigma_1(\Omega^*) \le \sigma_2(\Omega^*) \le \cdots$ be the eigenvalues of L, with corresponding eigenfunctions $\phi_1(\Omega^*)$, $\phi_2(\Omega^*) \cdots$ defined on $H(\Omega^*)$, then*

$$\sigma_n(\Omega^*) > \sigma_n(\Omega). \tag{26}$$

In particular, let $\sigma_1 \le \sigma_2 \le \cdots$ be the eigenvalues of L, with corresponding eigenvectors ϕ_n defined on H, then

$$\sigma_n(\Omega) > \sigma_n. \tag{27}$$

The following lemma states the maximum principle for unbounded domains, see [46, Theorem IX.27].

Lemma 5.5 (*The Maximum Principle for the Dirichlet problem*). *Let $\Omega \subset \mathbb{R}^d$ be an open nonempty set, possibly unbounded, with boundary of class C^1, and assume V satisfies hypothesis (2). Let $f \in L^2(\Omega)$ and $u \in H(\Omega, V)$ be such that (22) holds.*

Then

$$\min\{\inf_{\partial\Omega} u, \inf_{\Omega} f\} \le u \le \max\{\sup_{\partial\Omega} u, \sup_{\Omega} f\} \tag{28}$$

where sup = sup *ess and* inf = inf *ess. In particular, if*

$$u \ge 0 \quad \text{on } \partial\Omega, \quad \text{and} \quad f \ge 0 \quad \text{in } \Omega, \tag{29}$$

then

$$u \ge 0 \quad \text{in } \Omega, \text{ and} \tag{30a}$$

$$\|u\|_{L^\infty(\Omega)} \le \max\{\|u\|_{L^\infty(\partial\Omega)}, \|f\|_{L^\infty(\Omega)}\}. \tag{30b}$$

5.3. Main result

We now consider Eq. (6) as a bifurcation problem. Considering λ as a real parameter, we look for pairs $(\lambda, u_\lambda) \in \mathbb{R} \times H$ such that u_λ is a positive solution of (6).

As in Section 5.2, set $L := -\frac{1}{2}\Delta + V$, let σ_1 stand for the first eigenvalue of the eigenvalue problem

$$\left(-\frac{1}{2}\Delta + V(x)\right)\phi_1 := \sigma_1\phi_1, \quad x \in \mathbb{R}^d, \quad \phi_1 \in D(L), \tag{31}$$

and given an open regular enough domain $\Omega \subset \mathbb{R}^d$, let $\sigma_1(\Omega)$ stand for the first eigenvalue of the Dirichlet eigenvalue problem

$$\left(-\frac{1}{2}\Delta + V(x)\right)\phi_1 := \sigma_1\phi_1, \quad x \in \Omega, \quad \phi_1 \in D(L, \Omega), \tag{32}$$

where the first eigenfunction $\phi_1 = \phi_1(\Omega) > 0$.

Let Ω_0 be the interior of the set where g vanishes, defined by Eq. (8). We assume that Ω_0 is composed by a finite union of connected sets

$$\Omega_0 = \bigcup_{1 \le j \le J} \Omega_j, \quad \overline{\Omega_i} \cap \overline{\Omega_j} = \emptyset, \ i \ne j.$$

It is also assumed that each component Ω_j is regular enough and possibly some Ω_j unbounded.

Set σ_0 the minimum

$$\sigma_0 := \min\{\sigma_1(\Omega_i) : 1 \le j \le J\}, \tag{33}$$

thanks to the union being finite, the minimum σ_0 is attained, i.e. $\sigma_0 := \sigma_1(\Omega_j)$ for some Ω_j.

We next prove that the positive solutions diverge pointwise for each x in Ω_j. What we conclude in Theorem 5.6 is that if u_λ is a positive solution of Eq. (6), then

$$u_\lambda(x) \uparrow \infty \quad \text{as } \lambda \uparrow \sigma_0 \text{ for all } x \in \Omega_j.$$

Moreover, if $\sigma_0 = \sigma_1(\Omega_j) = \sigma_1(\Omega_i)$ with $i \ne j$ then the positive solution diverges pointwise for each $x \in \Omega_j \cup \Omega_i$. See [39] for an analogous result on bounded domains.

Theorem 5.6. *Problem (6) has a unique positive solution (λ, u_λ) if and only if*

$$\sigma_1 < \lambda < \sigma_0. \tag{34}$$

Moreover

$$\|u_\lambda\|_{L^\infty(\mathbb{R}^d)} \to 0, \quad \text{as } \lambda \downarrow \sigma_1, \tag{35a}$$

$$u_\lambda(x) \uparrow \infty, \quad \text{as } \lambda \uparrow \sigma_0, \forall x \in \Omega_j, \tag{35b}$$

Ω_j is the connected set where the minimum σ_0 is attained, i.e. $\sigma_0 = \sigma_1(\Omega_j)$. Moreover, if $\sigma_0 = \sigma_1(\Omega_j) = \sigma_1(\Omega_i)$ with $i \ne j$ then

$$u_\lambda(x) \uparrow \infty, \quad \text{as } \lambda \uparrow \sigma_0, \ \forall x \in \Omega_j \cup \Omega_i. \tag{36}$$

In the proof of this theorem, we need a technical lemma. An analogous result for bounded domains can be seen in [39, theorem 2.4].

Lemma 5.7. *Assume there exists a sequence of positive functions $q_i \in L^\infty(\mathbb{R}^d)$ such that*

$$q_i = 0 \quad \text{in } \Omega_0 = \bigcup_{1 \le j \le J} \Omega_j \tag{37a}$$

$$\min_{x \in K} q_i(x) \uparrow \infty, \quad \forall \text{ compact } K \subset \mathbb{R}^d \setminus \Omega_0. \tag{37b}$$

Then

$$\sigma_1(\mathbb{R}^d, V + q_i) \uparrow \sigma_0.$$

Proof. (I) At this step, we assume that Ω_0 is connected. First, let us observe that, thanks to $q_i \in L^\infty(\mathbb{R}^d)$, for each i, $H(V + q_i) = H(V)$.

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From the monotonicity of the first eigenvalue with respect to the domain, see Lemma 5.1,

$$\sigma_i := \sigma_1(\mathbb{R}^d, V + q_i) \leq \sigma_1(\Omega_0, V + q_i) =: \sigma_0. \tag{38}$$

Fix any $\varepsilon > 0$ and choose

$$\Omega_0 \subset \Omega_0^{\varepsilon/2} \subset \Omega_0^{\varepsilon}$$

such that

$$\sigma_1(\Omega_0^{\varepsilon}) < \sigma_0 < \sigma_1(\Omega_0^{\varepsilon}) + \varepsilon.$$

Set $\phi_0^{\varepsilon} > 0$ the first eigenfunction associated with $\sigma_1(\Omega_0^{\varepsilon})$ and choose a function $\overline{u} \in D(L)$ such that $\overline{u} = \phi_0^{\varepsilon}$ in $\Omega_0^{\varepsilon/2}$ and $(-\frac{1}{2}\Delta + V)\overline{u} = \mathrm{e}^{-|x|^2}$ in $\mathbb{R}^d \setminus \Omega_0^{\varepsilon}$, $\overline{u} \geq 0$. Then

$$\left(-\frac{1}{2}\Delta + V + q_i\right)\overline{u} = (\sigma_0 - \varepsilon)\overline{u} + f_i, \quad x \in \mathbb{R}^d \tag{39}$$

where

$$f_i = \left[\sigma_1(\Omega_0^{\varepsilon}) - (\sigma_0 - \varepsilon)\right]\phi_0^{\varepsilon} + q_i\phi_0^{\varepsilon}, \quad \text{in } \Omega_0^{\varepsilon/2} \tag{40a}$$

$$f_i = \mathrm{e}^{-|x|^2} + [q_i - (\sigma_0 - \varepsilon)]\overline{u}, \quad \text{in } \mathbb{R}^d \setminus \Omega_0^{\varepsilon} \tag{40b}$$

then $f_i > 0$ in $\Omega_0^{\varepsilon/2}$ and $f_i > 0$ for any compact set $K \subset \mathbb{R}^d \setminus \Omega_0^{\varepsilon}$, by continuity $f_i \geq 0$ in $\mathbb{R}^d$.

Set $\phi_i \in H(V) > 0$ to be the first eigenfunction associated with σ_i, choosing ϕ_i as a test function in the weak definition of (39), see (22), we deduce

$$\sigma_i \int \phi_i\overline{u} = (\sigma_0 - \varepsilon)\int \phi_i\overline{u} + \int f_i\phi_i \tag{41}$$

and therefore $\sigma_i \geq \sigma_0 - \varepsilon$.

(II) If $\Omega_0 = \cup_{1\leq j\leq J}\Omega_j$ then we only have to realize that, arguing as before for each Ω_j, $\sigma_i \leq \min_j \sigma_1(\Omega_j, V + q_i) =: \sigma_0$. The reverse inequality is obtained in the same way, changing Ω_0 by the set Ω_j where the min is attained. □

Proof of Theorem 5.6. From the Crandall–Rabinowitz bifurcation theorem [47], $(\sigma_1, 0)$ is a bifurcation point in $\mathbb{R} \times H$ i.e. there is a continuum of positive solutions, $(\lambda, u_\lambda) \to (\sigma_1, 0)$ in particular $\|u_\lambda\|_H \to 0$ as $\lambda \to \sigma_1$. Now an standard bootstrap argument implies that (35a) is accomplished.

Let u_λ be a positive solution of Eq. (6). Differentiating Eq. (6) with respect to λ formally we have

$$\left(-\frac{1}{2}\Delta + V + pgu_\lambda^{p-1}\right)\frac{\mathrm{d}u}{\mathrm{d}\lambda} = \lambda\frac{\mathrm{d}u}{\mathrm{d}\lambda} + u_\lambda, \quad x \in \mathbb{R}^d. \tag{42}$$

The uniqueness of the positive eigenfunction, see Lemma 5.4(iv), allows us to consider λ as an eigenvalue of a problem with a nonlinear potential, i.e.

$$\lambda = \sigma_1(\mathbb{R}^d, V + gu_\lambda^{p-1}). \tag{43}$$

The Rayleigh sup-inf characterization of the eigenvalues (21) sets that the eigenvalues are monotone respect to the potential, then as $p > 1$ we have $\sigma_1(\mathbb{R}^d, V + pgu_\lambda^{p-1}) > \lambda$ and Eq. (42) has a solution. The Maximum Principle states that $\mathrm{d}u/\mathrm{d}\lambda > 0$, therefore the branch of solutions, while it exists, is increasing in λ, moreover there are no turning points and for each λ in the branch of solutions, there is only one solution, denoted by u_λ.

By the monotonicity of the eigenvalue respect to the domain, by (8) and (33), we have

$$\lambda < \min_{1\leq j\leq J} \sigma_1(\Omega_j, V + gu_\lambda^{p-1}) = \sigma_0, \tag{44a}$$

moreover, by monotonicity with respect to the potential

$$\lambda > \sigma_1(\mathbb{R}^d, V) =: \sigma_1, \tag{44b}$$

then (34) is a necessary condition.

Now fix λ satisfying (34), let ϕ_1 be the positive eigenfunction of (31) associated with the first eigenvalue σ_1, for $\varepsilon 0$ small enough, $\varepsilon\phi_1$ is a strictly positive subsolution of (6).

Choose a sequence q_i under the hypothesis of Lemma 5.7. Fix some i big enough so that $\sigma_i := \sigma_1(\mathbb{R}^d, V + q_i) \geq \sigma_0 - \varepsilon > \lambda$. Now set ϕ_i to be the positive eigenfunction associated to the eigenvalue σ_i, choose a constant C such that $g(C\phi_i)^{p-1} \geq q_i$, then $C\phi_i$ is a strictly positive supersolution of (6). Now the the fact that the subsolution is strictly less than the supersolution proves the existence of a solution.

Now, the Rabinowitz theorem [48,49] implies that the set of solutions (λ, u_λ) is a continuum unbounded in $\mathbb{R} \times H$, then $\|u_\lambda\|_H \to \infty$ for $\lambda \uparrow \sigma_0$. Assume Ω_0 is connected. Let ϕ_0 be the positive eigenfunction of (32) for $\Omega = \Omega_0$, ϕ_0 is associated with the first eigenvalue σ_0, choose $\varepsilon > 0$ small enough so that $u_\lambda > \varepsilon\phi_0$ in Ω_0. Set $z = \frac{\varepsilon}{\sigma_0 - \lambda}\phi_0$, then z is a subsolution of (42) and $z(x) \uparrow \infty$ as $\lambda \uparrow \sigma_0$, $\forall x \in \Omega_0$, as a consequence

$$\frac{\mathrm{d}u_\lambda}{\mathrm{d}\lambda}(x) \uparrow \infty, \quad \text{as } \lambda \uparrow \sigma_0, \ \forall x \in \Omega_0, \tag{45}$$

and the pointwise unboundedness (35b) is accomplished ending the proof. If Ω_0 is not connected, set $\sigma_0 = \sigma_1(\Omega_j) = \sigma_1(\Omega_i)$, where the min is attained, we only have to reason on Ω_j and on Ω_i, as we have done in Ω_0. □

6. Conclusions and discussion

We have studied the ground state of nonlinear Schrödinger equations with confining potentials and repulsive interactions vanishing on nonempty sets Ω_0 and shown that there is a nonlinear localization phenomenon of the solution on this set. We have presented analytical formulae and numerical simulations showing it and provided a theorem which rigorously explains some of the observed features.

The results have interesting implications to the physics of Bose–Einstein condensates with repulsive spatially varying interactions because in that situation the atom density will localize dramatically near the regions where the interactions are close to zero when the nonlinear interactions are relevant enough. This behavior does not depend on the spatial dimensionality and can be used to design very effectively one-, two- or three-dimensional spatial distributions with large values of the atom density by acting on the control field, e.g. using micromagnets to change locally the magnetic field or localized laser beams.

One interesting question concerns the direct experimental realization of our predictions in real BECs. To answer this question we must first consider the possibility that experimentally it is very difficult to achieve exactly zero values but small values close to zero (either positive or negative). The localization phenomenon is also present when the values of the interactions are small and positive although the singular behavior disappears (i.e. the existence of a cutoff, etc). As to the possibility of having negative values we would expect the same qualitative results although then a large value of gN would drive the condensate to blow up and thus we would observe the phenomenon for a limited range of gN values. However, having very small negative values of the interactions g would not essentially affect our results since then a huge number of atoms would be required to achieve the blow-up. Thus we expect the localization phenomenon described in this paper to be valid in systems where the interactions are tuned to a reasonable limit of precision to zero. Some related abstract

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theoretical results for this problem valid *for bounded domains* have been published in Ref. [50].

We would like to emphasize that the behavior described in this paper cannot be achieved with ordinary potentials since due to tunneling of the wavefunction in linear potentials it is not possible to achieve such a high degree of localization. However, the nonlinear interactions here are essential for limiting the tunneling to the regions with larger values of the scattering length which is independent of the number of particles.

Our results could be useful in different applications of Bose–Einstein condensates such as for atom lithography, atom beam guiding or other applications where a precise control of the positioning of large values of the density of an atomic cloud is required.

These phenomena may appear in multicomponent condensates that offer a much wider range of possibilities for their ground states depending on the types of components and their relative interactions [51]. It would be interesting to study the situation in which the variations of the scattering length make the components miscible or immiscible in different spatial regions and, what is the geometry of the resulting domains.

Finally, it is interesting that the phenomena reported here could also be observed in other systems ruled by nonlinear Schrödinger equations similar to Eq. (4), for instance in nonlinear optical systems. Although ordinary optical materials have small nonlinearities where these phenomena could not be easily observed except for unrealistically large laser intensities, there are media with a giant nonlinear response [52,53] as happens when a probe laser beam propagates in a medium with transparency induced electromagnetically by a second coupling field. Therefore, by managing the parameters it may be possible to find an optical version of the phenomena presented here.

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