Universal Critical Power for Nonlinear Schrödinger Equations with a Symmetric Double Well Potential

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(Received 3 August 2009; published 5 November 2009)

Here we consider stationary states for nonlinear Schrödinger equations in any spatial dimension n with symmetric double well potentials. These states may bifurcate as the strength of the nonlinear term increases and we observe two different pictures depending on the value of the nonlinearity power: a supercritical pitchfork bifurcation, and a subcritical pitchfork bifurcation with two asymmetric branches occurring as the result of saddle-node bifurcations. We show that in the semiclassical limit, or for a large barrier between the two wells, the first kind of bifurcation always occurs when the nonlinearity power is less than a critical value; in contrast, when the nonlinearity power is larger than such a critical value then we always observe the second scenario. The remarkable fact is that such a critical value is *a universal constant* in the sense that it does not depend on the shape of the double well potential and on the dimension n.

DOI: 10.1103/PhysRevLett.103.194101 PACS numbers: 05.45.−a, 02.30.Oz, 03.65.Xp, 03.75.Lm

The spontaneous symmetry breaking phenomenon is a rather important effect that arises in a wide range of physical systems modeled by nonlinear equations. In classical physics, spontaneous symmetry breaking occurs in optics, and it has been experimentally observed for laser beams in Kerr media and focusing nonlinearity [1,2]. Another natural setting in which spontaneous symmetry breaking phenomenon may arise is for Bose-Einstein condensates with an effective double well formed by the combined effect of a parabolic-like trap and a periodical-like optical lattice [3–5]. Also, the study of gases of pyramidal molecules, such as the ammonia NH_3, is a topic where spontaneous symmetry breaking phenomenon plays a crucial role. A nonlinear mean field model of a gas of pyramidal molecules has been introduced in [6,7]; in this model spontaneous symmetry breaking explaining the presence of two asymmetrical degenerate ground states, corresponding to the different localization of the molecules, has been predicted with the full agreement with experimental data [7,8].

The n-dimensional linear Schrödinger equation with a symmetric double well potential has stationary states of a definite even and odd parity. However, the introduction of a nonlinear term (which usually models, in quantum mechanics, an interacting many-particle system) may give rise to asymmetrical states related to a spontaneous symmetry breaking effect. The governing nonlinear Schrödinger equations

$$i\hbar\partial_t\psi = H_0\psi + \epsilon|\psi|^{2\mu}\psi \tag{1}$$

are of Gross-Pitaevskii type, where ϵ is the strength of the nonlinear term, $\mu > 0$ is the nonlinearity power, and H_0 is the linear Hamiltonian with a symmetric double well potential. The wave function ψ belongs to the Hilbert space $L^2(\mathbf{R}^n)$ with norm $\|\cdot\|$, under the normalization to the unit $\|\psi\| = 1$. When $\mu = 1$ we have a cubic nonlinearity and the resulting equation has been largely studied [9–14]. Recently, for higher values of μ the resulting equation has been the object of an increasing interest with several interesting physical applications [15].

For cubic nonlinearities a family of asymmetric stationary states bifurcates when the adimensional nonlinear parameter η, associated with the strength ϵ of the nonlinear perturbation by (9), assumes the value $\eta^\star$ given by (12). The nonlinear ground state branch consists of states having the same symmetry of the linear stationary state, and typically we observe also an exchange of the stability properties. The symmetric stationary state is stable for η less than the value $\eta^\star$, and for η larger than $\eta^\star$ the symmetric stationary state becomes unstable and the new asymmetrical states are stable: that is we have a supercritical pitchfork bifurcation as in Fig. 1 panel (a) where the variable z belonging to the interval $[-1, +1]$ represents the *imbalance function*. The imbalance function, defined in Eq. (10), is related to the position of mean value of the stationary state: when $z = 0$ the state in invariant (up to a phase term) with respect to the symmetry of the double well potential. In contrast, when z takes the end-point values $z = \pm 1$ then the state is localized on one well (conventionally the right-hand side one for $z = +1$).

However, we should remark that the picture of Fig. 1 panel (a) still holds true also for other values of the nonlinearity power, for instance for $\mu = 2$ and $\mu = 3$, but for higher values of this parameter we observe a rather different picture [14]. In Fig. 1 panel (b) we consider the case of nonlinearity power $\mu = 5$, in such a case a couple of new asymmetrical stationary states sharply appear as saddle-node bifurcations when η is equal to a given value $\eta^+ \approx 4.41$; then, for increasing values of η, the two unstable solutions disappear at $\eta = \eta^\star = 6.4$ showing a subcritical pitchfork bifurcation. Thus, for η between the two values $\eta^+ \approx 4.41$ and $\eta^\star = 6.4$ we observe the co-

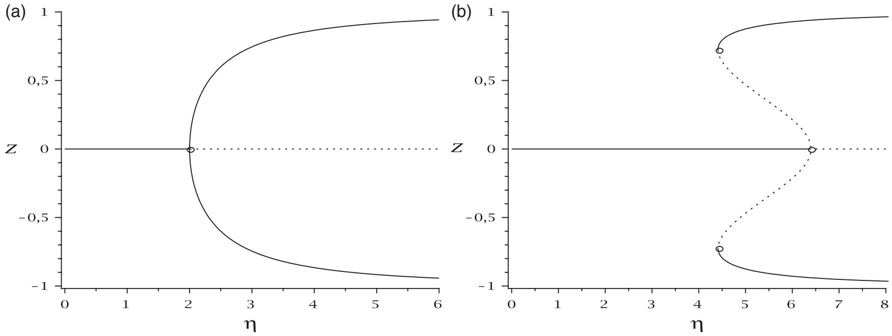

FIG. 1. In this figure we plot the graph of the stationary states around the minimum of the energy (full lines represent stable stationary states, broken lines represent unstable stationary states) as a function of the nonlinearity parameter η for cubic nonlinearity (i.e., for $\mu = 1$) in panel (a), and for higher nonlinearity power $\mu = 5$ in panel (b). The variable z represents the *imbalance function*.

existence of three stable stationary states: one of them corresponds to the symmetric stationary state which has the same symmetry properties of the potential, while the other two are localized on only one well.

In this Letter we investigate the bifurcation picture of the stable stationary states normalized to the L^2 unit of Eq. (1), for any positive value of the nonlinearity power μ, as a function of the parameter ϵ. In particular, in the semiclassical limit (or, equivalently, in the limit of large distance between the wells) we will see that the simple pitchfork bifurcation as in Fig. 1 panel (a) always occurs when the power μ is less than a critical value $\mu_{\text{threshold}}$, and the couple of saddle-node bifurcations with a subcritical pitchfork bifurcation as in Fig. 1 panel (b) always appears when the power μ is larger than $\mu_{\text{threshold}}$. The remarkable fact is that such a critical value $\mu_{\text{threshold}}$ is a *universal critical power*, in the sense that it does not depend on the shape of the double well potential and on the spatial dimension. Such a critical value is found to be equal to

$$\mu_{\text{threshold}} = (3 + \sqrt{13})/2. \qquad (2)$$

The linear Hamiltonian we consider,

$$H_0 = -\frac{\hbar^2}{2m}\Delta + V, \qquad (3)$$

has a symmetric double well potential $V(x) = V[\mathcal{S}(x)]$, where $\mathcal{S}(x)$ is the symmetric spatial inversion with respect to a given hyperplane Π of the space $\mathbf{R}^n$. The potential has two nondegenerate minima at $x = x_\pm$, $x_+ = \mathcal{S}(x_-)$, such that $V(x) > V(x_\pm)$, $\forall\ x \in \mathbf{R}^n \setminus \{x_\pm\}$, and $\nabla V(x_\pm) = 0$ and Hess $V(x_\pm) > 0$. If we consider the semiclassical limit of $\hbar$ small enough [14,16], or equivalently the limit of large distance between the two wells [11,17], then it is well known that the discrete spectrum of H_0 is given by a sequence of doublets. Let $\lambda_\pm$ be a doublet of nondegenerate eigenvalues ($\lambda_+ < \lambda_-$), for instance the lowest two eigenvalues of H_0, then

$$\inf_{\lambda\in\sigma(H_0)\setminus\{\lambda_\pm\}}[\lambda - \lambda_\pm] \geq C\hbar,$$

for some positive constant $C > 0$ independent of $\hbar$; $\sigma(H_0)$ is the spectrum of H_0. The *splitting* between the two eigenvalues $\omega = \frac{1}{2}(\lambda_- - \lambda_+)$ exponentially vanishes as $\hbar$ goes to zero [18]. The normalized eigenvectors $\varphi_\pm$ associated to $\lambda_\pm$ are even and odd real-valued functions with respect to the hyperplane Π: $\varphi_\pm[\mathcal{S}(x)] = \pm\varphi_\pm(x)$. The normalized right- and left-hand side vectors

$$\varphi_R = (\varphi_+ + \varphi_-)/\sqrt{2} \quad \text{and} \quad \varphi_L = (\varphi_+ - \varphi_-)/\sqrt{2},$$

usually named *single-well states*, are localized on only one well and their supports practically do not overlap in the sense that

$$\max_{x\in\mathbf{R}^n}|\varphi_R(x)\varphi_L(x)| = \mathcal{O}(e^{-C/\hbar}), \quad \text{as} \quad \hbar \to 0, \qquad (4)$$

for some positive constant C.

The time dynamics associated to the linear Hamiltonian (3) is well studied [19]: when the state ψ is initially prepared on the space spanned by the two vectors $\varphi_{R,L}$, then it performs a beating motion between the two wells with beating period $T = 2\pi\hbar/\omega$. Since the beating period T plays the role of the unit of time then we rescale the time $\tau = \omega t/\hbar$; furthermore, we also consider the gauge choice $\psi(x,t) \to e^{i\Omega t/\hbar}\psi(x,t)$, where $\Omega = (\lambda_+ + \lambda_-)/2$. Then Eq. (1) takes the form

$$i\omega\partial_\tau\psi = [H_0 - \Omega]\psi + \epsilon|\psi|^{2\mu}\psi \qquad (5)$$

where we apply the two-level approximation by restricting the wave function ψ to the space spanned by the two single-well states $\varphi_{R,L}$:

$$\psi = a_R\varphi_R + a_L\varphi_L, \qquad (6)$$

where a_R and a_L are unknown complex-valued functions depending on the time τ. In such an approximation we have neglected the contributions to the wave function ψ from the continuous spectrum and from the other discrete linear eigenstates; even if this approximation can be rigorously justified under some assumptions [11,14], here we do not dwell on these details. Since

$$H_0\psi = a_R[\Omega\varphi_R - \omega\varphi_L] + a_L[-\omega\varphi_R + \Omega\varphi_L]$$

then, by substituting (6) in (5) and projecting the resulting equation onto the one-dimensional spaces spanned by the single-well states φ_R and φ_L, it takes the form (hereafter $'$ denotes the derivative with respect to τ)

$$\begin{aligned} i\omega a_R' &= -\omega a_L + \epsilon\langle\varphi_R, |\psi|^{2\mu}\psi\rangle \\ i\omega a_L' &= -\omega a_R + \epsilon\langle\varphi_L, |\psi|^{2\mu}\psi\rangle \end{aligned} \qquad (7)$$

where $\langle\cdot,\cdot\rangle$ denotes the scalar product in the Hilbert space

$L^2(\mathbf{R}^n)$. From (4) and since $\varphi_R[\mathcal{S}(x)] = \varphi_L(x)$, then a straightforward calculation led us to the following results in the semiclassical limit:

$$\langle \varphi_R, |\psi|^{2\mu}\psi\rangle = c|a_R|^{2\mu}a_R + \mathcal{O}(e^{-C_R/\hbar})$$
$$\langle \varphi_L, |\psi|^{2\mu}\psi\rangle = c|a_L|^{2\mu}a_L + \mathcal{O}(e^{-C_L/\hbar})$$

for some positive constants C_R and C_L, and where the constant c is the same in both equations and it is given by

$$c = \langle \varphi_R, |\varphi_R|^{2\mu}\varphi_R\rangle = \langle \varphi_L, |\varphi_L|^{2\mu}\varphi_L\rangle.$$

Thus, the two-level approximation (7) takes the following form up to an exponentially small error as $\hbar$ goes to zero

$$ia_R' = -a_L + \eta|a_R|^{2\mu}a_R \qquad ia_L' = -a_R + \eta|a_L|^{2\mu}a_L \tag{8}$$

where

$$\eta = c\epsilon/\omega \tag{9}$$

is an adimensional parameter which only depends on the strength ϵ of the nonlinear term and, by means of the constant c and of the splitting ω, on the shape of the double well potential. We perform now the qualitative analysis of the two-level approximation (8) by looking for the stationary states and studying their dynamical stability/instability properties. To this end we assume, for the sake of definiteness, $\eta > 0$ and let

$$a_R = pe^{i\alpha}, \quad a_L = qe^{i\beta}, \quad z = p^2 - q^2, \quad \theta = \alpha - \beta \tag{10}$$

where p and q are such that $p^2 + q^2 = \|\psi\|^2 = 1$. The case of $\eta < 0$ is similarly treated; we may remark that in such a case Eq. (1) is of focusing type and blowup and instabilities could occur, actually in the semiclassical limit Eq. (1) is proved to be globally well posed for any η [14]. The imbalance function z takes value within the interval $[-1, 1]$, the phase θ is a torus variable with values in the interval $[0, 2\pi)$. Then, (8) takes the Hamiltonian form

$$\theta' = \partial_z\mathcal{H}, \qquad z' = -\partial_\theta\mathcal{H} \tag{11}$$

with Hamiltonian

$$\mathcal{H} = 2\sqrt{1-z^2}\cos\theta - \eta\frac{(1+z)^{\mu+1} + (1-z)^{\mu+1}}{2^\mu(\mu+1)}.$$

Equation (11) always has, respectively, symmetrical and antisymmetrical stationary solutions (θ_1, z_1) and (θ_2, z_2), where $\theta_1 = 0$ and $\theta_2 = \pi$ and where $z_1 = z_2 = 0$. Furthermore, asymmetrical stationary solutions may, respectively, occur for $\theta = 0$ and $\theta = \pi$ as solutions of equations $f_+(z) = 0$ and $f_-(z) = 0$, where

$$f_\pm(z) = \mp 2z/\sqrt{1-z^2} - \eta[(1+z)^\mu - (1-z)^\mu]2^{-\mu}.$$

Since we have assumed $\eta > 0$ then the derivative $\frac{df_+}{dz}$ takes only negative values for any $z \in [-1, +1]$ and thus $f_+(z) = 0$ has only the solution $z = 0$. On the other hand, equation $f_-(z) = 0$ might have other solutions coming from a pitchfork bifurcation of the stationary solution $z = 0$ as we can see in Fig. 1 panel (a) for η larger than the value

$$\eta^\star = \lim_{z\to 0}\eta(z) = 2^\mu/\mu \tag{12}$$

where $\eta(z)$ is obtained by solving equation $f_-(z) = 0$ with respect to η:

$$\eta(z) = 2^{\mu+1}z/\{\sqrt{1-z^2}[(1+z)^\mu - (1-z)^\mu]\}.$$

In particular, in Fig. 1 panel (b) we observe that in the case of $\mu = 5$ a couple of saddle-node bifurcations appears when $\eta \in (\eta^+, \eta^\star)$, where η^+ is a new critical value, and the unstable stationary solutions will merge with the antisymmetrical solution corresponding to $z = 0$ at $\eta = \eta^*$. We then observe a double saddle-node bifurcation and a subcritical pitchfork bifurcation. The couple of saddle-node bifurcations appears at η^+ where $\eta^+ = \eta(z^+)$ and z^+ is a zero of the derivative of $\eta(z)$; by means of a straightforward calculation it follows that z^+ actually is a nonzero real-valued solution within the interval $(0, +1)$ of the equation $g(z, \mu) = g(-z, \mu)$ where

$$g(z, \mu) = (z^2\mu - z\mu + 1)(1+z)^\mu.$$

For instance, we have that $\eta^+ = \sqrt{27/2} \approx 3.67$, for $\mu = 4$, and $\eta^+ \approx 4.41$ for $\mu = 5$.

We thus have a transition from the bifurcation picture as in panel (a) of Fig. 1 to the more complex bifurcation picture as in panel (b) of Fig. 1, and this transition occurs when the nonlinearity power μ is equal to a threshold value $\mu_{\text{threshold}}$ such that $\frac{d^2\eta(z)}{dz^2} = 0$ at $z = 0$, that is the two saddle nodes will merge with the stationary solution $z = 0$. Since

$$\left.\frac{d^2\eta(z)}{dz^2}\right|_{z=0} = \frac{2^\mu(3\mu + 1 - \mu^2)}{9\mu}$$

then the threshold value is given by (2). We may remark that this threshold in a *universal* value since it does not depend on the parameters of the double well model and on the spatial dimension.

The qualitative behavior of the solutions of Eq. (11) is then studied by means of the conservation of the energy $\mathcal{H}$ as done, for instance, by [6,13] for cubic nonlinearity (where $\mu = 1$). In Fig. 2 we plot the integral paths of the equation $\mathcal{H} = E$ for some values of the energy E, where $\mu = 5$. In panel (a) where $\eta = 2 < \eta^+ \approx 4.41$ we can only see closed curves corresponding to beating periodic motions between the two wells. In panel (b), where $\eta^+ \approx 4.41 < \eta = 5 < \eta^\star = 6.4$, we have three stable stationary solutions (circle points), two of them are localized on just one well and closed curves surrounding them correspond to periodic motions inside the well, without the beating effect. In panel (c), where $\eta^\star = 6.4 < \eta = 6.5$; we have two stable stationary solutions (circle points) localized on just one well and we do not observe a beating motion around the stationary solution at $z = 0$.

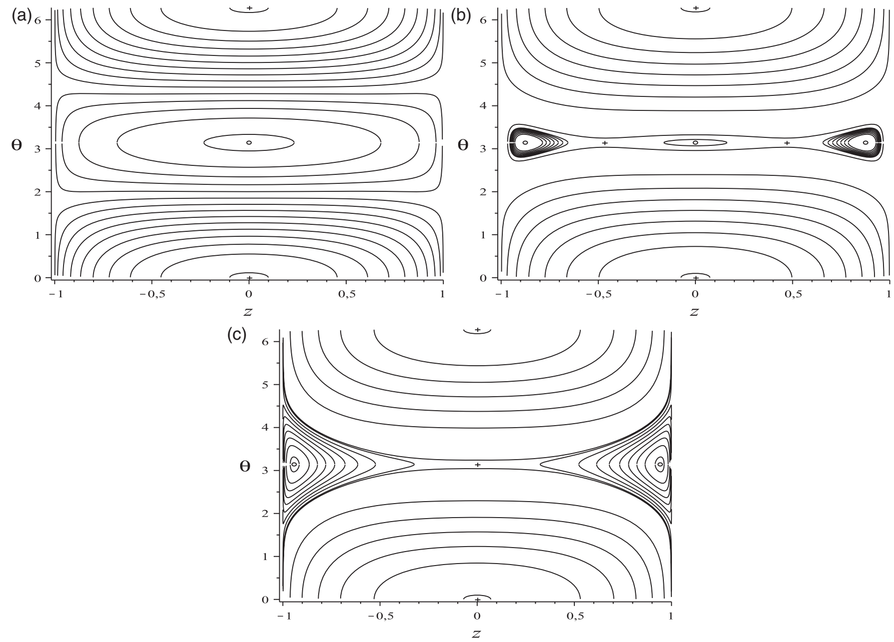

FIG. 2. Integral paths of the equation $\mathcal{H}(z,\theta) = E$ for some value of the energy E, where $\mu = 5$. Circle points and cross points, respectively, correspond to the stable and unstable stationary solutions. Panel (a) corresponds to $\eta = 2$, less than $\eta^{+} \approx 4.41$; panel (b) corresponds to $\eta = 5$, which lies between the two values η^{+} and $\eta^{\star} = 6.4$; panel (c) corresponds to $\eta = 6.5$ larger than $\eta^{\star} = 6.4$. For nonlinearity less than $\mu_{\text{threshold}}$ we only have the pictures of panels (a) and (c).

In conclusion, in this Letter we have proved the existence on a universal critical nonlinearity power (2) for nonlinear Schrödinger equations with double well potential in the semiclassical limit. For nonlinearity power below this value we always observe a supercritical pitchfork bifurcation phenomenon as the strength of the nonlinear perturbation increases, and the new asymmetrical stationary states gradually becomes localized on the single wells. In contrast, for nonlinearity power above (2) we always observe a more complicate scenario: the appearance of a couple of saddle-node bifurcations where the asymmetrical unstable stationary solutions will merge with the stationary solution at $z = 0$ drawing a subcritical pitchfork bifurcation as the strength of the nonlinear perturbation increases. The new physical relevant effect associated with such a new scenario is the sharp appearance of asymmetrical stationary solutions fully localized on the single wells.

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