Symmetry-breaking bifurcations in a double-well potential

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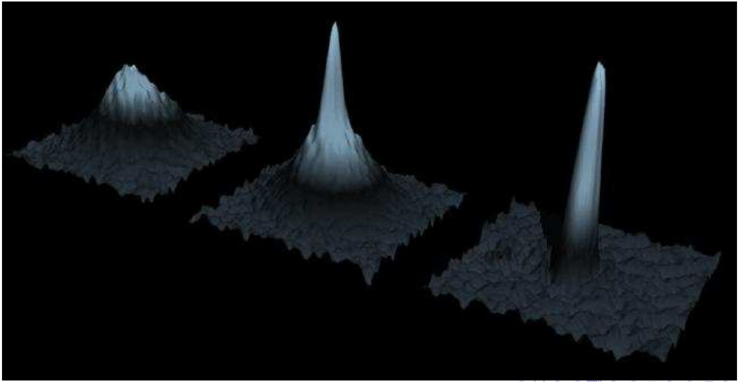
Bose–Einstein Condensation

1924: S. Bose and A. Einstein realize that Bose statistics predicts a maximum atom number in the excited states: a quantum phase transition.

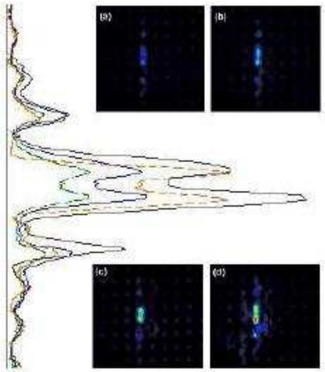
1995: E. Cornell, C. Wieman and W. Ketterle trapped BEC in a dilute gas of Rb^{87} and Na^{23}: 2001 Nobel Prize.

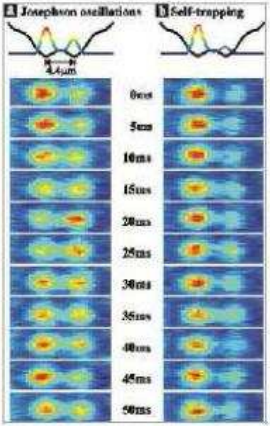
2010: 35 Experimental groups have achieved BEC (in Rb, Li, Na, H): $\mathcal{O}(10^4)$ theoretical and $\mathcal{O}(10^3)$ experimental papers were published!



Experiments on symmetry-breaking bifurcations

- M.Obertaler's group in Heidelberg, Germany (BECs)
- Z. Chen's group at San Francisco, USA (photonics)





Double-well potentials

Density waves in cigar–shaped Bose–Einstein condensates are modeled by the Gross-Pitaevskii equation

$$iu_t = -u_{xx} + V(x)u + \sigma|u|^{2p}u = 0,$$

where $\sigma \in \{1, -1\}$, $p > 0$, and $V(x) : \mathbb{R} \mapsto \mathbb{R}$ satisfies

(i) $V(x) \in L^\infty(\mathbb{R})$,

(ii) $\lim_{|x|\to\infty} V(x) = 0$,

(iii) $V(-x) = V(x)$ for all $x \in \mathbb{R}$.

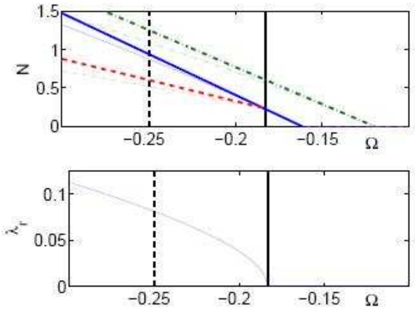
In particular, we consider the single-well potential splitting into two wells

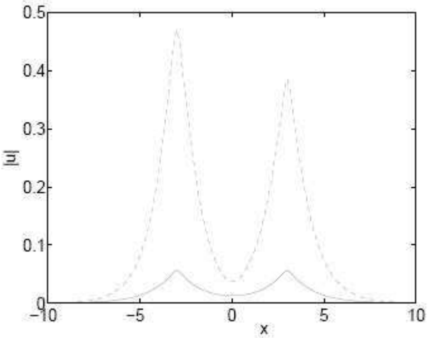
$$V(x) = \frac{1}{2}\left(V_0(x-s) + V_0(x+s)\right) \equiv V_s(x), \quad s \geq 0,$$

where $V_0(x) = -\mathrm{sech}^2(x)$.

Phenomenology

Let V_0 support exactly one negative eigenvalue of $L_0 = -\partial_x^2 + V_0(x)$ and s be large. Then, operator $L = -\partial_x^2 + V_s(x)$ has two negative eigenvalues with symmetric and anti-symmetric eigenfunctions.





Mathematical literature

2004: R.Jackson & M.Weinstein: Geometric analysis of existence of stationary states using two Dirac delta-function potentials.

2005: A. Sacchetti: Semiclassical analysis of symmetry-breaking bifurcation.

2008: E. Kirr, P. Kevrekidis, E. Schlizerman, & M. Weinstein: Derivation of normal form equations in the limit of large separation between the wells.

2009: A. Sacchetti: Threshold on the power p of nonlinearity that separates supercritical and subcritical symmetry-breaking bifurcations.

2010: J. Marzuola & M. Weinstein: Justification of normal form equations on long but finite times in the limit of large separation between the wells.

Existence of stationary states

Substitution $u(x,t) = e^{iEt}\phi(x)$ gives the stationary GP equation

$$-\phi''(x) + V(x)\phi(x) + \sigma|\phi(x)|^{2p}\phi(x) + E\phi(x) = 0, \quad x \in \mathbb{R},$$

where $E \in \mathbb{R}$ is arbitrary and $\phi(x) : \mathbb{R} \mapsto \mathbb{C}$ is the stationary state.

- Via standard regularity theory, if $V(x) \in L^\infty(\mathbb{R})$, then any weak solution $\phi(x) \in H^1(\mathbb{R})$ is a strong solution in $H^2(\mathbb{R})$.
- A strong solution in $H^2(\mathbb{R}) \hookrightarrow \mathcal{C}^1(\mathbb{R})$ is real-valued up to multiplication by $e^{i\theta}$, $\theta \in \mathbb{R}$.
- If $E > 0$, a strong solution in $H^2(\mathbb{R})$ decays exponentially fast to zero as $|x| \to \infty$.

Note: $-E$ is typically used as the chemical potential.

Stability of stationary states

Substitution

$$u(x,t) = e^{iEt}\left[\phi(x) + (u(x) + iw(x))e^{\lambda t} + (\bar{u}(x) + i\bar{w}(x))e^{\bar{\lambda} t}\right]$$

gives the spectral stability problem

$$L_+ u = -\lambda w, \quad L_- w = \lambda u,$$

where

$$\begin{cases} L_+ = -\partial_x^2 + E + V(x) + \sigma(2p+1)\phi^{2p}(x), \\ L_- = -\partial_x^2 + E + V(x) + \sigma\phi^{2p}(x), \end{cases}$$

- Eigenvalues λ occur in real and purely imaginary pairs or in complex quartets.
- If $\phi(x) > 0$ for all $x \in \mathbb{R}$, then operator L_- is positive and no complex quartets occur.

Stability of stationary states

- If operator L_+ has two or more negative eigenvalues, the stationary state ϕ is unstable because there exist real pairs of eigenvalues λ.
- If operator L_+ has one negative eigenvalue, the stationary state ϕ is stable if $N'(E) > 0$ and unstable if $N'(E) < 0$, where $N(E) = \|\phi\|_{L^2}^2$.
- If operator L_+ has no negative eigenvalues, the stationary state ϕ is unconditionally stable.

M. Weinstein (1985,1986); M. Grillakis, J. Shatah, & W. Strauss (1987,1990); M. Grillakis (1988,1990); V. Buslaev & G. Perelman (1993), D. Pelinovsky (2005), S. Cuccagna, D. Pelinovsky, & V. Vougalter (2005), T.Kapitula, P. Kevrekidis, & B. Sandstede (2004,2005), W. Schlag (2006), S.M. Chang, S. Gustafson, K. Nakanishi, & T.P. Tsai (2007), M. Chugunova & D. Pelinovsky (2010), and many others.

Plan of our work

Consider the focusing case with $\sigma = -1$:

$$-\phi''(x) + V(x)\phi(x) - \phi(x)^{2p+1} + E\phi(x) = 0, \quad x \in \mathbb{R}.$$

- Continue the symmetric state from the local bifurcation $E = E_0 > 0$ all way to $E = \infty$.
- Study existence of stationary states for large $E \to \infty$.
- Classify the pitchfork bifurcations for $E = E_*$, where $E_0 < E_* < \infty$.
- Obtain normal forms for the pitchfork bifurcations.

Note:
We shall make no assumption on large separation $s > 0$ between the wells.

Double-well potential

Recall again our double-well potential for numerical computations

$$V_s(x) \equiv \frac{1}{2}\left(V_0(x-s) + V_0(x+s)\right), \quad s \geq 0,$$

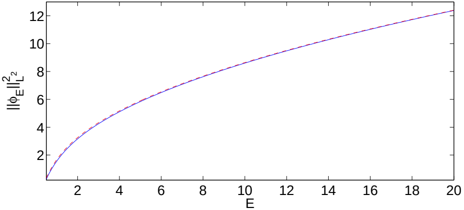
where $V_0(x) = -\mathrm{sech}^2(x)$.

$$V_s''(0) = V_0''(s) = 6\mathrm{sech}^4(s) - 4\mathrm{sech}^2(s).$$

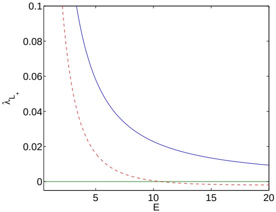
- For $s < s_* = \mathrm{arccosh}(\sqrt{3}/\sqrt{2}) \approx 0.66$, $V_s''(0) > 0$ and the potential $V_s(x)$ is still a single well centered at 0.
- For $s > s_* \approx 0.66$, $V_s''(0) < 0$ and the potential $V_s(x)$ contains two wells centered at $x \approx \pm s$.

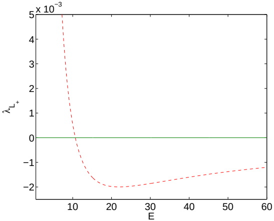
Numerical results: $-\phi''(x) + V_s(x)\phi(x) - \phi^3(x) + E\phi(x) = 0$

Blue: $s = 0.6 < s_*$. Red: $s = 0.7 > s_*$.



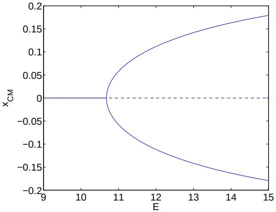
Second eigenvalue of $L_+ = -\partial_x^2 + E + V_s(x) - 3\phi^2(x)$

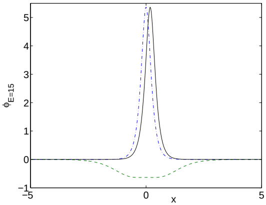




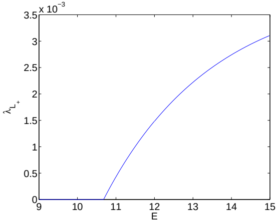
Numerical results: symmetric and asymmetric states

The location of the center of mass of the solution $\phi(x)$





Second eigenvalue of $L_+ = -\partial_x^2 + E + V_s(x) - 3\phi^2(x)$

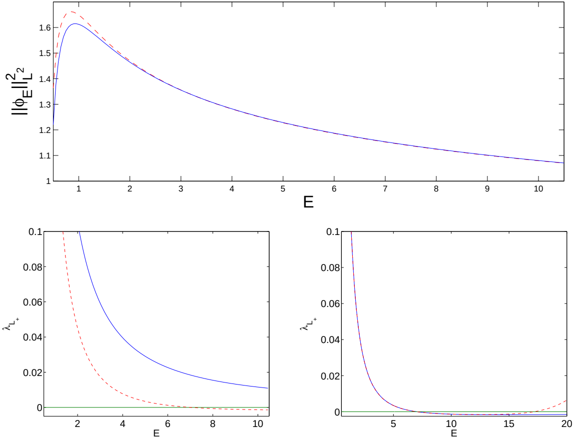


Numerical results: supercritical focusing NLS

$p = 3$:

$$-\phi''(x) + V_s(x)\phi(x) - \phi^7(x) + E\phi(x) = 0, \quad x \in \mathbb{R}.$$

Blue: $s = 0.6 < s_*$. Red: $s = 0.7 > s_*$.



Local bifurcation at $E = E_0$

Root-finding equation for $F(\phi, E) : H^2(\mathbb{R}) \times \mathbb{R} \mapsto L^2(\mathbb{R})$:

$$F(\phi, E) := (-\partial_x^2 + V(x) + E)\phi - \phi^{2p+1} = 0.$$

The Frechet derivative

$$D_\phi F(\phi, E) := -\partial_x^2 + V + E - (2p+1)\phi^{2p} \equiv L_+.$$

Let $-E_0 < 0$ be the smallest eigenvalue of $L_0 = -\partial_x^2 + V$ so that

$$\mathrm{Ker}(D_\phi(F(0, E_0))) = \mathrm{Ker}(L_0 + E_0) = \mathrm{span}\{\psi_0\}.$$

Let $Q : L^2 \mapsto \mathrm{Ran}(L_0 + E_0)$. Using the Lyapunov–Schmidt decomposition $\phi = a\psi_0 + \varphi$ with $\varphi \perp \psi_0$, we obtain

$$\begin{aligned} Q(L_0 + E)Q\varphi - Q(a\psi_0 + \varphi)^{2p+1} &= 0, \\ (E - E_0)a - \langle \psi_0, (a\psi_0 + \varphi)^{2p+1} \rangle &= 0. \end{aligned}$$

Local bifurcation at $E = E_0$

Theorem

There exist $\epsilon > 0$ and $C > 0$ such that for each E in the interval $\mathcal{I}_\epsilon = (E_0, E_0 + \epsilon)$, the stationary equation has a unique positive solution $\psi_E(x) \in H^2(\mathbb{R})$ such that

$$\|\psi_E\|_{H^2} \leq C|E - E_0|^{\frac{1}{2p}}.$$

Moreover the map $E \mapsto \psi_E$ is C^1 from $\mathcal{I}_\epsilon$ to H^2 and $\psi_E(x) = \psi_E(-x)$ for each $x \in \mathbb{R}$ and $E \in \mathcal{I}_\epsilon$.

Since

$$L_+ = L_- - 2p\psi_E^{2p} \quad \text{and} \quad L_-\psi_E = 0,$$

the lowest eigenvalue of L_+ is strictly negative for $E > E_0$.

The slope of $\|\psi_E\|_{L^2}^2$ in E is always positive for $E > E_0$ near $E = E_0$.

Bifurcation from infinity

As $E \to \infty$, we expect $\|\phi\|_{L^\infty} \to \infty$ and $\|\phi\|_{H^1} \to \infty$. Fix $a \in \mathbb{R}$ and consider the scaling transformation

$$E = \varepsilon^{-1} - V(a), \quad \xi = \varepsilon^{-1/2}(x - a), \quad \psi(\xi) = \varepsilon^{1/2p}\phi(x).$$

Then, $\psi(\xi)$ satisfies the rescaled equation

$$-\psi''(\xi) + \tilde{V}_\varepsilon(\xi)\psi(\xi) - \psi^{2p+1}(\xi) + \psi(\xi) = 0,$$

where

$$\tilde{V}_\varepsilon(\xi) = \varepsilon\left[V(a + \varepsilon^{1/2}\xi) - V(a)\right] \Rightarrow \|\tilde{V}_\varepsilon\|_{L^\infty} \to 0 \quad \text{as} \quad \varepsilon \to 0.$$

The truncated problem

$$-\psi_\infty''(\xi) - \psi_\infty^{2p+1}(\xi) + \psi_\infty(\xi) = 0$$

admits a unique (up to translation in $\xi \in \mathbb{R}$) positive solution

$$\psi_\infty = (1+p)^{\frac{1}{2p}} \,\mathrm{sech}^{\frac{1}{p}}(p\xi).$$

Bifurcation from infinity as $E \to \infty$

Theorem

Let $V(x) \in L^\infty(\mathbb{R}) \cap C^2(\mathbb{R})$. *For each* $a \in \mathbb{R}$ *such that* $V'(a) \neq 0$, *no solutions* $\psi(\xi) \in H^2(\mathbb{R})$ *of the stationary equation exist for small* $\varepsilon > 0$. *For each* $a \in \mathbb{R}$ *such that*

$$V'(a) = 0, \quad V''(a) \neq 0$$

there exists an $\varepsilon_0 > 0$ *such that for any* $\varepsilon \in (0, \varepsilon_0)$, *there exists a unique solution* $\psi(\xi) \in H^2(\mathbb{R})$ *of the stationary equation such that*

$$\exists C > 0 : \quad \|\psi - \psi_\infty\|_{H^2} \leq C\varepsilon^2.$$

Previous works:

1986 A.Floer & A. Weinstein: semi-classical analysis

2008 Y. Sivan, G. Fibich, N. Efremidis, & S. Bar-Ad: narrow lattice solitons in periodic potentials

Bifurcation from infinity as $E \to \infty$

Theorem

Let $V(x) \in L^\infty(\mathbb{R}) \cap C^2(\mathbb{R})$. There exists $\varepsilon_0 > 0$ such that for any $\varepsilon \in (0, \varepsilon_0)$, the second eigenvalue of L_+ is negative if $V''(a) < 0$ and positive if $V''(a) > 0$.

- Localized modes at the maximum of $V(x)$ are unstable.
- Localized modes at the minimum of $V(x)$ are stable if $\frac{d}{dE}\|\phi\|^2_{L^2} > 0$.

From the asymptotic scaling, we have

$$\|\phi\|^2_{L^2} = \varepsilon^{-\frac{1}{p}+\frac{1}{2}} \|\psi\|^2_{L^2} \sim E^{\frac{1}{p}-\frac{1}{2}} \|\psi_\infty\|^2_{L^2} \quad \text{as} \quad E \to \infty,$$

so that the localized modes are stable only if $p < 2$.

Pitchfork bifurcation at $E = E_* \in (E_0, \infty)$

Let $V_s(x)$ is a double-well potential for $s > s_*$ with the maximum at $x = 0$ and two symmetric minima at $x = \pm x_0$, $x_0 \approx s$.

- The symmetric state ψ_E centered at $x = 0$ bifurcates for $E > E_0$ and it is stable.
- The symmetric state ψ_E is unstable as $E \to \infty$ but two asymmetric states $\psi_E^{\pm}$ centered at $x = \pm x_0$ exist and stable if $p < 2$.

There exists $E_* \in (E_0, \infty)$, when the second eigenvalue of L_+ at ψ_E crosses zero and become negative for $E > E_*$. We anticipate bifurcation of asymmetric states from the symmetric state at $E = E_*$.

Assumption: There exists $\varphi_* \in H^2_{\rm odd}(\mathbb{R})$ such that $\mathrm{Ker}(L_+|_{E=E_*}) = \mathrm{span}\{\varphi_*\}$ and $\lambda'(E_*) < 0$, where $\lambda(E)$ is the second eigenvalue of L_+.

Pitchfork bifurcation at $E = E_* \in (E_0, \infty)$

Consider again

$$F(\phi, E) := (-\partial_x^2 + V(x) + E)\phi - \phi^{2p+1} = 0.$$

and let $\phi = \psi_* + a\varphi_* + \theta$, where $\psi_* \in H^2_{\rm even}(\mathbb{R})$ and $\phi_* \in H^2_{\rm odd}(\mathbb{R})$.

Then $F(\phi, E) = 0$ is equivalent to

$$\begin{array}{rcl} PL_* P\theta & = & -(E - E_*)P(\psi_* + \theta) + PN(a\varphi_* + \theta), \\ G(\theta, a, E) & := & -(E - E_*)a + \langle \varphi_*, N(a\varphi_* + \theta)\rangle_{L^2} = 0, \end{array}$$

where

$$N(\varphi) = (\psi_* + \varphi)^{2p+1} - \psi_*^{2p+1} - (2p+1)\psi_*^{2p}\varphi = \mathcal{O}(\|\varphi\|^2).$$

From the first equation, we have a unique C^3 map
$\mathbb{R}^2 \ni (a, E) \mapsto \theta = \theta_*(a, E) \in H^2$ near $a = 0$ and $E = E_*$.
We denote

$$G(a, E) \equiv G(\theta_*(a, E), a, E) : \mathbb{R}^2 \mapsto \mathbb{R}.$$

Pitchfork bifurcation at $E = E_* \in (E_0, \infty)$

From symmetries, we know that

$$G(0,E) = 0, \quad G(-a,E) = G(a,E), \quad (a,E) \in \mathbb{R}^2.$$

The near-identity transformation is needed to obtain the leading order of $G(a,E)$:

$$\theta = (E - E_*)\partial_E \psi_* + a^2(2p+1)pL_*^{-1}\psi_*^{2p-1}\varphi_*^2 + \mathrm{o}_{H^2}(|E - E_*|, a^2).$$

$G(a,E)$ reduces to the normal form

$$C(E - E_*)a + Qa^3 + \mathcal{O}((E-E_*)^2 a, (E-E_*)a^3, a^5) = 0,$$

where

$$C = 2p(2p+1)\langle \varphi_*^2, \psi_{E_*}^{2p-1}\partial_E \psi_{E_*}\rangle_{L^2} - 1 = -\lambda'(E_*) > 0$$

and

$$Q = 2p^2(2p+1)^2\langle \varphi_*^2\psi_{E_*}^{2p-1}, L_*^{-1}\psi_{E_*}^{2p-1}\varphi_*^2\rangle_{L^2} + \frac{1}{3}p(2p+1)(2p-1)\langle \varphi_*^2, \psi_{E_*}^{2p-2}\varphi_*^2\rangle_{L^2}$$

are numerical coefficients.

Pitchfork bifurcation at $E = E_* \in (E_0, \infty)$

Theorem

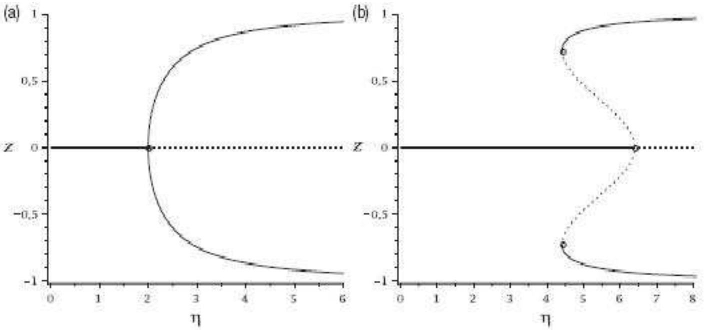
There exists $\epsilon > 0$ such that the branch of symmetric states (ψ_E, E) can be continued smoothly (C^1) on $(E_* - \epsilon, E_* + \epsilon)$. Moreover, there exist two branches of asymmetric states $(\psi_E^{\pm}, E)$ for $E \in \mathcal{I}_\epsilon = (E_* - \epsilon, E_*]$ if $Q > 0$ and for $E \in \mathcal{I}_\epsilon = [E_*, E_* + \epsilon)$ if $Q < 0$ such that

$$\exists C > 0: \quad \|\psi_E^{\pm} - \psi_{E_*}\|_{H^2} \leq C|E - E_*|^{1/2}.$$

Under conditions of the theorem, the second eigenvalue of $L_+ = D_\phi F(\psi_E^{\pm}, E)$ is negative for $Q > 0$ and is positive for $Q < 0$.

Pitchfork bifurcation at $E = E_* \in (E_0, \infty)$

Left: Supercritical bifurcation. Right: Subcritical bifurcation.



Here z is the center of localization and $\eta \equiv E$ is the bifurcation parameter.

What is the correct parameter for bifurcation and stability in the Gross–Pitaevskii equation?

Pitchfork bifurcation at $E = E_* \in (E_0, \infty)$

Question: What is the correct parameter for bifurcation and stability in the Gross–Pitaevskii equation?

Answer: $N = \|\phi\|_{L^2}^2$ (the power or charge invariant).

Under conditions of the theorem, near $E = E_*$, we have

- $\|\psi_E^\pm\|_{L^2}^2 < \|\psi_{E_*}\|_{L^2}^2$ if $R < 0$;
- $\|\psi_E^\pm\|_{L^2}^2 > \|\psi_{E_*}\|_{L^2}^2$ if $R > 0$,

where

$$R := -Q \frac{d}{dE} \|\psi_{E_*}\|_{L^2}^2 - C^2.$$

Pitchfork bifurcation at $E = E_* \in (E_0, \infty)$

As $s \to \infty$ (large separation between potential wells), we have

$$\psi_{E_*}(x) \sim \frac{1}{\sqrt{2}}(\varphi_0(x-s) + \varphi_0(x+s)), \quad \varphi_*(x) \sim \frac{1}{\sqrt{2}}(\varphi_0(x-s) - \varphi_0(x+s)).$$

In particular,

$$\varphi_*^2 \sim \frac{\psi_*^2}{\|\psi_*\|_{L^2}^2}.$$

Performing direct computations, we obtain

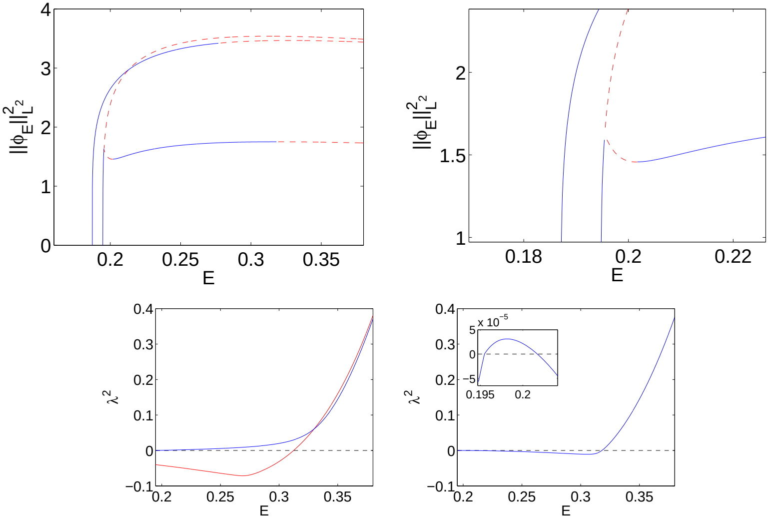
$$Q = -\frac{4p(p+1)(2p+1)}{3} \frac{\|\psi_*\|_{L^{2p+2}}^{2p+2}}{\|\psi_*\|_{L^2}^4} < 0, \quad R = -\frac{4}{3}(p^2 - 3p - 1).$$

Supercritical pitchfork occurs for $p < p_* \approx 3.5$.
Subcritical pitchfork occurs for $p > p_*$.

- A. Sacchetti, "Universal critical power for nonlinear Schrödinger equations with a symmetric double well potential", Phys. Rev. Lett. **103**, 194101 (4 pages) (December, 2009)

Numerical results in the focusing case

Subcritical pitchfork bifurcation for $p = 5$ and $s = 4$.



Conclusion

Summary:

- Existence and bifurcations of solution branches are studied from Lyapunov–Schmidt reductions applied to the stationary equation.
- Stability of solution branches is studied from the information on the number of negative eigenvalues of L_+ and the slope of $\|\phi\|_{L^2}^2$ versus E.
- Normal form dynamics should follow separately from the time-dependent Gross–Pitaevskii equation.

More results?

We proved a unique connection of the branch of symmetric states in the focusing case between local bifurcation at $E = E_0$ and bifurcation from infinity at $E = \infty$.