Global Bifurcations and Large Ground States in Nonlinear Schrödinger Equations

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The Nonlinear Schrödinger Equation

$$i\partial_t u(t,x) = (-\Delta_x + V(x))u + f(|u|^2)u \qquad (1)$$

- $u : \mathbb{R} \times \mathbb{R}^n \to \mathbb{C}$; $f : \mathbb{R} \to \mathbb{R}$;

- $V : \mathbb{R}^n \to \mathbb{R}$, $\lim_{|x|\to\infty} |V(x)| = 0$, $V, x \cdot \nabla V(x) \in L^\infty(\mathbb{R}^n)$

Results extend to $V, x{\cdot}\nabla V(x) \in L^q + L^r$, $\max\{1, n/2\} < q \le r \le \infty$.

Applications: Nonlinear Optics, Water Waves, Quantum Physics in particular Bose-Einstein Condensates.

In Quantum Physics

$$i\hbar\partial_t u(t,x) = -\frac{\hbar^2}{2m}\Delta_x u + V(x)u$$

basically means the total energy of a particle is equal to the kinetic plus the potential energy. Here

$|u(t,x)|^2 =$ probability density for the particle to be at time t

in position x. In analogy with photon propagation for which

$$u(t,x) = u_0 e^{\frac{i}{\hbar}(px-\mathcal{E}t)}$$

taking one derivative in time we get

$$\partial_t u(t,x) = -\frac{i}{\hbar}\mathcal{E}u(t,x)$$

or $i\hbar\partial_t u(t,x) = \mathcal{E}u(t,x)$. Similarly $-\frac{\hbar^2}{2m}\Delta u = \frac{p^2}{2m}u$.

The nonlinearity can be viewed as a the potential $f(|u|^2)$ induced by the particle, or, in Bose-Einstein Condensates, when many bosons converge to the same state (wave function $u(t,x)$) then the effect of the other particles on a given one is of the form

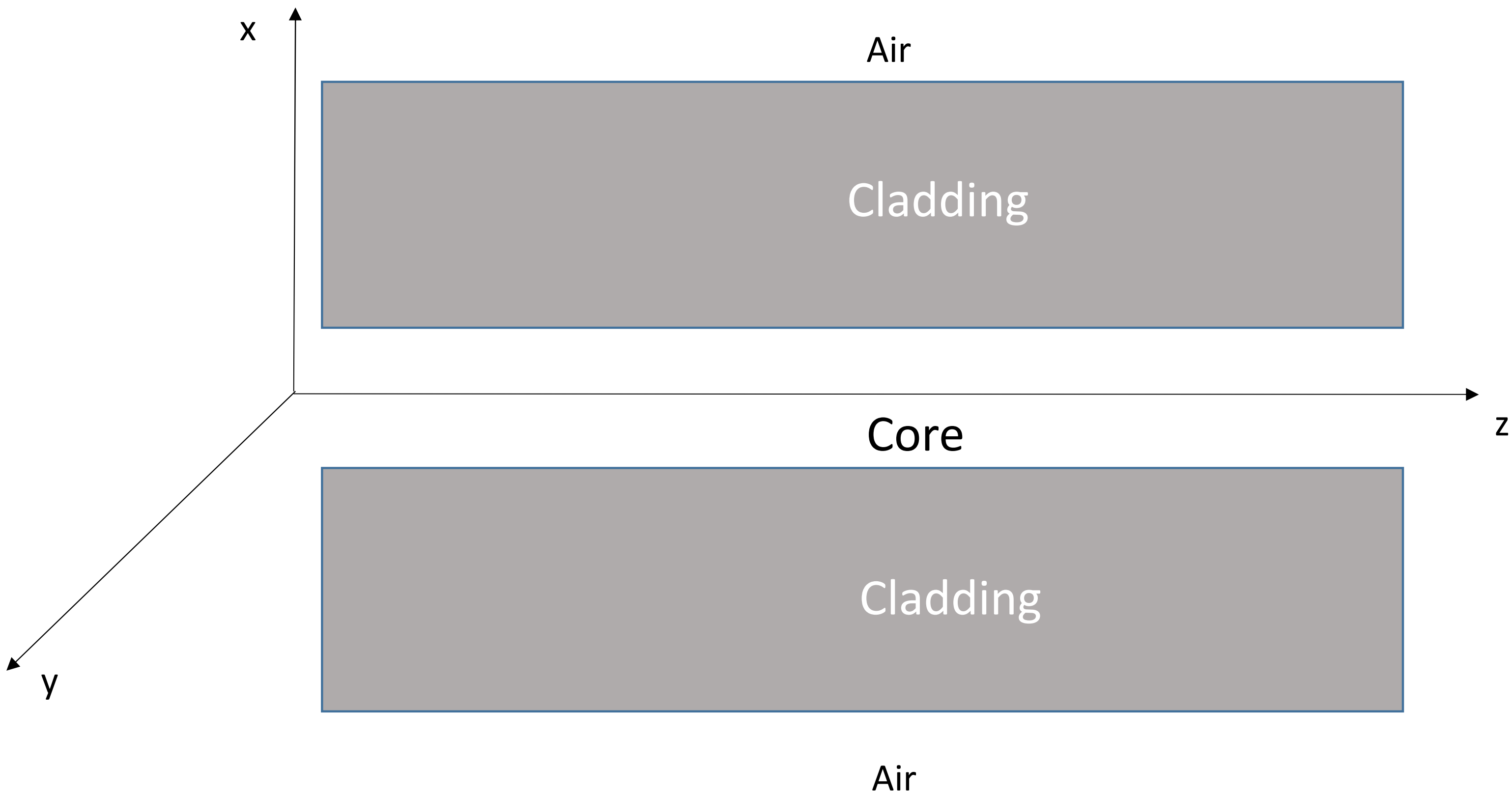
$$f(|u|^2)(x) = \int_{\mathbb{R}^n} K(|x-y|)|u(y)|^2 dy$$

where the interaction can be given by Coulomb potential $K(z) = \sigma/|z|$ giving the Hartree nonlinearity. However, in dilute gas approximation, $K(z) \approx \sigma\delta$ giving the power nonlinearity

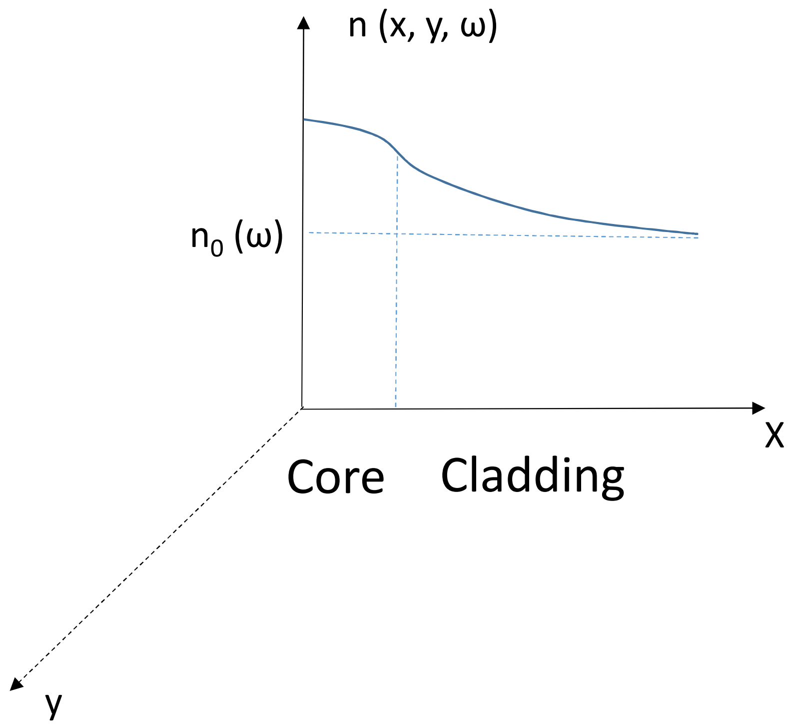
$$f(|u|^2)u = \sigma|u|^2 u$$

in which case the equation is sometimes called Gross-Pitaevskii. Higher power nonlinearities result when higher order interaction between particles dominates.

In Nonlinear Optics



Refractive Index:



Maxwell Equations:

$$
\begin{aligned}
\nabla \times \overrightarrow{E} &= -\partial_t \overrightarrow{B} \\
\nabla \cdot \overrightarrow{B} &= 0 \\
\nabla \cdot \overrightarrow{D} &= \rho \\
\nabla \times \overrightarrow{H} &= \partial_t \overrightarrow{D} + \overrightarrow{j}
\end{aligned}
$$

where:

$$
\begin{aligned}
\overrightarrow{D} &= \epsilon_0 \overrightarrow{E} + \overrightarrow{P} \\
\overrightarrow{H} &= \frac{1}{\mu_0}\overrightarrow{B} - \overrightarrow{M}
\end{aligned}
$$

with constitutive relations for dielectrics: $\rho = 0$, $\overrightarrow{j} = 0 = \overrightarrow{M}$, $\mu_0 = (\epsilon_0 c^2)^{-1}$, and

$$
\begin{aligned}
\frac{1}{\epsilon_0}\overrightarrow{P}(t) = &\int_{-\infty}^{t} \chi^1(t-\tau)\overrightarrow{E}(\tau)d\tau \\
&+ \int_{-\infty}^{t}\int_{-\infty}^{t}\int_{-\infty}^{t} \chi^3(t-\tau_1, t-\tau_2, t-\tau_3)\overrightarrow{E}(\tau_1)\cdot\overrightarrow{E}(\tau_2)\overrightarrow{E}(\tau_3)d\tau_1 d\tau_2 d\tau_3
\end{aligned}
$$

The Graded Optical Fiber Ansatz:

$$\begin{aligned}\overrightarrow{E} &= \varepsilon\overrightarrow{E_0} + \varepsilon^2\overrightarrow{E_1} + \varepsilon^3\overrightarrow{E_2} + \ldots \\ \overrightarrow{E_0} &= u(\varepsilon x, \varepsilon y, \varepsilon^2 z)e^{i(k(\omega_0)z - \omega_0 t)}\overrightarrow{e}\end{aligned}$$

leads to

$$i\partial_Z u = -\frac{1}{2k(\omega_0)}(\partial_{XX} + \partial_{YY})u - \frac{n^2 - n_0^2}{\varepsilon^2 n_0^2}u - \frac{k(\omega_0)n_2}{n}|u|^2 u$$

under the assumption $n^2 - n_0^2$ is of size ε^2 and slowly changes with $X = \varepsilon x,\ Y = \varepsilon y$. Note that:

$$\begin{aligned}n^2 &= 1 + \widehat{\chi^1} \\ 2n_0 n_2 &= 3\widehat{\chi}^3\end{aligned}$$

In Water Waves

Involves:

- multi-scale analysis (similar to the optical case described previously)

- the Dirichlet to Neumann map due to the free surface.

General Hamiltonian Formulation

The general Hamiltonian system:

$$\partial_t u = JD\mathcal{E}(u)$$

becomes equivalent to the nonlinear Schrödinger equation under the choices:

$$\begin{aligned} \mathcal{E}(u) \quad &= \quad \frac{1}{2}\int_{\mathbb{R}^n} |\nabla u|^2 dx + \frac{1}{2}\int_{\mathbb{R}^n} V|u|^2 dx + \frac{1}{2}\int_{\mathbb{R}^n} F(|u|^2) dx, \\ J \; = -i \; &= \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \end{aligned}$$

$\mathcal{E} : H^1(\mathbb{R}^n, \mathbb{C}) \mapsto \mathbb{R},\ J : H^1(\mathbb{R}^n, \mathbb{C}) \subset H^{-1}(\mathbb{R}^n, \mathbb{C}) \mapsto H^1(\mathbb{R}^n, \mathbb{C})$.

More generally, for X a real Hilbert space, $\mathcal{E} : X \mapsto \mathbb{R}$ a C^2 map and $J : D(J) \subset X^* \mapsto X$ a skew-adjoint operator the formulation covers a large class of wave equations e.g. Hartree, Dirac, Klein-Gordon, KdV, NW.

Gauge Symmetry

The energy is assumed invariant under the action of a continuous unitary group $T(\omega)$ on X i.e.

$$\mathcal{E}(T(\omega)u) = \mathcal{E}(u), \quad T(\omega)J = JT^*(-\omega),\ \omega \in \mathbb{R}.$$

This leads to a second conserved quantity (besides the energy):

$$\mathcal{N}(u) = \frac{1}{2}\langle Bu, u\rangle,$$

where $B : X \mapsto X^*$ is self-adjoint and JB extends $T'(0)$.

In the Schrödinger case $T(\omega)u = e^{-i\omega}u$ are rotations in the complex plane and

$$\mathcal{N}(u) = \frac{1}{2}\langle u, u\rangle = \frac{1}{2}\|u\|_{L^2}^2.$$

General Coherent Structures

are solutions of the form:

$$u(t) = T(\omega t)\psi_\omega, \qquad \psi_\omega \in X.$$

Hence ψ_ω satisfies in the weak sense:

$$JD\mathcal{E}(\psi_\omega) = \omega JD\mathcal{N}(\psi_\omega). \tag{2}$$

Note that for an one-to-one J the coherent states are critical points of the $\mathcal{E} - \omega\mathcal{N}$ functional.

Hence, variational methods have been successfully used to prove existence of coherent structures, especially "large" ones.

Existence of Coherent Structures. The Variational Method

Particular coherent structures (ground states) are solutions of:

$$\min_{\mathcal{N}(\psi)=const.} \mathcal{E}(\psi)$$

Successful in many problems, produces orbitally stable states, but it requires sophisticated compactness arguments e.g. *concentration compactness* (P. L. Lions '84), when the constrain $\mathcal{N}$ is *not weakly continuous* on X.

Delicate reformulations of the minimization problem are necessary in *critical and supercritical regimes* when $\mathcal{E}$ has *no minimizer* e.g. large power nonlinearities

$$F(|u|^2) = |u|^{2p+2}, \; p \geq 2/n$$

in NLS energy.

In this case one can use a different functional which is bounded from below (Rose-Weinstein '88):

$$\min_{\|\psi\|_{L^{2p+2}}=const.} \|\nabla\psi\|_{L^2}^2 + \int_{\mathbb{R}^n} V|\psi|^2 dx + E\|\psi\|_{L^2}^2$$

or Nehari manifolds, etc...

Limitations of the Variational Methods

- "artsy", non-systematic, identifies only special coherent states, minimizers or "mountain pass" (saddle) points of certain functionals.

- do not guarantee smooth dependence on parameters e.g. ω.

- if they rely on functionals unrelated to the dynamical invariants they provide no stability information.

Linear Bound-States in Schrödinger Eq.

$$\begin{aligned} i\partial_t u(t,x) &= (-\Delta_x + V(x))u \\ u(0,x) &= u_0(x) \end{aligned}$$

$-\Delta + V$ is a self adjoint operator on L^2 with domain H^2, and V is a relative compact perturbation of $-\Delta$. Hence

$$\text{Spectrum of } -\Delta + V = [0,\infty) \bigcup \sigma_{discrete}$$

where $\sigma_{discrete} = \{$isolated e-values with finite multiplicity$\}$. Via Stone's theorem for u_0 in L^2 :

$$u(t,x) = e^{i(\Delta - V)t}u_0 = \sum_{\omega \in \sigma_{discrete}} e^{-i\omega t}\mathsf{P}_\omega u_0 + e^{i(\Delta - V)t}\mathsf{P}_c u_0$$

Linear Evolution and Asymptotic Behavior.

Moreover $e^{i(\Delta-V)t}\mathsf{P}_c$ is unitary on L^2 but

$$\|e^{i(\Delta-V)t}\mathsf{P}_c u_0\|_{L^\infty} \leq (4\pi|t|)^{-n/2}\|u_0\|_{L^1}$$

The nonlinear variant of this result is a conjecture:

Asymptotic Completeness Conjecture: Any solution of (1) eventually converges to a superposition of nonlinear bound-states and a radiative part which disperses to infinity.

It is only proven for the integrable case $n = 1$, $V \equiv 0$, and $f(|u|^2)u = -|u|^2u$.

Existence of Coherent Structures. The Bifurcation Methods

Find zeroes of the map:

$$F : H^1(\mathbb{R}^n, \mathbb{C}) \times \mathbb{R} \mapsto H^{-1}(\mathbb{R}^n, \mathbb{C}),$$

$$F(\psi, E) = (-\Delta + V + E)\psi + \sigma|\psi|^{2p}\psi,$$

which is equivariant under the action of $O(2)$, i.e.:

$$F(e^{i\theta}\psi, E) = e^{i\theta}F(\psi, E),$$

$$F(\overline{\psi}, E) = \overline{F(\psi, E)}.$$

It is Fréchet differentiable over the *real* Banach spaces:

$$H^1(\mathbb{R}^n, \mathbb{C}) \cong H^1(\mathbb{R}^n, \mathbb{R}) \times H^1(\mathbb{R}^n, \mathbb{R}) \hookrightarrow H^{-1}(\mathbb{R}^n, \mathbb{R}) \times H^{-1}(\mathbb{R}^n, \mathbb{R}).$$

Linearization

For ψ real valued (hence $F(\psi, E)$ real valued) we have:

$$D_\psi F(\psi, E)[u + iv] = \begin{bmatrix} L_+(\psi, E) & 0 \\ 0 & L_-(\psi, E) \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix},$$

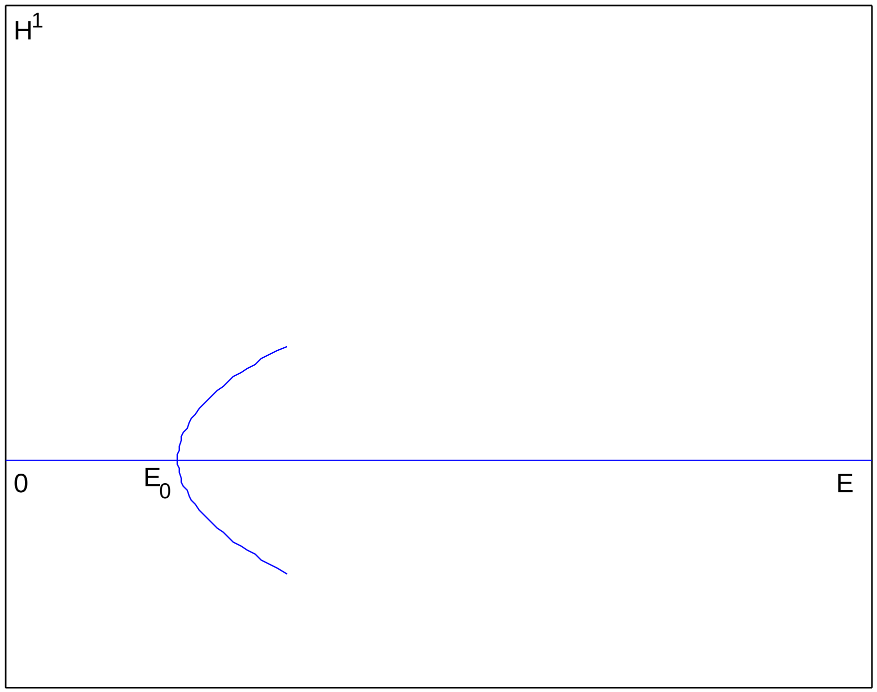
where

$$\begin{aligned} L_+(\psi, E)[u] &= (-\Delta + V + E)u + (2p+1)\sigma|\psi|^{2p}u \\ L_-(\psi, E)[v] &= (-\Delta + V + E)v + \sigma|\psi|^{2p}v \end{aligned}$$

In particular

$$L_\pm(0, E) = -\Delta + V + E$$

Bifurcation Diagram for Ground-States in NLS



where $-E_0 < 0$ is the lowest eigenvalue of the (unbounded) linear operator $-\Delta + V$ on L^2.

Preliminary Result: The solutions (ψ_E, E) of (**??**) in a (small) neighborhood of $(0, E_0) \in H^1(\mathbb{R}^n) \times \mathbb{R}$ where $-E_0$ is lowest e-value of $-\Delta + V$ (which is simple!) form a two dimensional C^1 manifold:

$$(E, \theta) \mapsto e^{i\theta}\psi_E, \ 0 \le \theta < 2\pi, \ \psi_E \text{ real valued},$$

called the *ground-state manifold.* Moreover $u(t,x) = e^{iEt+i\theta}\psi_E(x)$ are orbitally stable solutions of (1):

$$i\partial_t u = (-\Delta + V)u + \sigma|u|^{2p}u.$$

Questions: How far can we continue this manifold? Are there any bifurcations along it and/or changes of stability? Are there other ground-state manifolds not connected to this one?

Note: there are no nontrivial solutions near $(0, E_*)$ for $E_* > E_0$ since the linear operator $-\Delta + V + E_*$ is an isomorphism.

Results for Attractive Nonlinearity $\sigma < 0$:

- if $x \in \mathbb{R}$, $V(x) = V(-x)$, and V is strictly increasing for $x > 0$ then the ground state branch bifurcating from E_0 can be uniquely continued for all $E > E_0$ (Jeanjean & Stuart '99, monotonicity methods).

- if $V \equiv V_s(x) = V(x_1 + s, x_2, \ldots, x_n) + V(-x_1 + s, x_2, \ldots, x_n)$ then there exists s_* sufficiently large such that for all $s \geq s_*$ the *ground state manifold* suffers a pitchfork type bifurcation at a finite $E_* \gtrsim E_0$ (KKP '11, see also KKSW '08 and Heeyeon's thesis all based on perturbative analysis valid for small ground states or excited states).

- if $x \in \mathbb{R}$, $V(x) = V(-x)$, and V is twice differentiable at $x = 0$ with $\nabla^2 V(0) < 0$ then the *ground state manifold* suffers a pitchfork type bifurcation at a finite $E_* > E_0$ (KKP '11, extends to $x \in \mathbb{R}^n$).

- if $x \in \mathbb{R}^n$ then there is at least one ground state for each $E > E_0$ (Rose & Weinstein '88, variational methods).

- if V has more than one critical point then there are multipeak ground states and multiple ground states as $E \mapsto \infty$ (Dancer & Yan '01, Aschbacher & all '02, and more recently by T.-C. Lin, variational methods).

Global Bifurcation Theory

Topological Degree Method: If

$$S = \{(\psi, E) \mid F(\psi, E) = 0,\ \psi \not\equiv 0\}$$

then

$$S_0 = \text{ the connected component of } \overline{S} \text{ containing } (0, E_0)$$

either reaches the boundary of the domain where $D_\psi F$ is Fredholm or contains a solution $(0, E_1),\ E_1 \neq E_0$.

The method requires the introduction of a degree for $F(\cdot, E)$ i.e. certain compactness properties of the pre-images F^{-1}(bounded set). Such compactness result are not available for the attractive non-linearity. For the repelling case see Jeanjean at all '99.

Analytical Maps Method: If F is real analytic then the branch bifurcating from $(0, E_0)$ can be analytically continued until it forms a loop or reaches the boundary of the domain where $D_\psi F$ is Fredholm. Requires relative compactness of the connected component of the set of zeroes of F containing $(0, E_0)$:

Theorem 1. *(compactness): If* (ψ_{E_n}, E_n) *are zeroes of* F *in the connected component of* $(0, E_0)$ *and*

$$(\psi_{E_n}, E_n) \overset{H^1 \times \mathbb{R}}{\rightharpoonup} (\psi_{E_*}, E_*)$$

then there exists a subsequence $(\psi_{E_{n_k}}, E_{n_k})$ *such that*

- $\lim_{k\to\infty} \|\psi_{E_{n_k}} - \psi_{E_*}\|_{H^1} = 0$ *and*

- $F(\psi_{E_*}, E_*) = 0$.

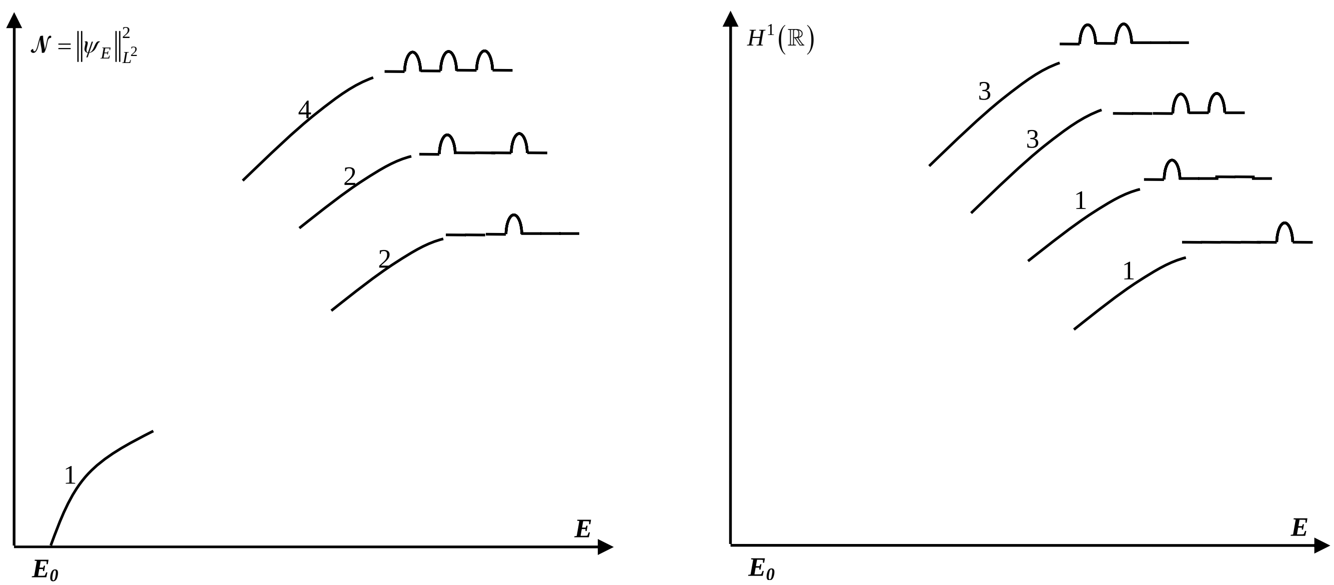
New Results (valid in any space dimension):

- No bound-state manifold blows up in L^2 (or H^1) norm at finite E. No ground state manifold goes to the left of E_0.

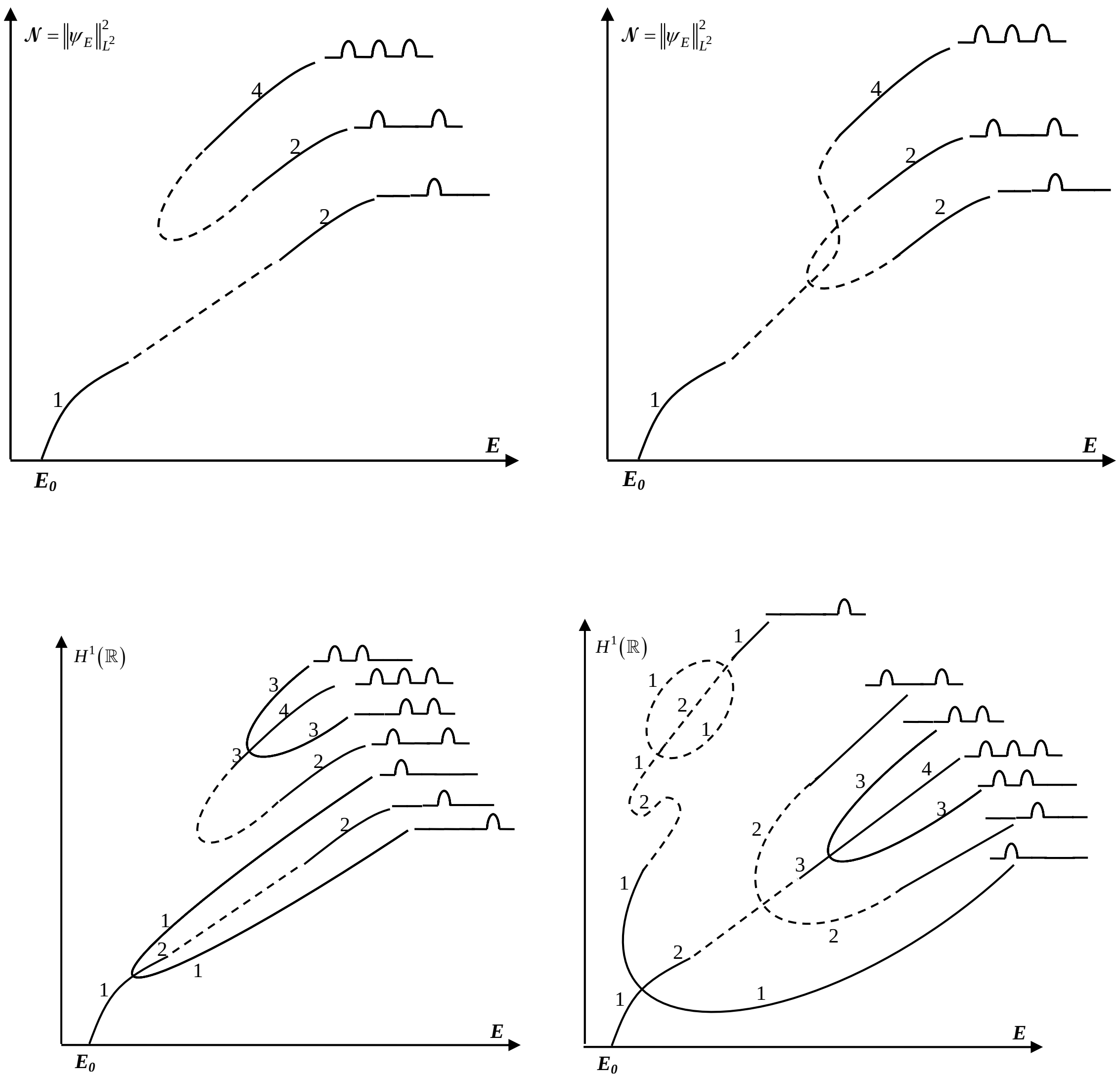
- We know *all* ground-state manifolds near $E = \infty$ in terms of the critical points of the potential provided the latter are all non-degenerate.

- In some situations we can establish how the ground-state manifolds near $E = \infty$ connect with the one near $E = E_0$, and with each other via bifurcations, hence we can find all ground-state branches.

Ground state manifolds near $E = E_0$ and $E = \infty$ for the double well potential (see Theorems 2 & 3)



(Almost) all ground state manifolds



Comments on the Example:

- the full picture depends on how manifolds near the boundary of the Fredholm domain connect among themselves i.e., in this example, how each symmetric ground state at $E = \infty$ turns around at certain finite E and connects to a different symmetric ground state as it returns to $E = \infty$; it turns out that these connections depend on the distance "s" between wells, see next numerical graph and animated picture thanks to P. Kevrekidis and J. Lee (UMass):

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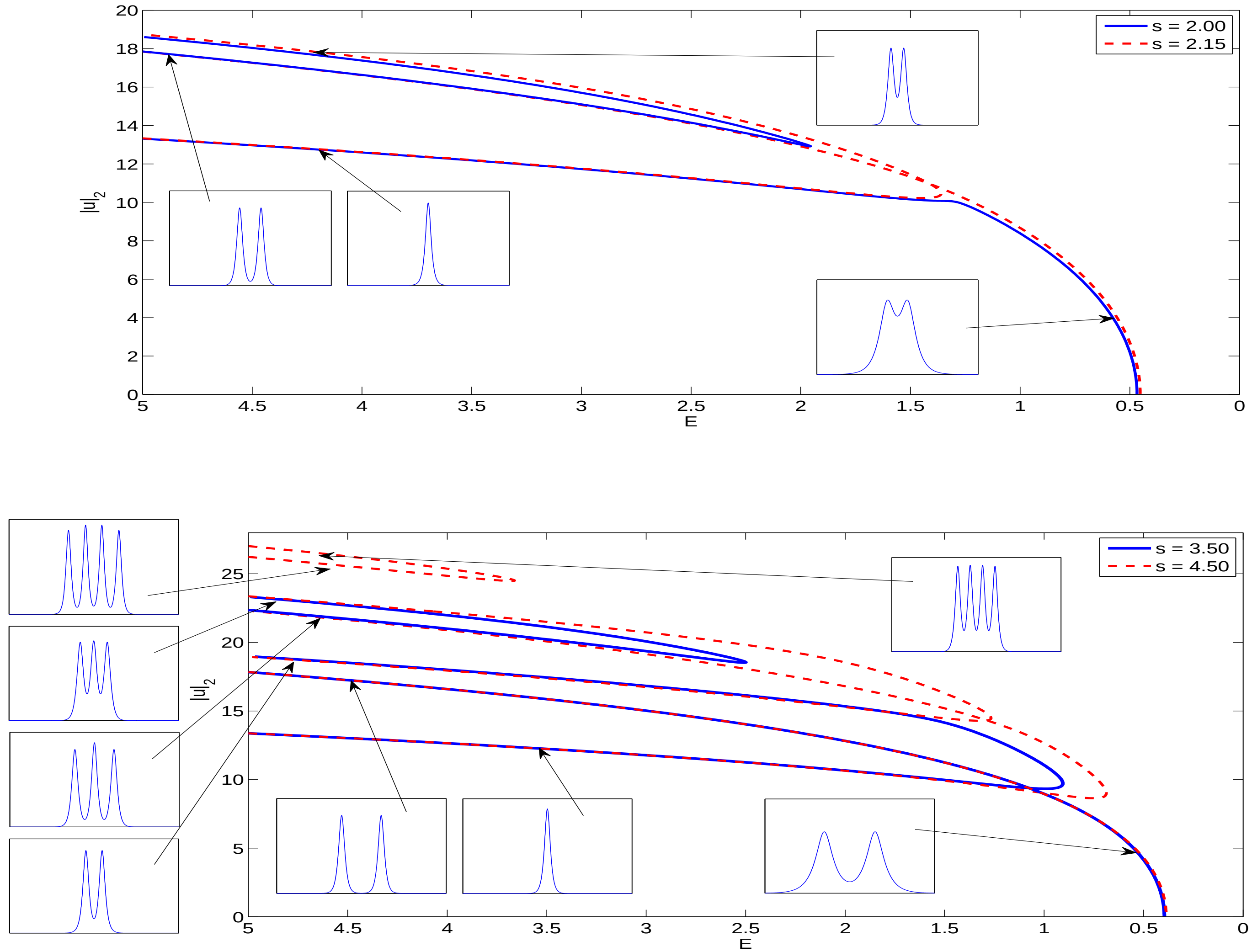

Conclusions:

- We are on the verge of understanding the correlation between critical points of the potential and the bifurcations along the ground-state (and excited-state) manifolds. The missing links are results on how multi-peak solutions, which approach the same critical point in the limit $E \to \infty$, connect, and a classification of possible bifurcations in higher dimensions when a multiple eigenvalue crosses zero.

- Once all bound-state manifolds have been identified one can approach the asymptotic completeness conjecture in NLS by starting with the dynamics near the bifurcation points.

- The technique is rather general for Hamiltonian PDE's, relying on energy estimates, analysis of the linearized operator, concentration compactness and properties of the limiting equation (as the parameter approaches a certain limit). Applications to general nonlinearities in NLS are almost finished (with V. Sadoveanu). Applications to rotating BEC's and coupled wave equations are underway.

Thank you!