CHAPTER 16

Extended Hamiltonian Systems

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1. Introduction

In this chapter we discuss Hamiltonian partial differential wave equations which are defined on unbounded spatial domains, a class of so-called *extended Hamiltonian systems*. The examples we consider are the nonlinear Schrödinger and Klein–Gordon equations defined on $\mathbb{R}^3$. These may be viewed as infinite-dimensional Hamiltonian systems, which have coherent solutions, e.g., spatially uniform equilibria, spatially nonuniform solitary standing waves.... Questions of interest include the dynamics in a neighborhood of these states (stability to small perturbations), stability under small Hamiltonian perturbations of the dynamical system, the behavior of solutions on short, intermediate and infinite time scales and the manner in which these coherent states participate in the structure of solutions on these time scales.

The contrast in dynamics between Hamiltonian systems of extended type and those of compact type is striking. Compact Hamiltonian systems arising, for example, from finite-dimensional Hamiltonian systems or Hamiltonian partial differential equations (PDEs) governing an evolutionary process defined on a bounded spatial domain, are systems governed by finite or infinite systems of ordinary differential equations (ODEs) with a *discrete* set of frequencies. Many fundamental phenomena and questions here involve the persistence or breakdown of regular (e.g., time periodic or quasiperiodic) solutions and their dynamical stability relative to small perturbations. A stable state of the system is one around which neighboring trajectories oscillate. KAM theory implies states persist in the presence of small Hamiltonian perturbations (structural stability) provided certain arithmetic *non-resonance* conditions on the set of frequencies of the unperturbed state hold [1,27,11,3].

In contrast, extended Hamiltonian systems arising from Hamiltonian PDEs are systems involving continuous as well as discrete spectra of frequencies. Stable states are expected to be *asymptotically stable*; states initially nearby the unperturbed state remain close and even converge to it in an appropriate metric. Since the flow is in an infinite-dimensional space, this does not contradict the Hamiltonian character of the phase flow, which in finite-dimensional spaces preserves volume. Convergence to an asymptotic state occurs through a mechanism of radiating energy to infinity. It is also possible that some states of the system are long-lived *metastable states*. These are states which persist on long time scales, but decay as $t \to \infty$. This structural instability due to Hamiltonian perturbations occurs due to nonlinearity induce resonances of states associated with discrete and continuous spectra, precisely that which is precluded in the setting of KAM theory.

2. Overview

We consider partial differential equations for which the linear part (the small amplitude limit) has spatially localized and time-periodic “bound state” solutions, which are dynamically stable. Such solutions of the linear dynamical system are associated with the discrete spectrum of linear self-adjoint operator generating the flow. Also associated with this operator, due to the unboundedness of the spatial domain, is continuous spectrum with corresponding spatially extended (nondecaying) radiation states. These bound and radiation states are central to the linear dynamics. Arbitrary finite energy initial conditions can, by the spectral theorem for self-adjoint operators, be decomposed into a superposition of discrete and continuous spectral states. Their amplitudes evolve with time according to an infinite system of decoupled linear ordinary differential equations. The discrete component of the solution is quasiperiodic in time and localized in space, while the continuous spectral component disperses to zero (e.g., in a local L^2 sense) as time advances. We seek to understand the dynamics in the *weakly nonlinear regime*, the regime where nonlinearity is present and where the initial data are small in an appropriately chosen norm.

Except in very special cases of integrable systems where, in an appropriate "nonlinear basis", bound (soliton) and radiation states evolve decoupled from one another, nonlinearity induces coupling and exchange of energy among bound and radiation states. It is this situation which interests us and we consider as examples the following two nonlinear wave equations of Hamiltonian type: the nonlinear Schrödinger equation (NLS) and the nonlinear Klein–Gordon equation (NLKG)[1]

$$\text{NLS}\quad i\partial_t\Phi = \big(-\Delta + V(x)\big)\Phi + g|\Phi|^2\Phi, \qquad \Phi(t,x)\in\mathbb{C},\ (t,x)\in\mathbb{R}^1\times\mathbb{R}^3 \tag{2.1}$$

$$\text{NLKG}\quad \big(\partial_t^2 - \Delta + m^2 + V(x)\big)u = gu^3, \qquad u = u(t,x)\in\mathbb{R},\ (t,x)\in\mathbb{R}^1\times\mathbb{R}^3. \tag{2.2}$$

The nonlinear coupling coefficient, g, is real and taken to be either zero or of order unity. The particular nonlinear Schrödinger equation, (2.1), with a nontrivial potential is also called the Gross–Pitaevskii equation (G–P). Applications, especially of the nonlinear Schrödinger equation, abound. These range from the fundamental physics of Bose–Einstein condensation [29,16] to nonlinear optics, e.g., nonlinear optical pulse propagation in inhomogeneous media [19,18].

The remainder of the chapter is outlined as follows:

- In Section 3 we shall introduce solitary wave solutions of the nonlinear Schrödinger equation, (2.1).
- We then discuss a variational approach to H^1 orbital Lyapunov stability of solitary waves in Section 4.
- The detailed behavior of solutions containing solitary wave components requires a detailed understanding of spectral properties of the solitary wave. The linearization about a stable solitary wave may have (a) discrete spectrum consisting of eigenstates with zero frequency associated with the equation's symmetries, and neutral ("internal") oscillatory eigenstates and (b) continuous spectrum associated with spatially extended radiation states. The presence or absence of these neutral oscillatory states, a property which is not derivable from the variational characterization the solitary wave, has an important effect on the dynamics on all time scales. Section 5 contains a discussion of asymptotic stability of solitary waves in the simple case where there are no neutral oscillations.

[1] Two other examples are cited at the end of this section. We have not attempted a comprehensive survey in this chapter.

- The case where there are neutral oscillatory eigenstates is considerably more rich in phenomena and requires deeper mathematical study. We shall see that these latter states typically decay to zero on very large time scales. The mechanism for decay is nonlinearity induced resonance of discrete and continuum states; the continuous spectral modes act as an effective dissipative heat bath with computable dissipation rate. In Section 6 the ideas and methods of analysis are introduced in the simpler context of the nonlinear Klein–Gordon equation. Then, in Section 7 we return to NLS/G–P to study the weakly nonlinear regime of multimode nonlinear Schrödinger equations.

A theme throughout this article is that we view each PDE as a Hamiltonian system comprised of two subsystems: (a) a finite-dimensional subsystem describing the evolution of coherent spatially localized states and (b) an infinite-dimensional part, governing the radiation of energy to spatial infinity. For a general small norm initial condition, the solution has different behaviors on different time scales: "initial phase", "large but finite time" and "infinite time". This behavior is elucidated by derivation of an appropriate *normal form*, which makes explicit the key mechanism for energy transfer among bound and radiation states. *The direction of energy flow is an emerging property, a consequence of the initial condition being localized, resonant coupling of bound to dispersive waves due to nonlinearity and the property of local decay of dispersive waves.*

There are close connections between these phenomena and their analysis with the computation of lifetimes of quantum states (transition theory), the perturbation theory of embedded eigenvalues in continuous spectra, and parametrically forced Hamiltonian systems; see, for example, [41–43,24,25,37,38].

In conclusion we remark that the asymptotic stability and scattering of coherent structures for infinite volume Hamiltonian systems has been considered in other contexts as well. Two important other studies are (i) the long time dynamics resulting from a classical particle interacting with a scalar wave field; see, for example, [26] and (ii) the stability of the Minkowski metric for the Einstein equations of the gravitational field [10].

3. Linear and nonlinear bound states

In this section we introduce bound states of the linear ($g = 0$) and nonlinear ($g \neq 0$) Schrödinger equation (2.1).

Bound states of the unperturbed problem

Let $H = -\Delta + V(x)$. We assume that $V(x)$ is smooth, real-valued and sufficiently rapidly decaying, so that H defines a self-adjoint operator in L^2. Additionally, we assume that the spectrum of H consists of continuous spectrum extending from zero to positive infinity and two discrete negative eigenvalues, each of multiplicity one[2]:

$$\sigma(H) = \{E_{0*}, E_{1*}\} \cup [0, \infty).$$

[2] The general case of any finite number of bound states can be considered as well. The case of $m \leqslant 2$ bound states captures all key phenomena we wish to discuss and keeps the presentation as simple as possible.

Therefore, there exist eigenstates, which smooth, square-integrable normalized functions, $\psi_{j*}(x),\ j = 0, 1$, such that

$$H\psi_{j*} = E_{j*}\psi_{j*}, \quad \langle\psi_{j*}, \psi_{k*}\rangle = \delta_{jk}. \tag{3.1}$$

We also introduce spectral projections onto the discrete eigenstates and continuous spectral part of H, respectively:

$$P_{j*}f \equiv \langle\psi_{j*}, f\rangle\psi_{j*}, \quad j = 0, 1,$$
$$P_{c*} \equiv I - P_{0*} - P_{1*}.$$

Nonlinear bound states

We seek solutions of (2.1) of the form

$$\phi = e^{-iEt}\Psi_E.$$

Substitution into (2.1) yields the following elliptic problem for the bound states of NLS

$$H\Psi_E + g|\Psi_E|^2\Psi_E = E\psi_E, \quad \psi_E \in H^1. \tag{3.2}$$

Note that if Ψ_E is any solution of (3.2) then for any $\theta \in \mathbb{R}$, $\Psi_E e^{i\theta}$ is a solution.

THEOREM 3.1 [35]. *For each $j = 0, 1$ we have a one-parameter family, bound states depending on the complex parameter α_j and defined for $|\alpha_j|$ sufficiently small*:

$$\Psi_{\alpha_j}(x) \equiv \alpha_j\bigl(\psi_{j*}(x) + \mathcal{O}\bigl(|\alpha_j|^2\bigr)\bigr),$$
$$E_j = E_{j*} + \mathcal{O}\bigl(|\alpha_j|^2\bigr).$$

For α_j complex and $|\alpha_j|$ small, the set $\{\Psi_{\alpha_0}\}$ is called the nonlinear ground state family and $\{\Psi_{\alpha_j}\colon\ j \geqslant 1\}$, the family of nonlinear excited states. Below, we shall also use the notation Ψ_{E_j} to denote a real-valued nonlinear bound state and parametrize the family of states by $\Psi_{E_j}(x)e^{i\theta},\ \theta \in \mathbb{R}$.

The proof uses standard bifurcation theory [31], which is based on the implicit function theorem. The analysis extends to the case of nonlocal nonlinearities.

In what follows we shall "time-modulate" these bound states. For convenience, we shall use the notation: $\Psi_j(t, x) = \Psi_{\alpha_j(t)}$ and $E_j(t) = E_j(|\alpha_j(t)|^2)$.

An alternative approach to the construction of nonlinear bound states is by *variational methods*. The variational characterization is of particular interest in the case of the ground state, due to its role in establishing its *dynamic* stability. Our point of departure for the variational approach is the observation that NLS has the following two conserved integrals, which are constant in time on solutions of NLS:

$$\mathcal{H}[\Phi] \equiv \int |\nabla\Phi|^2 + V(x)|\Phi|^2 + \frac{1}{2}g|\Phi|^4\,dx, \tag{3.3}$$

$$\mathcal{N}[\Phi] = \int |\Phi|^2\,dx, \tag{3.4}$$

$\mathcal{H}$ is a Hamiltonian, which generates NLS;

$$i\partial_t\Phi = \frac{\delta\mathcal{H}[\Phi,\Phi^*]}{\delta\Phi^*}.$$

Its time-invariance for the NLS flow is associated with time-translation symmetry, while the time-invariance of $\mathcal{N}$ is related to the phase symmetry $\Phi \mapsto \Phi e^{i\gamma}$, $\gamma \in \mathbb{R}$.

Nonlinear bound states of NLS are H^1 solutions, $F_\star$, of the elliptic equation

$$HF_\star + g|F_\star|^2F_\star = E_\star F_\star, \tag{3.5}$$

for some choice of E and can also be viewed as critical points of the functional

$$J_E[f] \equiv \mathcal{H}[F] + E\mathcal{N}[F]. \tag{3.6}$$

That is, we have that the first variation of $J_{E_\star}$ vanishes at $E_\star$, i.e. $\delta J_{E_\star}[F_\star] = 0$.

The nonlinear ground state has a characterization as a constrained minimizer

$$I_\theta = \inf\bigl\{\mathcal{H}[F]\colon\ F \in H^1,\ \mathcal{N}[F] = \theta\bigr\}. \tag{3.7}$$

For θ small, the minimum in (3.7) is attained at the ground state obtained in Theorem 3.1. The value of the frequency parameter of a ground state Ψ_E depends on θ.

4. Orbital stability of ground states

In this section we discuss the orbital Lyapunov stability of ground states of NLS. Note that by the phase invariance of NLS, we have that the *orbit* of the ground state

$$\mathcal{O}_{\mathrm{gs}} = \bigl\{\Psi_{E_0}(x)e^{i\gamma}\colon\ \gamma \in [0,2\pi)\bigr\} \tag{4.1}$$

is a one-parameter family of ground states. The ground state is stable in the following sense. If initially $\Phi(x,t=0)$ is H^1 close to some phase-translate of Ψ_{E_0} then, for all $t \neq 0$, $\Phi(x,t)$ is H^1 close to some (typically t dependent) phase-translate of Ψ_{E_0}. In order to make this precise, we introduce a metric which measures the distance from an arbitrary H^1 function to the ground state orbit:

$$\mathrm{dist}(u,\mathcal{O}_{\mathrm{gs}}) = \inf_\gamma \bigl\|u - \Psi_0 e^{i\gamma}\bigr\|_{H^1}. \tag{4.2}$$

Thus a more precise statement of stability is as follows. For any $\varepsilon > 0$ there is a $\delta > 0$ such that if

$$\mathrm{dist}\big(\Phi(\cdot,0),\mathcal{O}_{\mathrm{gs}}\big) < \delta \tag{4.3}$$

then for all $t \neq 0$

$$\mathrm{dist}\big(\Phi(\cdot,t),\mathcal{O}_{\mathrm{gs}}\big) < \varepsilon.$$

The proof of stability is now sketched. Let ε be an arbitrary positive number. We have for $t \neq 0$, by choosing δ in (4.3) sufficiently small

$$\begin{aligned}
\varepsilon^2 &\sim J_{E_0}\big[\Phi(\cdot,0)\big] - J_{E_0}[\Psi_0] \\
&= J_{E_0}\big[\Phi(\cdot,t)\big] - J_{E_0}[\Psi_0] \quad \text{by conservation laws} \\
&= J_{E_0}\big[\Phi(\cdot,t)e^{i\gamma}\big] - J_{E_0}[\Psi_0] \quad \text{by phase invariance} \\
&= J_{E_0}\big[\Psi_0 + u(\cdot,t) + iv(\cdot,t)\big] - J_{E_0}[\Psi_0] \\
&\quad \text{(definition of the perturbation } u+iv,\ u,v \in \mathbb{R}) \\
&\sim \big(L_+u(t),u(t)\big) + \big(L_-v(t),v(t)\big) \\
&\quad \text{(by Taylor expansion and } \delta J_{E_0}[\Psi_0] = 0).
\end{aligned} \tag{4.4}$$

The operators L_+ and L_- are, respectively, the real and imaginary parts of the second variational derivative of J_{E_0}, the linearized operator about the ground state. If L_+ and L_- were positive definite operators, implying the existence of positive constants C_+ and C_- such that

$$(L_+u,u) \geqslant C_+\|u\|_{H^1}^2, \tag{4.5}$$

$$(L_-v,v) \geqslant C_-\|v\|_{H^1}^2 \tag{4.6}$$

for all $u,v \in H^1$, then it would follow from (4.4) that the perturbation about the ground state, $u(x,t) + iv(x,t)$, would remain of order ε in H^1 for all time $t \neq 0$. The situation is however considerably more complicated. The relevant facts to note are as follows.

(1) $L_-\Psi_0 = 0$, with $\Psi_0 > 0$. Hence, Ψ_0 is the ground state of L_-, $0 \in \sigma(L_-)$, and L_- is a nonnegative with continuous spectrum $[|E_0|,\infty)$.

(2) For small L^2 nonlinear ground states, L_+ has exactly one strictly negative eigenvalue and continuous spectrum $[|E_0|,\infty)$.

The zero eigenvalue of L_- and the negative eigenvalue of L_+ constitute two *bad* directions, which are treated as follows, noting that $u(\cdot,t)$ and $v(\cdot,t)$ are not arbitrary H^1 functions but are rather constrained by the dynamics of NLS.

To control L_-, we choose $\gamma(t)$ so as to minimize the distance of the solution to the ground state orbit, (4.2). This yields the codimension one constraint on v: $(v(\cdot,t),\Psi_0) = 0$, subject to which (4.6) holds with $C_- > 0$.

To control L_+, we observe that since L^2 is invariant on solutions, we have the codimension constraint on u: $(u(\cdot,t),\Psi_0)=0$. Although Ψ_0 is not the ground state of L_+, it can be shown by constrained variational analysis that for small amplitude nonlinear ground states, $C_+>0$ in (4.5).

Thus, positivity (coercivity) estimates (4.5) and (4.6) hold and J_{E_0} serves as a Lyapunov functional which controls the distance of the solution to the ground state orbit. The argument presented here appears in greater detail and greater generality in [54], where it is proved that

$$\partial_E \|\psi_E\|_2^2 > 0 \tag{4.7}$$

implies orbital stability of any constrained energy *local* minimizers. The approach is inspired by the seminal article [2], who refers to origins in the work of Boussinesq. A general functional analytic setting is given in [20], where it is shown that (4.7) is necessary and sufficient for stability. See also the related compactness-based variational approach to stability in [9] for a proof of orbital stability of constrained *global* minimizers.

5. Asymptotic stability of ground states I. No neutral oscillations

The type of stability discussed in the previous section is that encountered in the setting of finite-dimensional Hamiltonian systems; if the initial conditions are close to the group orbit of the ground state, then the solution remains close for all time. *Asymptotic stability*, in which the solution asymptotically converges to the state of interest, cannot apply in finite-dimensional Hamiltonian systems as this would violate the volume preserving constraint on the phase flow. However, in an infinite-dimensional setting not all norms are equivalent and there are processes, namely radiation of energy to infinity, which facilitate asymptotic convergence to a preferred state.

We now discuss such a result for small amplitude ground states of NLS. The notion of stability can be seen as a natural refinement of the ideas of Section 4. Instead of freezing the “energy” E of the individual ground state, whose stability is under study, and allowing the phase, θ to evolve in order to *approximately* track the solution, we instead construct $E(t)$ and $\theta(t)$ to evolve in time in such a way that the deviation of the solution, $\phi(\cdot,t)$ and the *modulated* ground state $\Psi_{E(t)}e^{-i(\int_0^t E(s)\,ds-\theta(t))}$ tends to zero in an appropriate norm.

Before stating a result along these lines we need to briefly discuss some spectral properties of the ground state. Recall that by stability of the ground state (in the Lyapunov sense) it is necessary that all spectrum of the generator of the linearized flow, $-i\mathcal{H}_0$ about the ground state lie on the imaginary axis. Zero is an isolated eigenvalue, arising from symmetries of the equation and the continuous spectrum consists of vertical semi-infinite lines $[i|E_0|,i\infty)$ and $(-i\infty,-i|E_0|]$. The key hypotheses are: (i) that $\mathcal{H}_0$ has no nonzero eigenvalues in the gap between $-i|E_0|$ and $i|E_0|$, and thus solutions of the linearized evolution with periodic or quasiperiodic oscillations about the ground state are precluded (see $(h3)$ below), and (ii) that H has neither an eigenvalue nor a “resonance” at zero energy [21], a hypothesis on the behavior of $(H-zI)^{-1}$ as $z\to 0$, which holds for generic $V(x)$, and ensures sufficiently strong dispersive time-decay estimates of the linearized evolution.

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THEOREM 5.1 [39,40,32]. *Consider NLS in spatial dimension $n = 3$. Assume the following*

(h1) *The multiplication operator $f \mapsto \langle x\rangle^\sigma V(x) f$, where $\sigma > 3$ is bounded on $H^2(\mathbb{R}^3)$,*
(h2) *The Fourier transform of V, $\widehat{V} \in L^1(\mathbb{R}^3)$*
(h3) *Zero is neither an eigenvalue nor a resonance of the operator $H = -\Delta + V$.*
(h4) *H_0 acting on L^2 has exactly one negative eigenvalue $E_{0*} < 0$, with $H_0\psi_{0*} = E_{0*}\psi_{0*}$, $\|\psi_{0*}\|_2 = 1$.*

Let the initial condition ϕ_0 be sufficiently small in $H^1 \cap L^2(\langle x\rangle^2\,dx)$. Then, there exist smooth functions $E(t)$ and $\theta(t)$, such that $\lim_{t\to\pm\infty} E(t) = E^\pm$ and $\lim_{t\to\pm\infty}\theta(t) = \theta^\pm$ exist and

$$\lim_{t\to\pm\infty} \left\|\phi(\cdot,t) - e^{-i(\int_0^t E(s)\,ds-\theta(t))}\Psi_{E(t)}\right\|_{L^4(\mathbb{R}^3)} = 0. \tag{5.1}$$

To prove Theorem 5.1 we seek a solution in the form of a modulated nonlinear ground state and a dispersive correction:

$$\phi(x,t) = \Psi_{E(t)} e^{-i(\int_0^t E(s)\,ds-\theta(t))} + \eta(t). \tag{5.2}$$

Substitution into NLS and projection onto the subspaces associated with the discrete and continuum modes of the linearized flow yields a coupled system of equations for $E(t), \theta(t)$ and $\eta(t)$. Asymptotic convergence of $E(t)$ and $\theta(t)$, and decay of $\eta(\cdot,t)$ as $t\to\pm\infty$ are proved using local decay [21] and dispersive L^p, $p > 2$, estimates [22].

We postpone further discussion of this analysis to our discussion of the case where the linearized dynamics has neutral oscillations about the ground state, e.g., which may result from H possessing two or more eigenvalues; see Sections 6 and 7. The analogous coupled ODE–PDE system requires considerably deeper study. In the next section, Section 6, we discuss the metastability and decay of neutral oscillations in the context of the nonlinear Klein–Gordon equation. Then, in Section 7 we turn to the case of NLS, where the same mechanisms are at work.

6. Resonance and radiation damping of neutral oscillations—metastability of bound states of the nonlinear Klein–Gordon equation

Consider the nonlinear Klein–Gordon equation (NLKG) with a potential $V(x)$, assumed to be smooth and sufficiently rapidly decaying as $|x|\to\infty$:

$$\left(\partial_t^2 + B^2\right)u = gu^3. \tag{6.1}$$

Here, $B^2 = -\Delta + m^2 + V(x)$, is a strictly positive operator with a single eigenvalue, Ω^2, satisfying $0 < \Omega^2 < m^2$, with corresponding L^2-normalized eigenfunction $\varphi(x)$, which satisfies $B^2\varphi = \Omega^2\varphi$. We also assume that the essential spectrum of B^2 is absolutely continuous and is given by the semi-infinite interval $[m^2,\infty)$. The parameter, g, is taken to be real and either zero or of order unity.

Corresponding to the discrete spectral part of B^2 is a family of time-periodic and spatially localized solutions:

$$u_b(t,x;R,\theta) = R\cos(\Omega t+\theta)\varphi(x) \tag{6.2}$$

of the linear Klein–Gordon equation

$$\left(\partial_t^2 + B^2\right)u = 0. \tag{6.3}$$

For any sufficiently smooth and localized (finite energy) initial conditions, the solution to (6.3) has the decomposition:

$$u(t,x) = u_b(t,x;R_0,\theta_0) + \eta(t,x), \tag{6.4}$$

where R_0 and θ_0 are constants determined by the initial conditions and $\eta(t,x)$ disperses to zero as t tends to infinity.

QUESTION. What is the character of solutions to the *nonlinear* problem $g \neq 0$ for initial data which are small in an appropriate norm?

REMARK 6.1. This question is of independent interest for the nonlinear Klein–Gordon equation. We wish, however, to also point out the relation of this question to the large time asymptotics of NLS. Recall our assumption in Theorem 5.1 that H have only one eigenvalue, E_{0*}, which by Theorem 3.1, gives rise to a branch of nonlinear ground states. If H has two eigenvalues, then there is an additional branch of nonlinear excited states. For NLKG, the role of the nonlinear ground state is played by the zero solution and the dynamics of the nonlinear excited state can be understood by our analysis of how the unperturbed time-periodic bound state of the Klein–Gordon equation decays due to resonant energy transfer to radiation modes under a nonlinear Hamiltonian perturbation.

The following result [44] gives a detailed description of solutions.

THEOREM 6.1. *Consider the nonlinear Klein–Gordon equation* (6.1), *with* $V(x)$, *real-valued and satisfying*

(h1) *There exists* $\delta > 5$ *such that for all* $|\alpha| \leqslant 2$, $|\partial^\alpha V(x)| \leqslant C_\alpha \langle x\rangle^{-\delta}$.
(h2) $(-\Delta+1)^{-1}((x\cdot\nabla)^l V(x))(-\Delta+1)^{-1}$ *is bounded on* L^2 *for* $|l| \leqslant 10$.
(h3) *Zero is not a resonance of the operator* $-\Delta + V$, [21].
(h4) *Nonlinear analogue of the Fermi Golden Rule resonance condition*; *see, for example*, [42].

$$\Gamma \equiv \frac{\pi}{3\Omega}\left(P_c\varphi^3, \delta(B-3\Omega)P_c\varphi^3\right) \equiv \frac{\pi}{3\Omega}\left|\left(\mathcal{F}_c\varphi^3\right)(3\Omega)\right|^2 > 0.$$

Here, P_c *denotes the projection onto the continuous spectral subspace of* B *and* $\mathcal{F}_c$ *denotes the Fourier transform relative to the continuous spectral part of* B.

Assume that the initial data $u(x,0)$ *and* $\partial_t u(x,0)$ *are such that their norms are sufficiently small in* $W^{2,2} \cap W^{2,1}$ *and* $W^{1,2} \cap W^{1,1}$*, respectively. Then, the solution of the initial value problem with* $\lambda \neq 0$ *decays to zero as* $t \to \pm\infty$*. In particular,*

$$u(x,t) = R(t)\cos\bigl(\Omega t + \theta(t)\bigr)\varphi(x) + \eta(x,t),$$
$$\bigl|R(t)\bigr| \leqslant C|t|^{-1/4}, \ \bigl\|\eta(\cdot,t)\bigr\|_{L^8} \leqslant C|t|^{-3/4}. \tag{6.5}$$

To prove this result, it is natural to first decompose the solution into its discrete and continuous spectral components:

$$u(x,t) = a(t)\varphi(x) + \eta(x,t), \quad \bigl\langle \varphi, \eta(\cdot,t)\bigr\rangle = 0. \tag{6.6}$$

Then, a and η satisfy a coupled system equations, which in the zero amplitude limit is the decoupled linear system:

$$\bigl(\partial_t^2 + \Omega\bigr)a(t) = 0, \qquad \bigl(\partial_t^2 + B^2\bigr)\eta(t,x) = 0. \tag{6.7}$$

The latter has time-periodic and spatially localized solution $a(t) = R\cos(\Omega t + \theta)$, $\eta \equiv 0$, corresponding to (6.2). For small norm solutions, the equations for a and η are coupled, and can be analyzed by a variant of the arguments outlined in Section 7. We point out that the slow decay of the solution, $u(x,t)$, quantified in the estimates (6.5) is governed by the effective oscillator equation

$$\partial_t^2 a + \bigl(\Omega^2 + \mathcal{O}\bigl(|a|^2\bigr)\bigr)a \sim -\Gamma a^4 \partial_t a, \quad \Gamma > 0. \tag{6.8}$$

Equation (6.8) is a *damped* equation, which governs the transfer of energy from the oscillator to the dispersive wave-field. Γ is the derived nonlinear friction coefficient.

7. Asymptotic stability II. Multiple bound states and selection of the ground state in NLS

We now return to the nonlinear Schrödinger equation (NLS)

$$i\partial_t \Phi = H\Phi + g|\Phi|^2\Phi, \quad H = -\Delta + V. \tag{7.1}$$

In Section 5 we saw, in the case where H has exactly one bound state, that solutions with small initial conditions asymptotically, as $t \to \pm\infty$, approach an asymptotic ground state. In this section we consider the case where the Schrödinger operator $H = -\Delta + V(x)$ has multiple bound states.

For the linear Schrödinger equation ($g = 0$), the solution can be expressed as

$$e^{-iHt}\phi_0 = \sum_j \langle \psi_{j*}, \phi_0\rangle \psi_{j*} e^{-iE_{j*}t} + e^{-iHt}P_{c*}\phi_0, \tag{7.2}$$

where $e^{-iHt}P_{c*}\phi_0$ decays to zero as $t \to \pm\infty$. The time decay of the continuous spectral part of the solution can be expressed, under suitable smoothness, decay and genericity assumptions on $V(x)$, in terms of *local decay estimates* [21,30]:

$$\left\| \langle x \rangle^{-\sigma} e^{-iHt} P_{c*}\phi_0 \right\|_{L^2(R^3)} \leqslant C\langle t \rangle^{-3/2} \left\| \langle x \rangle^{\sigma} \phi_0 \right\|_{L^2(R^3)}, \tag{7.3}$$

$\sigma \geqslant \sigma_0 > 0$, and $L^1 \to L^\infty$ *decay estimates* [22,55]

$$\left\| e^{-iHt} P_{c*}\phi_0 \right\|_{L^\infty(R^3)} \leqslant C|t|^{-3/2} \, \|\phi_0\|_{L^1(R^3)}. \tag{7.4}$$

Therefore, the large time behavior of typical solutions of the linear Schrödinger equation ($g = 0$) is quasiperiodic.

Consider now the case of NLS with $g \neq 0$ and V is such that the Schrödinger operator H has exactly two bound states: $\psi_{0*}e^{-iE_{0*}t}$ and $\psi_{1*}e^{-iE_{1*}t}$, with $H\psi_{j*} = E_{j*}\psi_{j*}$, $\psi_{j*} \in L^2$. By Theorem 3.1 NLS has ground state and excited state branches of nonlinear bound states $\Psi_{\alpha_0}e^{-iE_0t}$ and $\Psi_{\alpha_1}e^{-iE_1t}$, with $\Psi_{\alpha_j} \in L^2$ satisfying

$$H\Psi_{\alpha_j} + g|\Psi_{\alpha_j}|^2\Psi_{\alpha_j} = E_j\Psi_{\alpha_j}. \tag{7.5}$$

Here, α_j denotes a coordinate along the jth nonlinear bound state branch and

$$E_j = E_{j*} + \mathcal{O}\big(|\alpha_j|^2\big).$$

We are interested in the behavior of solutions to NLS with initial conditions of small norm. In contrast to asymptotic quasiperiodic behavior (7.2)–(7.3), we find that the generic long time behavior is a ground state plus dispersive radiation [46]:

THEOREM 7.1. *Consider NLS with a $V(x)$ a smooth and short range (sufficiently decaying) potential supporting two bound states as described above. Furthermore, assume that the linear Schrödinger operator, H, has no zero energy resonance* [21]. *Assume the (generically satisfied) nonlinear Fermi golden rule resonance condition*[3]

$$\Gamma_{\omega_*} \equiv g^2\pi\big\langle \psi_{0*}\psi_{1*}^2, \delta(H - \omega_*)\psi_{0*}\psi_{1*}^2 \big\rangle > 0 \tag{7.6}$$

holds, where

$$\omega_* = 2E_{1*} - E_{0*} > 0. \tag{7.7}$$

Then, there exist constants $k_0 \geqslant 3$ and $\sigma_0 \geqslant 2$ such that for any $\sigma \geqslant \sigma_0$ and $k \geqslant k_0$, if $\|\langle x \rangle^\sigma \phi(0)\|_{H^k}$ is sufficiently small, we have the following characterization of the large time dynamics of the solution $\phi(t)$ of the initial value problem for NLS with initial data $\phi(0)$.

[3]The operator $f \mapsto \delta(H - \omega_*)f$ projects f onto the generalized eigenfunction of H with generalized eigenvalue ω_*. The expression in (7.6) is finite by local decay estimates (7.3); see, e.g., [42].

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As $t \to \infty$

$$\phi(t) \to e^{-i\omega_j(t)} \Psi_{\alpha_j(\infty)} + e^{i\Delta t}\phi_+, \tag{7.8}$$

in L^2, where either *$j = 0$ or $j = 1$. The phase ω_j satisfies*

$$\omega_j(t) = \omega_j^\infty t + \mathcal{O}(\log t). \tag{7.9}$$

Here, $\Psi_{\alpha_j(\infty)}$ is a nonlinear bound state (Section 3), with frequency $E_j(\infty)$ near E_{j*}. When $j = 0$, the solution is asymptotic to a nonlinear ground state, while in the case $j = 1$ the solution is asymptotic to a nonlinear excited state. Generically, $j = 0$.

See also the related results on [4–6,13,14,48,49]. Nongeneric solutions which converge asymptotically to an excited state were constructed in [50].

We give a sketch of the analysis. In analogy with the approach discussed in Section 5 for the one bound state case, we represent the solution in terms of the dynamics of the bound state part, described through the evolution of the *collective coordinates* $\alpha_0(t)$ and $\alpha_1(t)$, and a remainder ϕ_2, whose dynamics is controlled by a dispersive equation. In particular we have

$$\phi(t,x) = e^{-i\int_0^t E_0(s)\,ds - i\widetilde{\Theta}(t)} \big(\Psi_{\alpha_0(t)} + \Psi_{\alpha_1(t)} + \phi_2(t,x)\big). \tag{7.10}$$

We substitute (7.10) into NLS and use the nonlinear equations (7.5) for Ψ_{α_j} to simplify. Anticipating the decay of the excited state, we center the dynamics about the ground state. We therefore obtain for $\Phi_2 \equiv (\phi_2, \overline{\phi_2})^{\mathrm{T}}$ the equation:

$$i\partial_t \Phi_2 = \mathcal{H}_0(t)\Phi_2 + \mathcal{G}\big(t, x, \Phi_2; \partial_t\vec{\alpha}(t), \partial_t\vec{\alpha}, \partial_t\widetilde{\Theta}(t)\big), \tag{7.11}$$

where $\mathcal{H}_0(t)$ denotes the matrix operator which is the linearization about the time-dependent nonlinear ground state $\Psi_{\alpha_0(t)}$. The idea is that in order for $\phi_2(t,x)$ to decay dispersively to zero we must choose $\alpha_0(t)$ and $\alpha_1(t)$ to evolve in such a way as to remove all secular resonance terms from $\mathcal{G}$. Thus we require,

$$P_b\big(\mathcal{H}_0(t)\big)\Phi_2(t) = 0, \tag{7.12}$$

where $P_b(\mathcal{H}_0)$ and $P_c = I - P_b(\mathcal{H}_0)$ denote the discrete and continuous spectral projections of $\mathcal{H}_0$. Since the discrete subspace of $\mathcal{H}_0(t)$ is four-dimensional (consisting of a generalized null space of dimension two plus two oscillating neutral modes), (7.12) is equivalent to four orthogonality conditions implying four differential equations for α_0, α_1 and their complex conjugates. These equations are coupled to the dispersive partial differential equation for Φ_2. At this stage we have that NLS is equivalent to a dynamical system consisting of a finite-dimensional part governing $\vec{\alpha}_j = (\alpha_j, \overline{\alpha_j})$, $j = 0, 1$, coupled to an infinite-dimensional dispersive part governing Φ_2:

$$\begin{aligned} i\partial_t\vec{\alpha} &= \mathcal{A}(t)\vec{\alpha} + \vec{F}_\alpha, \\ i\partial_t\Phi_2 &= \mathcal{H}_0(t)\Phi_2 + \vec{F}_\phi. \end{aligned} \tag{7.13}$$

We expect $\mathcal{A}(t)$ and $\mathcal{H}_0(t)$ to have limits as $t \to \pm\infty$. We fix $T > 0$ arbitrarily large, and to study the dynamics on the interval $[0, T]$. In this we follow the strategy of [5,14]. We shall rewrite (7.13) as:

$$\begin{aligned} i\partial_t \vec{\alpha} &= \mathcal{A}(T)\vec{\alpha} + \big(\mathcal{A}(t) - \mathcal{A}(T)\big)\vec{\alpha} + \vec{F}_\alpha, \\ i\partial_t \Phi_2 &= \mathcal{H}_0(T)\Phi_2 + \big(\mathcal{H}_0(t) - \mathcal{H}_0(T)\big)\Phi_2 + \vec{F}_\phi \end{aligned} \tag{7.14}$$

and implement a perturbative analysis about the *time-independent* reference linear, respectively, matrix and differential, operators $\mathcal{A}(T)$ and $\mathcal{H}_0(T)$.

More specifically, we analyze the dynamics of (7.14) by using (1) the eigenvalues of $\mathcal{A}(T)$ to calculate the key resonant terms and (2) the dispersive estimates of $e^{-i\mathcal{H}_0(T)t}P_c(T)$ [13,17,33,34].

Next we explicitly factor out the rapid oscillations from α_1 and show that, after a near identity change of variables $(\alpha_0, \alpha_1) \mapsto (\tilde{\alpha}_0, \tilde{\beta}_1)$, that the modified ground and excited state amplitudes satisfy the perturbed *dispersive normal form*:

$$\begin{aligned} i\partial_t \tilde{\alpha}_0 &= (c_{1022} + i\Gamma_\omega)|\tilde{\beta}_1|^4 \tilde{\alpha}_0 + F_\alpha[\tilde{\alpha}_0, \tilde{\beta}_1, \eta, t], \\ i\partial_t \tilde{\beta}_1 &= (c_{1121} - 2i\Gamma_\omega)|\tilde{\alpha}_0|^2 |\tilde{\beta}_1|^2 \tilde{\beta}_1 + F_\beta[\tilde{\alpha}_0, \tilde{\beta}_1, \eta, t]. \end{aligned} \tag{7.15}$$

REMARK 7.1. For finite-dimensional Hamiltonian systems the normal form coefficients are real. That they are complex here, with imaginary part $\sim \Gamma_\omega$, is to due NLS being an infinite-dimensional Hamiltonian system with discrete spectral states resonating with continuum spectral states. The positivity of Γ_ω reflects the energy flow from the excited state to the ground state and continuum states, and the resulting damping of the nonlinear excited state.

It follows from (7.15) that a *Nonlinear Master Equation* governs $P_j = |\tilde{\alpha}_j|^2$, the power in the jth mode:

$$\begin{aligned} \frac{dP_0}{dt} &= 2\Gamma P_1^2 P_0 + R_0(t), \\ \frac{dP_1}{dt} &= -4\Gamma P_1^2 P_0 + R_1(t). \end{aligned} \tag{7.16}$$

Coupling to the dispersive part, Φ_2, is through the source terms R_0 and R_1. The expression "master equation" is used since the role played by (7.16) is analogous to the role of master equations in the quantum theory of open systems [15].

REMARK 7.2. An interesting phenomenon is anticipated by the system obtained from (7.16), by dropping the decaying correction terms $R_j(t)$:

$$\begin{aligned} \frac{dp_0}{dt} &= 2\Gamma p_1^2 p_0, \\ \frac{dp_1}{dt} &= -4\Gamma p_1^2 p_0. \end{aligned} \tag{7.17}$$

First, it is easy to see from (7.17) that $p_1(t)$ decays to zero as $t \to \infty$ unless $p_0(0) = 0$. Furthermore, note that the resulting equation has the conservation law $2p_0(t) + p_1(t) = 2p_0(0) + p_1(0)$, the "total energy". Therefore, since $p_1(t) \to 0$ as $t \to \infty$, we have

$$p_0(\infty) = p_0(0) + \frac{1}{2}p_1(0).$$

Thus we expect that half the energy in decaying excited state is transferred to the ground state and half to continuum radiation.

The detailed behavior of the system (7.16) coupled to the dispersive part can be characterized on short, intermediate and long time scales. We consider the system (7.16) on three time intervals: $I_0 = [0, t_0]$ (initial phase) $I_1 = [t_0, t_1]$ (embryonic phase) and $I_2 = [t_1, \infty)$ (selection of the ground state). A careful analysis reveals an effective finite-dimensional reduction to a system of equations for the "effective mode powers": $Q_0(t)$ and $Q_1(t)$, closely related to $P_0(t)$ and $P_1(t)$, whose character on different time scales dictates the full infinite-dimensional dynamics, in a manner analogous to role of a center manifold reduction of a dissipative system [7].

Initial phase—$t \in I_0 = [0, t_0]$. Here, I_0 is the maximal interval on which $Q_0(t) \leqslant 0$. If $t_0 = \infty$, then $P_0(t) = \mathcal{O}(\langle t\rangle^{-2})$ and the ground state decays to zero. In this case, we show that the excited state amplitude has a limit as well (with may or may not be zero). This case is nongeneric.

Embryonic phase—$t \in I_1 = [t_0, t_1]$. If $t_0 < \infty$, then for $t > t_0$:

$$\begin{aligned} \frac{dQ_0}{dt} &\geqslant 2\Gamma' Q_0 Q_1^2, \\ \frac{dQ_1}{dt} &\leqslant -4\Gamma' Q_0 Q_1^2 + \mathcal{O}\big(\sqrt{Q_0}Q_1^m\big), \quad m \geqslant 4. \end{aligned} \tag{7.18}$$

Therefore, Q_0 is monotonically increasing; *the ground state grows*. Furthermore, if Q_0 is small relative to Q_1, then

$$\frac{Q_0}{Q_1} \quad \text{is montonically increasing,}$$

in fact exponentially increasing; *the ground state grows rapidly relative to the excited state.*

Selection of the ground state $t \in I_2 = [t_1, \infty)$. There exists a time $t = t_1$, $t_0 \leqslant t_1 < \infty$, at which the $\mathcal{O}(\sqrt{Q_0}Q_1^m)$ term in (7.18) is dominated by the leading ("dissipative") term. For $t \geqslant t_1$ we have

$$\begin{aligned} \frac{dQ_0}{dt} &\geqslant 2\Gamma' Q_0 Q_1^2, \\ \frac{dQ_1}{dt} &\leqslant -4\Gamma' Q_0 Q_1^2. \end{aligned} \tag{7.19}$$

It follows that $Q_0(t) \to Q_0(\infty) > 0$ and $Q_1(t) \to 0$ as $t \to \infty$; *the ground state is selected.*

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Appendix. Notation

H^s denotes the Sobolev space of functions obtain via the closure of C_0^∞ in a norm: $\|f\|_{H^s}^2 = \sum_{|\alpha|\leqslant s} \|\partial^\alpha f\|_{L^2}^2$.

$P_{b*} = P_{b*}(A)$ denotes the projection onto the discrete spectral subspace of bound states (L^2 eigenstates) of an operator A. $P_{c*} = I - P_{b*}$ denotes the projection onto the continuous spectral subspace.

$H = -\Delta + V$, self-adjoint Schrödinger operator on L^2, with smooth, sufficiently decaying potential, $V(x)$.

$\mathcal{H}_0$ matrix linearization of NLS about the ground state.

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