Theory of Nonlinear Dispersive Waves and Selection of the Ground State

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A theory of time-dependent nonlinear dispersive equations of the Schrödinger or Gross-Pitaevskii and Hartree type is developed. The short, intermediate and large time behavior is found, by deriving nonlinear master equations (NLME), governing the evolution of the mode powers, and by a novel multitime scale analysis of these equations. The scattering theory is developed and coherent resonance phenomena and associated lifetimes are derived. Applications include Bose-Einstein condensate large time dynamics and nonlinear optical systems. The theory reveals a nonlinear transition phenomenon, "selection of the ground state," and NLME predicts the decay of excited state, with half its energy transferred to the ground state and half to radiation modes. Our results predict the recent experimental observations of Mandelik *et al.* in nonlinear optical waveguides.

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Recent experimental [1–4] and theoretical [5–9] breakthroughs in the field of Bose-Einstein condensates (BECs) and the intense interest in nonlinear optical devices [10] necessitates the detailed analysis of time-dependent nonlinear dispersive equations, such as the time-dependent Gross-Pitaevski (GP) and nonlinear Schrödinger (NLS) equations in one or more spatial dimensions. Also, new coherent phenomena in soft condensed matter, such as macroscopic resonances [11,12], DNA-denaturation dynamics, and macromolecule dynamics, have rekindled the need to determine the large time behavior of time-dependent Hartree-Fock (HF) type equations. In contrast to linear scattering, where time-independent methods are used to compute an approximate S matrix for general multichannel processes, nonlinear problems are not amenable to such theory, except in completely integrable cases. Thus, mainly large scale numerical methods have been applied so far.

In this Letter we describe and apply a rigorous time-dependent theory and approach developed in Ref. [13] to provide detailed explicit behavior for a class of nonlinear dispersive partial differential equations, which include NLS, GP, and HF, on short, intermediate and infinite time scales. We show, as a consequence of our analysis, that in a multimode nonlinear dispersive systems which has multiple nonlinear bound states, that nonlinear resonant interactions lead to a crystallization of the coherent and localized part of the solution on the nonlinear ground state (selection of the ground state); the nonlinear excited states are metastable and decay at a rate given by a nonlinear analogue of Fermi's golden rule.

In very recent experimental work [4] on CW beams centered at wavelength, $\lambda = 2\pi/k_0$, propagating in multimode nonlinear AlGaAs waveguides, the output distribution of optical power is measured, and ground state selection and the partition law (4) have been demonstrated. Our results predict these observations and can be used to interpret the earlier work on photorefractive waveguides [14].

For definiteness we consider the nonlinear Schrödinger equation in three space dimensions:

$$i\partial_t \phi = H_0 \phi + gF(|\phi|^2)\phi. \qquad (1)$$

F denotes the nonlinearity, here taken to be local, $F(|\phi|^2) = |\phi|^2$, but more generally, of Hartree-Fock type $F(|\psi|^2) \equiv \int G(x, y)|\psi(y)|^2 dy$ with, for example, $G(x, y) = |x - y|^{-\alpha} e^{-r|x-y|}$, $r \geq 0$. g denotes the coupling coefficient, related to the scattering length in BECs and, in optics, to $-n_2$, the nonlinear Kerr coefficient. $H_0 = -\Delta + V(x)$, where $V(x)$ denotes a potential which decays to zero sufficiently rapidly at infinity, and for which H_0 has two bound states (for simplicity); $H_0\psi_{j*} = E_{j*}\psi_{j*}$, $j = 0, 1$. Such equations appear in many applications in which coherent soliton-like structures and their internal modes [15] interact with dispersive waves, e.g., [7,10–12,16,17,24]. The effective equations of an atom in a field or active media is also of this form [12,18]. The requirement on $V(x)$ that H_0 have (at least) two bound states makes the model of general interest and the phenomena very rich.

Nonlinear bound state solutions bifurcate from linear bound states for weakly nonlinear perturbations [19] giving rise to nonlinear ground state family and nonlinear excited state families (for two bound state Hamiltonians). Specifically, for energies close to E_{0*} and E_{1*}, the eigenvalues of H_0, there are nonlinear bound states: $e^{-iE_0 t}\psi_{E_0}$, $\psi_{E_1} e^{-iE_1 t}$, which solve (1). ψ_{E_0} and ψ_{E_1} are complex-valued (exponentially) localized solutions of $(H_0 + gF(|\psi_{E_i}|^2))\psi_{E_i} = E_i \psi_{E_i}$. When $g = 0$, $E_0 = E_{0*}$ and $E_1 = E_{1*}$ are values for which there are nontrivial solutions. For $g \neq 0$ there is a solution for all E near E_{i*}. ψ_{E_j} can be thought of as a *pinned* soliton, ground ($j = 0$) or excited state ($j = 1$), within the support of $V(x)$. We assume $\omega_* \equiv 2E_{1*} - E_{0*} > 0$, ensuring coupling of bound states to the continuum at second order; analogous results with slower decay rates hold more generally.

The main results we establish concern the time evolution of solutions to (1) for all data (with small energy). The large time behavior is as follows: For any initial data, with small energy the solution $\psi(t)$ of (1) is asymptotically given by

$$\psi(t) \to e^{-i\theta_0^\pm(t)} e^{-iE_j^\pm t} \psi_{E_j^\pm} + e^{i\Delta t}\psi_\pm, \quad \text{as } t \to \pm\infty,$$

in L^2. Generically, $j = 0$, corresponding to the ground state, while there is a finite dimensional set of data for which $j = 1$. Thus, for typical initial conditions we have ground state selection. We analyze the detailed dynamics by reduction of the NLS to a finite dimensional system, which dominates the full dynamics.

The main second result concerns the transient, *finite* time, behavior of the system, which is very rich: There are *three* time scales, determined by the initial data. In the first time interval, the dynamics is dominated by radiative terms (formative stage); once the initial radiative part propagates far enough from the support of $V(x)$, the soliton's position, the second period (embryonic stage) begins. This is marked by a *monotonic* (exponentially fast) increase in the ground state amplitude, relative to the excited state amplitude. This stage proceeds as long as the excited state part is larger than some fraction of the ground state part. Once the ground state reaches a size comparable with some (fixed) fraction of the excited state, the third and final stage begins (ground state selection); the ground state amplitude increases monotonically and the excited state decreases monotonically, but at a polynomial rate as $t \to \infty$. (This describes the generic case; the asymptotic state is given by an excited state [20] whenever the first stage persists to time equal infinity.) A different approach, based on linearization around the excited state for intermediate times and around the ground state for large times, gives similar results [21].

This phenomenon is quantified by our derivation of the nonlinear master equations (NLME) that govern the dynamics of the coupled ground and excited state modes (and the radiation modes). If we denote by $P_0(t)$ and $P_1(t)$, respectively, the (up to near-identity transformations) squared projection of the system's state onto the ground state and excited states, at time t, we have

$$\begin{aligned} \partial_t P_0 &= 2\Gamma P_0 P_1^2 + \rho_0(t) P_0 P_1^{M_0} + \mathcal{O}(t^{-5/2}), \\ \partial_t P_1 &= -4\Gamma P_0 P_1^2 + \rho_1(t)\sqrt{P_0} P_1^{M_1} + \mathcal{O}(t^{-5/2}), \end{aligned} \tag{2}$$

$$\begin{aligned} \Gamma &= \pi g^2 |\mathcal{F}[dF[\psi_{0*}\psi_{1*}]\psi_{1*}](\omega_*)|^2, \\ dF[\psi_{0*}\psi_{1*}]\psi_{1*} &= \int G(x-y)\psi_{0*}(y)\psi_{1*}(y)dy\psi_{1*}(x). \end{aligned} \tag{3}$$

$\rho_{M_0}(t)$ and $\rho_{M_1}(t)$ are small oscillatory functions of time, $M_0, M_1 \geq 3$, and $\mathcal{F}[q](\omega)$ denotes the projection of q onto the generalized eigenfunction of H_0 at frequency ω. The crucial number Γ is (generically) positive and given explicitly in terms of known eigenstates of H_0. $\Gamma \neq 0$ is the nonlinear Fermi golden rule for such systems and it gives the rate of *decoherence* and relaxation [17,18,22–24]. The behavior of these master equations (2) reflects the three time scales mentioned above, on which the behavior is very different. For large enough time, in the third time domain, the last two terms in (2) can be ignored. In this latter regime, it is easy to see that $P_1(t) \to 0$ as $t \to \infty$ and $\partial_t(2P_0 + P_1) = 0$. Therefore, $2P_0(\infty) = 2P_0(t_0) + P_1(t_0)$. It follows that

$$P_0(\infty) = P_0(t_0) + \tfrac{1}{2}P_1(t_0); \tag{4}$$

half of the excited state energy flows to the ground state (the other half goes to radiation), a kind of energy equipartition. (The factor 2 also appears in the linear analysis, and is interpreted as the ratio of relaxation to decoherence time [18,23].) Furthermore, it follows that for any initial state $(P_0(t_0), P_1(t_0))$ with $P_0(t_0) \neq 0$ the system converges to $(P_0(\infty), 0)$ with a rate $\sim(1 + 4\Gamma P_0(\infty)P_1(t_0)t)^{-1}$ (selection of the ground state). Combining the analysis of the NLME (2) for all time scales with the previous statements gives a complete description of the solution for all time scales and, in particular, the asymptotic behavior, relaxation and decoherence rates, the asymptotic profile and energy of the soliton-ground state.

We sketch our method, for the special case of (1) with cubic nonlinearity, $F(|\phi|^2)\phi = |\phi|^2\phi$. Our approach makes use of ideas from Refs. [13,22,25–27]. We begin with the Ansatz $\phi(t) \equiv e^{-i\theta(t)}[\psi_0(t) + \psi_1(t) + \phi_2(t)]$ where $\psi_0(t) \equiv \psi_{E_0(t)}$ is a solution of the ground state eigenvalue equation with energy $E_0(t)$, at time t. $E_0(t)$ will be determined later by orthogonality conditions [13,22,26]. Similarly $\psi_1(t)$ is an excited state eigenvector with eigenvalue $E_1(t)$. $\theta(t) \equiv \theta_0(t) + \tilde{\theta}(t)$; $\theta_0(t) = \int_0^t E_0(s)ds$. $\tilde{\theta}(t)$ will be chosen appropriately; it includes a (logarithmic) divergent phase. Substitution of the above Ansatz for ϕ into (1), and complexifying the equations $[\phi_2 \to (\phi_2, \bar{\phi}_2) \equiv \Phi_2(t), (\psi_j \to (\psi_j, \bar{\psi}_j) \equiv \Psi_j(t)$ etc.] we derive

$$\begin{aligned} i\partial_t \Phi_2(t) &= \mathcal{H}_0(t)\Phi_2(t) - i\partial_t \Psi_0 \\ &\quad - [((E_0 - E_1) + \partial_t \tilde{\theta})\sigma_3 + i\partial_t]\Psi_1 + \vec{F}_{\rm NL}, \end{aligned} \tag{5}$$

where $\vec{F}_{\rm NL}$ is nonlinear in Φ_2, Ψ_0, Ψ_1, $\tilde{\theta}$ and $\mathcal{H}_0(t)$ is given by the matrix operator

$$\sigma_3 \begin{pmatrix} H - E_0(t) + 2g|\psi_0(t)|^2 & g\psi_0^2(t) \\ g\bar{\psi}_0^2(t) & H - E_0(t) + 2g|\psi_0(t)|^2 \end{pmatrix},$$

and σ_3 is the Pauli matrix diag$(1, -1)$. We consider the spectrum of $\mathcal{H}_0(t)$ for fixed t and $|\psi_0| \equiv |\alpha_0|$ small: (a) The continuous spectrum extends from $-|E_0|$ to $-\infty$, and $|E_0|$ to ∞. Let $\mu \equiv E_1 - E_0 + O(|\alpha_0|^2)$. The discrete spectrum is $\{0, -\mu, \mu\}$, with $0 < |\mu| < |E_0|$ by assumption. (b) Zero is a generalized eigenvalue of $\mathcal{H}_0$, with generalized eigenspace spanned by $\{\sigma_3\Psi_0, \partial_{E_0}\Psi_0\}$.

The discrete spectral subspace has dimension four. Therefore, Φ_2 which lies in the continuous spectral part of $\mathcal{H}_0(t)$, is constrained by four orthogonality conditions.

Furthermore, $\partial_t\tilde{\theta}$ is chosen to remove divergent logarithmic phase contributions. In the weakly nonlinear (perturbative) regime, bound states have expansions $\psi_{E_j} = \alpha_j(\psi_{j*}(x) + g|\alpha_j|^2\psi_j^{(1)}(x) + \mathcal{O}(g^2|\alpha_j|^4))$ and $E_g = E_{j*} + \mathcal{O}(|\alpha_j|^2)$. The system for Φ_2 and $\vec{\alpha} = (\vec{\alpha}_0, \vec{\alpha}_1)$ can be written in the form: $i\partial_t\vec{\alpha} = \mathcal{A}(t)\vec{\alpha} + F_\alpha$, $i\partial_t\Phi_2 = \mathcal{H}(t)\Phi_2 + F_\Phi$, where $\vec{\alpha}_j = (\alpha_j, \alpha_j^*)$.

To study the energy exchange between α_0 and α_1, it is important to express $\alpha_1(t)$ as a slow amplitude modulation of a rapidly varying phase. With this goal in mind, we study the equation for α_1, expressible as $i\partial_t\vec{\alpha}_1 = A(t)t\vec{\alpha}_1 + \vec{F}$. Freezing t at some arbitrary large time T in $A(t)$, we solve $i\partial_t\vec{\alpha}_1 = A(T)\vec{\alpha}_1$ in terms of the Floquet solution matrix $X(t)$. We use this to eliminate the (fast) oscillation in $\vec{\alpha}_1 \equiv X(t)\vec{\beta}_1$. The difference $A(t) - A(T)$ and other similar differences are higher order corrections, uniformly in t, as t, $T \to \infty$, and therefore can be neglected.

To proceed further we decompose Φ_2 into its continuous spectral (dispersive) part, η, relative to $\mathcal{H}_0(T)$, and its components along the discrete modes. The latter are higher order and controllable. Thus NLS at low energy is equivalent to a system of the form:

$$\begin{aligned} i\partial_t\eta &= \mathcal{H}_0(T)\eta + \mathcal{F}_\eta(t;\alpha_0,\beta_1,\eta), \\ i\partial_t\beta_1 &= 2g\langle\psi_{0*},\psi_{1*}^3\rangle|\beta_1|^2\alpha_0 e^{i(E_{1*}-E_{0*})t} \\ &\quad + 2g\langle\psi_{0*}\psi_{1*}^2,\pi_1\Phi_2\rangle\bar{\beta}_1\alpha_0 e^{2i(E_{1*}-E_{0*})t} + \mathcal{R}_0, \\ i\partial_t\alpha_0 &= g\langle\psi_{0*}^2,\psi_{1*}^2\rangle e^{-2i(E_{1*}-E_{0*})t}\beta_1^2\bar{\alpha}_0 \\ &\quad + g\langle\psi_{0*}\psi_{1*}^2,\Phi_2\rangle\beta_1^2 e^{-2i(E_{1*}-E_{0*})t} + \mathcal{R}_1, \end{aligned}$$

where $\mathcal{R}_j$ denotes corrections of a similar form and higher order.

The above system can be viewed as an infinite dimensional Hamiltonian system consisting of two subsystems: a finite dimensional subsystem governing "oscillators," (α_0, β_1), and an infinite dimensional subsystem governing the field, η. Although this system has time-rapidly varying coefficients and no evident direction of energy flow, we claim we have now made explicit the key aspects, which give rise to resonant energy exchange. This is achieved via a detailed analysis of nonresonant and resonant terms. *Nonresonant* oscillatory contributions can be transformed by successive near-identity changes of variables, $(\alpha_0, \beta_1) \mapsto (\tilde{\alpha}_0, \tilde{\beta}_1)$, to higher order in the energy of the data (assumed small) and perturbatively controlled. *Resonant* oscillatory terms cannot be transformed to higher order and contribute to the finite dimensional reduction.

To arrive at the reduction, we solve the η equation, making explicit all terms through second order in g, using the Green's function $G(t,t') = e^{-i\mathcal{H}_0(T)(t-t')}$. We focus on the key terms coming from the sources in $\mathcal{F}_\eta$ or the type $\alpha_0^i\alpha_1^j$, $0 \le i, j \le 2$ and having oscillatory phases $e^{im_{ij}(t)}$. Their contribution to η is of the form

$$\sim \int_0^t e^{-i\mathcal{H}_0(T)(t-t')}|\chi\rangle e^{im_{ij}(t')}\alpha_0^i(t')\alpha_1^j(t')dt' \qquad (6)$$

where α_0, α_1 is a component of either $\vec{\alpha}_0$ or $\vec{\alpha}_1$ and where $|\chi\rangle$ is an (exponentially localized) function of position, expressible in terms of ψ_{0*} and ψ_{1*}. We insert this solution into the α_0, α_1 equations, in place of Φ_2. We obtain integro-differential equations for α_0, α_1, (β_1). Terms of the form (6) are solutions to a forced linear system and among the forcing terms made explicit in (6) are oscillatory terms with the frequency ω_*, which are resonant with the continuous spectrum. Internal dissipation resulting in nonlinear resonant energy transfer from the excited state to the ground state and to dispersive radiation is derived from these resonant terms; see also the derivation of internal dissipation in both linear and nonlinear resonance theories, recently developed by us [17,22,24,25]. The dissipation coefficient is Γ, the rate of decoherence and relaxation. The above described scheme gives $i\partial_t\tilde{\alpha}_0 = (-\Lambda + i\Gamma)\times|\tilde{\beta}_1|^4\tilde{\alpha}_0 + \tilde{\mathcal{R}}_0(t)$, $i\partial_t\tilde{\beta}_1 = 2(\Lambda - i\Gamma)|\tilde{\alpha}_0|^2|\tilde{\beta}_1|^2\beta_1 + \tilde{\mathcal{R}}_1(t)$.

Introducing the squared projections of the system's state onto the ground state and excited states, $P_0 \equiv |\tilde{\alpha}_0|^2$, $P_1 \equiv |\tilde{\beta}_1|^2$ we obtain NLME, (2). The system (2) is analyzed in terms of renormalized powers, Q_0 and Q_1. It is shown that there exist transition times t_0 and t_1, such that: $Q_0(t)$ decays rapidly on $[0, t_0]$, $Q_0(t)/Q_1(t)$ grows rapidly on $[t_0, t_1]$, and then finally on $[t_1, \infty)$ the following system governs: $\partial_t Q_0 = 2\Gamma Q_0 Q_1^2$, $\partial_t Q_1 = -4\Gamma Q_0 Q_1^2$. This gives $Q_0 \uparrow Q_0(\infty)$ and $Q_1 \downarrow 0$ at rates discussed above.

The decay of the nonlinear excited state can also be understood as a linear instability. Let $\mathcal{H}_1$ denote the linearization about the nonlinear excited state, the operator in (5) with ψ_0 replaced by the excited state ψ_1. Since $\omega_* > 0$, in the limit of vanishing nonlinear terms, $\mathcal{H}_1$ has an embedded discrete eigenvalue in the continuous spectrum. Perturbation theory of embedded eigenvalues (see, for example, the time-dependent approach in Ref. [25,21]) can be applied to show that this embedded eigenvalue perturbs to a linear exponential instability with exponential rate $\sim\Gamma$ associated with the linear propagator $\exp(-i\mathcal{H}_1\tau)$.

In the context of nonlinear optical waveguide experiments, e.g., Ref. [4], our analysis gives the distance, L_{transf}, over which nonlinear resonant energy transfer occurs as $L_{\text{transf}}^{-1} = 4\Gamma P_0(\infty)P_1(0)$. Here $g = -n_2/\bar{n}_0$, n_2 $[m^2/W]$ is the Kerr nonlinear coefficient, and $P_j[V^2/m^2]$ is the square of the electric field projection onto state j. Γ is obtained from (3), where the states ψ_{j*} are those derived from the Hamiltonian, $H_0 = -2k_0^{-2}\Delta_x + V(x)$, with potential $V(x) = (1/2)(1 - (n_0(x)/\bar{n}_0)^2)$, with x the transverse coordinate. $n_0(x)$ and $\bar{n}_0$ are, respectively, the linear refractive index and its value at infinity. This implies $L_{\text{transf}}^{-1} \sim (4\pi k_0(2n_2/\varepsilon c\bar{n}_0^2)^2(Pwr/A_{\text{eff}})^2|\mathcal{F}[\psi_{0*}\psi_{1*}^2](\omega_*)|^2)$. For parameter values at wavelengths $\sim$1.5 μm and peak power levels at 10^3 W, L_{transf} of device size dimensions (100 μm to 1 mm) can be attained. The factor $\mathcal{F}[\cdot](\omega_*)$, which can be approximated by WKB, depends on the density of states of H_0 near ω_*, and can be tuned by varying the waveguide material and geometric parameters. A second application to optical devices is the use of periodic photonic microstructures with appropriately designed defects to trap coherent light pulses. For example, it has been shown theoretically that (Kerr) nonlinear and periodic structures support gap solitons [28] and trap pulses [29] traveling at any speed less than the speed of light. Experiments have demonstrated soliton propagation at about 50%c [30] and theoretical studies [31] show that gap solitons can be trapped with appropriately designed defects. This has potential applications to optical buffering, high-density storage and optical gates. The light stopping mechanism, is based on the transfer of energy from incoming solitons to the pinned nonlinear modes of the defect. The ground state selection phenomenon and the partition of excited state energy into pinned nonlinear ground state and radiation modes (4), described by NLME, quantify the rate of transfer and efficiency of trapping. For systems of BEC droplets in a potential well, the relaxation time to the ground state and the decoherence time due to the presence external perturbations, e.g., other droplets, are measurable and of fundamental importance related to Γ. For example, they are relevant to the construction and feasibility of quantum gates and memories.

Our analysis is applicable in Hamiltonian systems which can be decomposed into a lower dimensional dynamical system (oscillators) coupled to an infinite dimensional dynamical system (wave field), acting as a dispersive "heat bath,", e.g., how an open quantum system is effected by its environment. Γ is related to the rate of energy transfer or decoherence. In general, when a mean-field type approximation to the interaction with the environment describes the system, the above analysis can be used, e.g., to study wave function collapse in various systems.

To summarize, we have derived the behavior on all short, intermediate and infinite time scales of NLS type equations, in which general solutions involve an interaction among two families of nonlinear bound states (soliton-type) and dispersive radiation. We have derived nonlinear master equations, which govern the dynamics. The phenomenon of ground state selection was demonstrated, the rate of decay or relaxation was computed, and the energy distribution of the asymptotic state of the system was derived. These phenomena were recently observed experimentally in Ref. [4]. Finally, we have shown the applicability of our theoretical results to nonlinear optical devices and to BEC dynamics and decoherence phenomena.

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