Nonlinear Schrödinger Equation

Vassia Kyrieri

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1 Introduction

It is well known that the Newton's second law describes the motion of a particle x with mass m under the influence of a conservative force given by $F(x)$. The equation that describes particle's motion has the form [1]

$$m\frac{d^2x}{dt^2} = F(x). \tag{1}$$

This is a deterministic model and the dynamics can be easily analyzed using the conservation of energy law. Nevertheless, in the early 1900s, it was found that this classic model of motion fails on the atomic scale. At this point, the idea of quantum mechanics occurs and determine that the particle has no definite position or velocity; rather, it postulates a statistical or probabilistic interpretation of the state of the particle in terms of a wave function $u(x,t)$, which is complex. The solution to the question of how to find the wave function was given by Erwin Schrödinger. The equation that governs the evolution of a quantum mechanical system (the analog of Newton's law for the classic system) is the Schrödinger equation (linear), a second-order partial differential equation having the form

$$i\frac{\partial u}{\partial t} + \Delta u + V(\mathbf{x})u = 0, \tag{2}$$

where $V(\mathbf{r}) \in \mathbb{R}$ is the potential function depending on space and Δ is the Laplacian.

In many cases, such as propagation of a laser beam in a medium whose index of refraction is sensitive to the wave amplitude, the Nonlinear Schrödinger (NLS) equation is needed, which is a nonlinear variation of the Schrödinger equation. The NLS equation provides a canonical description of the envelope dynamics of a scalar dispersive wave train $\epsilon u e^{i(\mathbf{k}\cdot\mathbf{X}-\omega t)}$ with a small $\epsilon << 1$ but finite amplitude, slowly modulated in space and time, propagating in a conservative system. The NLS equation can take the simple form [2]

$$i\frac{\partial u}{\partial t} + \Delta u + \gamma|u|^2 u = 0, \tag{3}$$

with an attractive ($\gamma = 1$) or repulsive ($\gamma = -1$) nonlinearity. Here the potential may be proportional to the density of atoms $V = \gamma|u|^2$. In the next chapter, it will be explained how the NLS equation can be derived by the linear Schrödinger equation.

2 Derivation of the Nonlinear Schrödinger equation

Let us consider a scalar nonlinear wave equation written symbolically

$$L(\partial_t, \nabla)u + G(u) = 0 \tag{4}$$

where L is a linear operator with constant coefficients and G a nonlinear function of u and of its derivatives. The linear operator L, as well as the linear Schrödinger equation, has the form:

$$i\partial_t u + \Delta u + f(u) = 0 \tag{5}$$

where f is a linear function of u.

For a small-amplitude solution of magnitude $\epsilon << 1$, the nonlinear effects can first be neglected, and the equation admits approximate monochromatic wave solutions

$$u = \epsilon \psi e^{i(\mathbf{k}\cdot\mathbf{X}-\omega t)} \tag{6}$$

with a constant amplitude $\epsilon\psi$. The frequency ω and the wave vector $\mathbf{k}$ are real quantities related by the dispersion relation

$$L(-i\omega, i\mathbf{k}) = 0. \tag{7}$$

This (algebraic) equation may admit several solutions. We concentrate on one of them:

$$\omega = \omega(\mathbf{k}). \tag{8}$$

Although we assume a small-amplitude wave, cumulated nonlinear effects become significant on long time scales and large propagation distances. In order to solve the nonlinear equation, it will be used the perturbative expansion of the solution of (6), where the complex amplitude of the "carrying wave" (also called carrier) is no longer constant. Furthermore, the complex amplitude depends on the slow variables $T = \epsilon t$ and $X = \epsilon x$.

A simple heuristic argument can explain the canonical character of the NLS equation, viewed as the expansion at the lowest nontrivial order of a generalized weakly nonlinear dispersion relation. For this purpose, it is convenient to reinterpret the linear dispersion relation (8) in the form

$$(i\partial_t - \omega(-i\partial_{\mathbf{X}}))\psi e^{i(\mathbf{k}\cdot\mathbf{X}-\omega t)} = 0, \tag{9}$$

where $\partial_{\mathbf{X}}$ is the gradient with respect to $\mathbf{X}$ and $\omega(-i\partial_{\mathbf{X}})$ the pseudodifferential operator obtained by replacing k by $-i\partial_{\mathbf{X}}$ in $\omega(\mathbf{k})$.

In a weakly nonlinear medium, where the system is not transferring heat or mass between the system and its surroundings, the nonlinearity is expected to affect the dispersion relation of the carrying wave. For the nonlinear form the (complex) wave amplitude ψ is no longer a constant but is modulated in space and time, thus depending on the slow variables. Also, in (9) the derivatives ∂_t and $\partial_{\mathbf{X}}$ are thus to be replaced by $\partial_t + \epsilon\partial_T$ and $\partial_{\mathbf{X}} + \epsilon\nabla$, where ∇ now denotes the gradient with respect to the slow spatial variable $\mathbf{X}$. As a consequence, (9) is replaced by

$$[i\partial_t + i\epsilon\partial_T - \omega(-i\partial_{\mathbf{X}} - i\epsilon\nabla)]\psi e^{i(\mathbf{k}\cdot\mathbf{X}-\omega t)} = 0. \tag{10}$$

This approach with the small parameter ϵ expresses the modification of the wave amplitude. Specifically, there are two parts to the equation (10). Firstly, there are the terms (without ϵ) that look at the motion of the wave at the initial scale where modifications cannot be detected. The second part look at the wave at a larger scale where the terms modified with the parameter ϵ can detect the modification at the wave amplitude. These two parts can be managed separately.

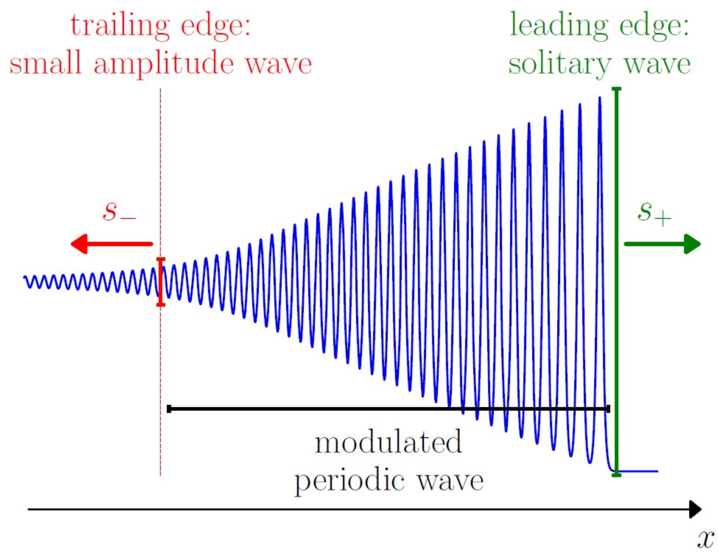

Figure 1: At this figure, the motion of the wave at the left of the red line is described by the linear part of the NLS equation and the right part of the motion by the terms modified with the parameter ϵ. [3]

If there were higher-order in powers of ϵ, the system could be looked at an even higher scale. In particular, the solution u could have the following form [3]:

$$u = u_0 + \epsilon u_1 + \epsilon^2 u_2 + \epsilon^3 u_3 + \cdots \tag{11}$$

where $u_1 = \psi(X,T)e^{i(\mathbf{k}\cdot\mathbf{X}-\omega t)}$. In our case, in order to eliminate secular terms at $O(\epsilon^3)$ and derive the NLS equation, we require that the solution satisfies the equation (10).

In addition, the frequency of the wave becomes dependent of the intensity and it leads to use the new frequency term $\Omega(-i\partial_{\mathbf{X}} - i\epsilon\nabla, \epsilon^2|\psi|^2)$ with $\Omega(-i\partial_{\mathbf{X}} - i\epsilon\nabla, 0) = \omega(-i\partial_{\mathbf{X}} - i\epsilon\nabla)$.

$$[\omega - i\epsilon\partial_T - \Omega(\mathbf{k} - i\epsilon\nabla, \epsilon^2|\psi|^2)]\psi e^{i(\mathbf{k}\cdot\mathbf{X}-\omega t)} = 0, \tag{12}$$

where $\omega = i\partial_t$ and $\mathbf{k} = -i\partial_{\mathbf{X}}$.

Taylor series expansion of multi-variable scalar-valued functions

A multi-variable function $f(x_1, \cdots, x_N) = f(\mathbf{x})$ can also be expanded by the Taylor series:

$$f(\mathbf{x}+\delta\mathbf{x}) = f(\mathbf{x}) + \sum_{j=1}^{N} \frac{\partial x}{\partial x_i \partial x_j} \delta x_i \delta x_j + \cdots$$

which can be expressed in vector form as:

$$f(\mathbf{x}+\delta\mathbf{x}) = f(\mathbf{x}) + \mathbf{g}^T \delta\mathbf{x} + \frac{1}{2}\delta\mathbf{x}^T \mathbf{H} \delta\mathbf{x} + \cdots$$

where $\delta\mathbf{x} = [\delta x_1, \cdots, \delta x_N]^T$ is a vector and $\mathbf{g}$ and $\mathbf{H}$ are respectively the gradient vector and the Hessian matrix (first and second order derivatives in single variable case) of the function defined as:

$$\mathbf{g} = \mathbf{g}_f(\mathbf{x}) = \triangledown f(\mathbf{x}) = \frac{d}{d\mathbf{x}} f(\mathbf{x}) = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \vdots \\ \frac{\partial f}{\partial x_N} \end{bmatrix}$$

$$\mathbf{H} = \mathbf{H}_f(\mathbf{x}) = \frac{d}{d\mathbf{x}} \mathbf{g}_f(\mathbf{x}) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_N} \\ \vdots & \ddots & \cdots \\ \frac{\partial^2 f}{\partial x_N^2} & \cdots & \frac{\partial^2 f}{\partial x_N \partial x_1} \end{bmatrix}$$

According to the previous paragraph, the following form has been derived from the Taylor expansion of the parameter Ω in equation (12):

$$i(\partial_T + \mathbf{v}_g \cdot \nabla)\psi + \epsilon\{\nabla \cdot (D\nabla\psi) + \gamma|\psi|^2\psi\} = 0, \tag{13}$$

where

$$\Omega(-i\partial_{\mathbf{X}} - i\epsilon\nabla, 0) = \omega(k - i\epsilon\nabla) = \omega - \nabla_{\mathbf{k}}\omega \cdot \nabla + \frac{1}{2}\epsilon\nabla \cdot [(\frac{\partial^2\omega}{\partial k_j \partial k_l})\epsilon\nabla] = \omega - \mathbf{v}_g \cdot \nabla + \epsilon^2 \nabla \cdot (D\nabla),$$

and $\mathbf{v}_g = \nabla_{\mathbf{k}}\omega$ is the group velocity and $D = (\frac{1}{2}\frac{\partial^2\omega}{\partial k_j \partial k_l})$, with $j, l = 1, \cdots d$, is defined as half the Hessian matrix of the frequency, both evaluated at the carrier wavevector $\mathbf{k} \in \mathbf{R}^d$, in the absence of nonlinearities.

If we set $\xi = \mathbf{X} - T\mathbf{v}_g$ and write the equation in a reference frame moving at the group velocity and also obtain the rescaling time $\tau = \epsilon T$, we get the NLS equation

$$\begin{aligned} i\frac{1}{\epsilon}\partial_T\psi + i\frac{1}{\epsilon}\mathbf{v}_g \cdot \nabla\psi + \nabla \cdot (D\nabla\psi) + \gamma|\psi|^2\psi = 0 \\ i\frac{1}{\epsilon}\partial_T\psi + i\frac{1}{\epsilon}\mathbf{v}_g \cdot \nabla\psi + \nabla \cdot (D\nabla\psi) + \gamma|\psi|^2\psi = 0 \\ i\frac{\partial\psi}{\partial\tau} + \nabla \cdot (D\nabla\psi) + \gamma|\psi|^2\psi = 0, \end{aligned} \tag{14}$$

with spatial derivatives with respect to ξ variable. The operator $T = \nabla \cdot (D\nabla)$ simplifies in isotropic media(which means having the same properties in all directions), where the frequency depends only on the modulus of the wave vector. Below, we give an example of a specific dispersion relation [3].

3 The Example of Optical Waves

At this example, the NLS equation will be derived in the context of an intense laser beam, propagating as weakly nonlinear waves of a paraxial approximation in an isotropic medium [4].

The propagation of an electromagnetic wave is governed by Maxwell's equations, which we will not explain at this project.

Lemma Let $\overrightarrow{\mathbf{E}}$ be solution of Maxwell's equations in vacuum. Then

$$\Delta\overrightarrow{\mathbf{E}} = \frac{1}{c^2}\frac{\partial^2\overrightarrow{\mathbf{E}}}{\partial t^2} \tag{15}$$

where $c = (\mu\epsilon)^{-\frac{1}{2}}$ is the speed of light in vacuum.

Assume the medium linear and steady. In the absence of fluctuations, the solution of the wave equation, and also of Maxwell's equations takes the form

$$\overrightarrow{\mathbf{E}} = (\mathbf{E_1}, 0, 0), \quad \mathbf{E_1}(x, y, z, t) = \mathcal{E}e^{i(k_0 z - \omega t)}, \tag{16}$$

where $\mathcal{E}$ is the constant amplitude of the wave and the wave vector $k_0^2 = \frac{\omega^2}{c^2}$.

Definition (*Linear polarization*) An electric field $\mathbf{E}$ is called linearly-polarized, if it points in a fixed direction, which is perpendicular to its direction of propagation [4].

The $\overrightarrow{\mathbf{E}} = (\mathbf{E_1}, \mathbf{E_2}, \mathbf{E_3})$ propagates in the z-direction, is localized in the transverse (x, y)-plane and is linearly-polarized in the x-direction.

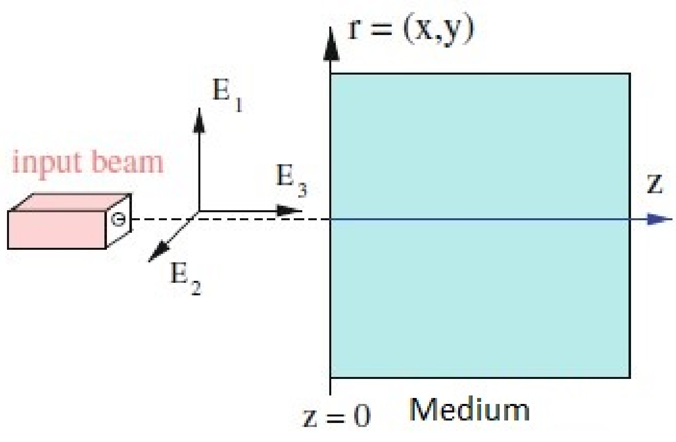

Figure 2: The coordinate system [3]

At "low" intensities of the electric field, the shift of the centers of the electron orbits, hence the polarization field, is linearly proportional to the electric field, i.e., $\mathbf{P} = \mathbf{P}_{lin} = c\mathbf{E}$. Hence, in case of a linear polarization field, the relation between $\mathbf{P}_{lin}$ and $\mathbf{E}$ is written as

$$\mathbf{P}_{lin} = \epsilon_0 \chi_0(\omega)\mathbf{E} \tag{17}$$

where χ_0 the first-order optical susceptibility, whose value depends on the frequency ω.

The only difference between Maxwell's equations in vacuum and in a linear dielectric is in the multiplicative term n_0^2, where n_0 is the (linear) index of refraction (or refractive index) of the medium. The value of n_0^2 is equal to one in vacuum, and is larger than one for dielectrics in their transparency spectrum and is given by

$$n_0^2 = 1 + \chi_0(\omega) \tag{18}$$

In electromagnetism, a dielectric (or dielectric material) is an electrical insulator that can be polarized by an applied electric field. When a dielectric material is placed in an electric field, electric charges do not flow through the material as they do in an electrical conductor, but instead only slightly shift from their average equilibrium positions, causing dielectric polarization.

The propagation of continuous wave linearly-polarized laser beams in a linear dielectric is governed by the scalar Helmholtz equation

$$\Delta\mathbf{E}(z, y, z) + k_0^2\mathbf{E} = 0, \quad k_0^2 = \frac{\omega^2}{c^2}n_0^2. \tag{19}$$

In an isotropic medium, the polarization field $\mathbf{P}$ is written as

$$\mathbf{P} = \mathbf{P}_{lin} + \mathbf{P}_{nl} \tag{20}$$

where the $\mathbf{P}_{nl} = \mathbf{P} - \mathbf{P}_{lin}$ is the nonlinear component of the polarization field. As noted, at low intensities, the dependence of P on the electric field $\mathbf{E}$ is linear. As $\mathbf{E}$ increases, the shift of the centers of the electrons orbits, hence the polarization field $\mathbf{P}$, begins to have a nonlinear dependence on $\mathbf{E}$. Let us consider the regime where $\mathbf{E}$ is sufficiently strong so that $\mathbf{P}_{nl}$ is no longer negligible, but not too strong so that $\mathbf{P}_{nl}$ is still much smaller than $\mathbf{P}_{lin}$, i.e.,

$$\mathbf{P}_{nl} \ll \mathbf{P}_{lin} \tag{21}$$

In other words, we consider the regime where the material response is weakly nonlinear. Therefore, we can expand $\mathbf{P}_{nl}$ in a Taylor series in $\mathbf{E}$, i.e.,

$$\mathbf{P}_{nl} = \chi_1(\omega)\mathbf{E}^2 + \chi_2(\omega)\mathbf{E}^3 \tag{22}$$

where χ_i is the i_{th}-order optical susceptibility. In the weakly-nonlinear regime, a "Taylor-series argument" implies that each additional term is substantially smaller than its predecessor. Therefore, the leading-order nonlinear material-response is quadratic in $\mathbf{E}$, i.e., $\mathbf{P}_{nl} \approx \chi_1\mathbf{E}^2$.

At the equation (19), if the index of refraction is typically weakly nonlinear and takes the form

$$n^2 = n_0^2 + 4N_1 n_0|\mathbf{E}|^2 \tag{23}$$

then the equation (19) is given by

$$\Delta\mathbf{E}(z,y,z)+k^2\mathbf{E}=0 \quad k^2=k_0^2(1+\frac{4n_1}{n_0}|\mathbf{E}|^2). \tag{24}$$

The NLS equation can be satisfied by ψ if we substitute $\mathbf{E}=e^{ik_0z}\psi$ in the equation (24) and apply the paraxial approximation $\psi_{zz}\ll k_0\psi_z$. The NLS equation takes the form

$$(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2})(e^{ik_0z}\psi)+k_0^2(1+\frac{4n_1}{n_0}|\psi|^2)(e^{ik_0z}\psi)=0 \implies$$

$$(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2})\psi e^{ik_0z}-k_0^2e^{ik_0z}\psi+2ik_0e^{ik_0z}\psi_z+e^{ik_0z}\psi_{zz}+k_0^2e^{ik_0z}\psi+k_0^2\frac{4n_1}{n_0}|\psi|^2\psi e^{ik_0z}=0\implies$$

$$(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2})\psi+2ik_0\psi_z+e^{ik_0z}\psi_{zz}+k_0^2\frac{4n_1}{n_0}|\psi|^2\psi=0\overset{\psi_{zz}\ll k_0\psi_z}{\implies}$$

$$\Delta_\perp\psi+2ik_0\psi_z+k_0^2\frac{4n_1}{n_0}|\psi|^2\psi=0. \tag{25}$$

4 Conclusions

The NLS equation is the fitting model to describe the propagation of intense linearly-polarized continuous-wave laser beams in a medium with no external charges or currents, in which the amplitude of electric field is slowly-varying, z is the direction of propagation and x and y are the coordinates in the transverse plane. Generally, The nonlinear Schrödinger equation models the slowly varying envelope dynamics of a weakly nonlinear quasi-monochromatic wave packet in dispersive media. This nonlinear evolution equation arises in various physical settings and admits a wide range of applications, including but not limited to, surface gravity waves, superconductivity, nonlinear optics, and Bose-Einstein condensate (BEC)[5]. For example, the NLS equation that can be modeled by a cubic nonlinearity sine-Gordon equation $\partial_t^2u-a\partial_x^2u+bu-\lambda u^3=0$ $a,b\geq 0$ and $u(x,0)=u_0,\partial_tu(x,0)=u_1$ is written as

$$i\partial_\tau A+\beta\partial_\xi^2A+\gamma|A|^2A=0, \quad \beta=\frac{1}{2}\omega''(k), \quad \gamma=\frac{3}{2}\frac{\lambda}{\omega(k)}. \tag{26}$$

A Bose-Einstein condensate (BEC) is a state of matter of a low density dilute gas, also known as bosons, for which cooling down to a nearly absolute zero temperature would cause them to condense into the lowest accessible quantum state. Ath this case the NLS equation is often referred to as the Gross-Pitaevskii equation (GPE)

$$i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t}=[-\frac{\hbar^2}{2m}\Delta+\mathbf{V}(\mathbf{r})+G|\Psi(\mathbf{r},t)|^2]\Psi(\mathbf{r},t). \tag{27}$$

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