Soliton Solutions of the Nonlinear Schrödinger Equation.

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Abstract

We integrate the nonlinear Schrödinger differential equation, looking for "lone wave" solutions, and then use the method of indeterminate coefficients. The integration is in closed form for the free particle, and then we integrate numerically for the particle subject to a weak periodic potential. In both cases, the system is one-dimensional.

1 The problem of initial conditions for the Schrödinger equation

Let us write the Schrödinger equation for a particle of mass m (without spin) constrained to move on the x-axis and subjected to a conservative force field of potential energy $V(x)$:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+V(x)\,\psi(x,t)=i\hbar\frac{\partial\psi}{\partial t} \tag{1}$$

The cases that interest us are: 1) free particle ($V(x)\equiv 0$); 2) particle in a one-dimensional lattice (periodic potential energy of period a: $V(x+na)\equiv V(x)$).

(1) is a linear partial differential equation of the second order in the derivative with respect to x, and of the first order in the time derivative. This last circumstance implies that a solution is uniquely determined by the initial condition $\psi(x,0)=\psi_0(x)$, where $\psi_0(x)$ is a given function (element of $\mathcal{L}^2(\mathbb{R})$). This can be seen by writing (1) in operational form:

$$\hat{H}\left|\psi(t)\right\rangle = i\hbar\frac{\partial\left|\psi(t)\right\rangle}{\partial t} \tag{2}$$

Here $\hat{H}=\frac{\hat{p}^2}{2m}+V(\hat{x})$ is the Hamiltonian operator of the particle. Given the initial state $|\psi_0\rangle$, (2) admits the unique solution

$$\left|\psi(t)\right\rangle = e^{-\frac{i}{\hbar}t\hat{H}}\left|\psi_0\right\rangle \tag{3}$$

(3) can be made explicit by expressing the initial state $|\psi_0\rangle$ as a combination of the energy eigenkets. For the hypotheses made on the potential $V(x)$, we have that the spectrum of $\hat{H}$ is purely continuous or at most given by the union of continuous bands separated by gaps. Therefore

$$|\psi_0\rangle = \int_{\sigma_c(\hat{H})} dE\,|E\rangle\underbrace{\langle E|\psi_0\rangle}_{c^{(0)}(E)}$$

Taking into account the completeness of the $\{|x\rangle\}$ system of position autokets. $\int_{-\infty}^{+\infty}dx\,|x\rangle\langle x|=\hat{1}$

$$c^{(0)}(E)=\langle E|\left(\int_{-\infty}^{+\infty}dx\,|x\rangle\langle x|\right)|\psi_0\rangle=\int_{-\infty}^{+\infty}\psi_0(x)\,u_E^*(x)\,dx$$

where $u_E(x)=\langle x|E\rangle$ are the eigenfunctions of energy. From (3)

$$|\psi(t)\rangle = e^{-\frac{i}{\hbar}t\hat{H}}\int_{\sigma_c(\hat{H})}dE\,|E\rangle\langle E|\psi_0\rangle=\int_{\sigma_c(\hat{H})}dE e^{-\frac{i}{\hbar}Et}\,|E\rangle\langle E|\psi_0\rangle$$

In x-representation i.e. by switching to the wave function:

$$\psi(x,t) = \int_{\sigma_c(\hat{H})} c^{(0)}(E)\, u_E(x)\, e^{-\frac{i}{\hbar}Et} dE \tag{4}$$

In the case of the free particle, we find a wave packet. Again in this case, the (1) can be solved directly by looking for solutions of the monochromatic plane wave type:

$$\psi_k(x,t) = Ae^{i(kx-\omega t)}, \quad \forall k \in \mathbb{R}$$

After simple steps:

$$\psi_k(x,t) = Ae^{i(kx-\omega(k)t)}, \quad \text{con } \omega(k) = \frac{\hbar k^2}{2m}$$

The linearity of the equation allows us to superimpose infinite solutions:

$$\psi(x,t) = \int_{-\infty}^{+\infty} A(k)\, e^{i(kx-\omega(k)t)} dk \tag{5}$$

where $A(k)$ is such that the integral converges. For the above, the (5) is a particular case of the (4). From (5) the initial profile follows:

$$\psi_0(x) = \int_{-\infty}^{+\infty} A(k)\, e^{ikx} dk \tag{6}$$

By the Fourier integral theorem:

$$A(k) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \psi_0(x)\, e^{-ikx} dk$$

So $A(k)$ is the Fourier transform of $\psi_0(x)$. So if we want to determine the temporal evolution of the wave function, it is necessary (and sufficient) to assign the initial profile of the wave packet (quantumly speaking this means assigning the initial state). Usually a Gaussian profile $G(x-x_0)$ centered at a given point x_0 is used as the modulation envelope of a sinusoidal oscillation. So

$$\psi_0(x) = G(x-x_0)\, e^{ik_0x} \tag{7}$$

In this case the Fourier transform $A(k)$ is still a Gaussian, centered at k_0 which therefore represents the dominant wave number. It follows that setting $k_0 = 0$ i.e. considering only the Gaussian as the initial impulse, implies that the Fourier transform $A(k)$ is centered at $k = 0$, and this is exactly what is expected because $\psi_0(x)$ does not contain sinusoidal oscillations (zero wave number). The widths of the respective Gaussians are such that $\Delta x \Delta k = 1/2$, where the first member is the uncertainty product relative to position x and wave number k (hence the impulse $p = \hbar k$). In other words, the Gaussian wave packet is the packet of minimum uncertainty. In fact, any other initial profile $\psi_0(x) = f(x)\, e^{ik_0x}$ is characterized by an uncertainty product $\Delta x \Delta k \geq 1/2$.

2 The nonlinear Schrödinger equation

(1) can be interpreted as the result of a linearization process of a nonlinear equation of the type:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\,\psi(x,t) - \beta\,|\psi(x,t)|^2\,\psi(x,t) = i\hbar\frac{\partial\psi}{\partial t} \tag{8}$$

where β is a non-zero real constant. This can be due to one of two factors: 1) interaction with other particles; 2) spontaneous local symmetry breaking [1].

In an attempt to integrate the (8) we start from the simplest case ($V(x) \equiv 0$), after which we consider a weak periodic potential $V(x)$, integrating numerically. For $V(x) \equiv 0$

$$\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + i\hbar\frac{\partial\psi}{\partial t} + \beta\left|\psi(x,t)\right|^2\psi(x,t) = 0 \tag{9}$$

We look for solutions of the "solitary wave" type (i.e. soliton):

$$\psi(x,t) = \frac{1}{\cosh(x - Vt)}e^{i(Kx-\Omega t)} \tag{10}$$

having denoted with capital letters the typical quantities that characterize the waves, to distinguish them from the case of so to speak, usual waves. We note incidentally that the nonlinearity of the (9) prevents linearly superimposing the solutions for different K. More specifically, the initial profile

$$\psi_0(x) = \frac{1}{\cosh x} \tag{11}$$

can be developed in Fourier integral, so that $\psi_0(x)$ is a superposition of infinite monochromatic components of wavenumbers $k \in (-\infty, +\infty)$. However, we cannot determine the time evolution $\psi(x,t)$ from this Fourier integral expansion because the differential equation is nonlinear.

Differentiating the (10) with respect to x:

$$\frac{\partial\psi}{\partial x} = F(x,t)\,e^{i(Kx-\Omega t)} \tag{12}$$

where

$$F(x,t) \overset{def}{=} \frac{G(x,t)}{\cosh^2(x - Vt)};\ G(x,t) \overset{def}{=} iK\cosh(x-Vt) - \sinh(x-Vt) \tag{13}$$

So

$$\frac{\partial^2\psi}{\partial x^2} = \left[\frac{\partial F}{\partial x} + iKF(x,t)\right]e^{i(Kx-\Omega t)} \equiv \chi(x,t)\,e^{i(Kx-\Omega t)} \tag{14}$$

having defined:

$$\chi(x,t) \overset{def}{=} \frac{\partial F}{\partial x} + iKF(x,t) \tag{15}$$

Differentiating the (13):

$$\frac{\partial F}{\partial x} = \frac{\phi(x,t)}{\cosh^3(x-Vt)} \tag{16}$$

where

$$\phi(x,t) \overset{def}{=} 2\sinh(x-Vt) - \cosh^2(x-Vt) - iK\sinh(x-Vt)\cosh(x-Vt) \tag{17}$$

Replacing (13)-(16) in (15):

$$\chi(x,t) = \frac{\phi(x,t) + iKG(x,t)\cosh(x-Vt)}{\cosh^3(x-Vt)} \tag{18}$$

So

$$\frac{\partial^2\psi}{\partial x^2} = \frac{\phi(x,t) + iKG(x,t)\cosh(x-Vt)}{\cosh^3(x-Vt)}e^{i(Kx-\Omega t)} \tag{19}$$

Let's move on to the derivative with respect to time:

$$\frac{\partial \psi}{\partial t} = \frac{V \sinh (x - Vt) - i\Omega \cosh (x - Vt)}{\cosh^2 (x - Vt)} e^{i(Kx - \Omega t)} \tag{20}$$

Replacing (19)-(20)-(10) in (9):

$$\frac{\hbar^2}{2m} \frac{\phi (x,t) + iKG (x,t) \cosh (x - Vt)}{\cosh^3 (x - Vt)} + i\hbar \frac{V \sinh (x - Vt) - i\Omega \cosh (x - Vt)}{\cosh^2 (x - Vt)} + \frac{\beta}{\cosh^3 x} = 0 \tag{21}$$

If in (21) we set $(x,t) = (0,0)$

$$\beta = \frac{\hbar^2 K^2}{2m} - \hbar\Omega \tag{22}$$

from which we see that in the linear case $\beta = 0$ we have $\Omega = \frac{\hbar K^2}{2m}$ which is precisely the dispersion law of the wave packet for the free particle. Therefore our procedure is correct. To determine the quantity V, we proceed in a similar way by setting $(x,t) = (x_0, 0)$ where $x_0 = \ln \left(1 + \sqrt{2}\right) \Longrightarrow \sinh x_0 = 1, \; \cosh x_0 = \sqrt{2}$. By doing the necessary steps you get:

$$V = \frac{\Omega}{K}$$

which is the (constant) speed of the wave described by (10).

If we now add a weak periodic potential:

$$V(x) = V_0 \left(1 - \cos\left(\frac{2\pi}{a} x\right)\right)$$

with $V_0 = 0.1$ (unità adimensionali). (dimensionless units). Integrating with *Mathematica*, we obtain the behavior of fig. 1 in the (t, x) plane.

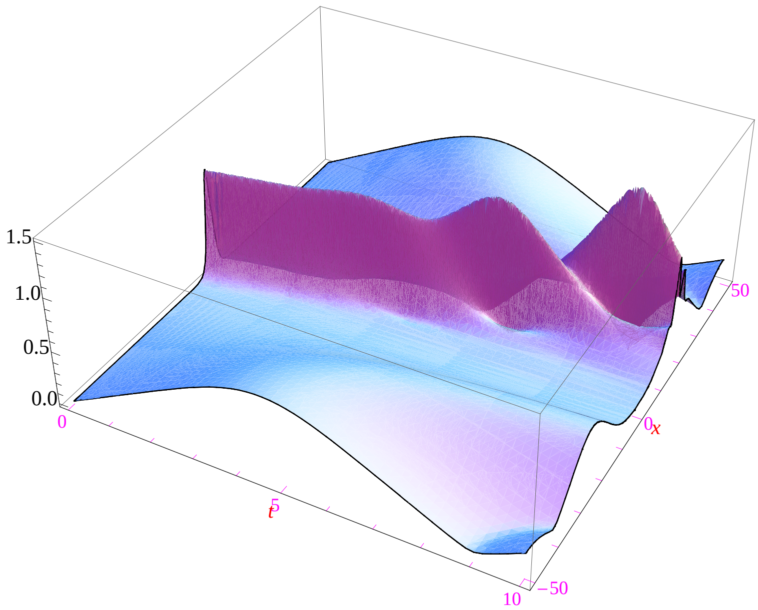

Figure 1: Trend of the solution with periodic potential, found with *Mathematica*.

References

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