Rayleigh-Schrödinger perturbation theory for nonlinear Schrödinger equations

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Abstract.

- We consider a nonlinear perturbation of a time-independent linear Schrödinger equation with isolated simple eigenvalues. It is proved that the associated Rayleigh-Schrödinger power series is convergent when the parameter representing the intensity of the nonlinear term is less in absolute value than a threshold value, and it gives a stationary solution to the nonlinear Schrödinger equation. This result is applied to simple models.

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Few words about NLS equation.

- NLS equations we consider here are given by

$$i\frac{\partial \psi}{\partial t} = H\psi + \nu|\psi|^{2\sigma}\psi\,,\ \sigma > 0\,,\ \mathrm{x} \in \mathbb{R}^d\,,$$

  where $H = -\Delta + V$ is a linear operator formally defined on $L^2(\mathbb{R}^d)$ with potential $V(\mathrm{x})$ and ν is the real-valued strength of the nonlinear perturbation. The units are such that $2m = 1$ and $\hbar = 1$.
- The parameter ν may assume both positive ($\nu > 0$ - *defocusing nonlinearity*) or negative ($\nu < 0$ - *focusing nonlinearity*) values.
- We look for solutions of the kind $\psi(\mathrm{x}, t) = e^{iEt}\psi(\mathrm{x})$, $E \in \mathbb{R}$, to the NLS equations. These solutions are called *standing waves*, or *bound states*, or *stationary solutions*.
- The profile $\psi(\mathrm{x})$ is time-independent and it satisfies to the time-independent NLS equation

$$H\psi + \nu|\psi|^{2\sigma}\psi = E\psi\,,\ \psi \in L^2(\mathbb{R}^d)\,. \tag{1}$$

Stationary solutions to NLS.

- Let us now focus our attention on the search for stationary solutions by making use of perturbation theory; that is the stationary solution can be written by means of a (possibly convergent) perturbation series.
- We discuss a perturbative method similar to Rayleigh-Schrödinger one for linear operators of the form $H_\nu := H + \nu W$ where ν is a "small parameter" and W is (relatively-)bounded perturbation.
- In our case the role of the "perturbation" is played by $|\psi|^{2\sigma}$. Since the this term depends on ψ, the context changes radically, necessitating the formulation of a specific theory for this case.

Stationary solutions via perturbation theory.

- Assumptions on the NLS (1):
- $\sigma = 1$ and $d = 1, 2, 3$. Limitation to $d \leq 3$ is due to the need to use the Gagliardo-Nirenberg inequality ($\| f \|_{L^p} \leq C_{p,d} \|\nabla f\|^\rho \|f\|^{1-\rho}$, $\rho = \frac{d}{2} - \frac{d}{p}$, $p \in [2, 2d/(d-2)]$ if $d > 2$ and $p \geq 2$ if $d = 1, 2$).
- The potential $V(x)$ is a real-valued piecewise continuous bounded function bounded from below:

$$V(x) \geq \Gamma \, , \ \forall x \in \mathbb{R}^d \, . \tag{2}$$

  Hence, H admits a self-adjoint extension on a domain $\mathcal{D}(H)$.
- The discrete spectrum of H is not empty, $\sigma_d(H) \neq \emptyset$, and admits a non degenerate eigenvalue e_0 with associated eigenvector ϕ_0:

$$H\phi_0 = e_0 \phi_0 \, , \ \phi_0 \in \mathcal{D}(H) \, , \ \|\phi_0\|_{L^2} = 1 \, .$$

  In fact, from the Gagliardo-Nirenberg inequality follows that $\phi_0 \in \mathcal{D}(H) \cap L^6(\mathbb{R}^d)$.
- We denote $\Lambda := \text{dist} \left[\sigma(H) \setminus \{e_0\}, e_0 \right] > 0$.

Formal solutions.

- The idea is that, when ν is small enough, the NLS equation

$$H\psi + \nu|\psi|^2\psi = E\psi$$

may have a solution $E := E(\nu)$ and $\psi(\mathrm{x}) := \psi(\mathrm{x}, \nu)$ close to the solution e_0 and ϕ_0 obtained when $\nu = 0$.

- ANSATZ: we look for a **formal solution** $E = \lim_{N\to+\infty} E_N$ and $\psi(\mathrm{x}) = \lim_{N\to+\infty} \psi_N(\mathrm{x})$ where the meaning of the limits will be specified later and where E_N and ψ_N are given by **formal** power series

$$E_N = \sum_{n=0}^{N} \nu^n e_n \quad \text{and} \quad \psi_N(\mathrm{x}) = \sum_{n=0}^{N} \nu^n \phi_n(\mathrm{x})$$

- The terms e_n and $\phi_n(\mathrm{x})$ are:
  - independent of ν;
  - e_0 and ϕ_0 coincide with the unperturbed eigenvalue and eigenvector of H;
  - e_n and $\phi_n \in \mathcal{D}(H) \cap L^6(\mathbb{R}^d)$, $\phi_n \perp \phi_0$ will be defined by induction for any $n \geq 1$.

Mathematical Induction.

- The iterative procedure is fairly standard: formal series are substituted into the equation, and terms with matching powers of ν are required to cancel each other out.
- Let e_ℓ and $\phi_\ell \in \mathcal{D}(H) \cap L^6(\mathbb{R}^d)$ be defined for any $\ell = 0, \ldots, n-1$ such that $\langle \phi_0, \phi_\ell \rangle = 0\,,\ \ell = 1, \ldots, n-1$. Then , let

$$
\begin{aligned}
v_{n-1} &= \sum_{m=0}^{n-1} \sum_{\ell=0}^{n-1-m} \phi_m \bar{\phi}_\ell \phi_{n-1-m-\ell} \in L^2 \\
u_n &= \sum_{m=1}^{n-1} e_m \phi_{n-m} \ \text{(where } u_1 \equiv 0) \ ,\ e_n = \langle \phi_0, v_{n-1} \rangle \\
\chi_n &= e_n \phi_0 + u_n - v_{n-1} \ \text{ such that } \ \langle \phi_0, \chi_n \rangle = 0 \\
\phi_n &= [H - e_0]^{-1} \chi_n \ \text{ where } \ \phi_n \perp \phi_0 \ \text{ and } \ \|\phi_n\|_{L^2} \leq \Lambda^{-1} \|\chi_n\|_{L^2}
\end{aligned}
$$

then $E_N = \sum_{n=0}^N \nu^n e_n$ and $\psi_N(x) = \sum_{n=0}^N \nu^n \phi_n(x)$ are such that

$$
r_N := H\psi_N + \nu |\psi_N|^2 \psi_N - E_n \psi_N = \mathcal{O}(\nu^{N+1}) \leftarrow \text{ formally!} .
$$

A comment: is e_n real-valued when $\nu \in \mathbb{R}$? Yes!

- In explicit models one can see that $e_n \in \mathbb{R}$. In fact, for $n = 1, 2, 3$ it easily follows, for $n \geq 4$ the check is harder.
- However, this property holds in general when ν is real-valued. To prove this fact, we choose the eigenvector ϕ_0 of the linear operator H to be real-valued. Hence:
  - v_0 and u_1 are real-valued;
  - $e_1 = \langle \phi_0, v_0 \rangle$ is real-valued;
  - $\chi_1 = e_1\phi_0 + u_1 - v_0$ is real-valued;
  - $\phi_1 = [H - e_0]^{-1}\chi_1$ is real-valued.

  and thus, by iteration, any ϕ_n is real-valued and then e_n is real-valued.

Main result.

- Here we state our main result:

Theorem (Thm 1)

There exixts $\nu^\star > 0$ such that for any $|\nu| < \nu^\star$ the power series

$$\psi(x,\nu) = \sum_{n=0}^{\infty} \nu^n \phi_n(x) \quad \textit{and} \quad E(\nu) = \sum_{n=0}^{\infty} \nu^n e_n$$

are strong (the first one) and in absolute value (the second one) convergent. Furthermore $\psi \in \mathcal{D}(H) \cap L^6(\mathbb{R}^d)$ and

$$H\psi + \nu|\psi|^2\psi = E\psi\,.$$

Comments to Theorem 1.

- We can conclude that any non-degenerate eigenvalue of H becomes a stationary solution of the NLS when the nonlinearity strength is, in absolute value, small enough.
- Our result is a rigorous proof of this fact and, much more, give a practical tool to calculate these stationary solutions with an estimate of how much the nonlinearity parameter ν can be large.
- Higher nonlinearity power, e.g. $\sigma = 2$ which correspond to the quintic nonlinearity, may be considered but in this case we have to estimate vectors in L^p for some $p > 6$ and so, in order to make use of the Gagliardo-Nirenberg inequality, we have to put some restriction to the dimension d; typically we have to assume that $d \leq 2$.

Can the stationary solution be normalized to 1? Yes!

- One may remark that ψ is NOT necessarily normalized to one. In fact, one can prove that

$$\|\psi\|_{L^2}^2 = 1 + \nu^2 g(\nu)$$

where $g(\nu)$ is a smooth function in a neighborhood of $\nu = 0$ such that $g(0) > 0$. Thus, $\tilde{\psi} = \psi / \|\psi\|_{L^2}$ is a NORMALIZED solution to

$$H\tilde{\psi} + \tilde{\nu}|\tilde{\psi}|^2\tilde{\psi} = E\tilde{\psi}\,, \text{ where } \tilde{\nu} := \tilde{\nu}(\nu) = \nu\left[1 + \nu^2 g(\nu)\right] .$$

- Since such a relation in invertible then let $\nu_+ := \tilde{\nu}^{-1}(\nu)$ and let $\psi_+ = \psi(x, \nu_+)$ and $E_+ = E(\nu_+)$ be the value obtained by means of the perturbative series and such that

$$H\psi_+ + \nu_+|\psi_+|^2\psi_+ = E_+\psi_+ .$$

Then $\psi = \psi_+ / \|\psi_+\|_{L^2}$ and $E = E_+$ is a normalized solution to

$$H\psi + \nu|\psi|^2\psi = E\psi .$$

Toy model 1: infinite well one-dimensional potential

- Let $V(x) = \begin{cases} 0 & \text{if } |x| \leq \pi \\ +\infty & \text{if } |x| > \pi \end{cases}$. That is $H\psi = -\psi''$ with Dirichlet BC $\psi(\pm\pi) = 0$. The spectrum of H is purely discrete $\sigma(H) = \{\frac{1}{4}j^2 \, , \; j = 1, 2 \ldots\}$.
- We are going to compute the perturbative series where $e_0 = \frac{1}{4}$ is, for instance, the first eigenvalue of H, with associated normalized eigenvector $\phi_0(x) = \frac{1}{\sqrt{2}} \cos(x/2)$.
- By means of a straightforward calculation the first terms follow:

$$
\begin{aligned}
e_1 &= \frac{3}{4\pi} \quad \text{and} \quad \phi_1(x) = -\frac{1}{8[\pi]^{3/2}} \cos\left(\frac{3}{2}x\right) \\
e_2 &= -\frac{3}{32\pi^2} \quad \text{and} \quad \phi_2(x) = \frac{1}{64\pi^{5/2}} \left[3\cos\left(\frac{3x}{2}\right) + \cos\left(\frac{5x}{2}\right)\right] \\
e_3 &= \frac{15}{256\pi^3} \quad \text{and} \quad \phi_3(x) = \ldots .
\end{aligned}
$$

Toy model 1: infinite well one-dimensional potential

- In Tables 1 we compute the values of E_N, $\|\psi_N\|_{L^2}$ and $\|r_N\|_{L^2}$, where r_N is the remainder term, for different values of N and for $\nu + 1$. It turns out that the formal power series rapidly converges and that the norm of the remainder term r_N rapidly decreases when N increases.

N	E_N	$\|\psi_N\|_{L^2}$	$\|r_N\|_{L^2}$
0	0.25	1	$0.25 \cdot 10^0$
1	0.488732	1.000791259	$0.16 \cdot 10^{-1}$
2	0.479234	1.000614941	$0.28 \cdot 10^{-2}$
3	0.481123	1.000634507	$0.48 \cdot 10^{-3}$
4	0.480777	1.000632165	$0.81 \cdot 10^{-4}$
5	0.480837	1.000632442	$0.13 \cdot 10^{-4}$
6	0.480827	1.000632410	$0.22 \cdot 10^{-5}$

Table: Infinite well potential - Table of values corresponding to the case of defocusing nonlinearities when $\nu = +1$.

Toy model 1: infinite well one-dimensional potential

- The solutions to the NLS $-\psi'' + \nu|\psi|^2\psi = E\psi$ with Dirichlet BC at $\mathrm{x} = \pm\pi$ can be explicitly computed.
- First of all one can prove that the solution ψ, if exists, is a real-valued function and thus the NLS equation becomes $-\psi'' + \nu\psi^3 = E\psi$ which general solution has the form

$$\psi(\mathrm{x}) = p\,\mathrm{sn}\left[\zeta(\mathrm{x} - \mathrm{x}_0), k\right]$$

where x_0 and ζ are arbitrary constants and where

$$k^2 = \frac{E - \zeta^2}{\zeta^2} \quad \text{and} \quad p^2 = 2\frac{E - \zeta^2}{\nu}\,.$$

- For $\nu = +1$ the Dirichlet BC implies that

$$k = 0.66823\ldots \quad \text{and} \quad E = 0.48082\mathbf{9}\ldots$$

and thus the value obtained by the perturbation theory given by $E_6 = 0.48082\mathbf{7}\ldots$ is in good agreement with the exact result.

Toy model 2: one-dimensional harmonic oscillator.

- Let $V(x) = x^2$. That is $H\psi = -\psi'' + x^2\psi$, $x \in \mathbb{R}$. The spectrum of H is purely discrete $\sigma(H) = \{2j-1\,,\ j=1,2\ldots\}$.
- We compute the perturbative series where $e_0 = 1$ is the first eigenvalue with associated normalized eigenvector $\phi_0(x) = \frac{1}{\sqrt[4]{\pi}} e^{-x^2/2}$.

N	E_N	$\|\psi_N\|_{L^2}$	$\|r_N\|_{L^2}$
0	1	1	$0.43 \cdot 10^{0}$
1	1.398942280	1.000653715	$0.23 \cdot 10^{-1}$
2	1.382389419	1.000599885	$0.24 \cdot 10^{-2}$
$\cdots$	$\cdots$	$\cdots$	$\cdots$
6	1.383922248	1.000602043	$0.17 \cdot 10^{-6}$

Table: Harmonic oscillator potential - table of values corresponding to the case of defocusing nonlinearities when $\nu = +1$.

- As in the previous example it turns out that the formal series rapidly converges.

Sketch of the Proof of Thm 1 - preliminary estimates.

- The proof is quite technical and I only try to give the main idea.
- Let Γ be the lower bound of the potential, let Λ be the distance between e_0 and the remainder of the spectrum of H and let $C_{p,d}$ be the numerical constant in the Gagliardo-Nirenberg inequality. Then one can prove the following a priori estimates:

$$\|\phi_n\|_{H^1} \leq \mu_1 \|\chi_n\|_{L^2} \quad \text{and} \quad \|\phi_n\|_{L^p} \leq \mu_2(p,d) \|\chi_n\|_{L^2}$$

where $\phi_n = [H - e_0]^{-1} \chi_n$, $\rho = \frac{d}{2} - \frac{d}{p}$ and where

$$\mu_1 = \left[\frac{1}{\Lambda^2} + \frac{1}{\Lambda} + \frac{e_0 - \Gamma}{\Lambda^2} \right]^{1/2} \quad \text{and} \quad \mu_2(p,d) = \frac{C_{p,d}}{\Lambda^{1-\rho}} \left[\frac{1}{\Lambda} + \frac{e_0 - \Gamma}{\Lambda^2} \right]^{\rho/2} .$$

- As a result, for $p = 6$ then it follows that $\phi_n \in \mathcal{D}(H) \cap L^6(\mathbb{R}^d)$.

Sketch of the Proof of Thm 1 - iterative scheme.

- We recall the iterative scheme. Let e_ℓ and $\phi_\ell \in \mathcal{D}(H) \cap L^6(\mathbb{R}^d)$ be defined for any $\ell = 0, \ldots, n-1$ such that

$$\langle \phi_0, \phi_\ell \rangle = 0\,,\ \ell = 1, \ldots, n-1\,.$$

- Let

$$\begin{aligned} v_{n-1} &= \sum_{m=0}^{n-1} \sum_{\ell=0}^{n-1-m} \phi_m \bar{\phi}_\ell \phi_{n-1-m-\ell} \in L^2 \\ u_n &= \sum_{m=1}^{n-1} e_m \phi_{n-m} \ \ (\text{where } u_1 \equiv 0) \\ e_n &= \langle \phi_0, v_{n-1} \rangle \\ \chi_n &= e_n \phi_0 + u_n - v_{n-1} \ \ \text{such that } \ \langle \phi_0, \chi_n \rangle = 0 \\ \phi_n &= [H - e_0]^{-1} \chi_n \ \ \text{where } \ \phi_n \perp \phi_0\,, \end{aligned}$$

then $E_N = \sum_{n=0}^N \nu^n e_n$ and $\psi_N(x) = \sum_{n=0}^N \nu^n \phi_n(x)$ are such that

$$H\psi_N + \nu |\psi_N|^2 \psi_N - E_n \psi_N = \mathcal{O}(\nu^{N+1}) \leftarrow \text{ formally!}\,.$$

Sketch of the Proof of Thm 1 - iterative scheme.

- In order to study the convergence of the iterative scheme let

$$c_n := \|\phi_n\|_{L^2}\,,\ \ b_n := |e_n|\,,\ \ n = 1, 2, \ldots$$

and

$$d_n := \|\phi_n\|_{L^6}\,,\ \ n = 0, 1, 2, \ldots\ ,$$

- Then, we can obtain the following estimates of the terms b_n, c_n and d_n:

$$\begin{aligned}
b_n &\leq \sum_{m=0}^{n-1} d_m \sum_{\ell=0}^{n-1-m} d_\ell d_{n-1-\ell-m} \\
c_n &\leq \frac{1}{\Lambda}\left[2\sum_{m=0}^{n-1} d_m \sum_{\ell=0}^{n-1-m} d_\ell d_{n-1-\ell-m} + \sum_{m=1}^{n-1} b_m c_{n-m}\right] \\
d_n &\leq \mu_2\left[2\sum_{m=0}^{n-1} d_m \sum_{\ell=0}^{n-1-m} d_\ell d_{n-1-\ell-m} + \sum_{m=1}^{n-1} b_m c_{n-m}\right]
\end{aligned}$$

Sketch of the Proof of Thm 1 - iterative estimates.

- Preliminarly we prove that (recall that $d_j = \|\phi_j\|_{L^6}$)

Lemma

Let us assume that for some $n \geq 1$ and some $\alpha \in \mathbb{R}$

$$d_j \leq \delta e^{\alpha j} \frac{1}{(j+1)^2}\,,\ j = 0, \ldots, n-1\,,\ \delta = d_0\,. \tag{3}$$

Then there exists a positive constant C_1 independent of n such that

$$\sum_{m=0}^{n-1} d_m \sum_{\ell=0}^{n-1-m} d_\ell d_{n-1-\ell-m} \leq C_1 \delta^3 e^{\alpha(n-1)} \frac{1}{(n+1)^2}\,.$$

- The constant $C_1 \leq 4 \cdot 4.7^2$ (actually $C_1 \approx 10.45$) is such that

$$C_1 = \sup_n (n+1)^2 \sum_{m=0}^{n-1} \frac{1}{(m+1)^2} \sum_{\ell=0}^{n-1-m} \frac{1}{(\ell+1)^2(n-m-\ell)^2}\,.$$

Sketch of the Proof of Thm 1 - iterative estimates.

- Then (recall that $c_j = \|\phi_j\|_{L^2}$ and $b_j = |e_j|$)

Lemma

Let us assume that for some $n \geq 1$

$$b_j \leq \beta e^{\alpha(j-1)} \frac{1}{(j+1)^2} \text{ and } c_j \leq \gamma e^{\alpha j} \frac{1}{(j+1)^2}, \; j = 1, \ldots, n-1, \qquad (4)$$

for $\beta = \max[4b_1, C_1\delta^3]$ and $\gamma = \max[4c_1, 1]$, where α has been introduced in the previous Lemma. Then there exists a positive constant C_2 independent of n such that

$$\sum_{m=1}^{n-1} b_m c_{n-m} \leq C_2 \frac{\beta\gamma}{(n+1)^2} e^{\alpha(n-1)}, \; C_2 = \sup_n \sum_{m=1}^{n-1} \frac{(n+1)^2}{(m+1)^2(n-m+1)^2}.$$

- One can estimate $C_2 \leq 2.7$ (actually $C_2 \approx 1.52$).

Sketch of the Proof of Thm 1 - convergence of the iterative scheme.

- We remark that (3) holds true for $j=0$ and that (4) hold true for $j=1$ for any α by means of the choice of β, γ and δ. So:

Lemma

Let (3) holds true for $j=0,1,\dots n-1$ and that (4) hold true for $j=1,2,\dots,n-1$, for some $n\geq 1$. Let $C_3=2C_1\delta^3+C_2\beta\gamma$ and let α satisfying (3) and (4) and large enough such that

$$e^{-\alpha}\leq \min\left[C_3^{-1}\gamma\Lambda, C_3^{-1}\mu_2(6,d)^{-1}\delta\right] \tag{5}$$

then (3) and (4) hold true for $j=n$.

- Thus, if $|\nu|\leq e^{-\alpha}$, the formal power series $E_N=\sum_{n=0}^N \nu^n e_n$ and $\psi_N=\sum_{n=0}^N \nu^n\phi_n(x)$ converge. From the value of β, γ, δ, Λ, C_1, C_2, $e_0-\Gamma$ and $\mu_2(6,d)$ an estimate of the radius of convergence can be given.

Sketch of the Proof of Thm 1 - conclusion.

- In order to be more precise, we have that for $|\nu| \leq e^{-\alpha}$, where α satisfies (5), we can prove that the previous power series converge and that there exists $E \in \mathbb{R}$ and $\psi \in L^2 \cap \mathcal{D}(H)$ such that

$$E_N \to E\,,\ \psi_N \to \psi \ \text{ in } \ L^2 \cap L^6 \cap H^1\,,\ H\psi_N \to H\psi \ \text{ in } \ L^2$$

  as N goes to ∞.
- Furthermore, in the limit we also have that

$$r_N := H\psi_N + \nu|\psi_N|^2\psi_N - E_N\psi_N \to 0 \ \text{ in } \ L^2\,,$$

  and thus

$$H\psi + \nu|\psi|^2\psi - E\psi = 0\,.$$

- Hence ψ is a stationary solution with associated “energy” E. Theorem 1 is so proved.
- **Thank you for your kind attention.**