Statistical Mechanics of Nonlinear Waves: Growth and Decay of Coherent Structures Interacting with Random Waves

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STATISTICAL MECHANICS OF NONLINEAR WAVES: GROWTH AND DECAY OF COHERENT STRUCTURES INTERACTING WITH RANDOM WAVES

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STATISTICAL MECHANICS OF NONLINEAR WAVES: GROWTH AND DECAY OF COHERENT STRUCTURES INTERACTING WITH RANDOM WAVES

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by

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High-amplitude coherent structures have been observed in many nonlinear wave systems, ranging from fluids, plasmas to optical waves. In this dissertation, we explore the interaction of Rayleigh-Jeans distributed low-amplitude random waves with coherent solitary structures in a nonintegrable and non-collapsing version of the nonlinear Schrödinger equation. We try to understand if such an interaction enhances or erodes the coherent structures with the method of statistical mechanics. We find the threshold of the growth and decay of the coherent structure by equating the phase frequency of the coherent structure to the chemical potential of low-amplitude weakly nonlinear random waves. If the phase frequency exceeds the critical threshold value, the coherent structure accumulates wave action from random waves while transferring energy to random waves and then grows. Otherwise it decays. We also verify this finding with numerical simulations and the numerical results match our theoretical prediction.
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This thesis is dedicated to my family and best friends.
1.1. An Observation: Regular Waves Immersed in Random Waves

A cnoidal wave is a nonlinear and exact periodic wave solution of the Korteweg–de Vries (KdV) equation $\phi_t + \phi_{xxx} - 6\phi\phi_x = 0$, where $\phi(x, t)$ is a complex variable. They are used to describe surface gravity waves of long wavelength, as compared to the water depth. Cnoidal wave solutions can appear in other applications besides surface gravity waves. For instance, they can be used to describe ion acoustic waves in plasma physics. Cnoidal wave solutions of the KdV equation are stable with respect to small perturbations. From figure 1.1, we can see that cnoidal waves can coexist with irregular waves. What is the impact of such a coexistence for these two types of waves?

Figure 1.1: Cnoidal waves coexisting with irregular waves. Cnoidal waves are those periodic waves while irregular waves are the ones between the cnoidal waves in the picture. Source: Wikipedia

The next observation will be related to optical waves. The propagation of an optical wave in a medium is usually described by the Maxwell equation. The following figure shows
the coexistence of a high-amplitude optical spike surrounded by random optical vortices. In this case, the regular structure is the high-amplitude spike. Again, what is the long-term impact of such a coexistence?

Figure 1.2: A high-amplitude optical spike is surrounded by random optical vortices. This peak is also called the rogue wave and it is the result of small vortex collision. The figure is from [18].

So it is natural to see that high-amplitude coherent structures are immersed in a sea of low-amplitude random waves in many physical systems such as fluids, plasmas, optics and lasers, etc.. Coherent structures are regular nonlinear structures that persist for a long period of time. These high-amplitude coherent structures are known as solitons, solitary waves, breathers, vortices etc.. Solitons of integrable nonlinear systems are persistent pulses that are robust under interactions with waves or other solitons. Solitary waves are similar structures that exist in more generic cases of nonintegrable equations of motion. They may change their shapes when they interact with other localized or extended waves. Breathers are localized periodic solutions of either continuous media equations or discrete lattice equations.

1.2. What Draws Our Attention?

Although KdV and Maxwell equations are fundamental equations, they are not what interest us at this time. What draws our attention is the coexistence of the high-amplitude regular waves and small-amplitude random waves from the above figures. We can see the
high-amplitude regular waves are immersed in a sea of low-amplitude random waves. What will happen in the long run? Will there be only random waves? Will both regular waves and random waves keep the current state without any changes? Will the large regular waves absorb small random waves and get even larger? These possibilities are the focus of our interest. It seems to be true from the point of entropy that only random waves can stay as a result of the interaction between these two waves since regular waves contribute little to the entropy of the system. But we are able to draw such a conclusion with the above examples as the KdV equation is integrable, so it is a special case. Optical waves are also the solutions of some integrable nonlinear equations. So can we make a more general statement that small random waves always destroy the large regular waves even in nonintegrable systems.

Both the KdV equation and the cnoidal wave solutions or the Maxwell equations and the optical waves are not what we will explore. We are interested in another system consisting of a different equation and different wave solutions but displays similar coexistence of large regular waves and small random waves. We will try to answer the question: will the high-amplitude regular waves always be eroded by small-amplitude random waves as a result of entropy maximization?

1.3. Our Situation: Non-equilibrium of Random Waves and Solitary Waves

In our case, we will consider the Rayleigh-Jeans distributed random waves. The wave amplitudes are Gaussian distributed and the modes are Rayleigh-Jeans distributed. The special feature of the Rayleigh-Jeans distributed random waves is that they can coexist with the high-amplitude coherent structures in an equilibrium state.

There are some other possible distributions of random waves besides the Rayleigh-Jeans distribution. One possibility is the Kolmogorov-Zakharov distribution in which the energy will flow through the wavenumber space and this is called the wave turbulence. Our result can be applied to the Kolmogorov-Zakharov distributed waves as well.

We will study the long-term impact of the interactions between these regular coherent structures and random waves. An isolated coherent structure would be persistent, but the
one surrounded by random waves might change.

In the system governed by the discrete nonlinear Schrödinger equation, it turns out that the high-amplitude coherent structure (soliton) can be either eroded or enhanced by low-amplitude random waves, depending on the dynamical property of the coherent structure and the statistical properties of random waves [24,42–44,47,48]. The dynamical property of the coherent structure is the phase frequency $\Omega_s$. The two statistical properties of random waves are the temperature $\beta^{-1}$ and the chemical potential $\mu$. Both the dynamical property and the statistical properties are unit free. They are just numbers. We will discuss these properties in detail in later chapters. The conclusion for the discrete nonlinear Schrödinger equation is that the threshold between growth and decay of the coherent structure is when $\mu = \Omega_s$. If $\mu > \Omega_s$, the solitary wave grows. Otherwise, it decays [43]. The temperature $\beta^{-1}$ is not involved in the determination of the growth or decay of the coherent structure, but controls the amplitudes of random waves. The method that we use to explain these two scenarios is statistical mechanics [31,45,50].

The main contribution of this dissertation is that we extend the conclusion from the discrete system to the continuous one, which means that we also find an analytical result for the growth or decay of the coherent structure interacting with random waves. Both the growth and decay situations are possible, still depending on the dynamical property of the coherent structure and statistical properties of random waves. But unlike the discrete system, there are some challenges with the continuous case. First, the continuous system is integrable, so there are infinitely many conserved quantities that partition the phase space and the dynamics of the system is relatively regular, which prevents us from explaining the growth or decay of the coherent structure using statistical mechanics. Second, wavenumbers of the continuous system can be infinitely large, which produces infinitesimally short wavelengths. Since we have an infinite number of wavelengths with the same energy, the energy will diverge. This phenomenon is also known as the “ultraviolet catastrophe”. Third, the connection of the conserved quantities in the continuous system is different from that of the discrete system. In the discrete system, the energy is proportional to the square of the wave action while in
the continuous system governed by the nonlinear Schrödinger equation (NLSE), the energy is proportional to the cube of the wave action. To solve these challenges, we construct a modified version of the NLSE for the continuous system. We first design the nonlinearity to make the modified NLSE nonintegrable so that there are only three conserved quantities of the system: Hamiltonian, wave action and momentum. The Hamiltonian and wave action are directly related to the growth and decay of the high-amplitude coherent structure. We discard very short waves to avoid the ultraviolet catastrophe as the physical relevance of these short waves is limited. The following figure shows two time-space plots of the interaction between a non-travelling solitary wave and random waves. The left plot shows the growth case and the right one shows the decay case.

Figure 1.3: Results of two numerical experiments in one dimension. The experiment processes will be described in chapter 5. Both plots show the spatial intensity distribution over time. The intensity is encoded in the grey scale and dark colors indicate high intensity. The solitary wave remains the same in both experiments, but the initial conditions of random waves are different in statistical properties. The left plot shows the growth of the solitary wave surrounded by random waves. The solitary wave always exists and the surrounding waves contribute powers to it. The right plot shows the decay case. The solitary wave lose much intensity and it will disappear eventually. It is possible for the formation of some small solitary waves during the interactions. These small solitary waves may collide with each other or collide with the initial solitary wave. But the collisions or the formations of these solitary waves do not prevent us from observing the final results. The final results are still two possible outcomes: a larger solitary wave after growing and only random waves after decaying.
1.4. Chapter Introduction

This rest of the dissertation is divided into 6 chapters.

Chapter 2 introduces the derivation of the NLSE from optics, the conserved quantities of the system, the lower boundary of the Hamiltonian and the modified version of the NLSE that we will use in the research work.

Chapter 3 introduces the high-amplitude solitary wave, the energy of it, the statistical mechanics of small-amplitude random waves, the derivation of the wave entropy from the Jaynes’s principle and the Rayleigh-Jeans distribution.

Chapter 4 introduces the thermodynamic model that is a simplification of the full system for the interaction between the solitary wave and random waves, alternative approaches besides our thermodynamic model, the growth and decay scenarios. We also explain the threshold between the growth and decay of the solitary wave as a saddle point.

Chapter 5 introduces numerical experiments that we perform to verify our theoretical prediction.

Chapter 6 introduces the further discussion on the generalization of our theory on higher dimension or when additional terms or effects are included.

Chapter 7 gives the conclusion.
2.1. Overview of the Nonlinear Schrödinger Equation

We review some fundamental knowledge about the NLSE, including a heuristic derivation of the NLSE in nonlinear optics, the difference between self-focusing and self-defocusing equations, the Hamiltonian and conserved quantities of the NLSE and the lower bound of the Hamiltonian.

2.1.1. The NLSE as an envelope equation in nonlinear optics

A sketch of a derivation of the NLSE in nonlinear optics is given.

Detailed derivations of the NLSE from both the dispersion relation and the variational approach have been discussed in [30, 55]. Kelly [25] gives a heuristic derivation of the NLSE for optical beams. We first introduce the Kerr effect. The Kerr effect describes a change in the refractive index of certain materials (carbon disulfide, polar liquid nitrobenzene, etc.) caused by electric fields, and is proportional to the square of the electric field strength [9]. The refractive index \( n \) can be expanded in terms of field strength as

\[
n = n_0 + n_2 E^2 + ...
\]  

(2.1)

Now we can move on with the derivation of the NLSE. The Kerr effect can be caused by an external electric field, but also by an electromagnetic wave that propagates through a Kerr-nonlinear medium. In this case the electromagnetic wave changes the optical properties of the medium, which yields a nonlinear wave equation [9]

\[
\nabla^2 \vec{E} - \frac{\epsilon^{(0)}}{c^2} \frac{\partial^2 \vec{E}}{\partial t^2} - \frac{\epsilon^{(2)}}{c^2} \frac{\partial^2 (E^2 \vec{E})}{\partial t^2} = 0
\]  

(2.2)
where $\vec{E}(x, y, z, t)$ is the electric field and $\epsilon^{(0)}$ and $\epsilon^{(2)}$ are permittivities. Permittivity is the ratio of the electric displacement and the corresponding electric field within a material. $c$ is the velocity of light in vacuum. The first two terms in (2.2) are just the wave equation while the third term means that the refractive index can grow as function of the strength of the electrical field.

Suppose there is a linearly polarized wave of frequency $\omega$ and propagating along the $z$ axis, so that

$$
\vec{E} = \frac{\hat{e}}{2} \left( \phi e^{i(kz-\omega t)} + c.c. \right)
$$

(2.3)

where linear polarization means the electric field is confined to a single plane along the direction of propagation. $k = \sqrt{\epsilon^{(0)} \omega / c}$ and $\hat{e}$ is a unit vector pointing the direction of the electric field. The factor $e^{i(kz-\omega t)}$ represents the propagating part of the wave. $\phi(x, y, z)$ is the slowly varying part and is a complex quantity. We then put (2.3) into (2.2) and ignore the third harmonic term, which gives

$$
\left\{ \begin{array}{l}
\frac{\partial^2 \vec{E}}{\partial t^2} = \frac{\hat{e}}{2} \left( -\omega^2 \phi e^{i(kz-\omega t)} \right) \\
\frac{\partial^2 \vec{E}}{\partial x^2} = \frac{\hat{e}}{2} \left( \frac{\partial^2 \phi}{\partial x^2} e^{i(kz-\omega t)} \right) \\
\frac{\partial^2 \vec{E}}{\partial y^2} = \frac{\hat{e}}{2} \left( \frac{\partial^2 \phi}{\partial y^2} e^{i(kz-\omega t)} \right) \\
\frac{\partial^2 \vec{E}}{\partial z^2} = \frac{\hat{e}}{2} \left( \frac{\partial^2 \phi}{\partial z^2} e^{i(kz-\omega t)} + 2ik \frac{\partial \phi}{\partial z} e^{i(kz-\omega t)} - k^2 \phi \right) \\
\end{array} \right.
$$

(2.4)

Next, we assume the term in the second $z$ derivative of $\phi$ to be small since $\phi$ is the slow modulation part and drop it, which gives

$$
2ik \frac{\partial \phi}{\partial z} + \left( \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial z^2} \right) + \frac{3\epsilon^{(2)} k^2}{4\epsilon_0} |\phi|^2 \phi = 0
$$

(2.5)

(2.5) is the NLSE in three dimension. The Kerr effect can cause highly intense optic beams to focus themselves without the use of a focusing lens in any medium, where a
focusing lens can be acted by a medium whose refractive index increases as a function of the electric field intensity.

The NLSE can also be applied to various physical systems in the description of nonlinear waves [13] such as propagation of light in nonlinear optical fibers, Bose–Einstein condensates, small-amplitude gravity waves on the surface of an ideal fluid [64], and plasma waves. It provides a canonical description of the envelope dynamics of small-amplitude dispersive waves, slowly modulated in space and time, propagating in a conservative system when dissipation is negligible [5, 30].

2.1.2. Focusing and defocusing NLSEs

The NLSE can be reduced to focusing and defocusing cases. We will review these two cases.

At variance to (2.5), we now consider a first-order time derivative and only one spatial dimension. The one dimensional NLSE is

$$i \phi_t + \phi_{xx} \pm |\phi|^2 \phi = 0 \quad (2.6)$$

where \( \phi(x, t) \) is a complex variable. We can re-scale the space and time to eliminate all coefficients.

There are two types of the NLSE: focusing and defocusing. The case with positive cubic nonlinearity in (2.6) is self-focusing and allows for bright soliton solutions which are localized in space and decay towards infinity [58].

The other case, with negative nonlinearity, is the self-defocusing NLSE which has dark soliton solutions. Dark solitons have constant amplitudes even at infinity [1].

2.1.3. Hamiltonian and conserved quantities of the NLSE

In addition to the Hamiltonian, the NLSE in one dimension conserves an infinite number of quantities.
The focusing NLSE is a nonlinear Hamiltonian partial differential equation and it follows from the Hamiltonian (2.7) and the canonical equations of motion (2.8-2.9) below

$$\mathcal{H}[\phi, \phi^*] = \int_{-\infty}^{\infty} |\phi_x|^2 - \frac{1}{2} |\phi|^4 \, dx$$

(2.7)

We will refer to the first part as the kinetic energy and the second part as the potential energy.

$$\begin{align*}
    i\phi_t &= \frac{\delta \mathcal{H}}{\delta \phi^*} \\
    i\phi^*_t &= -\frac{\delta \mathcal{H}}{\delta \phi}
\end{align*}$$

(2.8)

(2.9)

$$\frac{d\mathcal{H}}{dt} = \frac{\partial \mathcal{H}}{\partial t} = 0$$

(2.10)

Equation (2.10) shows that there is no explicit time dependence in the Hamiltonian function, so the Hamiltonian (2.7) is a conserved quantity of the NLSE. The Hamiltonian function is not the physical energy in all cases. We refer to the value of the Hamiltonian function as the energy in our case.

Conserved quantities are related to continuous symmetries [6, 17,55]. Conservation laws are of great importance for the analysis of the NLSE. A conservation law states that some measurable physical property does not change in the course of time within an isolated physical system. In general, whenever the system exhibits a continuous symmetry, there is an associated conserved quantity [55].

The conservation of the Hamiltonian is associated to the invariance by the infinitesimal time translation [55].

Another two fundamental conserved quantities are the wave action (or particle number, modulus squared norm) and the momentum. The wave action is defined as

$$\mathcal{A}[\phi, \phi^*] = \int_{-\infty}^{\infty} |\phi|^2 \, dx$$

(2.11)

The conservation of the wave action is associated to the invariance by the phase shift transformation [55].
The momentum is defined as

\[ P[\phi, \phi^*] = i \int_{-\infty}^{\infty} \phi_x \phi^* - \phi \phi_x^* \, dx \]  

(2.12)

The conservation of the momentum is associated to the invariance by the infinitesimal space translation \[55\].

We denote the fixed values of these conserved quantities as \( \mathcal{H} = E, \mathcal{A} = A \) and \( \mathcal{P} = P \).

There is an infinite number of conserved quantities in this equation that are related to less-obvious symmetries. The property makes this equation integrable and it can be solved by the inverse scattering method \[67\].

2.1.4. Lower bound of the Hamiltonian

We discuss the lower bound of the Hamiltonian of the NLSE, the homoclinic orbit of the potential energy, the ratio between \( E_s \) and \( A_s \).

For the wave action \( A_s \) being fixed, the Hamiltonian is unbounded from above since the kinetic energy term \( |\frac{\partial \phi}{\partial x}|^2 \) can become infinitely large when \( k \) is made infinitely large for \( \phi = a e^{ikx} \):

\[ |\phi_x|^2 = k^2 a^2 \]  

(2.13)

\[ \int_{-\infty}^{\infty} |\phi_x|^2 \, dx = k^2 A_s \]  

(2.14)

The quartic energy term is then \( |\phi|^4 \sim a^4 \). If \( A_s = a^2 L \) where \( L \) is the size of the system then

\[ \frac{1}{2} \int_{-\infty}^{\infty} a^4 \, dx = \frac{1}{2} \int_{-\infty}^{\infty} \left( \frac{A_s}{L} \right)^2 \, dx = \frac{A_s^2}{2L} \]  

(2.15)

The total energy now becomes \( E = k^2 A_s + \frac{A_s^2}{2L} \). Obviously, it diverges to \( \infty \) for \( k \to \infty \).

But the Hamiltonian is bounded from below if \( A_s \) is fixed. The variation of the Hamiltonian given the wave action being fixed \[30\] where \( \Omega_s \) is a Lagrange multiplier

\[ \delta(\mathcal{H} - \Omega_s \mathcal{A}) = 0 \]  

(2.16)

where
\( \mathcal{H} - \Omega_s A = \int_{-\infty}^{\infty} |\phi_x|^2 - \frac{1}{2} |\phi|^4 - \Omega_s |\phi|^2 \, dx \)

(2.16) yields the Euler-Lagrange equation

\[ \left( \frac{\partial}{\partial \phi^*} - \frac{\partial}{\partial x} \frac{\partial}{\partial \phi^*} \right) \left( \frac{\partial \phi}{\partial x} \right)^2 - \frac{1}{2} |\phi|^4 - \Omega_s |\phi|^2 \right) = 0 \]  

(2.17)

\[ \left( \frac{\partial}{\partial \phi^*} - \frac{\partial}{\partial x} \frac{\partial}{\partial \phi^*} \right) \left( \frac{\partial \phi}{\partial x} \phi^* - \frac{1}{2} \phi^2 (\phi^*)^2 - \Omega_s \phi \phi^* \right) = 0 \]  

(2.18)

\[
\begin{aligned}
\frac{\partial}{\partial \phi^*} \left( \frac{\partial \phi}{\partial x} \right) & = \frac{\partial}{\partial \phi^*} \left( \frac{\partial \phi}{\partial x} \right) \\
\frac{\partial}{\partial \phi^*} \left( -\frac{1}{2} \phi^2 (\phi^*)^2 \right) & = -\phi^2 \phi^* \\
\frac{\partial}{\partial \phi^*} \left( -\Omega_s \phi \phi^* \right) & = -\Omega_s \phi \\
\frac{\partial}{\partial x} \frac{\partial}{\partial \phi^*} \left( \frac{\partial \phi}{\partial x} \phi^* \right) & = -\frac{\partial}{\partial x} \left( \frac{\partial^2 \phi}{\partial \phi^* \partial x} \frac{\partial \phi}{\partial x} \phi^* \phi^* - \frac{\partial}{\partial x} \frac{\partial}{\partial x} \frac{\partial}{\partial \phi^*} \phi^* \phi^* \phi^* \phi^* \right) - \frac{\partial^2 \phi}{\partial x^2} \\
\frac{\partial}{\partial x} \frac{\partial}{\partial \phi^*} \left( -\frac{1}{2} \phi^2 (\phi^*)^2 \right) & = \frac{1}{2} \frac{\partial}{\partial x} \frac{\partial}{\partial \phi^*} (\phi^*)^2 + \frac{1}{2} \frac{\partial}{\partial x} \phi^2 (\phi^*)^2 \\
\frac{\partial}{\partial x} \frac{\partial}{\partial \phi^*} \left( -\Omega_s \phi \phi^* \right) & = \Omega_s \phi \phi^* + \Omega_s \phi \phi^* = 0
\end{aligned}
\]

Therefore, we can have the equation

\[ -\frac{\partial^2 \phi}{\partial x^2} - \phi^2 \phi^* - \Omega_s \phi = 0 \]

(2.19)

(2.19) is a condition for the extrema of the Hamiltonian.

Let us now seek a solution for \( i\phi_t + \phi_{xx} + |\phi|^2 \phi = 0 \) in the form \( \phi(x, t) = u(x) e^{-i\Omega t} \). The \( x \) dependence of the solution does not change and it just rotates. The function \( u \), which is the real amplitude, is determined from the equation

\[ \Omega_s u + u_{xx} + u^3 = 0 \]

(2.20)

and represents a stationary point of \( E_s \) given \( A_s \) is fixed. Solutions of (2.20) also satisfy (2.19).
(2.20) is analogous to the dynamics of a mass point in a potential when we interpret $u$ as the location of the mass point and $x$ as time

$$u_{xx} = -\Omega_s u - u^3 = -\frac{\partial V}{\partial u}$$

(2.21)

$$V(u) = \frac{\Omega_s}{2} u^2 + \frac{1}{4} u^4$$

(2.22)

Figure 2.1: The dynamics of the potential energy for $\Omega_s = -\frac{9}{5}$. The mass point starts at the saddle point $u = 0$ and then comes back to this point. This is a homoclinic orbit. The minimum of $V(u)$ yields a center.

The wave action is finite if the waves are solitary, i.e. $u(x)$ decays quickly enough as $x \to \pm \infty$. Such waves correspond to homoclinic orbits that connect the fixed point $u = 0$ to itself. $u$ needs to be a saddle point, which requires that $\Omega_s < 0$. Such waves are called “solitons”. A soliton refers to a solitary wave solution of an integrable equation. The soliton solution of an integrable equation can be obtained by using the inverse scattering method. Solitons have the property that they can interact with other solitons such that they emerge following a collision without changing shapes and speeds, apart for a short delay.

The relationship between $E_s$ and $A_s$ can be found with the help of the soliton solution $u(x) = \sqrt{-2\Omega_s} \text{sech}(\sqrt{-\Omega_s}x)$ of (2.6):
\[ E_s = \int_{-\infty}^{\infty} |u_x|^2 - \frac{|u|^4}{2} \, dx \]
\[ = \int_{-\infty}^{\infty} 2\Omega_s \tanh^2(\sqrt{-\Omega_s}x) \text{sech}^2(\sqrt{-\Omega_s}x) - 2\Omega_s^2 \text{sech}^4(\sqrt{-\Omega_s}x) \, dx \]
\[ = \frac{4}{3}(-\Omega_s)^{3/2} \tanh^3(\sqrt{-\Omega_s}x) - 2(-\Omega_s)^{3/2} \tanh(\sqrt{-\Omega_s}x) \bigg|_{-\infty}^{\infty} \]
\[ = -\frac{4}{3}(-\Omega_s)^{3/2} \]

The wave action is

\[ A_s = \int_{-\infty}^{\infty} |u|^2 \, dx \]
\[ = \int_{-\infty}^{\infty} -2\Omega_s \text{sech}^2(\sqrt{-\Omega_s}x) \, dx \]
\[ = 2(-\Omega_s)^{1/2} \tanh(\sqrt{-\Omega_s}x) \bigg|_{-\infty}^{\infty} \]
\[ = 4(-\Omega_s)^{1/2} \]

Since \( A_s = 4(-\Omega_s)^{1/2} \), then \((\Omega_s)^{1/2} = \frac{A_s}{4} \) and \((\Omega_s)^{3/2} = \left( \frac{A_s}{4} \right)^3 \). The lower bound of the Hamiltonian \( E_s \) is therefore

\[ E_s = -\frac{4}{3} \left( \frac{A_s}{4} \right)^3 = -\frac{A_s^3}{48} \quad (2.23) \]
Figure 2.2: It shows the relationship between $E_s$ and $A_s$. Each point on this line corresponds to one solitary wave that has a phase frequency $\Omega_s$. The lower bound of the Hamiltonian is the curve. Any smaller energy below the curve is not feasible.

Since the soliton solution corresponds to the lower bound of the Hamiltonian, the solution is relatively stable and keeps its form unchanged. The frequency $\Omega_s = \frac{dE_s}{dA_s} = -\frac{A_s^2}{16}$ is the change of the Hamiltonian per the change of wave action. It can also be viewed as the slope of $E_s$ as a function of $A_s$.

The ratio of $E_s$ and $A_s$ for the solution (2.19) has been discussed in [30]

$$E_s = \Omega_s \frac{d - 2}{4 - d} A_s$$

(2.24)

from which we know only when dimension $d = 1$ the Hamiltonian is bounded from below. When $d = 2$, there will be wave collapse and $E_s$ is always 0. But 0 is not the lower limit of the energy. There will be different solutions for higher dimensional cases.
2.2. Nonintegrable Version of the Nonlinear Schrödinger Equation

A nonintegrable and noncollapsing version of the self-focusing NLSE is introduced.

2.2.1. Modified NLSE and re-scaling

The NLSE is a generic equation for the envelope of dispersive nonlinear Hamiltonian waves, but its property of the integrability is not generic. Nonintegrable versions of the NLSE are actually more common.

The integrability of the NLSE is an exceptional property, with a few exceptions modified nonlinearities will give nonintegrable equation. For example, additional terms like $|\phi|^4\phi$ will destroy most of the conserved quantities. Such terms are commonly skipped in derivations as they will (for small amplitudes) be relevant only on long time scales. However, they cause a fundamental change of the dynamics from regular quasi-periodic behavior to high-dimensional Hamiltonian chaos. To study this type of dynamics we use this nonintegrable version throughout the research.

\[
i\phi_t = \phi_{xx} + |\phi|^2\phi - |\phi|^4\phi \tag{2.25}
\]

It can be obtained by re-scaling an equation with arbitrary coefficients $a_0 > 0$, $b_0 > 0$, $c_0 > 0$ and $d_0 > 0$.

\[
i a_0 \psi_t = b_0 \psi_{xx} + c_0 |\psi|^2\psi - d_0 |\psi|^4\psi \tag{2.26}
\]

Let $\psi(x,t) = a_1 \phi(b_1 x, b_2 t) = a_1 \phi(X,T)$, where $X = b_1 x$ and $T = b_2 t$ then we can write the original equation (2.26) as

\[
i b_2 a_0 a_1 \phi_T = b_1^2 a_1 b_0 \phi_{XX} + a_1^3 c_0 |\phi|^2\phi - a_1^5 d_0 |\phi|^4\phi \tag{2.27}
\]

(2.25) is the result of re-scaling of (2.27) by first choosing the constants $a_1$, $c_0$ and $d_0$ which make the coefficients of cubic and quintic terms equal. Next we can choose $b_0$ and $b_1$ which gives the same coefficient as the one of the cubic and quintic terms. We then divide by this same coefficient to make the coefficients of these three terms to be 1. Finally, we can re-scale
to make its coefficient also be 1. The equation under investigation includes a quintic order term that enables additional interactions of waves and destroys most conserved quantities.

The conserved quantities for the modified NLSE are the Hamiltonian, the wave action and the momentum as the symmetries still exist. The wave action and the momentum are still of the same form as (2.11) and (2.12) respectively.

2.2.2. Lower bound of the Hamiltonian for the modified NLSE

(*Thanks to the 6th power of the Hamiltonian, the Hamiltonian is bounded from below in any dimensions.)*

The Hamiltonian of (2.25) is

$$\mathcal{H} = \int_0^L |\phi_x|^2 - \frac{|\phi|^4}{2} + \frac{|\phi|^6}{3} \, dx$$  \hspace{1cm} (2.28)

where \(L\) is the large system size with periodic boundary conditions. Periodic boundary conditions are chosen to approximate our large system with a single interval.

The Hamiltonian of the modified NLSE is also bounded from below. Let

$$- \frac{|\phi|^4}{2} + \frac{|\phi|^6}{3} \geq -\alpha |\phi|^2$$  \hspace{1cm} (2.29)

for some \(\alpha > 0\). Then (2.29) reduces to

$$- \frac{|\phi|^2}{2} + \frac{|\phi|^4}{3} \geq -\alpha$$  \hspace{1cm} (2.30)

by dividing \(|\phi|^2\). We compute the minimum of the left part of the inequality by making its derivative be 0, which gives

$$\frac{d}{d|\phi|^2} (- \frac{|\phi|^2}{2} + \frac{|\phi|^4}{3}) = 0$$  \hspace{1cm} (2.31)

Then we have \(|\phi|^2 = \frac{3}{4}\). Putting this value into (2.30) gives \(\alpha \leq \frac{3}{16}\).

The kinetic part of the Hamiltonian is always positive. The potential part is
\[ E_p = \int_0^L -\frac{\phi^4}{2} + \frac{\phi^6}{3} \, dx \]
\[ \geq -\frac{3}{16} \int_0^L |\phi|^2 \, dx \]
\[ \geq -\frac{3}{16} A_s \]

Therefore the Hamiltonian

\[ E_s \geq \int_0^L |\phi_x|^2 \, dx - \frac{3}{16} A_s \quad (2.32) \]

has a lower bound.
3.1. Solitary Waves

A solitary wave is a wave which propagates without changing its shape or size. The envelope of the wave has one global peak and decays at infinity. Solitary waves arise in many contexts, including the elevation of the surface of water and the intensity of light in optical fibers.

3.1.1. Features of solitons and solitary waves

Solitary waves are localized high-amplitude waves of some partial differential equations while solitons are solitary waves in integrable systems.

Solitons were discussed in the previous chapter. Solitons are some stable solutions of integrable equations. When two solitons collide, they propagate with their original shapes and speeds. By solitary waves one usually means some special solutions of nonlinear nonintegrable equations which are spatially localized and keep their forms. But when two solitary waves collide, their shapes change. The one with the higher amplitude grows and the one with the smaller amplitude decays [14]. The main difference between solitons and solitary waves is on the integrability.

The amplitude of a solitary wave decays exponentially on either side of the maximum point. There are two types of solitary waves: travelling and non-travelling. Non-travelling waves have zero momentum while travelling solitary waves have nonzero momentum. In our research, we consider a zero momentum non-travelling solitary wave. The long-time behavior of solutions of some nonlinear equations whose initial conditions are close to a stable solitary wave have been studied. Pego and Weinstein [35] proved the asymptotic stability of the
solitary wave solutions of the KdV equations. Buslaev and Sulem [8] investigated and showed the asymptotic stability of stable solitary wave solutions of the NLSE. So the asymptotic stability is also a property of stable solitary waves.

3.1.2. The solitary wave solution of the modified NLSE

In the previous chapter, we introduced the modified version of the NLSE and it will be used throughout the research. We now check the existence of the solitary wave solution of the modified NLSE.

The reason why we consider the solitary wave solution is that it lies on the lower bound of the Hamiltonian and therefore it is a stable solution. The existence of the solitary wave solution is a precondition of our research.

The solitary wave can be obtained with the same variation method as how the soliton was obtained in the previous chapter. The minimal energy \( \mathcal{H} = E_s(A_s) \) given the wave action being fixed from the variation method is

\[
\delta(\mathcal{H} - \Omega_s A) = 0 \tag{3.1}
\]

with the multiplier \( \Omega_s \). The variation yields

\[
\left( \frac{\partial}{\partial \phi^*} - \frac{\partial}{\partial x} \frac{\partial}{\partial \phi^*_x} \right) \left( |\phi|^2 - \frac{1}{2} |\phi|^4 + \frac{1}{3} |\phi|^6 - \Omega_s |\phi|^2 \right) = 0 \tag{3.2}
\]

\[
\phi_{xx} + |\phi|^2 \phi - |\phi|^4 \phi = -\Omega_s \phi \tag{3.3}
\]

We consider the solution of the same form as the NLSE, which is \( \phi(x, t) = u(x)e^{-i\Omega_s t} \).

The real amplitude \( u(x) \) is governed by the equation

\[
u_{xx} = -\Omega_s u - u^3 + u^5 = -\frac{\partial V}{\partial u} \tag{3.4}\]

\[
V(u) = \frac{\Omega_s}{2} u^2 + \frac{1}{4} u^4 - \frac{1}{6} u^6 \tag{3.5}
\]
3.1.3. Energy of the solitary waves

We showed the existence of the solitary wave solution of the modified NLSE in the previous subsection. Now we give the specific range of values of the phase frequency required for the existence of the solitary wave solution.

The potential $V(u)$ in (3.5) has a minimum value at $u_1 > 0$ and a maximum value at $u_2 > u_1 > 0$ depending on the values of $\Omega_s$. Homoclinic orbits exist only if $V(u_2) > 0$. A homoclinic orbit has an amplitude $u_a$ when $V(u_a) = 0$. Then we can derive the scale of $\Omega_s$ from these conditions. Let $V(u_a) = 0$ in (3.5), then the discriminant is

$$\Delta = \left(\frac{1}{4}\right)^2 - 4 \left(-\frac{1}{6}\right) \frac{\Omega_s}{2}$$

(3.6)

Since $\Delta \geq 0$, then $\Omega_s \gtrsim -\frac{3}{16}$ and $u_a \lesssim \frac{\sqrt{3}}{2}$. When $\Omega_s = -\frac{3}{16}$, the potential $V$ has two maximum values at $V(u_0) = 0$ and $V(u_2 = u_a) = 0$ (the red curve in figure 3.2). So there is a pair of heteroclinic orbits that corresponds to domain walls between the domains $u = 0$
for $x \to \mp\infty$ and $u_2 = u_a = \frac{\sqrt{3}}{2}$ for $x \to \pm\infty$.

Figure 3.2: It shows the potential $V(u)$ in (3.5) for $\Omega_s = -\frac{1}{10}$ and $\Omega_s = -\frac{3}{16}$. $u_1$ is the minimum and $u_2$ is the maximum. $V(u_a) = 0$. In the case of $\Omega_s = -\frac{3}{16}$, $u_2 = u_a$.

Figure 3.3: The homoclinic orbits for $\Omega_s = -\frac{1}{10}$ and $\Omega_s \approx -\frac{3}{16}$. $\Omega_s = -\frac{1}{10}$ corresponds to a non-travelling solitary wave with the shape similar to the soliton solution of the focusing nonlinear Schrödinger equation with a small distortion by the $u^6$ term of the potential. The homoclinic orbit for $\Omega_s \approx -\frac{3}{16}$ is close to heteroclinic orbits that connect the two saddle points $u = 0$ and $u_2 = u_a \approx \frac{\sqrt{3}}{2}$. It corresponds to a non-travelling solitary wave with a broad plateau near its maximum.
For $0 < -\Omega_s \ll \frac{3}{16}$ the quintic term is small and therefore has a negligible influence. The energy of the solitary wave is the same as that of the soliton $u(x) = \sqrt{-2\Omega_s} \text{sech}(\sqrt{-\Omega_s}x)$ of the focusing nonlinear Schrödinger equation, which is computed in the previous chapter and $E_s \gtrsim -\frac{A^3}{48}$.

For $\Omega_s \approx -\frac{3}{16}$, the amplitude $u_a$ of the homoclinic orbit is close to $u_2$. The solitary wave has a broad plateau with $u(x) \approx \frac{\sqrt{3}}{2}$ and a width $\Delta x$ that diverges to infinity for $\Omega_s \to -\frac{3}{16}$. The kinetic energy of the walls

$$\int_0^L |\phi_x|^2 dx$$

(3.7)

can be negligible for broad solitary wave. The bulk energy

$$\int_0^L \left( -\frac{1}{2} |\phi|^4 + \frac{1}{3} |\phi|^6 \right) dx = \frac{9}{64} \Delta x$$

(3.8)

scales as

$$E_s \approx \left( -\frac{1}{2} u_2^4 + \frac{1}{3} u_2^6 \right) \Delta x$$

(3.9)

and the bulk wave action as

$$A_s \approx u_2^2 \Delta x = \frac{3}{4} \Delta x$$

(3.10)

It then follows

$$E_s \approx -\frac{3}{16} A_s$$

(3.11)

It is convenient to have an analytical approximation for the energy and the frequency as a function of the wave action. We can compute the energy for both small and large wave actions then match them, which gives

$$E_s(A_s) \approx \frac{3}{16} \left( \sqrt{3} \arctan \left( \frac{A_s}{\sqrt{3}} \right) - A_s \right)$$

(3.12)

The corresponding frequency is

$$\Omega_s = \frac{dE_s(A_s)}{dA_s} \approx -\frac{3A_s^2}{48 + 16A_s^2}$$

(3.13)
Figure 3.4 shows the lower boundary of the Hamiltonian for (2.25) and figure 3.5 shows the relationship between the phase frequency $\Omega_s$ and wave action $A_s$ for (2.25).

Figure 3.4: Lower boundary of the Hamiltonian $E_s(A_s)$ for (3.12), points on the line correspond to non-travelling solitary waves. Any other states (travelling solitary waves, spatially extended waves, etc.) correspond to points above this line. The Hamiltonian cannot have values below this line.

Figure 3.5: The relationship between frequency $\Omega_s$ and wave action $A_s$ for (3.13). As we can see, $\Omega_s$ is strictly decreasing as a function of $A_s$. The wave action $A_s$ diverges to infinity when $\Omega_s$ approaches to $-\frac{3}{16}$, which corresponds to an infinitely broad solitary wave.
3.2. Statistical mechanics of random waves

3.2.1. Overview of random waves

*The interaction of small-amplitude random waves is weakly nonlinear.*

We express the amplitudes of random waves as \( \phi = \sum_k a_k e^{i k x} \), where \( a_k \) is a Fourier mode of wavenumber \( k \). The amplitudes are assumed to be small almost everywhere and the average wave action \( \langle |\phi|^2 \rangle = A/L \ll 1 \). So the system is weakly nonlinear except for regions where the solitary wave exists, which suggests that the Hamiltonian of random waves can be approximated by

\[
H_2[\phi, \phi^*] = \int |\phi_x|^2 dx \tag{3.14}
\]

The nonlinearity is neglected due to small wave amplitudes and it allows only the weak interaction between modes to achieve thermal equilibrium by randomizing the phases and redistributing energy and wave action. Small amplitudes of random waves allow the linear approximation \( a_k \sim e^{i \omega_k t} \) with the frequencies \( \omega_k = k^2 \). The energy and wave action of random waves are

\[
E_w = \sum_k \omega_k n_k \tag{3.15}
\]

\[
A_w = \sum_k n_k \tag{3.16}
\]

where \( n_k = \langle |a_k|^2 \rangle \) is the mean density of the wave action.

3.2.2. Wave entropy

*We review the derivation of wave entropy from the Jaynes’ principle.*

Wave entropy is an important quantity as it is related to the growth or decay of the solitary wave directly. It is a function of the mean density of wave action in ray phase space \( \bar{J}(k, x) \) and increases monotonically in time as the mean density evolves [24]. The standard choice [11] is

\[
S(\bar{J}) = \int \ln \bar{J}(k, x) \, d^3x d^3k/(2\pi)^3 \tag{3.17}
\]
Taking the logarithm transformation of $\bar{J}$ allows us to compute the total wave entropy of the system by adding the entropy of subsystems instead of multiplying. A classic derivation based on Jayne’s maximum-entropy principle [40] provides illustration of the utility of the principle.

Kaufman [24] assumes that $(k, x)$ space is not continuous, but a set of cells. So (3.17) can be written as

$$S(\bar{J}) = \sum \ln \bar{J}_k \quad (3.18)$$

where $\bar{J}_k$ is the mean action in the $k^{th}$ cell. We will show how (3.18) is derived. But in our case, we do not consider the $(k, x)$ space.

Before we continue, we need to introduce the action-angle variables. The setup is that there are linear oscillators with dispersion. We assume that the oscillators can maximize the entropy. The linear equation for the mode $a_k$ with the wave number $k$ is

$$ia_k = \omega_k a_k \quad (3.19)$$

(3.19) is an approximation of the Hamiltonian. There are some coupling terms which contain little energy, but allow the transfer of energy between these oscillators.

(3.19) is an integrable system and the solution of it is

$$\begin{cases} a_k(t) = a_k(0)e^{i\psi_k(t)} \\ \psi_k(t) = -\omega_k t \end{cases} \quad (3.20)$$

The action variable is $J_k = |a_k|^2$ and the angle variable is $\psi_k$.

The Hamiltonian is now

$$H(J_1, ..., J_N) = \sum_k J_k \omega_k \quad (3.22)$$

and it is transferred from the original Hamiltonian which consists of $2N$ variables.

The Hamilton equations are

$$\begin{cases} \dot{\psi}_k = -\frac{\partial H}{\partial J_k} = -\omega_k \\ \dot{J}_k = \frac{\partial H}{\partial \psi_k} = 0 \end{cases} \quad (3.23)$$

26
So

\[ \psi_k(t) = \psi_k(0) - \omega_k t \]  (3.25)
\[ J_k = \text{constant} \]  (3.26)

The probability density \( \rho(J_1, \ldots, J_N) \) is

\[ \rho(J_1, \ldots, J_N) = \prod_k \rho_k(J_k, \psi_k) \]  (3.27)

It is easy to show that \( \rho_k \) is uniformly distributed over \( \psi_k \), so we use \( \rho_k(J_k) \) instead of \( \rho_k(J_k, \psi_k) \) for simplicity. The average of the wave action is then

\[ \bar{J}_k = \int_0^\infty \rho_k(J_k) J_k dJ_k \]  (3.28)

The Jaynes principle is to introduce Gibbs-Shannon entropy \( S(\rho) \) as a functional of the system distribution function \( \rho \) over the whole space \( \Gamma \)

\[ S(\rho) = - \int \rho \ln \rho \, d\Gamma \]
\[ = - \sum_k \int_0^\infty \rho_k \ln \rho_k dJ_k \]  (3.29)

The extremum of the entropy under the constraint that \( \Sigma_k \int_0^\infty \rho_k J_k dJ_k = \text{constant} \) (This means the total wave action \( \sum_k < |a_k|^2 > \) has a constant value) is

\[ \delta \left( S - \gamma \sum_k \int_0^\infty \rho_k J_k dJ_k \right) = 0 \]  (3.30)

where \( \gamma \) is a Lagrange multiplier. With

\[ \delta(\rho_k \ln \rho_k) = (\ln \rho_k + 1)\delta \rho_k \]  (3.31)

(3.30) yields

\[ (\ln \rho_k + 1 + \gamma J_k) \delta \rho_k = 0 \]  (3.32)

The solution of (3.32) is

\[ \rho_k = e^{-1-\gamma J_k} \]  (3.33)
With normalizing the density and the definition of average wave action being given by

\[
\begin{align*}
\int_0^\infty \rho_k dJ_k &= 1 \quad (3.34) \\
\int_0^\infty \rho_k J_k dJ_k &= \bar{J}_k \quad (3.35)
\end{align*}
\]

We can determine the coefficient \( \gamma = \frac{J_k - \bar{J}_k}{\bar{J}_k} \).

So we have

\[
\rho_k = \frac{1}{\bar{J}_k} e^{-J_k / \bar{J}_k} \quad (3.36)
\]

Now (3.29) becomes

\[
S = -\int \rho \ln \rho \prod_k dJ_k \\
= -\sum_k \int_0^\infty \rho_k \ln \rho_k dJ_k \\
= -\sum_k \int_0^\infty \frac{1}{\bar{J}_k} e^{-J_k / \bar{J}_k} \left( -\frac{J_k}{\bar{J}_k} - \ln \bar{J}_k \right) dJ_k \\
= -\sum_k \left( -\int_0^\infty \frac{J_k}{\bar{J}_k} e^{-J_k / \bar{J}_k} \left( \frac{J_k}{\bar{J}_k} \right) - \ln \bar{J}_k - \int_0^\infty e^{-J_k / \bar{J}_k} \left( \frac{J_k}{\bar{J}_k} \right) \right) \\
= \sum_k 1 + \ln \bar{J}_k \\
= \sum_k \ln n_k + \text{constant} \quad (3.37)
\]

where \( n_k = \bar{J}_k = \langle |a_k|^2 \rangle \). After we discard the constant term in (3.37), we will have the expression in (3.18)

\[
S(E_w, A_w) = \sum_k \ln n_k \quad (3.38)
\]

Wave entropy measures the number of microstates associated with a macrostate in the system. It is not clear if the high-amplitude solitary wave will be enhanced or melted by random waves, which means that we cannot predict if the growth or decay process is dominant in the system. But it is always the case that the solitary wave changes in the direction to maximize the wave entropy. In other words, if the solitary wave grows, then the growth process increases the wave entropy. Otherwise, the decay process increases the
wave entropy. The detailed discussion will be given in the next chapter with the help of a thermodynamic model.

3.2.3. Random waves contain most wave entropy

*Random waves contribute most entropy for the full system while the solitary wave contributes a negligible amount of entropy.*

Random waves contribute to the energy, wave action and the most wave entropy of the whole system as they have their own phases and amplitudes. The solitary wave contributes to the energy and the wave action but a negligible amount of the wave entropy on the other hand as it has few degrees of freedom.

The dynamics of the solitary wave can be represented by a nonlinear oscillator with a Hamiltonian $E_s(A)$ where $A$ and $\alpha$ are action-angle variables. The canonical equations are

$$
\begin{align*}
\dot{\alpha} &= -\frac{\partial E_s(A)}{\partial A} = \Omega_s \\
\dot{A} &= \frac{\partial E_s(A)}{\partial \alpha} = 0
\end{align*}
$$

(3.39)

(3.40)

The microcanonical partition function is

$$
\omega = \int_0^{2\pi} \int_0^\infty \delta(E_s(A) - E_s(A_s))dAd\alpha
$$

$$
= 2\pi \left| \frac{\partial A_s}{\partial E_s(A_s)} \right|
$$

$$
= \frac{2\pi}{|\Omega_s|}
$$

The translational degree of freedom yields the system size as an irrelevant factor of this number. Although the fact that this single oscillator system is far from the thermodynamic limit, we introduce an entropy

$$
\ln \omega = -\ln|\Omega_s| + constant
$$

(3.41)
This entropy is extremely small as it is associated with only one degree of freedom. So the entropy of the solitary wave can be neglected.

3.2.4. The Rayleigh-Jeans distribution of random waves

The Rayleigh-Jeans distribution of the wave action of random waves is the distribution that maximizes the wave entropy. We can compute the Rayleigh-Jeans distribution under the constraints of fixed $E_w$ and $A_w$.

We compute the extreme value of the wave entropy under the constraints of fixed energy $E_w$ and wave action $A_w$ by introducing Lagrange multipliers $\beta$ and $\mu$

$$\delta(S - \beta(E_w - \mu A_w)) = 0$$

$$\delta \left( \sum_k \ln n_k - \beta \sum_k \omega_k n_k + \beta \mu \sum_k n_k \right) = 0$$

$$\sum_k \left( \frac{\delta n_k}{n_k} - \beta \omega_k \delta n_k + \beta \mu \delta n_k \right) = 0$$

$$\delta n_k \left( \frac{1}{n_k} - \beta \omega_k + \beta \mu \right) = 0$$

Therefore, we have the Rayleigh-Jeans distribution of the wave action of random waves as

$$n_k = \frac{1}{\beta(\omega_k - \mu)}$$

where $\beta^{-1}$ and $\mu$ are the temperature and the chemical potential of random waves, respectively. $n_k > 0$ indicates $\mu < 0$. The inverse temperature measures the change of wave entropy per the change of energy, which is

$$\beta = \frac{\partial S}{\partial E_w}$$

The chemical potential measures the change of energy per the change of wave action with the wave entropy being constant \[10\], which is

$$\mu = \frac{\partial E_w}{\partial A_w} \bigg|_{S=\text{constant}}$$
So we have

$$\beta \mu = -\frac{\partial S}{\partial A_w}$$  \hspace{1cm} (3.46)

The Rayleigh-Jeans distribution describes the wave action as a function of the wavenumber $k$. For each $k$, we have a Gaussian distribution of the amplitudes and a uniform distribution of the phases. This is the state with the maximum entropy given the constraints that the energy and the wave action are fixed.

3.2.5. Maximum entropy for the Rayleigh-Jeans distribution

*We computed the Rayleigh-Jeans distribution in the previous section. We now show the Rayleigh-Jeans distribution maximizes the wave entropy.*

We can show that the Rayleigh-Jeans distribution of wave action gives the maximal wave entropy by the quadratic expansion. We first put (3.43) into the wave entropy (3.38), which gives

$$S = \sum_k \ln n_k$$

$$= -\sum_k \ln (\beta(\omega_k - \mu))$$

The wave action and energy are redistributed on small-amplitude random waves with the constraints of fixed energy and wave action, which indicates

$$\begin{cases} 
\sum_k \omega_k \delta n_k = 0 \\
\sum_k \delta n_k = 0 
\end{cases} \hspace{1cm} (3.47)$$

$$\sum_k \delta n_k = 0 \hspace{1cm} (3.48)$$
This gives a change of the wave entropy

\[
\delta S = \sum_k \delta (\ln n_k) \\
= \sum_k n_k^{-1} \delta n_k \\
= \beta \sum_k \omega_k \delta n_k - \beta \mu \sum_k \delta n_k \\
= 0
\] (3.49)

\[
\delta^2 S = \sum_k n_k^{-1} \delta n_k - \frac{1}{2} n_k^{-2} \delta n_k^2 \\
= \beta \sum_k \omega_k \delta n_k - \beta \mu \sum_k \delta n_k - \frac{1}{2} \beta^2 \sum_k (\omega_k - \mu)^2 \delta n_k^2 \\
= -\frac{1}{2} \beta^2 \sum_k (\omega_k - \mu)^2 \delta n_k^2 \\
< 0
\] (3.50)

Since the linear order is 0 and the quadratic order is negative, the Rayleigh-Jeans distribution does provide the maximal wave entropy. Therefore, any deviations from the Rayleigh-Jeans distribution will decrease the wave entropy.

3.2.6. Divergence of energy for the Rayleigh-Jeans distribution

The “ultraviolet catastrophe” describes the energy divergence in the Rayleigh-Jeans distribution for the continuous system. We discard very short waves to solve this problem.

As a general feature of the classical equilibrium statistics of continuous dynamical systems, the energy \( E_w \) diverges for a grandcanonical ensemble where \( \beta^{-1} \neq 0 \) and \( \mu \) are fixed. In other words, if the wave system is coupled to an infinite reservoir of energy and wave action, modes that are associated with infinitesimal wavelengths absorb an infinite amount of energy from the reservoir. For a microscopical ensemble (energy and wave action of the waves are fixed), the energy spreads out over all modes, in which each mode absorbs only an infinitesimal amount of these quantities.
In our case with the Rayleigh-Jeans distribution, the energy of each mode

\[ E_w = \omega_k n_k \]

\[ = \frac{\omega_k}{\beta(\omega_k - \mu)} \]

\[ \rightarrow \frac{1}{\beta} \quad (3.51) \]

for \( \omega_k \to \infty \), which means all modes (infinitely many) have the same energy. The energy will diverge as a result.

However, the physical relevance of these very short waves is limited since envelope equations like the NLSE describe long modulations of a shorter carrier wave. We then introduce a finite cut-off wavenumber \( |k_{\text{max}}| = \frac{\pi}{2} \) to avoid ultraviolet divergence. \( |k_{\text{max}}| = \frac{\pi}{2} \) is the half length of the Brillouin Zone, which is a compromise between enough modes and less short waves. This is not the only choice for the cut-off, but a good choice in the numerical experiments in our case. Any higher values of wavenumbers will be discarded.

The left plot in the figure 3.6 shows the Rayleigh-Jeans distribution as a function of the wavenumber \( k \) while the right plot shows the energy \( E_w \) of random waves as a function of \( k \).

![Figure 3.6](image)

Figure 3.6: The left plot shows the relationship between \( n_k \) and wavenumber \( k \) while the right one shows the relationship between the energy \( E_w \) and \( k \). In both figures, \( \beta = 0.1 \) and \( \mu = -1 \) for the display purpose only. The right figure tells that as \( k \) gets larger, the influence of \( \omega_k = k^2 \) is more important than that of \( \mu \). \( E_w \) converges to \( \frac{1}{\beta} = 10 \), which matches (3.51).
4.1. Interaction Between a Solitary Wave and Random Waves

*We treat the solitary wave and random waves as two subsystems. They are allowed to exchange both energy and wave action in a way that increases the total wave entropy.*

4.1.1. Alternative approaches

*Besides the thermodynamic model that we will use, there are some other approaches to study the solitary wave interacting with random waves. We explain why these alternatives are not appropriate here.*

The standard statistical approach is to compute the phase space which is available under the constraints of fixed values of energy and wave action. The microcanonical partition function is

$$\Omega = \int \int \delta(H - E) \delta(A - A) dAdE$$  \hspace{1cm} (4.1)

The total entropy follows directly as

$$S = \ln \Omega$$  \hspace{1cm} (4.2)

A technically more feasible approach is often to constrain not the conserved quantities, but the associated intensive parameters (the temperature and the chemical potential in our case). The physical interpretation of this approach is that the system is not isolated, but coupled to external reservoirs of energy and wave action, which yields the grand canonical
partition function

\[ y = \int e^{-\beta H - \mu A} d\phi d\phi^* \]

\[ = \int e^{-\beta \left( \int_{-\infty}^{\infty} |\phi_x|^2 - |\phi|^4/2 + |\phi|^6/3dx \right)} - \mu \int_{-\infty}^{\infty} |\phi|^2 dx d\phi d\phi^* \quad (4.3) \]

Both methods as well as a hybrid approach (one conserved quantity and one temperature are fixed) can be applied with some approximations \[21,31\].

4.1.2. The thermodynamic model

*We introduce a thermodynamic model which truncates some parts of the Hamiltonian and explain the transfer of conserved quantities when the growth or decay process occurs.*

We take a different approach by introducing a thermodynamic model that corresponds to a simplified Hamiltonian. This model consists of two subsystems in which each subsystem can still be represented by its own Hamiltonian

- A high-amplitude non-travelling solitary wave which corresponds to the Hamiltonian at the lower boundary as described in section (3.1)
- Low-amplitude random waves with the quadratic approximation \( \int |\phi_x|^2 dx \) as the Hamiltonian and it was described in section (3.2)

The omitted terms of the Hamiltonian are taken into account only as a weak coupling of these two subsystems, but not as a significant contribution to the energy. The effect of the coupling is that the energy and wave action of each subsystem can exchange. The main advantage of this approach is that it allows us to compute metastable states that correspond to local maximum of the entropy. Figure 4.1 gives the thermodynamic model.
4.1.3. Discussion on the transfer of the conserved quantities

In this section, we discuss seven possible ways of the transfer of the conserved quantities between the two subsystems and some of the transfers are not allowed.

- Is it possible to transfer only the energy from random waves to the solitary wave? Yes, it is possible but not favorable. The solitary wave absorbs energy and then changes its shape, which means it is not a solitary wave anymore as it is not at the lower boundary of the Hamiltonian. From the figure 3.4, we can see when the solitary wave absorbs energy only from random waves, it moves up from the lower boundary of the Hamiltonian, which is feasible. But taking energy from random waves without giving wave action to them will decrease the wave entropy ($\beta > 0$). So this process will not happen.
Figure 4.2: The simplified version of figure 3.4. It is the lower boundary of the Hamiltonian and the region below this line is not feasible. The x-axis is the wave action $A_s$ and the y-axis is the energy $E_s$. The solitary wave absorbs energy only from random waves, it moves up from the lower boundary of the Hamiltonian, which is feasible.

- Is it possible to transfer only the energy from the solitary wave to random waves? No, it is not possible as the solitary wave is already at the lower boundary of the Hamiltonian. So decreasing the energy of the solitary wave is not allowed.

Figure 4.3: The solitary wave is already at the lower boundary of the Hamiltonian. So it is not allowed to transfer energy to random waves.

- Is it possible to transfer only the wave action from random waves to the solitary wave? Yes, it is possible but not favorable. This situation is similar to the first one. Random waves can give only wave action to the solitary wave, which makes the solitary wave leave the lower boundary of the Hamiltonian and therefore it is not a solitary wave anymore. From the figure 3.4, we can see when the solitary wave absorbs wave action only from random waves, it moves to the right of the lower boundary of the Hamiltonian, which is again feasible. However, the process will not happen as taking the wave action from random waves will again decrease the wave entropy for $-\beta \mu > 0$. 

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Figure 4.4: The solitary wave absorbs wave action only from random waves, it moves to the right from the lower boundary of the Hamiltonian, which is possible.

- Is it possible to transfer only the wave action from the solitary wave to random wave? It is similar to the second situation, so it is not possible as the solitary wave is not allowed to move to the left from the lower boundary of the Hamiltonian in the figure 3.4.

Figure 4.5: The solitary wave is already at the lower boundary of the Hamiltonian. So it is not allowed to transfer wave action to random waves.

- Is it possible to transfer both energy and wave action from random waves to the solitary wave? Again it is possible but not favorable. The solitary wave can receive both quantities at the same time and moves to the upper right of the lower boundary of the Hamiltonian. However, transferring both quantities to the solitary wave decreases the wave entropy of the system. So this process will not happen.
Figure 4.6: The solitary wave can absorb both energy and wave action from random waves, but the process decrease the wave entropy. So the process is not allowed.

- Is it possible to transfer both quantities only from the solitary wave to random waves at the same time? As discussed before, transferring any one of the quantities from the solitary wave to random wave is not allowed. So this rule applies to the transfer of two conserved quantities at the same time as well. So it is not possible.

Figure 4.7: The region below the line is not feasible.

- Is it possible to transfer both quantities in the opposite directions? Yes, it is possible and will be the most likely cases for the system. The transfer direction of each conserved quantity depends on if the wave entropy can be maximized by such a combination of the transfer. Also, the transfer of the two conserved quantities will result in the changes of the solitary wave, namely the growth and decay. We will discuss these two possible changes of the solitary wave in the following subsections.

4.1.4. The change of the wave entropy

*We derive the change of the wave entropy as a function of both the chemical potential $\mu$ of random waves and the phase frequency $\Omega_s$ of the solitary wave. Their values can be used to decide the growth or decay of the solitary wave.*
The total energy and wave action of the combined system keeps constant, which means

\[ E = E_w + E_s \]  \hspace{1cm} (4.4)

\[ A = A_w + A_s \]  \hspace{1cm} (4.5)

remains conserved for all time. As mentioned in the section 4.1.2, some parts of the complete Hamiltonian are skipped in the thermodynamic model but are taken into account by the coupling of the two subsystems.

Either the growth or decay of the solitary wave corresponds to the transfer of these two quantities at the same time. We consider the situation where the wave action \( A_w \gg A_s \) and energy \( E_w \gg |E_s| \). Whether the solitary wave grows or decays depends on the change of the total wave entropy of random waves. The change of the wave entropy \( S(E_w, A_w) \) is

\[ dS = \beta(dE_w - \mu dA_w) \]  \hspace{1cm} (4.6)

Changes of energy when the wave action changes for the solitary wave is

\[ dE_s - \Omega_s dA_s = 0 \]  \hspace{1cm} (4.7)

With the total energy and wave action being conserved

\[ dE_w + dE_s = 0 \]  \hspace{1cm} (4.8)

\[ dA_w + dA_s = 0 \]  \hspace{1cm} (4.9)

The entropy of random waves then changes as

\[ dS = \beta(\mu - \Omega_s)dA_s \]  \hspace{1cm} (4.10)

Now the change of entropy is related to the chemical potential \( \mu \) of random waves and the phase frequency \( \Omega_s \) of the solitary wave. Also, the change of entropy is accompanied by the change of wave action of the solitary wave \((dA_s > 0 \text{ or } dA_s < 0)\). There are two opposite scenarios follow from (4.10).
4.1.5. The growth case

*We discuss how the transfer of two conserved quantities in the growth case.*

When $\Omega_s < \mu < 0$, $\mu - \Omega_s > 0$, the solitary wave grows. The growth process indicates that the wave action is transferred from random waves to the solitary wave ($dA_s > 0$) while the energy is transferred in the opposite direction (figure 4.8). The energy of the solitary wave will then become more strongly negative as it loses energy. The entropy of random waves decreases when they lose wave action but increases when they receive energy. The growth process occurs only if the energy gain of random waves has a greater entropic effect than that of their loss of the wave action ($dS > 0$).

![Figure 4.8](image)

*Figure 4.8: Growth case of a solitary wave interacting with random waves. The solitary wave absorbs wave action from random wave while it releases energy to random waves. The entropic effect of receiving energy is greater than that of the loss of wave action for random waves.*

4.1.6. The decay case

*We discuss how the transfer of two conserved quantities in the decay case.*

When $\mu < \Omega_s < 0$, $\mu - \Omega_s < 0$, the solitary wave decays. The decay process indicates that the wave action is transferred from the solitary wave to random waves ($dA_s < 0$) while the energy is transferred in the opposite direction (figure 4.9). The energy of the solitary wave will then become less strongly negative as it absorbs energy. The entropy of random
waves at this time increases when they obtain wave action but decreases when they lose energy. The decay process occurs only if the gain of wave action of random waves has a greater entropic effect than that of their loss of energy \((dS > 0)\).

![Diagram of wave action and energy transfer](image)

Figure 4.9: Decay case of a solitary wave interacting with random waves. The solitary wave absorbs energy from random wave while it releases wave action to random waves. The entropic effect of receiving wave action is greater than that of the loss of energy for random waves.

From both the growth and decay processes of the solitary wave, we know that entropy of random waves increases as a result. Random waves transfer conserved quantities to the solitary wave only when these transfers help increase its entropy.

4.1.7. A concrete example

*We give a visualization of the growth and decay of the solitary wave.*

We now consider the limit of a large system with a single solitary wave being immersed in a sea of low-amplitude random waves. As we discussed in the previous sections, most wave action and energy are contained in random waves, which means \(A_w \gg A_s\) and \(E_w \gg E_s\). If the solitary wave is melted by random waves, wave action is transferred from the solitary wave to random waves while the energy is transferred from the opposite direction.

With random waves being a large reservoir of the two conserved quantities, their temperature and chemical potential will be effectively unchanged. The same is true if the solitary
wave grows by such an interaction moderately, meaning that the transfer of the conserved quantities is moderate compared to their amount being stored in random waves. In either case, the entropy of random waves can be described by the linear approximation

\[ S(E_w, A_w) = \beta(E_w - E - \mu(A_w - A)) + \text{constant} \]  

(4.11)

Figure 4.10(b) gives the entropy surface (4.11) with \( E_w - E = -E_s \) and \( A_w - A = -A_s \) for a constant chemical potential \( \mu = -0.05 \) and temperature \( \beta = 20 \) as an example (Other values of \( \beta \) merely re-scale the entropy axis with no qualitative effect).

The curve \( E_s(A_s) \) from figure 4.10(a) is projected on the entropy surface in figure 4.10(b). The dotted line is an isentrope with \( \frac{dE_w}{dA_w} = \mu = -0.05 \). This isentrope is tangential to the projection of the curve \( E_s(A_s) \) at the point \( \Omega_s = \mu \), which corresponds to \( A_s = A - A_w = \sqrt{12/11} \) from the equation (3.13). The entropy at this point is the lowest along the curve \( E_s(A_s) \). The region beyond the boundary line (corresponding to higher entropy) is not accessible. The region below this line has a lower entropy and corresponds to a solitary wave whose energy is not extreme. Entropy maximization pushes the solitary wave to the boundary. In other words, the solitary wave is stabilized by the thermodynamic forces \( \beta \) and \( \mu \).
Figure 4.10: (a) Lower boundary $E_s(A_s)$ of the energy of the solitary wave. (b) Wave entropy surface $S(E, A)$ of random waves for $\beta = 20$ and $\mu = -0.05$. The dotted line is an isentrope $S = \text{constant}$ with $\frac{dE_w}{dA_w} = \mu$. The energy and wave action of random waves can change by transferring these two quantities from or to a growing or decaying solitary waves. This corresponds to a time evolution along the boundary curve from (a) projected onto the entropy surface. Growth of the large solitary wave ($\Omega_s < \mu < 0$) increases the entropy (blue curve) and decay of the small solitary wave ($\mu < \Omega_s < 0$) increases the entropy (red curve). The tangential point $\Omega_s = \mu = -0.05$ ($E_s = E - E_w = -0.0196$, $A_s = A - A_w = \sqrt{\frac{12}{11}}$) corresponds to an equilibrium of the solitary wave and random waves.

A solitary wave with small values of $|E_s|$ and $A_s$ will be melted as a consequence of the interaction with random waves: the entropy of random waves increases as the wave action increases. The solitary wave evolves along the red part of the curve $E_s(A_s)$ towards $A_s = 0$ and $E_s = 0$, which means $E_w = E$ and $A_w = A$.

A solitary wave with $E_s$ and $A_s$ above the tangential point grows by interacting with random waves: it transfers energy to random waves which increases the entropy. The solitary wave evolves along the blue part of the curve $E_s(A_s)$. The growth of the solitary wave is expected to continue until there is an equilibrium. This equilibrium can only be achieved by transferring so much energy and wave action so that the chemical potential of the waves
approaches the extremum of $\Omega_s$, namely $-\frac{a}{16}$. The system is then in a two-phase state: one low-amplitude phase and one high-amplitude phase with $|\phi| \approx \sqrt{\frac{3}{2}}$.

The entropy of random waves increases both as a function of the wave action and energy. Gain of energy is associated with the loss of the wave action and vice versa. The entropic effect of the energy prevails for solitary waves with $|\Omega_s| > |\mu|$ while the entropic effect of the wave action prevails for solitary waves with $|\Omega_s| < |\mu|$.

4.2. Saddle point at $\Omega_s = \mu$

The transition point $\Omega_s = \mu$ is a saddle point of the wave entropy.

The entropy does not change in linear order when $\Omega_s = \mu$. A quadratic expansion shows that the point $\Omega_s = \mu$ is a saddle point for small solitary waves and a maximum for solitary waves with high amplitudes.

We compute the quadratic expansion of the wave entropy when the wave action and energy are transferred to or from the solitary wave. With

$$\Omega_s \approx \mu + \frac{d\Omega_s}{dA_s} dA_s$$  \hspace{1cm} (4.12)

The change of the wave entropy is

$$d^2S = -\beta \frac{d\Omega_s}{dA_s} dA_s^2$$  \hspace{1cm} (4.13)

From (3.13), we know $\frac{d\Omega_s}{dA_s} = \frac{d^2E_s}{dA_s^2} < 0$, so (4.12) becomes

$$d^2S = -\beta \frac{d^2E_s}{dA_s^2} dA_s^2 > 0$$  \hspace{1cm} (4.14)

This shows that the wave entropy is minimal with respect to the growth or decay processes of the solitary wave. $\Omega_s = \mu$ is a saddle point of the wave entropy in the sense that

- Any redistribution (3.50) of wave action within random waves will lead to a quadratic decrease of the entropy as Rayleigh-Jeans distribution already gives the best distribution which maximizes the entropy.

- Changing the shape of the solitary wave with wave action being fixed but transferring
energy also decreases the wave entropy. This situation was discussed in section 4.1.3 already. The solitary wave is not at the lower boundary of the Hamiltonian any more. This process takes energy away from random waves, so the entropy decreases.

- Changing the shape of the solitary wave with the energy being fixed but varying the wave action also decreases the wave entropy. This situation was also discussed in section 4.1.3. This process takes wave action away from random waves.

- The transfer of wave action (4.14) either to \((dA_s > 0)\) or from \((dA_s < 0)\) the solitary wave will lead to a quadratic increase of the wave entropy since both two conserved quantities can be transferred between two subsystems.

\[\Omega_s = \mu\] is a threshold that separates domains of growth and decay of the solitary wave.
Chapter 5

NUMERICAL EXPERIMENTS

We perform numerical simulations of the full system. For the modified NLSE, we deal with the linear and nonlinear part with different techniques. The numerical results match our theoretical prediction.

5.1. Initial Conditions

5.1.1. The initial condition for the solitary wave

We employ the finite difference method for the space variable to solve the ODE (3.4) as the initial condition for the solitary wave.

For the modified NLSE (2.25), we seek a solution in the form \( \phi(x,t) = u(x)e^{-i\Omega s t} \) and obtain the equation (3.4). The finite difference discretization for the second derivative is

\[
 u_{xx} \approx \frac{u_{n+1} - 2u_n + u_{n-1}}{h^2} \tag{5.1}
\]

where \( h \) is the step size. In our case, we consider \( h = 1 \).

The full scheme to solve (3.3) will then be the map

\[
\begin{aligned}
 p_{n+1} &= u_n \\
 u_{n+1} &= h^2(-\Omega s u_n - u_n^3 + u_n^5) + 2u_n - p_n
\end{aligned} \tag{5.2}
\]

The fixed point of the map is

\[
\begin{aligned}
 p_{n+1} &= 0 \\
 u_{n+1} &= 0
\end{aligned} \tag{5.3}
\]

So there is an unstable manifold. We start with this manifold and we will have the homoclinic orbit.
Figure 5.1: The left plot is the homoclinic orbit of the map. The right plot is the solution of the map with $\Omega_s = -0.04$ as an example initial condition. This initial solitary wave is not related to later experiments.

But if we set the $\Omega_s = -\frac{3}{16}$. Then the map will be two heteroclinic orbits which connect two fixed points of $u = 0$ and $u = \frac{\sqrt{3}}{2}$. In our numerical simulations, we only consider the homoclinic orbit.

Figure 5.2: The heteroclinic orbit of the map (5.2) when $\Omega_s = -\frac{3}{16}$.
5.1.2. The initial condition for random waves

We first use random number generator to generate random numbers between (0, 1) and use Box-Muller method to generate a Gaussian distribution of amplitudes for random waves. The Rayleigh-Jeans distribution of modes requires to multiply additional terms.

Small random waves have random phases, a Gaussian distribution of amplitudes and a Rayleigh-Jeans distribution of modes for $-\frac{\pi}{2} \leq k \leq \frac{\pi}{2}$. Waves with $\frac{\pi}{2} < |k| \leq \pi$ have zero amplitudes initially. This cut-off reduces the aliasing error, where some modes may be indistinguishable at some discrete grid points. We can create a Gaussian distribution $y$ from a uniform distribution $x$ using the Box-Muller [37] method $y = \sqrt{-2 \ln x}$. Since the Fourier modes are complex, we need to multiply a factor to give them random phases. We
also multiply a factor $\sqrt{\frac{T}{\mu + \omega_k}}$ to have the Rayleigh-Jeans distribution of modes.

\[
Re(a_k) = \sqrt{-2 \ln x_1} \cos \left( 2\pi x_2 \sqrt{\frac{T}{\mu + \omega_k}} \right)
\]
(5.4)

\[
Im(a_k) = \sqrt{-2 \ln x_1} \sin \left( 2\pi x_2 \sqrt{\frac{T}{\mu + \omega_k}} \right)
\]
(5.5)

where $T = \frac{1}{k_B \beta}$ and $k_B$ is the Boltzmann constant. In our case, $k_B = 1$.

Figure 5.4: The initial condition of the Rayleigh-Jeans distributed random waves in the first Brillouin Zone $[-\pi, \pi]$. It is an example only and not related to later numerical simulations.

5.1.3. Superposition of a solitary wave and random waves

There are different ways to combine the solitary wave and random waves. For example, we can add up everything to build one combined system. But this is not the best way.

The initial condition is a state with one solitary wave which is immersed in a sea of small-amplitude random waves. This combination is not a simple addition of these two components since addition would significantly change the shape and energy of the solitary wave. Instead, the solitary wave replaces random waves at the locations where the amplitude of the solitary wave exceeds those of the random waves. Our simulations show that a small amount of wave action flows into the region $\frac{\pi}{2} < |k| \leq \pi$. The spreading of energy to very
short waves is a comparatively slow process.

Figure 5.5: The initial condition for the combined system.

5.2. Solving the Modified NLSE

5.2.1. The finite number of modes and periodic boundary conditions

*We have a finite number of Fourier modes in the simulations and impose the periodic boundary conditions. The code used here is adapted from the code originally written for [46, 49].*

Given the modified NLSE (2.25), we Fourier transform it into the wavenumber space. If we let $\mathcal{F}$ be the operator of the Fourier transform and $a_k(t)$ be the Fourier modes of $\phi(x,t)$, then we have the time derivative as

$$
\mathcal{F}(i\phi_t) = i \int \frac{\partial}{\partial t} \phi(x,t) e^{-ikx} \, dx
$$

$$
= i \int \frac{\partial}{\partial t} [\phi(x,t) e^{-ikx}] \, dx
$$

$$
= i \frac{\partial}{\partial t} a_k
$$
The Fourier transform of the space derivative $\phi_{xx}$ is

$$F(\phi_{xx}) = \int \phi_{xx}(x, t)e^{-ikx}dx$$

$$= -\int \phi_x(x, t)(-ik)e^{-ikx}dx$$

$$= (ik)^2 \int \phi(x, t)e^{-ikx}dx$$

$$= -k^2a_k$$

The Fourier transform of the nonlinear part is just $F(|\phi|^2\phi) - F(|\phi|^4\phi)$.

So the complete equation after the Fourier transform of (2.25) is

$$i\frac{\partial}{\partial t}a_k = -k^2a_k + F(|\phi|^2\phi) - F(|\phi|^4\phi) \quad (5.6)$$

We have the finite number of $k$ in the interval $[-\pi, \pi]$. In our case, the number of modes is equal to the system size $N$. The distance between each wavenumber $k_i$ is $\frac{2\pi}{N}$ for $i = 1, ..., N$. Also, each mode has the same distance. Periodic boundary conditions are used in the simulations to avoid the issues with boundary effects caused by the finite size of the system and make the system more like an infinite one.

5.2.2. Stiffness of linear differential equations

The stiffness index measures the ratio of the largest and smallest eigenvalues. The stiffness is an issue for using numerical methods.

The eigenvalues of (5.6) are purely imaginary and vary from small to large values, which gives the problem of the stiffness. The stiffness comes from the dispersion relation $k^2$ and it can affect the stability of the numerical methods. As a result, we need to solve it before employing the numerical schemes.

We can remove the linear part of (5.6) by introducing an integrating factor to solve the stiffness problem [33]

$$b_k(t) = e^{-ik^2t}a_k(t) \quad (5.7)$$
Then equation (5.6) becomes

\[ i \frac{\partial}{\partial t} (b_k e^{ik^2 t}) = -k^2 (b_k e^{ik^2 t}) + \tilde{F}(|\phi|^2 \phi) - \tilde{F}(|\phi|^4 \phi) \]  

(5.8)

\[ i \left( \frac{\partial}{\partial t} b_k \right) e^{ik^2 t} - k^2 b_k e^{ik^2 t} = -k^2 (b_k e^{ik^2 t}) + \tilde{F}(|\phi|^2 \phi) - \tilde{F}(|\phi|^4 \phi) \]  

(5.9)

where \( \tilde{F} \) represents the Fourier transform of the nonlinear part with \( b_k \).

The remaining equation is

\[ i \left( \frac{\partial}{\partial t} b_k \right) e^{ik^2 t} = \tilde{F}(|\phi|^2 \phi) - \tilde{F}(|\phi|^4 \phi) \]  

(5.10)

5.2.3. Dealing with the nonlinear part

If we compute the nonlinear part in the Fourier space directly, the computation process will be extremely slow as the number of modes will be large for the 3rd and 5th powers.

A spectral method is to represent the solution of a differential equation in terms of a basis of some vector space and then reduce the differential equations to an ODE system for the coefficients. The pseudospectral method is a special spectral method which represents the solution in terms of the basis but imposes the equation only at discrete points. The ‘pseudospectral’ in the method refers to the spatial part of a PDE.

We use the FFTPACK written by Paul Swarztrauber and Dick Valent for the Fast Fourier Transform (FFT). The process is as follows

- Compute \( \tilde{F}(|\phi|^2 \phi) - \tilde{F}(|\phi|^4 \phi) \) in the real space.
- Transform the results back in the Fourier space again with FFT.

5.2.4. Multistep Adams method

The remaining ODE equations for the modes can be solved by multistep Adams method.

We use a multistep Adams method for the last computation part. Since the linear part has been removed, there will be no stiffness problem. There are two advantages of the multistep Adams method. First, the Adams method is efficient for solving non-stiff
equations. Second, unlike the one-step method, we evaluate the equation only once in each step with the multistep method. So we compute fewer Fourier transforms, which is less computationally expensive. The equations of motion for the modes are integrated with the code ODE written by Lawrence Shampine and Marilyn Gordon in this part.

5.3. Numerical Results

We give the results of the numerical experiments with discussions.

The system size is $N = 2^{12}$ with $2^{12}$ modes and periodic boundary conditions. This system size is large enough to make the numerical results applicable to complex systems. The interaction of the solitary wave and random waves is weak so that the integration times are long and the integration needs to be relatively accurate. We use the conservation of wave action $A$ as a measure to monitor the numerical accuracy. The relative error is less than $10^{-4}$ over the integrations. The results have been verified for larger ($N = 2^{14}$) system size and for various numerical accuracies. The codes have also been tested for solitary waves without the surrounding random waves.

Figure 5.6 and 5.7 give results for the same set of 21 numerical simulations for different chemical potentials varying from $\mu = -0.2$ to $\mu = 0$ with an increment of 0.01. The average squared amplitude of random waves is $\langle |\phi_w|^2 \rangle = 0.012$ in the initial conditions for all simulations. This can be achieved by adjusting the value of temperature for each simulation. The purpose of having the same initial squared amplitudes is to make the time scale of growth or decay processes for different values of $\mu$ more comparable without influencing the transition behavior. The solitary wave has an initial phase frequency $\Omega_s = -0.1$ in each simulation. About 4 percent of the total wave action is stored in the solitary wave and 96 percent is stored in random waves for these initial conditions. The chemical potential and temperature change only slightly when the solitary wave is eroded.
Figure 5.6: Time evolution of the maximum amplitudes of $|\phi|^2$ for a solitary wave with the phase frequency $\Omega_s = -0.1$ and an initial squared amplitude $u^2 = 0.24$ (corresponding to the smaller solitary wave in Figure 3.3) immersed in a sea of small-amplitude random waves with different temperatures and chemical potentials. The temperatures are chosen so that the average squared amplitude is $\langle |\phi_w|^2 \rangle = 0.012$ for all simulations. The curves are running time averages over 2000 time units. The 10 red curves correspond to random waves with chemical potentials from $-0.2 \leq \mu < -0.1$. The 10 blue curves correspond to values $-0.1 < \mu \leq 0$. The black curve corresponds to $\mu = -0.1$. Increases of the curves indicate the growth of the solitary waves and they approach to the larger one in figure 3.3. Decreases means the decay of the solitary waves and eventually the solitary waves will have a smaller amplitudes than random waves.

Figure 5.6 shows the time evolution of the spatial maximum amplitudes of the solitary wave $|\phi|^2$ for 21 simulations. Red curves correspond to $-0.2 \leq \mu < -0.1$. Blue curves correspond to $-0.1 < \mu \leq 0$. The black curve corresponds to $\mu = -0.1$. Figure 5.7 displays the end points of these simulations as a function of $\mu$. 
The numerical experiments show that solitary waves grow for $\mu < -0.1$ with the exception of one outlier at $\mu = -0.11$ that decays. Solitary waves with $\mu > -0.1$ grow with the exception of one outlier at $\mu = -0.08$. We find that such outliers occur occasionally near the transition at $\mu = \Omega_s = -0.1$. These outliers are the consequence of the finite amplitude of random waves that can push the initial solitary wave just above or below the threshold.

Growing solitary waves will develop to approach a broad plateau similar to the bigger solitary wave in figure 3.3 while decaying solitary waves will be melted and have a smaller amplitudes than those of the random waves eventually.

So the numerical experiments help confirm the theoretical prediction: If the phase frequency of the solitary wave is greater than the chemical potential of random waves, the solitary wave accumulates wave action while transferring the energy to random waves and grows. If the phase frequency is smaller, then the decay process occurs and two conserved quantities are transferred in the opposite direction.

It is notable that small solitary waves may emerge during the interaction. In our numerical experiments, when the chemical potential is small, we can see the formation of some
small solitary waves. These solitary waves may collide with the initial high-amplitude solitary wave. But this collision does not affect our prediction, we still can see the results of either a larger solitary wave after growing or just random waves after decaying. Our theory argues from the entropy of the final result.
Chapter 6

FURTHER DISCUSSION

6.1. Generalization to Higher Dimensional Cases

We briefly discuss how our model and results can be generalized in two and three dimensional cases.

Besides the solitary waves, there are other coherent structures. The unique feature that distinguishes the solitary waves from other coherent structures is that solitary waves have the lowest possible energy for a fixed amount of wave action, which makes it thermodynamically favorable. The thermodynamic forces temperature $\beta$ and chemical potential $\mu$ push coherent structures towards the lower bound of the Hamiltonian.

Small solitary waves with $\mu < \Omega_s < 0$ decay when they interact with random waves. In this case, the entropic effect of transferring wave action to random waves is more dominant than transferring energy in the opposite direction. This leads to a metastable state of random waves without the coherent structures. A metastable state is also a stable state other than the state with the least energy. The entropy of the metastable state is only locally maximal and its contribution to the microcanonical ensemble is insignificant.

Large solitary waves with $\Omega_s < \mu < 0$ grow when they interact with random waves. In this case, the entropic effect of transferring energy to random waves is dominant compared with transferring wave action to the solitary waves, which leads to a sustained growth of the coherent structures.

A solitary wave is in an unstable equilibrium state with random waves if

$$\Omega_s = \frac{dE_s}{dA_s} = \frac{dE_w}{dA_w} = \mu$$

(6.1)
The entropic effect of transfer of wave action and energy under the growth or decay of the coherent structure cancel each other in linear order. By (4.13), when \( \frac{\partial^2 E_s}{\partial A_s^2} < 0 \), this is a minimum of the entropy along the lower bound of the Hamiltonian and marks the transition between growth and decay processes. At the same time, it is maximal with respect to variations

\[
\begin{cases}
  dA_s > 0 \quad \text{with} \quad dE_s = 0 \\
  dE_s > 0 \quad \text{with} \quad dA_s = 0
\end{cases}
\]

(6.2) (6.3)

In this sense, it is a saddle point. The assumption [29] that this is the maximum of entropy is true for a coherent structure with the property \( \frac{\partial^2 E_s}{\partial A_s^2} > 0 \).

Our arguments are based only on the entropic effect of the transfers of the two conserved quantities to random waves and the coherent structure. This is independent of the details of the interaction of the coherent structure and random waves. One such mechanism is the spontaneous formation of solitary waves when \( |\mu| \) is small. This formation occurs randomly. In this case, high-amplitude regions may exceed the growth condition for a small \( |\mu| \). When such small solitary waves collide with a larger solitary wave, they transfer wave action to the larger one [14,63].

Are these results applicable to two or three spatial dimensions? The focusing nonlinear Schrödinger Hamiltonian is bounded from below in one dimension (2.6) to have stable ground state solitons. But in two and three dimensions, the Hamiltonian is not bounded from below, so stable solitons at the lower boundary do not exist. Instead, there are finite-time blow-ups in two and three dimensions. But in the counterpart of (2.25) in two and three dimensions, the Hamiltonian is still bounded from below due to the \( |\phi|^6 \) term. In particular, broad solitary waves with \( E_s = -\frac{3}{16} A_s \) similar to the one-dimensional case of figure 3.3 still exist. The mechanism of the growth and decay of the coherent structures described before can still be applied with the two and three dimensional cases.
6.2. Nonzero Momentum

In our previous discussion, we only considered the standing solitary wave with zero momentum. What about the nonzero case?

Since our study contains the zero momentum solitary wave, we can only observe slow motions of the solitary wave caused by interactions with random waves. Nonzero momentum could be incorporated in both the solitary wave and random waves, which will lead to an additional balance of the speed of the solitary wave and a parameter \( v \) of the Rayleigh-Jeans distribution

\[
n_k = \frac{1}{\beta(\omega_k - vk - \mu)}
\]  

(6.4)

\( vk \) shifts the Rayleigh-Jeans distribution in wavenumber space and absorbs some energy. But we think the nonzero momentum case will not violate our previous findings. We still should be able to find the growth or decay of the solitary wave as momentum only gives the initial speeds for both the solitary wave and random waves. There will be an offset during the interaction at some point. We will investigate the nonzero momentum case in a more detailed way in the future.

6.3. Physical Status of Classical Thermal Equilibrium in Hamiltonian PDEs

The physical relevance of the statistically attracting set is not this state itself but in its influence on physically relevant states that are far apart from it. They may be studied either by including short-scale dissipation or a cut-off in the initial conditions.

For a canonical ensemble where a system is coupled with an external heat bath with a temperature \( \beta^{-1} \), the infinitesimal degrees of freedom absorb an infinite amount of energy. If energy and wave action are both fixed, the finite coupling energy is shared by all modes, so it flows to infinitesimal wavelengths. The physical relevance of the attracting set is its influence on the dynamics at the scale where the wave equation is applicable. Spatial fluctuations on short (and certainly on infinitesimal) scales are outside the applicability of the wave equations. In particular, the nonlinear Schrödinger equation describes the envelope
dynamics of a shorter carrier wave. At even shorter scales, various microscopic effects like dissipation and thermal noise (in fluids), quantum corrections (in optical waves) as well as the spatial discreteness (in crystals) become relevant.

The method of introducing a cut-off in the initial conditions is self-consistent as spreading of energy into the short-scale range turns out to be a slow process compared to growth or decay of the coherent structures. The cut-off can also have direct physical relevance: in photonics a natural cut-off has been found as a result of higher-order dispersion terms that lead to truncated [3] or anomalous [57] thermalization. Another effective cut-off can be caused by proximity to the integrable case [56]. Finally, spatial discreteness of lattices confines the wavenumber to the Brillouin-zone.

6.4. Dissipation Effect: Non-equilibrium Spectra

We now discuss the situations when dissipation is taken into consideration.

Dissipation at short scales can lead to a state of wave turbulence in which energy flows from long scales into the dissipation range. The second conserved quantity wave action flows towards small $k$ in an inverse cascade. A stationary non-equilibrium state can be achieved when both quantities are fed into the system at an intermediate length scale. It also requires nontrivial resonances of interacting modes, which is easier to achieve in two or three spatial dimensions than in one. Kolmogorov-Zakharov distributed waves with

$$n_k \sim \frac{1}{\omega_k^q}, \quad q > 1$$

(6.5)
can in principle support growth of coherent structures even more strongly than Rayleigh-Jeans distributed waves. The build-up of coherent structures is then a strongly nonlinear mechanism that feeds energy into the waves and that can coexist with the interaction of weakly correlated waves of turbulence [49]. The formation of localized structures can be a relevant contributor to dissipation [23].
What makes our findings unique is that there is a real threshold $\Omega_s = \mu$ which can be verified by numerical simulations for complex dynamical systems. We have found the growth and decay of a coherent structure interacting with random waves in a generic nonintegrable and non-collapsing nonlinear Schrödinger equation. The threshold of these two types of dynamics depends on the statistical property of random waves and the dynamical property of the coherent structure, namely the chemical potential of random waves and the phase frequency of the coherent structure.

The growth process is the result of an interaction with surrounding random waves which transfers wave action to the coherent structure. The decay process drives random waves into a metastable state. The threshold between growth and decay represents an unstable equilibrium. The solitary wave is a thermal structure which will also grow in non-thermal (turbulent) wave backgrounds with a Komogorov-Zakharov spectrum. The behaviors that we have found are the consequence of the entropy maximization under the constraints of conserved quantities. These behaviors are expected to happen in different equations, dimensions and with different types of spectra of the surrounding waves. In the discrete system, there are other transitions from negative to positive temperatures, but we do not have this concern in the continuous system.

The possible future work will be to add the nonzero momentum into consideration. We may also consider the multi- solitary-wave solutions or change the NLSE to other equations.
BIBLIOGRAPHY


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