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Formalism of the nonlinear Schrödinger equations

Make everything as simple as possible, but not simpler.
– Albert Einstein.

Someone told me that each equation I included in the book would halve the sales.
– Stephen Hawking.

When the author was a graduate student, introductions to texts on nonlinear evolution equations contained a long description of physical applications, numerous references to the works of others, and sparse details of the justification of analytical results. Times have changed, however, and the main interest in the nonlinear evolution equations has moved from modeling to analysis. It is now more typical for applied mathematics texts to start an introduction with the main equations in the first lines, to give no background information on applications, to reduce the list of references to a few relevant mathematical publications, and to focus discussions on technical aspects of analysis.

Since this book is aimed at young mathematicians, we should reduce the background information to a minimum and focus on useful analytical techniques in the context of the nonlinear Schrödinger equation with a periodic potential. It is only in this introduction that we recall the old times and review the list of nonlinear evolution equations that we are going to work with in this book. The few references will provide a quick glance at physical applications, without distracting attention from equations.

The list of nonlinear evolution equations relevant to us begins with the nonlinear Schrödinger equation with an external potential,

$$\mathrm{i}u_t = -\Delta u + V(x)u + \sigma|u|^2 u,$$

where $\Delta = \partial_{x_1}^2 + \cdots + \partial_{x_d}^2$ is the Laplacian operator in the space of d dimensions, $u(x,t) : \mathbb{R}^d \times \mathbb{R} \to \mathbb{C}$ is the amplitude function, $V(x) : \mathbb{R}^d \to \mathbb{R}$ is a given potential, and $\sigma \in \{1, -1\}$ is the sign for the cubic nonlinearity. If $\sigma = -1$, the nonlinear Schrödinger equation is usually called focusing or attractive, whereas if $\sigma = +1$, it is called defocusing or repulsive. The names differ depending on the physical applications of the model to nonlinear optics [5], photonic crystals [192], and atomic physics [171].

It is quite common to use the name of the *Gross–Pitaevskii equation* if this equation has a nonzero potential $V(x)$ and the name of the *nonlinear Schrödinger* *equation* if $V(x) \equiv 0$. Historically, this terminology is not justified as the works of E.P. Gross and L.P. Pitaevskii contained a derivation of the same equation with $V(x) \equiv 0$ as the mean-field model for superfluids [83] and Bose gas [170]. However, given the number of physical applications of this equation with $V(x) \equiv 0$ in nonlinear optics, photonic crystals, plasma physics, and water waves, we shall obey this historical twist in terminology and keep reference to the Gross–Pitaevskii equation if $V(x)$ is *nonzero* and to the nonlinear Schrödinger equation if $V(x)$ is *identically zero*.

Several recent books [2, 30, 133, 199, 201] have been devoted to the nonlinear Schrödinger equation and we shall refer readers to these books for useful information on mathematical properties and physical applications of this equation. As a main difference, this book is devoted to the Gross–Pitaevskii equation with a *periodic* potential $V(x)$.

We shall study localized modes of the Gross–Pitaevskii equation with the periodic potential. These localized modes are also referred to as the *gap solitons* or *discrete breathers* because they are given by time-periodic and space-decaying solutions of the Gross–Pitaevskii equation. In many of our studies, we shall deal with localized modes in one spatial dimension. Readers interested in analysis of vortices in the two-dimensional Gross–Pitaevskii equation with a harmonic potential may be interested to read the recent book of Aftalion [3].

Many other nonlinear evolution equations with similar properties actually arise as asymptotic reductions of the Gross–Pitaevskii equation with a periodic potential, while they merit independent mathematical analysis and have independent physical relevance. One such model is a system of two *coupled nonlinear Schrödinger* equations,

$$\begin{cases} \mathrm{i}u_t = -\Delta u + \sigma\left(|u|^2 + \beta|v|^2\right)u, \\ \mathrm{i}v_t = -\alpha\Delta v + \sigma\left(\beta|u|^2 + |v|^2\right)v, \end{cases}$$

where α and β are real parameters, $\sigma \in \{1, -1\}$, and $(u, v)(x, t) : \mathbb{R}^d \times \mathbb{R} \to \mathbb{C}^2$ stand for two independent amplitude functions. The number of amplitude functions in the coupled nonlinear Schrödinger equations can exceed two in various physical problems. However, two is a good number both from the increased complexity of mathematical analysis compared to the scalar case and from the robustness of the model to the description of practical problems. For instance, two polarization modes in a birefringent fiber are governed by the system of two coupled nonlinear Schrödinger equations and so are the two resonant Bloch modes at the band edge of the photonic spectrum [7].

When the coupled equations for two resonant modes in a periodic potential are derived in the space of one dimension ($d = 1$), the group velocities of the two modes are opposite to each other and the coupling between the two modes involves linear terms. In this case, the system takes the form of the *nonlinear Dirac* equations,

$$\begin{cases} \mathrm{i}(u_t + u_x) = \alpha v + \sigma\left(|u|^2 + \beta|v|^2\right)u, \\ \mathrm{i}(v_t - v_x) = \alpha u + \sigma\left(\beta|u|^2 + |v|^2\right)v, \end{cases}$$

where α and β are real parameters, $\sigma \in \{1, -1\}$, and $(u, v)(x, t) : \mathbb{R} \times \mathbb{R} \to \mathbb{C}^2$ are the amplitude functions for two resonant modes. Two counter-propagating waves coupled by the Bragg resonance in an optical grating is one of the possible applications of the nonlinear Dirac equations [197]. We recall from quantum mechanics that the Dirac equations represent the relativistic theory compared to the Schrödinger equations that represent the classical theory.

The list of nonlinear evolution equations for this book ends at the spatial discretization of the nonlinear Schrödinger equation, which is referred to as the *discrete nonlinear Schrödinger* equation. This equation represents a system of infinitely many coupled differential equations on a lattice,

$$\mathrm{i}\dot{u}_n = -(\Delta u)_n + \sigma |u_n|^2 u_n,$$

where $(\Delta u)_n$ is the discrete Laplacian operator on the d-dimensional lattice, $\sigma \in \{1, -1\}$, and $\{u_n(t)\} : \mathbb{Z}^d \times \mathbb{R} \to \mathbb{C}$ is an infinite set of amplitude functions. The discrete nonlinear Schrödinger equation arises in the context of photonic crystal lattices, Bose–Einstein condensates in optical lattices, Josephson-junction ladders, and the DNA double strand models [110].

Modifications of the nonlinear evolution equations in the aforementioned list with a more general structure, e.g. with additional linear terms and non-cubic nonlinear functions, are straightforward and we adopt these modifications throughout the book if necessary. It is perhaps more informative to mention other nonlinear evolution equations, which are close relatives to the nonlinear Schrödinger equation. Among them, we recall the *Klein–Gordon*, *Boussinesq*, and other nonlinear dispersive wave equations. In the unidirectional approximation, many nonlinear dispersive wave equations reduce to the *Korteweg–de Vries* equation. It would take too long, however, to list all other nonlinear evolution equations, their modifications, and the relationships between them, hence we should stop here and move to the mathematical analysis of the Gross–Pitaevskii equation with a periodic potential. For the sake of clarity, we work with the simplest mathematical models keeping in mind that the application-motivated research in physics leads to more complicated versions of these governing equations.

1.1 Asymptotic multi-scale expansion methods

Our task is to show how the Gross–Pitaevskii equation with a periodic potential can be approximated by the simpler nonlinear evolution equations listed in the beginning of this chapter. To be able to perform such approximations, we shall consider a powerful technique known as the *asymptotic multi-scale expansion method*. This method is applied in a certain asymptotic limit after all important terms of the primary equations are brought to the same order, while all remaining terms are removed from the leading order.

The above strategy does not sound like a rigorous mathematical technique. If power expansions in terms of a small parameter are developed, only a few terms are actually computed in the asymptotic multi-scale expansion method, while the remaining terms are cut down in the hope that they are small in some sense. In the time evolution of a hyperbolic system with energy conservation, it is not unusual to bound the remaining terms at least for a finite time (Sections 2.2–2.4). In the time evolution of a parabolic system with energy dissipation, the theory of invariant manifolds and normal forms is often invoked to obtain global results for all positive times, as we shall see in the same sections in the context of a time-independent elliptic system (which is a degenerate case of a parabolic system).

It is still true that a formal approximation of the asymptotic multi-scale expansion method is half way to the rigorous analysis of the asymptotic reduction. Another way to say this: if you do not know how to solve a problem rigorously, first solve it formally! In many cases, the formal solution may suggest ways to rigorous analysis.

The above slogan explains why, even being unable to analyze asymptotic approximations thirty or even twenty years ago, applied mathematicians tried nevertheless to formalize the asymptotic multi-scale expansion method in many details to avoid misleading computations and failures. The method has been described in several books [143, 199] and the number of original publications in the context of physically relevant equations is truly uncountable!

We shall look at the three different asymptotic limits separately for the reductions of the Gross–Pitaevskii equation with a periodic potential to the nonlinear Dirac equations, the nonlinear Schrödinger equation, and the discrete nonlinear Schrödinger equation. Our approach is based on the classical asymptotic multi-scale expansion method, which has been applied to these three asymptotic reductions in the past [152].

The starting point for our asymptotic analysis is the Gross–Pitaevskii equation in one spatial dimension,

$$\mathrm{i}u_t = -u_{xx} + V(x)u + \sigma|u|^2u, \tag{1.1.1}$$

where $u(x,t) : \mathbb{R}\times\mathbb{R} \to \mathbb{C}$, $\sigma \in \{1,-1\}$, and $V(x+2\pi) = V(x)$ is a bounded 2π-periodic potential.

Three different asymptotic limits represent different interplays between the strength of the periodic potential $V(x)$ and the strength of the nonlinear potential $\sigma|u|^2$ affecting existence of localized modes in the Gross–Pitaevskii equation (1.1.1). These asymptotic limits are developed for small-amplitude potentials (Section 1.1.1), finite-amplitude potentials (Section 1.1.2), and large-amplitude potentials (Section 1.1.3). In each case, we derive the leading-order asymptotic reduction that belongs to the list of nonlinear evolution equations in the beginning of this chapter.

1.1.1 The nonlinear Dirac equations

In the limit of small-amplitude periodic potentials, the Gross–Pitaevskii equation (1.1.1) can be rewritten in the explicit form,

$$\mathrm{i}u_t = -u_{xx} + \epsilon V(x)u + \sigma|u|^2u, \tag{1.1.2}$$

where ϵ is a small parameter. If the nonlinear term $\sigma|u|^2u$ is crossed over and ϵ is set to 0, equation (1.1.2) becomes the linear Schrödinger equation

$$\mathrm{i}u_t = -u_{xx}, \tag{1.1.3}$$

which is solved by the Fourier transform as

$$u(x,t) = \int_{\mathbb{R}} a(k) e^{\mathrm{i}kx - \mathrm{i}\omega(k)t} dk,$$

where $\omega(k) = k^2$ is the dispersion relation for linear waves and $a(k) : \mathbb{R} \to \mathbb{C}$ is an arbitrary function, which is uniquely specified by the initial condition $u(x,0)$. Since $V(x+2\pi) = V(x)$ for all $x \in \mathbb{R}$, we can represent $V(x)$ by the Fourier series

$$V(x) = \sum_{m \in \mathbb{Z}} V_m e^{\mathrm{i}mx}.$$

For any fixed $k \in \mathbb{R}$, the Fourier mode $e^{\mathrm{i}kx - \mathrm{i}\omega(k)t}$ in $u(x,t)$ generates infinitely many Fourier modes in the term $\epsilon V(x)u(x,t)$ at the Fourier wave numbers $k_m = k + m$ for all $m \in \mathbb{Z}$. These Fourier modes are said to be in *resonance* with the primary Fourier mode $e^{\mathrm{i}kx - \mathrm{i}\omega(k)t}$ if

$$\omega(k_m) = \omega(k), \quad m \in \mathbb{Z},$$

which gives us an algebraic equation $m(m+2k) = 0$, $m \in \mathbb{Z}$. Thus, if $2k$ is not an integer, none of the Fourier modes with $m \neq 0$ are in resonance with the primary Fourier mode, while if $2k = n$ for a fixed $n \in \mathbb{N}$, the Fourier mode with $m = -n$ is in resonance with the primary mode with $m = 0$. In terms of the Fourier harmonics, the two resonant modes have $k = \frac{n}{2}$ and $k_{-n} = k - n = -\frac{n}{2}$.

In the asymptotic method, we shall zoom in the two resonant modes at $k = \frac{n}{2}$ and $k_{-n} = -\frac{n}{2}$ by a scaling transformation and obtain a system of nonlinear evolution equations for mode amplitudes by bringing all important terms to the same first order in ϵ, where the resonance is found. The important terms to be included in the leading order are related to the nonlinearity, dispersion, and interaction of the resonant modes, as well as to their time evolution. To incorporate all these effects, we shall look for an asymptotic multi-scale expansion in powers of ϵ,

$$u(x,t) = \epsilon^p \left[\left(a(X,T) e^{\frac{\mathrm{i}nx}{2}} + b(X,T) e^{-\frac{\mathrm{i}nx}{2}} \right) e^{-\frac{\mathrm{i}n^2 t}{4}} + \epsilon u_1(x,t) + \mathcal{O}(\epsilon^2) \right], \tag{1.1.4}$$

where $X = \epsilon^q x$, $T = \epsilon^r t$, (p,q,r) are some parameters to be determined, $n \in \mathbb{N}$ is fixed, $(a,b)(X,T) : \mathbb{R} \times \mathbb{R} \to \mathbb{C}^2$ are some amplitudes to be determined, $\epsilon u_1(x,t)$ is a first-order remainder term, and $\mathcal{O}(\epsilon^2)$ indicates a formal order of truncation of the asymptotic expansion. When the asymptotic expansion (1.1.4) is substituted into the Gross–Pitaevskii equation (1.1.2), the exponents are chosen from the condition that terms coming from derivatives of (a,b) in (X,T) and terms coming from powers of (a,b) enter the same order of the asymptotic expansion. This procedure sets uniquely $p = \frac{1}{2}$ and $q = r = 1$.

The simple choice of the exponents (p,q,r) may fail to bring all terms to the same order. For instance, coefficients in front of the first derivatives of (a,b) or the powers of (a,b) can be zero for some problems. Such failures typically indicate that (p,q,r) must be chosen smaller so that the coefficients in front of the higher-order derivatives of (a,b) or the higher-order powers of (a,b) are nonzero. Therefore, similarly to the technique of integration, the asymptotic multi-scale expansion method is a laboratory, in which a researcher plays an active role by employing the strategy of trials and errors until he or she manages to bring all important terms to the same order.

Setting $p=\frac{1}{2}$, $q=r=1$ and truncating the terms of the order of $\mathcal{O}(\epsilon^2)$, we write a linear inhomogeneous equation for $u_1(x,t)$,

$$\begin{aligned}\left(\mathrm{i}\partial_t+\partial_x^2\right)u_1 &= -\mathrm{i}(a_T\mathbf{e}_+ + b_T\mathbf{e}_-) - \mathrm{i}n(a_X\mathbf{e}_+ - b_X\mathbf{e}_-)\\ &\quad + V(a\mathbf{e}_+ + b\mathbf{e}_-) + \sigma\left|a\mathbf{e}_+ + b\mathbf{e}_-\right|^2(a\mathbf{e}_+ + b\mathbf{e}_-), \qquad (1.1.5)\end{aligned}$$

where $\mathbf{e}_\pm \equiv e^{\pm\frac{\mathrm{i}n}{2}x-\frac{\mathrm{i}n^2}{4}t}$ satisfy the linear Schrödinger equation (1.1.3). If terms proportional to either $\mathbf{e}_+$ or $\mathbf{e}_-$ occur on the right-hand side of the linear inhomogeneous equation (1.1.5), the solution $u_1(x,t)$ becomes unbounded in variables (x,t), e.g. $u_1(x,t)\sim t\mathbf{e}_\pm$. Since secular growth is undesired as it destroys the applicability of the asymptotic solution (1.1.4) already at the first order in ϵ, one needs to eliminate the resonant terms on the right-hand side of (1.1.5). This is possible if the amplitudes (a,b) satisfy the system of first-order semi-linear equations,

$$\left\{\begin{array}{l}\mathrm{i}(a_T+na_X)=V_0a+V_nb+\sigma(|a|^2+2|b|^2)a,\\ \mathrm{i}(b_T-nb_X)=V_{-n}a+V_0b+\sigma(2|a|^2+|b|^2)b,\end{array}\right. \qquad (1.1.6)$$

where V_0, V_n, and V_{-n} are coefficients of the Fourier series for $V(x)$. The amplitude equations (1.1.6) are nothing but the nonlinear Dirac equations.

Because the linear Schrödinger equation (1.1.3) is dispersive with $\omega''(k)=2\neq 0$, the other Fourier modes on the right-hand side of (1.1.5) which are different from $\mathbf{e}_\pm$ do not produce a secular growth of $u_1(x,t)$. Therefore, the system (1.1.6) gives the necessary and sufficient condition that $u_1(x,t)$ is bounded for all $(x,t)\in\mathbb{R}^2$. Indeed, we can find the explicit bounded solution of the inhomogeneous equation (1.1.5),

$$\begin{aligned}u_1(x,t) = &-\sum_{m\notin\{-n,0\}}\frac{V_ma}{m(m+n)}e^{\mathrm{i}\left(m+\frac{n}{2}\right)x-\frac{\mathrm{i}n^2t}{4}} - \sum_{m\notin\{0,n\}}\frac{V_mb}{m(m-n)}e^{\mathrm{i}\left(m-\frac{n}{2}\right)x-\frac{\mathrm{i}n^2t}{4}}\\ &-\frac{1}{2n^2}\left(a^2\bar{b}e^{\frac{3\mathrm{i}nx}{2}}+b^2\bar{a}e^{-\frac{3\mathrm{i}nx}{2}}\right)e^{-\frac{\mathrm{i}n^2t}{4}}.\end{aligned}$$

This expression suggests that the asymptotic solution (1.1.4) to the original equation (1.1.2) may be factored by $e^{-\frac{\mathrm{i}n^2t}{4}}$. After the bounded solution is found for the first-order remainder term, one can continue the formal asymptotic solution (1.1.4) to the next order of $\mathcal{O}(\epsilon^2)$.

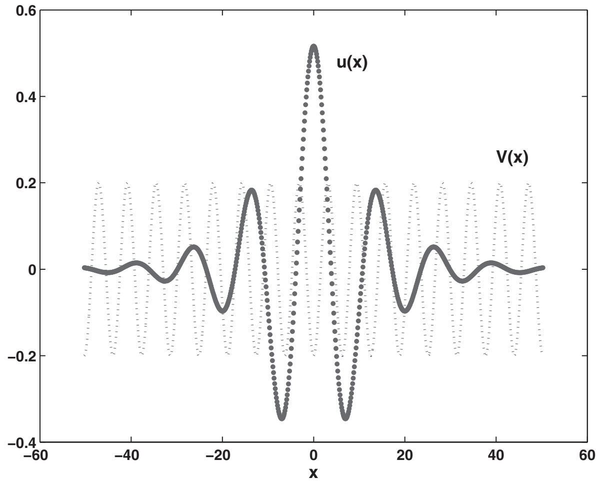

Figure 1.1 Schematic representation of the leading order in the asymptotic solution (1.1.4).

In view of so many restrictive assumptions and so many truncations made in the previous computations, it might be surprising to know that the nonlinear Dirac equations can be rigorously justified for small-amplitude periodic potentials (Section 2.2). Stationary localized modes to the nonlinear Dirac equations (1.1.6) can be constructed in explicit form (Section 3.3.4).

Figure 1.1 shows the leading order of the asymptotic solution (1.1.4) with $p = \frac{1}{2}$ and $q = r = 1$, when (a, b) is the stationary localized mode of the nonlinear Dirac equations (1.1.6) for $V(x) = -2\cos(x)$, $\sigma = -1$, $n = 1$, and $\epsilon = 0.1$.

Exercise 1.1 Consider the nonlinear Klein–Gordon equation,

$$u_{tt} - u_{xx} + u + \sigma u^3 + \epsilon V(x) u = 0,$$

where $u(x,t) : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$, $\sigma \in \{1, -1\}$, and $V(x + 2\pi) = V(x)$ is bounded, and derive the nonlinear Dirac equations in the asymptotic limit $\epsilon \to 0$.

Exercise 1.2 Consider the nonlinear wave–Maxwell equation,

$$E_{xx} - \left(1 + \epsilon V(x) + \sigma |E|^2\right) E_{tt} = 0,$$

where $E(x,t) : \mathbb{R} \times \mathbb{R} \to \mathbb{C}$, $\sigma \in \{1, -1\}$, and $V(x + 2\pi) = V(x)$ is bounded, and derive the nonlinear Dirac equations in the asymptotic limit $\epsilon \to 0$. Show that the first-order correction is not a bounded function for all $(x,t) \in \mathbb{R}^2$ because the linear wave equation $E_{xx} - E_{tt} = 0$ has no dispersion and infinitely many Fourier modes are in resonance with the primary Fourier mode.

Exercise 1.3 Consider the Gross–Pitaevskii equation with periodic coefficients,

$$\mathrm{i} u_t = -u_{xx} + \epsilon V(x) u + G(x) |u|^2 u,$$

where $u(x,t) : \mathbb{R} \times \mathbb{R} \to \mathbb{C}$, $V(x+2\pi) = V(x)$ and $G(x+2\pi) = G(x)$ are bounded, and derive an extended system of nonlinear Dirac equations in the asymptotic limit $\epsilon \to 0$.

Exercise 1.4 Repeat Exercise 1.3 with even $V(x)$ and odd $G(x)$ and derive the nonlinear Dirac equations with quintic nonlinear terms.

1.1.2 The nonlinear Schrödinger equation

We shall now assume that the 2π-periodic potential $V(x)$ is bounded but make no additional assumptions on the amplitude of $V(x)$. Let us rewrite again the Gross–Pitaevskii equation (1.1.1) in the explicit form,

$$\mathrm{i}u_t = -u_{xx} + V(x)u + \sigma|u|^2 u. \tag{1.1.7}$$

If the nonlinear term $\sigma|u|^2u$ is crossed over, equation (1.1.7) becomes a linear Schrödinger equation with a periodic potential

$$\mathrm{i}u_t = -u_{xx} + V(x)u. \tag{1.1.8}$$

The linear modes are now given by the quasi-periodic Bloch waves in the form

$$u(x,t) = \psi_k(x)e^{-\mathrm{i}\omega(k)t},$$

where $\psi_k(x)$ is a solution of the boundary-value problem for the second-order differential equation

$$\begin{cases} -\psi_k''(x) + V(x)\psi_k(x) = \omega(k)\psi_k(x), \\ \psi_k(x+2\pi) = e^{2\pi\mathrm{i}k}\psi_k(x), \end{cases} \qquad x \in \mathbb{R}.$$

Here k is real and $\omega(k)$ is to be determined (Section 2.1.2).

The asymptotic multi-scale expansion method is now developed in a neighborhood of a particular linear Bloch wave for a given value (k_0, ω_0), where $\omega_0 = \omega(k_0)$. Guided by the asymptotic method from Section 1.1.1, we shall try again the asymptotic multi-scale expansion in powers of ϵ,

$$u(x,t) = \epsilon^p \left[a(X,T)\psi_{k_0}(x)e^{-\mathrm{i}\omega_0 t} + \epsilon u_1(x,t) + \mathcal{O}(\epsilon^2) \right], \tag{1.1.9}$$

where $X = \epsilon^q x$, $T = \epsilon^r t$, (p,q,r) are some parameters to be determined, $a(X,T) : \mathbb{R} \times \mathbb{R} \to \mathbb{C}$ is an envelope amplitude to be determined, $\epsilon u_1(x,t)$ is a first-order remainder term, and $\mathcal{O}(\epsilon^2)$ is a formal order of truncation of the asymptotic expansion.

When the asymptotic expansion (1.1.9) is substituted into the Gross–Pitaevskii equation (1.1.7), we can set the exponents as $p = \frac{1}{2}$ and $q = r = 1$, similarly to the previous section. We will see however that this choice is not appropriate and the values for the exponents (p,q,r) will have to be changed.

Setting the exponents $p = \frac{1}{2}$, $q = r = 1$ and truncating the terms of the order of $\mathcal{O}(\epsilon^2)$, we write a linear inhomogeneous equation for $u_1(x,t)$,

$$\left(\mathrm{i}\partial_t + \partial_x^2 - V\right) u_1 = \left(-\mathrm{i}a_T\psi_{k_0} - 2a_X\psi_{k_0}' + \sigma|a|^2 a|\psi_{k_0}|^2\psi_{k_0}\right) e^{-\mathrm{i}\omega_0 t}. \tag{1.1.10}$$

The right-hand side of (1.1.10) produces a secular growth of $u_1(x,t)$ in variables (x,t) because $\psi_{k_0}(x)e^{-i\omega_0 t}$ is a solution of the homogeneous equation (1.1.8). Looking for a solution in the form $u_1(x,t) = w_1(x)e^{-i\omega_0 t}$, we obtain an ordinary differential equation on $w_1(x)$,

$$\left(-\partial_x^2 + V + \omega_0\right) w_1 = \mathrm{i} a_T \psi_{k_0} + 2a_X \psi_{k_0}' - \sigma |a|^2 a |\psi_{k_0}|^2 \psi_{k_0}. \qquad (1.1.11)$$

Multiplying the left-hand side of (1.1.11) by $\bar{\psi}_{k_0}$ and integrating on $[0,2\pi]$ we note that if $w_1(x)$ belongs to the same class of functions as $\psi_{k_0}(x)$, then

$$\int_0^{2\pi} \bar{\psi}_{k_0} \left(-\partial_x^2 + V + \omega_0\right) w_1 dx = -\left(\bar{\psi}_{k_0} w_1' - \bar{\psi}_{k_0}' w_1\right)\Big|_{x=0}^{x=2\pi} = 0.$$

Multiplying now the right-hand side of (1.1.11) by $\bar{\psi}_{k_0}$ and integrating on $[0,2\pi]$, we obtain a nonlinear evolution equation on the amplitude $a(X,T)$,

$$\mathrm{i} a_T = -\frac{2\langle \psi_{k_0}', \psi_{k_0} \rangle_{L^2_{\mathrm{per}}}}{\|\psi_{k_0}\|^2_{L^2_{\mathrm{per}}}} a_X + \sigma \frac{\|\psi_{k_0}\|^4_{L^4_{\mathrm{per}}}}{\|\psi_{k_0}\|^2_{L^2_{\mathrm{per}}}} |a|^2 a. \qquad (1.1.12)$$

If the nonlinear evolution equation (1.1.12) is violated, then either $w_1(x)$ becomes unbounded on $\mathbb{R}$ because of a linear growth as $|x| \to \infty$ or $u_1(x,t)$ grows secularly in time t as $t \to \infty$.

Equation (1.1.12) is a scalar semi-linear hyperbolic equation, which is easily solvable. Because of the periodic boundary conditions of $|\psi_{k_0}(x)|^2$ on $[0,2\pi]$, the coefficient $\langle \psi_{k_0}', \psi_{k_0} \rangle_{L^2_{\mathrm{per}}}$ is purely imaginary, so that the X-derivative term can be removed by the transformation $a(X,T) = a(X - c_g T, T)$, where

$$c_g = \frac{2\langle \psi_{k_0}', \psi_{k_0} \rangle_{L^2_{\mathrm{per}}}}{\mathrm{i}\|\psi_{k_0}\|^2_{L^2_{\mathrm{per}}}} \in \mathbb{R}$$

has the meaning of the group velocity of the Bloch wave $u(x,t) = \psi_{k_0}(x)e^{-i\omega_0 t}$. After the transformation, the nonlinear evolution equation on $a(X - c_g T, T)$ does not have X-derivative terms and can be immediately integrated.

Exercise 1.5 Find the most general solution of the amplitude equation (1.1.12).

The amplitude equation (1.1.12) does not capture effects of dispersion of the Bloch wave at the same order where the effects of nonlinearity, time evolution, and group velocity occur. This outcome of the asymptotic multi-scale expansion method indicates that the leading-order balance misses an important contribution from the wave dispersion which is modeled by the second-order X-derivative terms on $a(X,T)$. Therefore, we have to revise the exponents (p,q,r) of the asymptotic expansion in order to bring all important effects to the same order.

Let us keep the exponent $q = 1$ in the scaling of $X = \epsilon^q x$ for convenience. Since the linear second-order derivative terms are of the order ϵ^{2+p}, while the cubic nonlinear terms are of the order ϵ^{3p}, a non-trivial balance occurs if $p = 1$. The time evolution is of the order ϵ^{q+p} and it matches the balance if $q = 2$. In addition, we need to remove the group-velocity term by the transformation

$$a(X,T) \to a(X - c_g T, T).$$

Combining all at once, we revise the asymptotic expansion (1.1.9) as

$$u(x,t) = \epsilon\left[a(X - c_g T, \tau)\psi_{k_0}(x)e^{-\mathrm{i}\omega_0 t} + \epsilon u_1(x,t) + \epsilon^2 u_2(x,t) + \mathcal{O}(\epsilon^3)\right], \qquad (1.1.13)$$

where $T = \epsilon t$, $\tau = \epsilon^2 t$, and $\mathcal{O}(\epsilon^3)$ indicates a new order of truncation of the asymptotic expansion. When the asymptotic multi-scale expansion (1.1.13) is substituted into the Gross–Pitaevskii equation (1.1.7), we obtain the first-order correction term in the explicit form

$$u_1(x,t) = \varphi_1(x) a_X(X - c_g T, \tau) e^{-\mathrm{i}\omega_0 t},$$

where $\varphi_1(x)$ solves

$$\left(-\partial_x^2 + V + \omega_0\right)\varphi_1 = -\mathrm{i}c_g\psi_{k_0} + 2\psi_{k_0}'.$$

Note that the choice of c_g provides a sufficient condition that $\varphi_1(x)$ belongs to the same class of functions as $\psi_{k_0}(x)$. The second-order remainder term $u_2(x,t)$ satisfies now the linear inhomogeneous equation

$$\left(\mathrm{i}\partial_t + \partial_x^2 - V\right)u_2 = \left(-\mathrm{i}a_\tau\psi_{k_0} + (\mathrm{i}c_g\varphi_1 - 2\varphi_1' - \psi_{k_0})a_{XX} + \sigma|a|^2 a|\psi_{k_0}|^2\psi_{k_0}\right)e^{-\mathrm{i}\omega_0 t}.$$

Looking for a solution in the form $u_2(x,t) = w_2(x)e^{-\mathrm{i}\omega_0 t}$, we obtain an ordinary differential equation on $w_2(x)$:

$$\left(-\partial_x^2 + V + \omega_0\right)w_2 = \mathrm{i}a_\tau\psi_{k_0} - (\mathrm{i}c_g\varphi_1 - 2\varphi_1' - \psi_{k_0})a_{XX} - \sigma|a|^2 a|\psi_{k_0}|^2\psi_{k_0}.$$

Using the same projection algorithm as for equation (1.1.11), we obtain a nonlinear evolution equation on the amplitude $a(X - c_g T, \tau)$,

$$\mathrm{i}a_T = \alpha a_{XX} + \sigma\beta|a|^2 a, \qquad (1.1.14)$$

where

$$\alpha = \frac{\mathrm{i}c_g\langle\varphi_1,\psi_{k_0}\rangle_{L^2_{\mathrm{per}}} - 2\langle\varphi_1',\psi_{k_0}\rangle_{L^2_{\mathrm{per}}}}{\|\psi_{k_0}\|^2_{L^2_{\mathrm{per}}}} - 1, \quad \beta = \frac{\|\psi_{k_0}\|^4_{L^4_{\mathrm{per}}}}{\|\psi_{k_0}\|^2_{L^2_{\mathrm{per}}}}.$$

The amplitude equation (1.1.14) is nothing but the nonlinear Schrödinger (NLS) equation. The asymptotic reduction to the NLS equation is rigorously justified (Section 2.3). The stationary localized mode of the NLS equation (1.1.14) exists in explicit form (Section 1.4.1).

Figure 1.2 shows the leading order of the asymptotic solution (1.1.13), when a is the stationary localized mode of the nonlinear Schrödinger equation (1.1.14) for $V(x) = 0.2(1 - \cos(x))$, $\sigma = -1$, $k_0 = 0$, and $\epsilon = 0.1$. The localized mode corresponds to the lowest Bloch wave.

Exercise 1.6 Consider the nonlinear Klein–Gordon equation,

$$u_{tt} - u_{xx} + u + \sigma u^3 + V(x)u = 0,$$

where $u(x,t) : \mathbb{R}\times\mathbb{R} \to \mathbb{R}$, $\sigma \in \{1,-1\}$, and $V(x + 2\pi) = V(x)$ is bounded, and derive the cubic nonlinear Schrödinger equation for a Bloch wave $u(x,t) = \psi_{k_0}(x)e^{-\mathrm{i}\omega_0 t}$.