19

Asymptotic Reductions of the Gross–Pitaevskii Equation

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Various analytical techniques are reviewed in the context of asymptotic reductions of the Gross–Pitaevskii (GP) equation, which is the nonlinear Schrödinger (NLS) equation with an external potential. When the external potential is periodic, the GP equation can be reduced to the coupled-mode (Dirac) system, the continuous NLS equation and the discrete NLS equation by using formal multi-scale expansion methods and their rigorous mathematical analogues. When the external potential is decaying at infinity, finite-dimensional reductions of the GP equation can be derived for modeling of dynamics of localized modes. When the external potential is confining, the GP equation can be recovered from the multi-particle linear Schrödinger equation.

19.1 Introduction

The main part of this book is devoted to characterization of various properties of localized and periodic modes trapped by external potentials in the physics of Bose–Einstein condensation. Localized and periodic modes are modeled typically by the dimensionless Gross–Pitaevskii (GP) equation

$$\mathrm{i}u_t = -\Delta u + V(x)u + \sigma|u|^2 u, \quad x \in \mathbf{R}^N, \;\; t \geq 0, \;\; u \in \mathbf{C}, \tag{19.1}$$

where $\Delta = \partial_{x_1}^2 + \cdots + \partial_{x_N}^2$, $\sigma = \pm 1$, and $V(x)$ is an external potential. Many theoretical results described in other chapters of this book are of numerical nature. For instance, various software packages are employed to run the time evolution problem (19.1) or fixed-point iterations of the stationary problem

$$\omega\phi = -\Delta\phi + V(x)\phi + \sigma\phi^3, \quad x \in \mathbf{R}^N, \;\; \phi \in \mathbf{R}, \;\; \omega \in \mathbf{R}. \tag{19.2}$$

Other theoretical results are based on robust computational methods beyond the numerical simulations such as variational approximations, energy estimations, and asymptotic multi-scale expansions. This chapter is intended to link some of these methods with modern mathematical analysis of the GP equation. The presentation will remain on the "physical" level with sparse technical details, but links to rigorous mathematical techniques with relevant references, if available, will be made. It should be pointed out that the system of amplitude equations derived with few lines of formal computations can sometimes be proved by careful functional analysis over a hundred of journal pages.

A natural question that would arise is: *Why would we care about asymptotic reductions of the GP equation (19.1)?* The answer follows from understanding that the GP equation (19.1) is a space-inhomogeneous infinite-dimensional dynamical system, which is often unsuitable for direct analysis. On the other hand, some reductions of the GP equation are derived in the form of space-homogeneous differential or difference equations or in terms of finite-dimensional dynamical systems, which may possess exact or approximate solutions. For instance, existence of gap solitons (decaying solutions in periodic potentials) was proved in the stationary problem (19.2) from the elliptic theory [1], bifurcation methods [2, 3] and the variational theory [4] but the localized solutions are not available in a closed analytic form. On the other hand, approximations of the gap solitons in the closed analytic form can be obtained from the asymptotic reductions of the stationary equation (19.2) to the coupled-mode system [5] or to the continuous NLS equation [6].

The main part of this chapter consists of three sections; each section is devoted to a different class of the potential function $V(x)$. I shall start with a class of periodic potentials and describe simplifications of the GP equation to one of the three models: the coupled-mode system of Dirac equations, the continuous nonlinear Schrödinger (NLS) equation and its discrete counterpart, the discrete NLS equation. I will then consider the class of decaying potentials and describe the finite-dimensional models for localized modes of the GP equation. Finally, I will review other results relevant for the class of confining potentials.

Most results discussed in this chapter are based on consideration of the one-dimensional problem ($N = 1$), while open questions are mentioned about extensions of these results to multi-dimensional problems ($N \geq 2$). The main focus of this chapter is at the approximations of the localized modes of the stationary equation (19.2), while fewer details will be given on the derivation of the time-evolution versions of the reduced systems from the time-dependent GP equation (19.1).

19.2 Class of Periodic Potentials

We shall assume here that $V(x + d) = V(x)$ is a bounded periodic potential with the smallest irreducible period d. Depending on the strength of the potential amplitude $V_\infty = \|V\|_{L^\infty}$, one can develop three different reductions of the time-dependent GP equation (19.1) and the stationary problem (19.2). The crucial information for derivation of these reductions comes from the spectrum of the linear operator $L = -\Delta + V(x)$ in the space of infinitely smooth, compactly supported functions. It is well-known that the spectrum of L denoted by $\sigma(L)$ is purely continuous, consisting of a sequence of spectral bands located on a subset of real axis. For one-dimensional potentials ($N = 1$), the spectral bands do not overlap and may allow for existence of non-empty gaps between two adjacent bands. In general, the one-dimensional Hill's equation

$$L\psi(x) = -\psi''(x) + V(x)\psi(x) = \omega\psi(x) \tag{19.3}$$

has bounded solutions $\psi(x)$ called the Bloch functions if and only if ω is in the union of spectral bands

$$\sigma(L) = [\omega_0, \omega_1] \cup [\omega_2, \omega_3] \cup [\omega_4, \omega_5] \cup \ldots,$$

where $\omega_{2m-2} < \omega_{2m-1} \leq \omega_{2m}$, $m \in \mathbf{N}$ and $\omega_m \to \infty$ as $m \to \infty$. For a fixed ω in the interior point of the nth spectral band of $\sigma(L)$, both fundamental solutions of the Hill's equation (19.3) are quasi-periodic in x and have the representation

$$\psi = u^{\pm}_{n,k}(x)\mathrm{e}^{\pm \mathrm{i}kx},$$

where k is the quasi-momentum defined in the fundamental interval $k \in \left[-\frac{\pi}{d}, \frac{\pi}{d}\right]$, and

$$u^{\pm}_{n,m}(x + d) = u^{\pm}_{n,m}(x)$$

are bounded periodic functions satisfying the relations $u^{-}_{n,m}(x) = \overline{u}^{+}_{n,m}(x)$. Let us represent the nth spectral band of $\sigma(L)$ by the dispersion relation $\omega = \omega_{n,k}$. Then $\omega_{n,k}$ can be extended into an even periodic function of $k \in \mathbf{R}$ with period $2\pi/d$, according to the Fourier series

$$\omega_{n,k} = \sum_{l \in \mathbf{Z}} \hat{\omega}_{n,l}\mathrm{e}^{\mathrm{i}kld},$$

where the real Fourier coefficients $\hat{\omega}_{n,l}$ satisfy the relations $\hat{\omega}_{n,l} = \hat{\omega}_{n,-l}$.

For a fixed $\omega \in \mathbf{R} \setminus \sigma(L)$, the two fundamental solutions of the Hill's equation (19.3) grow exponentially either in x or $-x$ and have the representation $\psi = \phi_{\pm}(x)\mathrm{e}^{\pm\kappa x}$, where $\phi_{\pm}(x) = \phi_{\pm}(x+d)$ and κ depends on $\omega \in \mathbf{R}\setminus\sigma(L)$. When $\omega = \omega_0$ represents a particular end-point of a spectral band of $\sigma(L)$, one of the solutions $\psi = \psi_0(x)$ is either d-periodic (corresponding to $k = 0$) or d-antiperiodic (corresponding to $k = \pi/d$) and the other fundamental solution ψ grows linearly in x.

It has been shown numerically in [5, 6] that localized solutions of the nonlinear problem (19.2) (so-called gap solitons) exist in any finite gap of the spectrum $\sigma(L)$ and in the semi-infinite gap in the focusing case $\sigma = -1$. A rigorous theorem on existence of gap solitons was proved in [4]. Analytical approximations of the gap solitons with the coupled-mode theory and the discrete NLS equation were considered in [5], while those with the continuous NLS equation were described in [6]. We shall focus on these three approximations in the remainder of this section.

19.2.1 Small Strength: Coupled-Mode Equations

Coupled-mode equations have been exploited traditionally in the context of nonlinear optics [7] and photonic crystals [8]. Extensions of the standard one-dimensional coupled-mode equations to the higher-dimensional couplings between advective and dispersive terms were recently modeled in [9]. The role of the coupled-mode equations is fundamental: they provide normal forms for Bragg resonances of periodic or anti-periodic Bloch waves in a nonlinear system with a *small* periodic potential $V(x)$, when $V_\infty = \|V\|_{L^\infty}$ is a small parameter. We shall review the derivation of the coupled-mode equations by working with the Lyapunov–Schmidt reduction technique, similar to the analysis of [10]. In particular, we shall consider the stationary problem (19.2) in one dimension $N = 1$ and apply either periodic or anti-periodic boundary conditions to the solution $\phi(x)$. Let $V(x)$ and $\phi(x)$ be expanded into the Fourier series

$$V(x) = \sum_{m \in \mathbf{Z}} v_{2m} \mathrm{e}^{(2\pi \mathrm{i} m x)/d}, \quad \phi(x) = \sum_{m \in \mathbf{Z}'} \phi_m \mathrm{e}^{(\pi \mathrm{i} m x)/d}, \tag{19.4}$$

where $\mathbf{Z}'$ contains all even numbers for periodic $\phi(x)$ and all odd numbers for anti-periodic $\phi(x)$ and $\phi_{-m} = \bar{\phi}_m$ for real-valued $\phi(x)$. After substitution of (19.4) into (19.2), the differential equation (19.2) with $N = 1$ becomes the lattice problem:

$$\left(\omega - \frac{\pi^2 m^2}{d^2}\right) \phi_m = \sum_{m_1 \in \mathbf{Z}'} v_{m-m_1} \phi_{m_1} + \sigma \sum_{m_1 \in \mathbf{Z}'} \sum_{m_2 \in \mathbf{Z}'} \phi_{m_1} \phi_{m_2} \phi_{m-m_1-m_2}, \tag{19.5}$$

where $m \in \mathbf{Z}'$ and the convolution sums are closed both in periodic and anti-periodic cases since $V(x)\phi(x)$ and $\phi^3(x)$ are periodic or anti-periodic if $\phi(x)$ is periodic or anti-periodic, respectively. The left-hand-side of the nonlinear lattice equation (19.5) is represented by an infinite-dimensional matrix operator which is singular if and only if $\omega = \omega_n$, where $\omega_n = \left(\frac{\pi n}{d}\right)^2$ for some $n \in \mathbf{N}$. If $\omega \neq \omega_n$, the matrix operator is invertible and the zero solution $\phi_m = 0$, $\forall m \in \mathbf{Z}'$ is uniquely continued in the nonlinear lattice equation (19.5) according to the Implicit Function Theorem. No bifurcations of nonlinear periodic or anti-periodic solutions are possible for $\omega \neq \omega_n$. However, if $\omega = \omega_n$, some eigenvectors (one for $n = 0$ or two for $n \neq 0$) belong to the kernel of the singular matrix operator, and the non-zero solutions may bifurcate due to the presence of the right-hand-side terms of the lattice equation (19.5). The method of Lyapunov–Schmidt reductions provide the decomposition of the infinite-dimensional vector $\boldsymbol{\phi} = (..., \phi_{-2}, \phi_{-1}, \phi_0, \phi_1, \phi_2, ...)^{\mathrm{T}}$ into the finite-dimensional and infinite-dimensional parts along the kernel and its compliment, the construction of the mapping of the infinite-dimensional part in coordinates of the finite-dimensional part by using the Implicit Function Theorem, and finally the projections of the full system (19.5) to the reduced bifurcation equations [11]. Using this method for $n \neq 0$, we represent the vector $\boldsymbol{\phi}$ and the parameter ω in the form

$$\boldsymbol{\phi} = a\mathbf{e}_n + b\mathbf{e}_{-n} + \boldsymbol{\varphi}, \quad \omega = \left(\frac{\pi n}{d}\right)^2 + \Omega,$$

where $\mathbf{e}_{\pm n}$ are unit eigenvectors in the space of infinite-dimensional vectors, $(a,b) \in \mathbf{C}^2$ are coordinates of the kernel of the matrix operator, $\boldsymbol{\varphi}$ belongs to the orthogonal complement of the kernel, and Ω is a parameter. Due to the requirement that $\phi(x)$ is real-valued, we note the symmetry constraint $b = \bar{a}$. By the Implicit Function Theorem in the space $l_s^2(\mathbf{Z})$ with the norm

$$\|\boldsymbol{\phi}\|_{l_s^2}^2 = \sum_{m \in \mathbf{Z}} (1+m^2)^s |\phi_m|^2 < \infty$$

for $s > \frac{1}{2}$, a smooth mapping $\boldsymbol{\varphi} = \boldsymbol{\varphi}(a,b;\Omega,\mathbf{v})$ exists in a local neighborhood of $(a,b) = (0,0)$ for small values of Ω and $\|\mathbf{v}\|_{L^1}$ [11]. As a result, the bifurcation equations for $(a,b) \in \mathbf{C}^2$ becomes closed. The truncated equations at the leading order take the explicit form:

$$\Omega a = v_0 a + v_{2n} b + \sigma(|a|^2 + 2|b|^2)a, \quad \Omega b = v_{-2n} a + v_0 b + \sigma(2|a|^2 + |b|^2)b, \quad (19.6)$$

where the truncation error is of the order of $\mathrm{O}(\|\mathbf{v}\|_{L^1}^2, (|a|+|b|)^5)$. Since $v_{-2n} = \bar{v}_{2n}$, the symmetry constraint $b = \bar{a}$ is satisfied and one equation (19.6) is redundant.

It is a subject of ongoing studies to derive a full time-dependent version of the coupled-mode equations (19.6) which would be valid in the energy space $(a,b) \in H^1(\mathbf{R}, \mathbf{C}^2)$ on the infinite line $x \in \mathbf{R}$. The formal derivation is based on the asymptotic multi-scale expansions [8], which result in the coupled-mode system

$$\begin{aligned} \mathrm{i}\,(\partial_t + \partial_x)\, a &= v_0 a + v_{2n} b + \sigma(|a|^2 + 2|b|^2)a, \\ \mathrm{i}\,(\partial_t - \partial_x)\, b &= v_{-2n} a + v_0 b + \sigma(2|a|^2 + |b|^2)b, \end{aligned} \quad (19.7)$$

where (x,t) are rescaled space-time variables. The presence of exact localized solutions in the coupled-mode equations (19.7) makes this reduced model particularly useful for analysis of existence, stability and time evolution of gap solitons [12]. Other rigorous methods for justification of the coupled-mode equations (19.7) can be found in [13,14], where localized modes are controlled up to a finite-time interval and up to a small error (which may not be localized in space).

Coupled-mode equations are formally extended in the space of two and three dimensions [8], e.g., for four counter-propagating waves in the GP equation with $N = 2$. The system of four coupled-mode equations may possess a gap in the continuous spectrum [8], where stationary two-dimensional gap solitons may reside. However, since no gaps may exist in a two-dimensional periodic potential $V(x_1, x_2)$ in the limit of small strength $V_\infty = \|V\|_{L^\infty}$ [15], these gap solitons cannot be fully localized in the original GP equation (19.1). Therefore, the breakup in convergence of iterations is expected when the methods of Lyapunov–Schmidt reductions are applied to the higher-dimensional GP equation (19.1) with $N \geq 2$.

19.2.2 Moderate Strength: Continuous NLS Equations

The envelope approximation for modulated nonlinear dispersive waves was used to simplify problems of nonlinear optics, plasma physics, and water-waves since the works of Leontovich in 1930s and Talanov in 1960s [16]. In the simplest situation, this approximation results in a reduction of the second-order time-evolution partial differential equations (PDEs), such as the Maxwell equations, into the first-order time-evolution PDE represented by the nonlinear Schrödinger (NLS) equation. The NLS equation is different from the GP equation (19.1) in that the potential term $V(x)$ is absent. In the context of the *finite* periodic potentials, the NLS equation was derived formally in [6] near the band edges of the spectral bands but earlier works on the use of the NLS approximation in the same context have been known for quite some time, e.g. in [17]. We shall justify the NLS approximation for the stationary problem (19.2) in one dimension $N = 1$ by using elements of the Floquet theory and dynamical systems, similar to [18]. The two Floquet multipliers of the Hill's equation (19.3) associated with the periodic potential $V(x)$ belong to the unit circle when ω is in the interior point of $\sigma(L)$, collide at $+1$ or -1 when ω is at the band edge of $\sigma(L)$ and split along positive or negative real axis outside and inside the unit circle when ω is in the point of a spectral gap. We shall consider a transformation of the stationary problem (19.2) when ω is close to a particular band edge ω_0. For instance, let $\omega = \omega_0 + \epsilon^2 \Omega$, where ϵ is a small parameter to measure the deviation $|\omega - \omega_0|$. Let us introduce two functions $\psi_0(x)$ and $\psi_1(x)$ from the solutions of the ODEs:

$$-\psi_0'' + V(x)\psi_0 = \omega_0 \psi_0, \quad -\psi_1'' + V(x)\psi_1 = \omega_0 \psi_1 + 2\psi_0'. \tag{19.8}$$

These functions are either periodic or anti-periodic on $x \in [0, d]$, depending on the band edge ω_0. The second eigenfunction $\psi_1(x)$ called the generalized Bloch function solves the inhomogeneous Hill's equation.

Let us represent the solution $\phi(x)$ of the stationary problem (19.2) in the form

$$\phi(x) = \epsilon \left[a(x)\psi_0(x) + b(x)\psi_1(x) \right]$$

subject to the constraint $a'\psi_0 + b'\psi_1 = b\psi_0$. Another constraint on the normal coordinates (a, b) follows from the ODE (19.2):

$$a'\psi_0' + b'(\psi_1' + \psi_0) = b\psi_0' - \epsilon^2 \Omega (a\psi_0 + b\psi_1) + \epsilon^2 \sigma (a\psi_0 + b\psi_1)^3. \tag{19.9}$$

The determinant of the coefficient matrix in the left-hand-side of the system (19.9) is

$$D(x) = \psi_0(x)\psi_1'(x) - \psi_0'(x)\psi_1(x) + \psi_0^2(x).$$

It is easy to check by direct differentiation that the determinant is x-independent, such that $D(x) = D_0$. We will assume here that $D_0 \neq 0$ and show later that this condition gives a sufficient condition for existence of the gap on one side of the point $\omega = \omega_0$. By diagonalizing the system (19.9) and rescaling the variables $X = \epsilon x$, $a = A(X)$ and $b = \epsilon B(X)$, we rewrite the system (19.9) in an equivalent form:

$$\dot{A} = B + \frac{\epsilon}{D_0}\left[\sigma\psi_1(A\psi_0 + \epsilon B\psi_1)^3 - \Omega\psi_1(A\psi_0 + \epsilon B\psi_1)\right],$$

$$\dot{B} = -\frac{1}{D_0}\left[\sigma\psi_0(A\psi_0 + \epsilon B\psi_1)^3 - \Omega\psi_0(A\psi_0 + \epsilon B\psi_1)\right], \qquad (19.10)$$

where the dots $(\dot{A}, \dot{B})$ denote derivatives in $X = \epsilon x$, while the functions ψ_0 and ψ_1 depend on $x = X/\epsilon$. Therefore, a regular averaging method is applied to decompose (A, B) into the mean-field and varying parts, so that the varying part is defined uniquely in terms of the mean-field part [19]. Furthermore, the ODE system (19.10) is associated with the Jordan block for a double zero eigenvalue, which is brought into a normal form by a standard normal form transformation [18]. By using these two rigorous techniques, the truncated normal form at the leading order is written as follows:

$$D_0\ddot{A} - \Omega A(\psi_0, \psi_0)_{[0,d]} + \sigma A^3(\psi_0^2, \psi_0^2)_{[0,d]} = 0, \qquad (19.11)$$

where

$$(u, v)_{[0,d]} = \frac{1}{d}\int_0^d u(x)v(x)\mathrm{d}x$$

is the averaging operator. Depending on the signs between D_0, Ω and σ, the averaged second-order ODE (19.11) may have a homoclinic orbit expressed in terms of the hyperbolic sech-function. According to the asymptotic procedure above, the sech-soliton of the reduced problem (19.11) resembles the gap soliton of the stationary problem (19.2) near the band edge $\omega = \omega_0$.

In order to relate the quantity D_0 to the linear spectrum of $L = -\partial_x^2 + V(x)$, we shall consider the Bloch function

$$\psi = u_{n,k}^{\pm}(x)\mathrm{e}^{\pm \mathrm{i}kx}$$

of the spectral band $\omega = \omega_{n,k}$ near the band edge $\omega = \omega_0$. At $\omega = \omega_0$, the quasi-momentum is $k = 0$ if $\psi_0(x)$ is a periodic Bloch function and $k = \pi/d$ if $\psi_0(x)$ is an anti-periodic function. Therefore, by abusing slightly notations we can represent the solution of the Hill's equation (19.3) for $\omega = \omega_{n,k} \equiv \omega_k$ in the form $\psi \equiv \phi_k(x)\mathrm{e}^{\mathrm{i}kx}$, where k is now near zero if ω_k is near ω_0 and $\phi_k(x)$ is either periodic or anti-periodic function, which satisfies the generalized Hill's equation

$$-\phi_k'' + V(x)\phi_k = \omega_k \phi_k + 2\mathrm{i}k\phi_k' - k^2\phi_k. \tag{19.12}$$

Because of analyticity of $\phi_k(x)$ and ω_k with respect to k (see [20]), one can expand

$$\omega_k = \omega_0 + \frac{1}{2}\omega_k'' k^2 + \mathrm{O}(k^3)$$

and

$$\phi_k = \psi_0(x) + \mathrm{i}k\psi_1(x) + k^2\psi_2(x) + \mathrm{O}(k^3)$$

and derive the inhomogeneous problem for ψ_2:

$$-\psi_2'' + V(x)\psi_2 = \omega_0\psi_2 + \frac{1}{2}\omega_k''\psi_0 - 2\psi_1' - \psi_0. \tag{19.13}$$

The function $\psi_2(x)$ is periodic or anti-periodic if and only if the right-hand-side of the ODE (19.13) is orthogonal to $\psi_0(x)$ on $x \in [0,d]$. This condition results in the constraint

$$\frac{1}{2}\omega_k''(\psi_0,\psi_0)_{[0,d]} = (\psi_0,\psi_0)_{[0,d]} + 2(\psi_0,\psi_1')_{[0,d]} = (1,D)_{[0,d]} = D_0.$$

With this relation, the stationary equation (19.11) can be rewritten in the form

$$\frac{1}{2}\omega_k''\ddot{A} - \Omega A + \sigma\chi A^3 = 0, \qquad \chi = \frac{(\psi_0^2,\psi_0^2)_{[0,d]}}{(\psi_0,\psi_0)_{[0,d]}} > 0. \tag{19.14}$$

If $\omega_k'' \neq 0$, the gap exists on the other side of the point $\omega = \omega_0$ relative to the band $\omega = \omega_k$ and the gap solitons bifurcate as solutions of the truncated problem (19.14) under the conditions that ω_k'', Ω and σ are of the same signs.

Localized modes of the stationary problem (19.2) associated with the periodic potential $V(x)$ have their linear counterparts, called *defect modes*, which are bound states of the linear Schrödinger operator with a sum of periodic and small decaying potentials. For instance, one can look for localized solutions of the linear problem

$$-\phi'' + V(x)\phi + \epsilon W(x)\phi = \omega\phi, \tag{19.15}$$

where $V(x)$ is a bounded periodic potential, ω is in the gap of the spectrum $L = -\partial_x^2 + V(x)$, $W(x)$ is a bounded exponentially decaying potential, and ϵ is small parameter. The first rigorous works on analysis of isolated eigenvalues in the linear Schrödinger problem (19.15) are dated back to 1980s [21], while recent activities on this subject are motivated by studies of defect modes in nonlinear photonic lattices [22, 23].

The problem of bifurcations of isolated eigenvalues of the spectral problem (19.15) can be effectively solved with the Evans function method. The Evans function was successfully used in a similar context of the edge bifurcation from the continuous spectrum [24]. Let $L = -\partial_x^2 + V(x)$, $\omega \notin \sigma(L)$, and consider two particular solutions $\phi_{1,2}(x)$ of the linear problem (19.15), so that $\phi_1(x)$ converges to the Bloch functions $\phi_+(x)\mathrm{e}^{\kappa x}$ as $x \to -\infty$ and $\phi_2(x)$ converges to the Bloch function $\phi_-(x)\mathrm{e}^{-\kappa x}$ as $x \to +\infty$, respectively. Such solutions are well-defined for $\mathrm{Re}\,\kappa > 0$ by the ODE theory [25]. The parameter $\mathrm{Re}\,\kappa > 0$ is called the Lyapunov exponent and it depends on ω, such that $\mathrm{Re}\,\kappa \to 0$ as $\omega \to \omega_0$, where ω_0 is a particular band edge of the spectrum of $\sigma(L)$.

Let the spectral band $\omega = \omega_{n,k} \equiv \omega_k$ be represented by

$$\omega_k = \omega_0 + \frac{1}{2}\omega_k'' k^2 + \mathrm{O}(k^3)$$

on one side of the point $\omega = \omega_0$, where k is near zero and $\omega_k'' \neq 0$. By abusing notations again we can consider κ to be a small real parameter on the other side of the point $\omega = \omega_0$. The inverse dependence of $\kappa(\omega)$ for $\omega \notin \sigma(L)$ is defined by the expansion

$$\omega = \omega_0 - \frac{1}{2}\omega_k'' \kappa^2 + \mathrm{O}(\kappa^3).$$

The Evans function $E(\kappa, \epsilon)$ is the 2×2 Wronskian determinant of the 2-vector extensions of the two fundamental solutions $\phi_1(x)$ and $\phi_2(x)$. When $E(\kappa_*, \epsilon_*) = 0$ for some $\kappa_* \in \mathbf{C}$ with $\mathrm{Re}\,\kappa > 0$ and $\epsilon_* \in \mathbf{R}$, the two solutions become linearly dependent. They span an exponentially decaying solution $\phi(x)$ of the spectral problem (19.15) on $x \in \mathbf{R}$ for the corresponding value ω_* which is found from the dependence $\omega_* = \omega(\kappa_*)$. It is proved in standard analysis [25] that $E(\kappa, \epsilon)$ is analytic with respect to κ and ϵ for $\mathrm{Re}\,\kappa > 0$ and $\epsilon \in \mathbf{R}$ and it can be analytically extended in κ near $\kappa = 0$.

Since $\phi_+(x)$ and $\phi_-(x)$ are linearly dependent at $\kappa = 0$ and $\epsilon = 0$, then $E(0,0) = 0$. If $\partial_\kappa E(0,0) \neq 0$, the zero $\kappa = 0$ is continued into a simple zero $\kappa = \kappa_*$ of $E(\kappa, \epsilon)$ near $\kappa = 0$ and $\epsilon = 0$ by using the Implicit Function Theorem and the expansion

$$E(\kappa, \epsilon) = \kappa \partial_\kappa E(0,0) + \epsilon \partial_\epsilon E(0,0) + \mathrm{O}(\kappa^2, \epsilon\kappa, \epsilon^2).$$

If $\mathrm{Re}\,\kappa_* > 0$, the zero of $E(\kappa, \epsilon)$ corresponds to the eigenvalue of (19.15) with an exponentially decaying eigenfunction $\phi(x)$. First derivatives of $E(\kappa, \epsilon)$ are computed explicitly at $(\kappa, \epsilon) = (0, 0)$. Since

$$E(\kappa, 0) = \begin{vmatrix} \phi_+(x) & \phi_-(x) \\ \phi_+'(x) + \kappa\phi_+(x) & \phi_-'(x) - \kappa\phi_-(x) \end{vmatrix} = \phi_+\phi_-' - \phi_-\phi_+' - 2\kappa\phi_+\phi_-$$

and $\phi_\pm(x) = \psi_0(x) \pm \kappa\psi_1(x) + \mathrm{O}(\kappa^2)$, then

$$\partial_\kappa E(0,0) = 2\psi_1\psi_0' - 2\psi_0\psi_1' - 2\psi_0^2 = -2D_0 = -\omega_k''(\psi_0, \psi_0)_{[0,d]}.$$

On the other hand,

$$\partial_\epsilon E(\kappa,0) = (\phi_2'\partial_\epsilon\phi_1 - \phi_2\partial_\epsilon\phi_1') - (\phi_2\partial_\epsilon\phi_1' - \phi_1\partial_\epsilon\phi_2') = -\int_{-\infty}^{\infty} W(x)\phi_1\phi_2 \mathrm{d}x,$$

where $\phi_1(x)$ and $\phi_2(x)$ are the two fundamental solutions of the ODE (19.15) so that $\phi_{1,2} \to \psi_0(x)$ as $\epsilon \to 0$ and $\kappa = 0$. Therefore,

$$\partial_\epsilon E(0,0) = -(\psi_0, W(x)\psi_0)_{\mathbf{R}}.$$

The root of $E(\kappa,\epsilon)$ near $(\kappa,\epsilon) = (0,0)$ bifurcates in the domain $\kappa > 0$ if the matrix element $(\psi_0, \epsilon W(x)\psi_0)_{\mathbf{R}}$ has the opposite sign to the sign of ω_k''. The leading-order approximation for the root follows from the expansions above:

$$\omega = \omega_0 - \frac{\epsilon^2}{2\omega_k''}\left|\frac{(\psi_0, W(x)\psi_0)_{[0,d]}}{(\psi_0,\psi_0)_{[0,d]}}\right|^2 + \mathrm{O}(\epsilon^3). \tag{19.16}$$

The same formula was derived in [22] with a decomposition technique when a localized solution $\phi(x)$ is represented in terms of the complete set of Bloch functions over the spectrum $\sigma(L)$ and the asymptotic analysis of integrals with pole singularities is performed in the limit $\epsilon \to 0$ and $\omega \to \omega_0$. The asymptotic analysis is based on a rigorous technique, when the integral is decomposed into a rank-one singular and infinite-dimensional non-singular parts and the non-singular part is estimated in terms of the single component of the singular part of the integral [26]. This technique is similar to the method of Lyapunov–Schmidt reductions for integral equations.

The time-dependent version of the stationary equation (19.14) is the NLS equation

$$\mathrm{i}A_t = \frac{1}{2}\omega_k'' A_{XX} + \sigma\chi|A|^2 A. \tag{19.17}$$

Rigorous justification of the NLS equation (19.17) was reported in [27] from the Maxwell equations with nonlocal terms and in [28] from a lattice system that models the Fermi–Pasta–Ulam problem. These results are valid in the space of continuous functions on a finite time interval, where the spatial decay rate of the error terms can not be controlled.

Formal extensions of the NLS equation (19.17) in two and three dimensions can be developed when the dispersion surface $\omega = \omega_{\mathbf{k}}$ of the multi-dimensional periodic potential $V(\mathbf{x})$ admits extremal points $\omega = \omega_0$ where $\nabla_{\mathbf{k}}\omega_{\mathbf{k}} = \mathbf{0}$ and the Hessian matrix of $\omega_{\mathbf{k}}$ is sign-definite. A spectral gap exists on the other side of the extremal point $\omega = \omega_0$ relative to the band $\omega = \omega_{\mathbf{k}}$. Bifurcations of the multi-dimensional gap solitons near the band edge $\omega = \omega_0$ can be described by the multi-dimensional NLS equation, e.g. for $N = 2$:

$$\mathrm{i}A_t = \frac{1}{2}\left(\omega_{k_1}'' A_{X_1X_1} + \omega_{k_2}'' A_{X_2X_2}\right) + \sigma\chi|A|^2 A, \tag{19.18}$$

where (X_1, X_2) are appropriate coordinates which diagonalize the Hessian matrix of $\omega_{\mathbf{k}}$. Since ω_{k_1}'' and ω_{k_2}'' are of the same sign near the band edge, bifurcation of two-dimensional NLS solitons occurs when the NLS equation (19.18) is of the focusing type. However, such solutions are unstable and the critical blow-up occurs in the time-evolution of the two-dimensional NLS equation (19.18) in finite time [16]. On the other hand, no finite-time blow up occurs in the defocusing GP equation (19.1) with $\sigma = +1$, so that the correspondence between the GP equation and the NLS equation is lost for $N \geq 2$.

19.2.3 Large Strength: Discrete NLS Equations

Discrete NLS equations were used for modeling of various physical problems involving arrays of coupled oscillators [29]. Similar to this traditional application of the lattice equations, periodic continuous problems with *large* spacing between wells of the periodic potential $V(x)$ or *large* strength $V_\infty = \|V\|_{L^\infty}$ can also be reduced to the discrete problems in a so-called tight-binding approximation [5]. The Wannier function decomposition method was shown in [30] to be relevant for the derivation of the discrete NLS equation from the continuous GP equation (19.1).

We shall describe the Wannier function decomposition based on the analysis of [20]. Let us consider the stationary problem (19.2) in one dimension $N = 1$ and recall the construction of the Bloch functions $\psi = u^{\pm}_{n,k}(x)\mathrm{e}^{\pm \mathrm{i}kx}$ and the spectral band $\omega = \omega_{n,k}$ of the operator $L = -\partial_x^2 + V(x)$. By a definition, the Wannier function $a_n(x)$ for the nth spectral band $\omega = \omega_{n,k}$ is constructed from the Bloch function

$$\psi_{n,k} \equiv u^{+}_{n,k}(x)\mathrm{e}^{\mathrm{i}kx}$$

by

$$a_n(x) = \left(\frac{d}{2\pi}\right)^{1/2} \int_{-\pi/d}^{\pi/d} \psi_{n,k}(x)\mathrm{d}k. \tag{19.19}$$

It is proved in [20] for a class of symmetric potentials $V(-x) = V(x)$ that there exists only one Wannier function $a_n(x)$ for each $n \geq 0$, so that $a_n(x)$ is a real function, $a_n(x)$ is either even or odd about $x = 0$, and $a_n(x)$ decays exponentially as $|x| \to \infty$. Because of the decay, the set of Wannier functions $\{a_{n,l}(x)\}_{n\geq 0, l\in \mathbf{Z}}$ with $a_{n,l}(x) \equiv a_n(x - ld)$ provide a nice basis for decomposition of any function in $L^2(\mathbf{R})$ provided that the set is complete. Completeness of the set of Wannier functions follows from the Shannon's Sampling Theorem which relates the Fourier transform of a discrete unbounded sequence of functions and the Fourier transform of a continuous, compactly supported function. Indeed, since

$$\sum_{l\in\mathbf{Z}} \mathrm{e}^{\mathrm{i}ld(k'-k)} = \frac{2\pi}{d}\delta(k'-k),$$

$$\forall k, k' \in \left[-\frac{\pi}{d}, \frac{\pi}{d}\right],$$

where $\delta(k)$ is the Dirac delta function, one can find a pair of Fourier transforms between the Wannier functions $a_{n,l}(x)$ and the Bloch functions $\psi_{n,k}(x)$:

$$a_{n,l}(x) = \left(\frac{d}{2\pi}\right)^{1/2} \int_{-\pi/d}^{\pi/d} \psi_{n,k}(x) e^{-ikld} dk, \quad \psi_{n,k}(x) = \left(\frac{d}{2\pi}\right)^{1/2} \sum_{l \in \mathbf{Z}} a_{n,l}(x) e^{ilkd}.$$

Let us normalize the Bloch functions by the Dirac's orthogonality relations

$$(\psi_{n',k'}, \psi_{n,k})_{\mathbf{R}} = \int_{\mathbf{R}} \psi_{n',k'}(x) \bar{\psi}_{n,k}(x) dx = \delta_{n',n} \delta(k'-k),$$

where $\delta_{n',n}$ is the Kronecker delta symbol. It follows by direct computation that the set of Wannier functions

$$\{a_{n,l}(x)\}_{n \geq 0, l \in \mathbf{Z}}$$

satisfies the orthogonality relations

$$(a_{n',l'}, a_{n,l})_{\mathbf{R}} = \delta_{n',n} \delta_{l',l}.$$

Any function in $L^2(\mathbf{R})$ can be uniquely represented in terms of the set of Wannier functions

$$\{a_{n,l}(x)\}_{n \geq 0, l \in \mathbf{Z}}.$$

For instance, a solution $\phi(x)$ of the stationary problem (19.2) can be represented by

$$\phi(x) = \sum_{n \geq 0} \sum_{l \in \mathbf{Z}} c_l a_{n,l}(x),$$

where

$$\{c_{n,l}\}_{n \geq 0, l \in \mathbf{Z}}$$

is the set of projection coefficients. Using this representation, we reduce the stationary problem (19.2) to the nonlinear lattice problem

$$\omega c_{n,l} = \sum_{l_1 \in \mathbf{Z}} c_{n,l_1} \hat{\omega}_{n,l-l_1} + \sigma \sum_{(n_1,n_2,n_3) \geq 0} \sum_{(l_1,l_2,l_3) \in \mathbf{Z}^3} W_{l_1,l_2,l_3,l}^{n_1,n_2,n_3,n} c_{n_1,l_1} c_{n_2,l_2} c_{n_3,l_3}, \tag{19.20}$$

where

$$W_{l_1,l_2,l_3,l}^{n_1,n_2,n_3,n} = (a_{n_1,l_1} a_{n_2,l_2}, a_{n_3,l_3} a_{n,l})_{\mathbf{R}}$$

are matrix elements of the projections and $\hat{\omega}_{n,l}$ are Fourier coefficients for the spectral band

$$\omega_{n,k} = \sum_{l \in \mathbf{Z}} \hat{\omega}_{n,l} e^{ikld}.$$

In the limit of large $V_\infty = \|V\|_{L^\infty}$, the coefficients $\hat{\omega}_{n,l}$ are large at $l = 0$ and negligibly small at $l \neq 0$. Similarly, the matrix elements $W_{l_1,l_2,l_3,l}^{n_1,n_2,n_3,n}$ are large at $l_1 = l_2 = l_3 = l$ and $n_1 = n_2 = n_3 = n$ and negligibly small at

$|l_j - l| \neq 0$ and $|n_j - n| \neq 0$, $\forall j = 1, 2, 3$. Using these properties and the renormalization $\omega = \hat{\omega}_{n,0} + \Omega$, the truncated system of ODEs (19.20) at the leading order can be written as the tridiagonal system

$$\Omega c_{n,l} = \hat{\omega}_{n,1} \left(c_{n,l+1} + c_{n,l-1} \right) + \sigma W_{l,l,l,l}^{n,n,n,n} |c_{n,l}|^2 c_{n,l}. \tag{19.21}$$

By rescaling of Ω and $c_{n,l}$, the coefficients of the tridiagonal system (19.21) can be normalized to ± 1. The tridiagonal system (19.21) is formally extended to the time-evolution system called the discrete NLS equation

$$\mathrm{i}\dot{\psi}_l = \epsilon \left(\psi_{l+1} + \psi_{l-1} \right) + \sigma |\psi_l|^2 \psi_l, \tag{19.22}$$

where

$$\psi_l(t) = c_{n,l} \mathrm{e}^{-\mathrm{i}\Omega t} / \sqrt{W_{l,l,l,l}^{n,n,n,n}}$$

and $\epsilon = \hat{\omega}_{n,1}$. No works on rigorous justification of the discrete NLS equation (19.22) from the time-dependent GP equation (19.1) have been reported so far. A straightforward formal method was proposed in [31], where the periodic potential of a large strength V_∞ was approximated by a sequence of Dirac delta functions

$$V(x) = -V_\infty \sum_{l \in \mathbf{Z}} \delta(x - ld).$$

The individual delta-function potential $V(x) = -V_\infty \delta(x)$ admits the ground state

$$\phi_0(x) = \mathrm{e}^{-\frac{1}{2} V_\infty |x|}$$

for the lowest eigenvalue $\omega_0 = -\frac{1}{4} V_\infty^2$. The direct decomposition of the solution of the GP equation (19.1) is based on the representation

$$\psi(x,t) = \sum_{l \in \mathbf{Z}} c_l(t) \phi_0(x - ld).$$

Although the basis functions $\{\phi_0(x - ld)\}_{l \in \mathbf{Z}}$ are not orthogonal to each other, the inner product of

$$(\phi_0(x - ld), \phi_0(x - l'd))_{\mathbf{R}}$$

is $2/V_\infty$ for $l' = l$ and exponentially small in terms of $1/V_\infty$ for $l' \neq l$, e.g.

$$(\phi_0(x - ld), \phi_0(x - (l \pm 1)d))_{\mathbf{R}} = \frac{2 + dV_\infty}{V_\infty} \mathrm{e}^{-\frac{1}{2} V_\infty d}.$$

By substituting the decomposition for $\psi(x,t)$ into the GP equation (19.1) and by using the projection algorithm, one can find the leading-order amplitude equations for $c_l(t)$:

$$\mathrm{i}\dot{c}_l + \frac{1}{4} V_\infty^2 c_l = -\frac{1}{4} V_\infty^2 \left(1 + \frac{1}{2} dV_\infty \right) \mathrm{e}^{-\frac{1}{2} V_\infty d} (c_{l+1} + c_{l-1}) + \frac{1}{2} \sigma |c_l|^2 c_l. \tag{19.23}$$

Under the transformation

$$c_l(t) = \sqrt{2}\psi_l(t)\mathrm{e}^{\frac{\mathrm{i}}{4}V_\infty^2 t},$$

the system (19.23) becomes the discrete NLS equation (19.22) with

$$\epsilon = -\frac{1}{4}V_\infty^2\left(1 + \frac{1}{2}dV_\infty\right)\mathrm{e}^{-\frac{1}{2}V_\infty d}.$$

The discrete NLS equation (19.21) has an exponentially small coupling term ϵ in terms of $1/V_\infty$. The limit of zero coupling term ($\epsilon = 0$) is referred to as the *anti-continuum limit*. It has been used successfully in the proof of existence [32] and stability [33] of discrete solitons in one spatial dimension. Extensions of this method have been reported in the context of two-dimensional [34, 35] and three-dimensional [36] vortices. Since localized modes of the discrete NLS equation and the eigenvalues of the relevant linearizations are known at $\epsilon = 0$, the method of Lyapunov–Schmidt reductions can be used to derive the conditions when these localized modes and their corresponding eigenvalues can be continued in $\epsilon \neq 0$. Power series expansions in ϵ are constructed and studied in the technical implementation of the algorithm. It is however clear that the second-order terms $\mathrm{O}(\epsilon^2)$ of the Lyapunov–Schmidt reductions in [33–36] are comparable with the terms proportional to $\hat{\omega}_{n,2}$, which are truncated beyond the tridiagonal system (19.21). Therefore, some discrepancies may occur between the predictions of the continuous GP equation (19.1) and those of the discrete NLS equation (19.22).

The situation becomes worse in the space of higher dimensions. By using the same technique, the discrete NLS equation (19.22) with $N = 1$ is extended to the two-dimensional lattice with $N = 2$ in the form

$$\mathrm{i}\dot{\psi}_{l,m} = \epsilon\left(\psi_{l+1,m} + \psi_{l-1,m} + \psi_{l,m+1} + \psi_{l,m-1}\right) + \sigma|\psi_{l,m}|^2\psi_{l,m}, \qquad (19.24)$$

where the spectral band $\omega_{\mathbf{k}}$ is assumed to be isotropic so that the Fourier coefficients for $\omega_{n,\mathbf{k}}$ satisfy the conditions $\hat{\omega}_{n,1,0} = \hat{\omega}_{n,-1,0} = \hat{\omega}_{n,0,1} = \hat{\omega}_{n,0,-1}$. The two-dimensional discrete NLS equation (19.24) takes into account the horizontal and vertical couplings between adjacent sites. The next-order term contributing to the discrete NLS equation on a square lattice is the diagonal coupling term which is proportional to the coefficients

$$\hat{\omega}_{n,1,1} = \hat{\omega}_{n,1,-1} = \hat{\omega}_{n,-1,1} = \hat{\omega}_{n,-1,-1}.$$

If $\hat{\omega}_{n,1,0} \sim \mathrm{e}^{-V_\infty d}$ for large V_∞, then

$$\hat{\omega}_{n,1,1} \sim \mathrm{e}^{-\sqrt{2}V_\infty d},$$

i.e. $\hat{\omega}_{n,1,1}$ is much larger than

$$\hat{\omega}_{n,1,0}^2, \hat{\omega}_{n,2,0} \sim \mathrm{e}^{-2V_\infty d}.$$

If the Lyapunov–Schmidt reductions would depend crucially on the results of the second-order computations, the predictions without the account of the diagonal couplings between two-dimensional lattice sites could be incorrect.

19.3 Class of Decaying Potentials

We shall assume here that $V(x)$ is a decaying potential at infinity, which is given by a continuously differentiable function on $x \in \mathbf{R}^N$. If the potential $V(x)$ is absent, the stationary problem (19.2) admits a solution $\phi_0(x)$ decaying to zero as $|x| \to \infty$ in the focusing case with $\sigma = -1$ and $\omega < 0$. In the space of one dimension $N = 1$, this solution is nothing but the sech-soliton $\phi_0 = \sqrt{2|\omega|}\mathrm{sech}(\sqrt{|\omega|}x - s)$, where $s \in \mathbf{R}$ is an arbitrary translation parameter. We shall ask if the solution $\phi_0(x)$ persists in the full stationary problem (19.2) with a given potential $V(x)$. To answer this question, let us assume the existence of the localized solution of the stationary problem (19.2) with $\omega \notin \sigma(L)$ which is given by a continuously differentiable function $\phi(x)$ on $x \in \mathbf{R}^N$. We multiply the stationary problem (19.2) by $\partial_{x_j}\phi(x)$, $j = 1, ..., N$ and integrate over $x \in \mathbf{R}^N$. Since $\phi(x)$ decays to zero at infinity with an exponential rate for $\omega \notin \sigma(L)$, contributions from $(N-1)$-dimensional integrals vanish at infinity. As a result, the following integrals must be identically zero

$$\int_{\mathbf{R}^N} \phi^2(x)\partial_{x_j}V(x)\mathrm{d}x = 0, \qquad j = 1, ..., N. \tag{19.25}$$

Of course, these conditions give simply constraints on the profile of the classical solution $\phi(x)$ of the stationary problem (19.2), which *has been assumed* to exist. However, in two special cases, one can use the leading-order approximation $\phi(x) = \phi_0(x - s)$ with $s \in \mathbf{R}^N$ obtained for $V(x) = 0$ in the integral (19.25) and interpret the corresponding conditions as the persistence equations for continuation of $\phi_0(x - s)$ into a full solution $\phi(x)$ of the stationary problem (19.2) with $V(x) \neq 0$.

The special cases when the integrals (19.25) are small occur for *small* or *wide* potentials $V(x)$ relative to the amplitude or width of the stationary solution $\phi_0(x)$. In the first case, one can use the representation $V = \epsilon W(x)$, such that the conditions (19.25) have the magnitude of $\mathrm{O}(\epsilon)$ [37]. At the second case, one can use the representation $V = W(\epsilon x)$, such that the same conditions occur also at $\mathrm{O}(\epsilon)$ [38]. In either case, the rigorous technique for finding of the necessary condition for persistence of stationary solutions is based on the method of Lyapunov–Schmidt reductions [37, 38]. Moreover, the same technique can be extended to derive the sufficient condition for persistence, to study stability of the persistent configurations and to approximate the time-evolution dynamics of localized modes in the external potential $V(x)$ with the Newton's equation of motion

$$m_0\ddot{s} = -\nabla U(s), \tag{19.26}$$

where m_0 is an effective mass, s is the position of the localized mode on $x \in \mathbf{R}^N$, and $U(s)$ is an effective potential given by

$$U(s) = \frac{\int_{\mathbf{R}^N} V(x)\phi_0^2(x - s)\mathrm{d}x}{\int_{\mathbf{R}^N} \phi_0^2(x)\mathrm{d}x}. \tag{19.27}$$

Due to the Galilean translation of solutions of the GP equation

$$u(x,t) \mapsto \mathrm{e}^{\frac{\mathrm{i}}{2} v\cdot x - \frac{\mathrm{i}}{4}|v|^2 t} u(x - vt, t),$$

the constant m_0 is found to be $m_0 = 1/2$ independently of N [38]. In the space of one dimension $N = 1$, it follows from the Newton's equation of motion (19.26) that the localized mode $\phi_0(x - s)$ persists at the particular value $s = s_0$ with $U'(s_0) = 0$ if $U''(s_0) \neq 0$, it is stable if $U''(s_0) > 0$ and unstable if $U''(s_0) < 0$ and the long-term dynamics of localized mode is described by the long-term oscillations in the case $U''(s_0) > 0$. If there are several points s_0 with $U'(s_0) = 0$, the Newton's equation of motion (19.26) provides global information on stability of each equilibrium configuration and local dynamics in a neighborhood of the equilibria. In the space of two and three dimensions $N \geq 2$, the Newton's equation of motion (19.26) is not applicable for predictions of dynamics of localized modes due to spectral instabilities of solitons $\phi_0(x)$ of the multi-dimensional focusing NLS equation (19.1) with $V(x) = 0$ and $\sigma = -1$.

The formal derivation of the Newton's equation of motion (19.26) for dynamics of a localized mode in an external potential $V(x)$ was developed first in [39, 40] by using asymptotic multi-scale expansions. This formal technique is recovered from the Ehrenfest's theorem

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{\mathbf{R}^N} \frac{\mathrm{i}}{2} \left(\bar{u}\nabla u - u\nabla \bar{u}\right) \mathrm{d}x = \int_{\mathbf{R}^N} |u|^2 \nabla V(x) \mathrm{d}x \tag{19.28}$$

for any continuously differentiable solution $u(x,t)$ of the GP equation (19.1). The slow dynamics of a localized mode is supported by the smallness of the right-hand-side of (19.28), which occurs generally if $\nabla V(x)$ is small (either $V = \epsilon W(x)$ or $V = W(\epsilon x)$ with a small parameter ϵ). In this case, the leading-order solution $u(x,t)$ is an orbit of the moving soliton

$$u = \mathrm{e}^{\frac{i}{2} v\cdot x - \mathrm{i}\theta} \phi_0(x - s)$$

with $\dot{s} = v$ and $\dot{\theta} = \omega + \frac{|v|^2}{4}$, where all parameters (s, v, θ, ω) are (slow) functions of time t. (If $V = W(\epsilon x)$, one can shift parameters of $\phi_0(x)$ to remove $W(0)$ from the leading-order solution.) The balance equation (19.28) reduces in this leading-order approximation to the Newton's equation of motion (19.26).

Although the decomposition of the asymptotic multi-scale expansion method may seem rough and inaccurate, it has been rigorously proved in the case $V = W(\epsilon x)$ by two methods. The weak variational formalism was employed in [41] to prove convergence of the GP equation in the semi-classical limit to the set of Newton's equations of motion for a superposition of localized modes. The skew-orthogonal projection method, Lyapunov–Schmidt decompositions, and lower-upper bound estimates on the energy functional were developed in [38] for dynamics of a single localized mode. The same authors also extended their method to the case of confining potentials in [42] and derived the same Newton's equation of motion (19.26).

The other case $V = \epsilon W(x)$ with decaying $W(x)$ is even easier since the technique of [38] would work without any modifications. For instance, the sufficient condition of persistence of localized solutions, i.e. $U'(s_0) = 0$ and $U''(s_0) \neq 0$, follows from a classical application of Lyapunov–Schmidt reductions to the elliptic problem (19.2) with a perturbation term in $H^2(\mathbf{R})$ [37]. This method was recently applied to the case of dark solitons which are localized solutions with non-zero boundary conditions existing in the defocusing case $\sigma = 1$ and $\omega > 0$. Recent work [43] contains a rigorous proof of persistence and stability of dark solitons in small decaying potentials $V = \epsilon W(x)$ and numerical evidences that the Newton's law of motion modified by the radiative terms is relevant for slow dynamics of dark solitons. Following discussions in [44], we mention that the Ehrenfest's theorem (19.28) is not relevant for the derivation of the Newton's equation of motion for dark solitons as it gives a wrong value of the mass constant m_0.

A very similar technique can be developed to deal with localized modes of the GP equation when the decaying potential $V(x)$ is represented by a superposition of K identical single-well potentials $W(x)$ located on an equal *large* distance s far from each other:

$$V(x) = \sum_{k=1}^{K} W(x - (k-1)s). \tag{19.29}$$

The localized modes of the stationary problem (19.2) with the potential $V(x)$ in the form (19.29) persist and evolve according to an effective interaction potential. This theory of interaction of localized modes distant from each other was elaborated long ago by using formal methods in [40] and it was rigorously verified recently by using geometric constructions in [45].

In order to place this theory on mathematical footing, let us assume that the operator $L = -\partial_x^2 + W(x)$ associated with each potential well $W(x)$ has a number of isolated eigenvalues and the corresponding bound states. By using the classical Lyapunov–Schmidt reductions [11], each bound state for a simple isolated eigenvalue is uniquely continued into a nonlinear localized mode of the nonlinear problem (19.2) with $V = W(x)$. The ground state for the smallest eigenvalue is typically of the highest interest due to its stability with respect to time evolution in the nonlinear GP equation (19.1).

We now consider the stationary problem (19.2) with the potential $V(x)$ in the form (19.29) in the limit of large s. First, let us neglect the nonlinear terms and consider the splitting of eigenvalues of the linear operator $L = -\partial_x^2 + V(x)$. When $s = \infty$, the smallest eigenvalue of L has multiplicity K. However, the multiplicity of the eigenvalue of L is broken when $s \neq \infty$. Detailed computations for the case $K = 3$ were performed in [46] where a general geometric method of [45] for construction of multi-pulse solutions was employed to the analysis of splitting of eigenvalues of L. As a result of the reductive procedure, the bifurcating eigenvalues with the corresponding eigenfunctions are computed in the form

$$\lambda = \lambda_0 \pm 2\sqrt{2}\psi_0\left(\frac{s}{2}\right)\psi_0'\left(\frac{s}{2}\right): \quad \psi_{\pm} = \frac{1}{2}\left(\pm\,\psi_0(x) + \sqrt{2}\psi_0(x-s) \pm \psi_0(x-2s)\right),$$

while the persistent eigenvalue with the corresponding eigenfunction is

$$\lambda = \lambda_0: \quad \tilde{\psi}_0 = \frac{1}{\sqrt{2}}\left(\psi_0(x) - \psi_0(x-2s)\right),$$

where λ_0 and $\psi_0(x)$ are the smallest eigenvalue and the corresponding ground state of the linear operator $L = -\partial_x^2 + W(x)$. Using projections to the three eigenstates for sufficiently large s and employing the method of Lyapunov–Schmidt reductions in the nonlinear stationary problem (19.2), the authors of [46] found a system of nonlinear equations for projections and classified all coupled localized modes that exist in the three-well potential, including their spectral stability and predicted time evolution. A similar method was employed in [47] to consider continuations of eigenvalues of the linear problem associated with a confining potential due to the perturbation of a small periodic potential.

19.4 Class of Confining Potentials

We shall assume here that $V(x)$ is a confining potential in the sense that $\inf_{|x|\geq R} V(x) \to \infty$ as $R \to \infty$. Since most experimental settings are based on the so-called harmonic traps, a typical approximation of the general confining potentials is a quadratic function

$$V(x) = \frac{1}{2}\sum_{j=1}^{N} \omega_j^2 x_j^2$$

with parameters $(\omega_1, ..., \omega_N)$. The Schrödinger operator $L = -\nabla^2 + V(x)$ associated with the quadratic function $V(x)$ possesses an exact set of eigenvalues and bound states written in terms of the Gauss–Hermite polynomials.

Gauss–Hermite polynomials can be used for decomposition of the solution of the time-dependent GP equation (19.1) with the quadratic potential function $V(x)$ and reduction of the time-evolution PDE problem to the equivalent lattice problem. This approach was used in [48], where the lattice problem was truncated in the Galerkin approximation at the two dominant modes. The two-mode approximation was shown to represent adequately all main dynamical phenomena associated with existence, stability and evolution of localized modes in the confining potentials.

In all asymptotic reductions of this chapter up to this point, we have taken the GP equation (19.1) and its stationary counterpart (19.2) as starting equations of analysis and performed some actions to simplify them to other reduced equations. On the other hand, the GP equation (19.1) is itself a reduction of the primary equations of physics, which are based on the multi-particle wave-function formalism in the system of interacting bosons. One can ask therefore if the GP equation (19.1) can be derived rigorously from equations of multi-particle quantum mechanics.

These questions were answered for the stationary problem (19.2) with $N = 3$ in [49]. Extensions of this work for $N = 1, 2$ and for other physical settings are given in the stream of subsequent publications reviewed in [50]. The authors of [49] considered the Hamiltonian operator of n identical bosons

$$H = \sum_{j=1}^{n} \left[-\nabla_i^2 + V(x_i) \right] + \sum_{i<j} v(|x_i - x_j|), \tag{19.30}$$

where $V(x)$ is the confining potential, $v(|x|)$ is an interaction potential and $x_j \in \mathbf{R}^3$ for all $j = 1, ..., n$. The ground state of the Hamiltonian operator H is a totally symmetric square integrable wavefunction denoted by $\Psi(x_1, x_2, ..., x_n)$. It exists for the eigenvalue (energy level) $E_{\rm QM}(n, a)$, where a is the scattering length defined by the formula

$$a = \lim_{r\to\infty} \left(r - u(r)/u'(r) \right)$$

from the solution $u(r)$ of the boundary-value problem

$$-u''(r) + \frac{1}{2} v(r) u(r) = 0$$

with $u(0) = 0$.

The main results of [49] (and equivalent theorems in [50]) are proved in the limit of many particles $n \to \infty$ and zero scattering length $a \to 0$, such that na is fixed. In particular, it is proved that

$$\forall a_1 > 0 : \quad \lim_{n\to\infty} \frac{1}{n} E_{\rm QM}\left(n, \frac{a_1}{n}\right) = E_{\rm GP}(1, a_1), \tag{19.31}$$

where $E_{\rm GP}(n, a)$ is the energy of a solution of the stationary problem (19.2) defined by

$$E_{\rm GP}(n, a) = \int_{\mathbf{R}^3} \left(|\nabla \phi|^2 + V(x)|\phi|^2 + 4\pi a |\phi|^4 \right) {\rm d}x, \tag{19.32}$$

subject to the normalization condition

$$\int_{\mathbf{R}^N} |\phi|^2 {\rm d}x = n.$$

The ground state solution $\phi(x)$ is defined by the minimal value of $E_{\rm GP}$ subject to the fixed L^2-norm. Not only the energy level $E_{\rm QM}$ of the multi-particle Hamiltonian H in (19.30) converges to the energy level $E_{\rm GP}$ of the ground state solution of the stationary problem (19.2) but also the solutions converge weakly in $L^2(\mathbf{R}^{3n})$, i.e.

$$\forall a_1 > 0, a = \frac{a_1}{n} : \quad \lim_{n \to \infty} \int_{\mathbf{R}^{3n-3}} |\Psi(x, x_2, ..., x_n)|^2 \mathrm{d}x_2 ... \mathrm{d}x_n = \phi^2(x), \tag{19.33}$$

in the sense that the integral of the difference between the left-hand-side and right-hand-side terms of the equality (19.33) on $x \in \mathbf{R}^3$ converges to zero as $n \to \infty$.

The results of [49, 50] are only proved for stationary solutions of the GP equation (and only for the ground state solutions). The time-dependent GP equation (19.1) was considered recently in [51] within a similar asymptotic limit $n \to \infty$ under the constraint that $n^{\epsilon} a$ is fixed with $0 < \epsilon < 3/5$. It is proved that the limit points of the k-particle density matrices of the multi-particle wavefunction $\Psi(x, x_2, ..., x_n, t)$ solve asymptotically the GP equation and the associated hierarchy of evolution equations. Thus, only proved rigorously in 2006, the Gross–Pitaevskii model has been widely used in atomic physics since the pioneer works of Gross and Pitaevskii in 1960s.

Conclusions

I have described reductions of the stationary and time-dependent GP equations used for analysis of existence, stability and dynamics of localized modes in external potentials. Depending on the properties of the potential $V(x)$, the spatially inhomogeneous GP equation (19.1) reduces either to the homogeneous PDEs such as the coupled-mode system or the continuous NLS equation or to differential-difference equations such as the discrete NLS equation or to finite-dimensional models such as the Newton's equations of motion or the ODE system for truncated Gauss–Hermite polynomials.

The limited space of the chapter does not allow me to consider other asymptotic reductions relevant for physics of Bose–Einstein condensation, such as reductions of the time-periodic GP equation relevant for the Feshbach resonance management of the Bose–Einstein condensates (see, e.g., [52]). I conclude by saying that ways of rigorous analysis remain opened for further work in the context of the Gross–Pitaevskii equation. Some of the open problems have been mentioned explicitly in this chapter. Some other problems will show up themselves to young researchers who will take the risk to get involved into challenging topics of the modern mathematical physics.

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