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# Derivation of the Tight-Binding Approximation for Time-Dependent Nonlinear Schrödinger Equations

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**Abstract.** In this paper, we consider the nonlinear one-dimensional time-dependent Schrödinger equation with a periodic potential and a bounded perturbation. In the limit of large periodic potential, the time behavior of the wavefunction can be approximated, with a precise estimate of the remainder term, by means of the solution to the discrete nonlinear Schrödinger equation of the tight-binding model.

**Mathematics Subject Classification.** 35Q55, 81Qxx, 81T25.

## 1. Introduction

Here we consider the nonlinear one-dimensional time-dependent Schrödinger equation with a cubic nonlinearity, a periodic potential $V$ and a perturbing potential $W$

$$\begin{cases} i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + \frac{1}{\epsilon} V\psi + \alpha_1 W\psi + \alpha_2 |\psi|^2\psi, \psi(\cdot, t) \in L^2(\mathbb{R}) \\ \psi(x,0) = \psi_0(x) \end{cases} \tag{1}$$

in the limit of large periodic potential, i.e., $0 < \epsilon \ll 1$; $\alpha_1$ represents the strength of the perturbing potential $W$ and $\alpha_2$ represents the strength of the nonlinearity term. Equation (1) is the so-called Gross–Pitaevskii equation for Bose–Einstein condensates where $\hbar$ is the Planck's constant and $m$ is the mass of the single atom. Such a model describes, for instance, one-dimensional Bose–Einstein condensates in an optical lattice and under the effect of an external field with potential $\alpha_1 W$; in particular, when such a perturbing potential is a Stark-type potential, that is, it is locally linear, then recently has been shown

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the existence of Bloch oscillations for the wavefunction condensate and a precise measurement of the gravity acceleration has given [10,19].

In the physical literature, a standard way to study Eq. (1) consists in reducing it to a discrete Schrödinger equation taking into account only nearest neighbor interactions, the so-called *tight-binding model* [3]. The validity of such an approximation is, as far as we know, not yet rigorously proved in a general setting.

Recently, it has been proved that (1) admits a family of stationary solutions by reducing it to discrete nonlinear Schrödinger equations [11,18,23]. Concerning the reduction of the time-dependent equation to a discrete time-dependent nonlinear Schrödinger equation, much less is known and rigorous results are only given under some conditions: for instance, in [4], the authors prove the validity of the reduction to discrete nonlinear Schrödinger equations for large times when $V$ is multiple-well trapped potential; while, in [17] a similar result for periodic potentials $V$ satisfying a sequence of specific technical conditions (see Theorem 2.5 [16] for a resume) is obtained. We must also recall the papers [1,2,5] where applications of the orbital functions in a similar context is developed; in particular, in [2], the authors prove the validity of the reduction to discrete nonlinear Schrödinger equations of the Gross–Pitaevskii equation with a periodic linear potential and a sign-varying nonlinearity coefficient. In [5], the authors consider the case of a two-dimensional lattice; in particular, they show that tight-binding approximation is justified for simple and honeycomb lattices provided that the initial wavefunction is exponentially small.

In this paper, we are able to show that the reduction of (1) to the time-dependent discrete nonlinear Schrödinger equations properly works with a precise estimate of the error, and that we do not need of special technical assumptions on the shape of the initial wavefunction and/or on the periodic potential; in fact, we have only to assume that the initial wavefunction is prepared on one band of the Bloch operator, let us say for argument's sake the first one.

By introducing the new semiclassical parameter

$$h = \hbar\sqrt{\epsilon/2m}, \tag{2}$$

the new time variable

$$\tau = \frac{\hbar}{h} t$$

and the effective perturbation and nonlinearity strengths

$$F = \alpha_1 \frac{2mh^2}{\hbar^2} \quad \text{and} \quad \eta = \alpha_2 \frac{2mh^2}{\hbar^2}, \tag{3}$$

then Eq. (1) takes the semiclassical form

$$ih\frac{\partial \psi}{\partial \tau} = -h^2 \frac{\partial^2 \psi}{\partial x^2} + V\psi + FW\psi + \eta |\psi|^2 \psi \tag{4}$$

with $h \ll 1$.

In the tight-binding approximation, solutions to (4) are approximated by solutions to the time-dependent discrete nonlinear Schrödinger equation

$$i h \dot{g}_n = -\beta (g_{n+1} + g_{n-1}) + F \xi_n g_n + \eta C_1 |g_n|^2 g_n,\ n \in \mathbb{Z}, \tag{5}$$

where $\beta \sim \mathrm{e}^{-S_0/h}$ is an *exponentially small* positive constant in the semiclassical limit $h \ll 1$ (in fact, $S_0 > 0$ is the Agmon distance between two adjacent wells, and for a precise estimate of the coupling parameter $\beta$ we refer to (13)). Furthermore, $\xi_n = \langle u_n, W u_n \rangle$ and $C_1 = \|u_n\|_{L^4}^4$ where, roughly speaking (a precise definition for $u_n$ is given by [9,11,23]), $\{u_n\}_{n\in\mathbb{Z}}$ is an orthonormal base of vectors of the eigenspace associated to the first band of the Bloch operator such that $u_n \sim \psi_n$ as $h$ goes to zero; where $\psi_n$ is the ground state with associated energy $\Lambda_1$ of the Schrödinger equation with a single-well potential $V_n$ obtained by filling all the wells, but the $n$th one, of the periodic potential $V$:

$$- h^2 \frac{\partial^2 \psi_n}{\partial x^2} + V_n \psi_n = \Lambda_1 \psi_n. \tag{6}$$

In fact, the linear operator $-h^2 \frac{\partial^2}{\partial x^2} + V_n$ has a single-well potential, and thus, it has a not empty discrete spectrum, we denote by $\Lambda_1$ the first eigenvalue (which is independent on the index $n$ by construction).

We must underline that usually the tight-binding approximation is constructed by making use of the Wannier's functions instead of the vectors $u_n$ [3,16]. Indeed, the decomposition by means of the Wannier's functions turns out to be more natural and it works for any range of $h$; on the other hand, the use of a suitable base $\{u_n\}_{n\in\mathbb{Z}}$ in the semiclassical regime of $h \ll 1$ has the great advantage that the vectors $u_n$ are explicitly constructed by means of the semiclassical approximation. In fact, Wannier's functions may be approximated by such vectors $u_n$ as pointed out by [14].

The analysis of the discrete nonlinear Schrödinger Eq. (5) depends on the relative value of the perturbative parameters $F$ and $\eta$ with respect to the coupling parameter $\beta$. In this paper, we consider two situations.

In the first case, named *model 1* corresponding to Hypothesis (3a), we assume that $\alpha_1$ and $\alpha_2$ are fixed and independent of $\epsilon$. In such a case, we have that $\beta \ll |F|$ and $\beta \ll C_1|\eta|$ and then the analysis of (5) is basically reduced to the analysis of a system on infinitely many decoupled equations. Indeed, the perturbative terms with strength $F$ and $\eta$ dominate the coupling term with strength $\beta$ between the adjacent wells. In fact, this model has some interesting features; for instance, when $W$ represents a Stark-type perturbation then the analysis of the stationary solutions exhibits the existence of a cascade of bifurcations [22,23]. On other hand, due to the fact that the perturbation is *large*, when compared with the coupling term, the validity of the tight-binding approximation is justified only for time intervals rather small.

In the second case, named *model 2* corresponding to Hypothesis (3b), we assume that both $\alpha_1$ and $\alpha_2$ go to zero when $\epsilon$ goes to zero. In particular, we assume that

$$F = \mathcal{O}(\beta) \ \text{ and } \ C_1 \eta = \mathcal{O}(\beta).$$

That is the perturbative terms are of the same order of the coupling term. In such a case, the validity of the tight-binding approximation holds true for times of the order of the inverse of the coupling parameter $\beta$, that is the time interval is exponentially large.

We must remark that one could consider, in principle, other limits for $\alpha_1$ and $\alpha_2$ when $h$ goes to zero and Theorem 6 is very general and it holds true under different assumptions concerning $\alpha_1$ and $\alpha_2$ provided that $F = \mathcal{O}(h^2)$ and $\eta = \mathcal{O}(h^2)$. In fact, Hyp. (3a) and Hyp. (3b) represents, in some sense, two opposite situations concerning the choice of the parameters.

In Sect. 2, we state the assumptions on Eq. (4) and we state our main results in Theorems 1 and 2, they follow from a more technical Theorem 6 we state and prove in Sect. 5. In Sect. 3, we prove a priori estimate of the wavefunction $\psi$ and of its gradient $\nabla\psi$. In Sect. 4, we formally construct the discrete nonlinear Schrödinger equations; in this section we make use of some ideas already developed by [11,23] and we refer to these papers as much as possible. We must underline that in [11,23] the estimate of the remainder terms is given in the norm $\ell^1$, while in the present paper estimates in the norm $\ell^2$ are necessary and thus most of the material of Sect. 3, and in particular Lemmata 2, 3, 4, 5 and 6, is original and it cannot be simply derived from the papers quoted above. In Sect. 5, we finally prove the validity of the tight-binding approximation with a precise estimate of the error in Theorem 6, the method used is based on an idea already applied by [21] for a double-well model and now applied to a periodic potential; in particular, in Sect. 5.1, we consider the case where $\alpha_1$ and $\alpha_2$ are fixed, i.e., *model 1*, and in Sect. 5.2, we consider the case where $\alpha_1$ and $\alpha_2$ goes to zero as $\epsilon$ goes to zero in a suitable way, i.e., *model 2*.

## 2. Description of the Model and Main Results

### 2.1. Assumptions

Here, we consider the nonlinear Schrödinger Eq. (1) where the following assumptions hold true.

**Hypothesis 1.** *$V(x)$ is a smooth, real-valued, periodic and non-negative function with period $a$, i.e.,*

$$V(x) = V(x+a),\ \forall x \in \mathbb{R},$$

*and with minimum point $x_0 \in \left[-\frac{1}{2}a, +\frac{1}{2}a\right)$ such that*

$$V(x) > V(x_0),\ \forall x \in \left[-\frac{1}{2}a, +\frac{1}{2}a\right) \setminus \{x_0\}.$$

*For argument's sake, we assume that $V(x_0) = 0$ and $x_0 = 0$.*

*Remark 1.* We could, in principle, adapt our treatment to a more general case where $V(x)$ has more than one absolute minimum point in the interval $\left[-\frac{1}{2}a, +\frac{1}{2}a\right)$.

**Hypothesis 2.** *The perturbation $W(x)$ is a smooth real-valued function. We assume that $W \in L^\infty(\mathbb{R})$.*

Concerning the parameters $m$, $\hbar$, $\alpha_1$, $\alpha_2$ and $\epsilon$ we make the following assumption

**Hypothesis 3.** *We assume the semiclassical limit of large periodic potential, i.e., $\epsilon$ is a real and positive parameter small enough*

$$\epsilon \ll 1.$$

*Concerning the other parameters we assume that:*

(a) *The parameters $m$, $\hbar$, $\alpha_1$, $\alpha_2$ are real-valued and independent of $\epsilon$; or*

(b) *The parameters $m$, $\hbar$ are real-valued and independent of $\epsilon$ while the parameters $\alpha_1$, $\alpha_2$ are real-valued and they go to zero as $\epsilon$ goes to zero; in particular, we assume that there exist $\epsilon^\star > 0$ and a positive constant $C$ such that for any $0 < \epsilon < \epsilon^\star$ then*

$$|F| \leq C|\beta| \quad \text{and} \quad |C_1 \eta| \leq C|\beta|,$$

*where $F$ and $\eta$ are defined in (3), and where the parameters $\beta$ and $C_1$ depend on $\epsilon$ (by means of $h$) and they are defined by (13) and (14).*

*For argument's sake, we assume in both cases that $\alpha_1 \geq 0$; hence $F \geq 0$.*

*Remark 2.* In both cases, we have that $0 \leq F \leq Ch^2$ and $|\eta| \leq Ch^2$ for some positive constant $C$. In the case (b), in particular, $F$ and $\eta$ are exponentially small when $h$ goes to zero.

Let $H_B$ be the Bloch operator formally defined on $L^2(\mathbb{R}, \mathrm{d}x)$ as

$$H_B := -h^2 \frac{d^2}{\mathrm{d}x^2} + V. \tag{7}$$

It is well known that this operator admits self-adjoint extension on the domain $H^2(\mathbb{R})$, still denoted by $H_B$, and its spectrum is given by bands:

$$\sigma(H_B) = \cup_{\ell=1}^\infty [E_\ell^b, E_\ell^t], \quad \text{where} \quad E_\ell^t \leq E_{\ell+1}^b < E_{\ell+1}^t.$$

The intervals $(E_\ell^t, E_{\ell+1}^b)$ are named gaps; a gap may be empty, that is $E_{\ell+1}^b = E_\ell^t$, or not. It is well known that in the case of one-dimensional crystals all the gaps are empty if, and only if, the periodic potential is a constant function. Because we assume that the periodic potential is not a constant function then one gap, at least, is not empty (for a review of Bloch operator we refer to [20]). In particular, when $h$ is small enough then the following asymptotic behaviors [24,25]

$$\frac{1}{C} h \leq E_1^b \leq Ch \quad \text{and} \quad \frac{1}{C} h \leq E_2^b - E_1^t \leq Ch \tag{8}$$

hold true for some $C > 1$; hence, the first gap between $E_1^t$ and $E_2^b$ is not empty in the semiclassical limit.

Let $\Pi$ the projection operator associated to the first band $[E_1^b, E_1^t]$ of $H_B$ and let $\Pi_\perp = \mathbb{1} - \Pi$. Let

$$\psi = \psi_1 + \psi_\perp \quad \text{where } \psi_1 = \Pi\psi \quad \text{and} \quad \psi_\perp = \Pi_\perp \psi. \tag{9}$$

We assume that

**Hypothesis 4.** $\Pi_\perp \psi_0 = 0$, *where* $\psi_0(x) = \psi(x, 0)$; *that is the wave function* $\psi$ *is initially prepared on the first band. Through the paper we assume, for argument's sake, that* $\psi_0$ *is normalized, i.e.,* $\|\psi_0\|_{L^2} = 1$.

### 2.2. Main Results

Here, we state our main results; they are a consequence of a rather technical Theorem 6 we postpone to Sect. 5. Let $\mathbf{g} \in C(\mathbb{R}, \ell^2(\mathbb{Z}))$ be the solution to the tight-binding model, that is the discrete nonlinear Schrödinger Eq. (5); let $\psi(\tau, x) \in C(\mathbb{R}, H^1(\mathbb{R}))$ be the solution to the nonlinear Schrödinger Eq. (4) with initial condition $\psi_0(x) = \sum g_n(0) u_n(x)$, let us recall (2) and, finally, let $\Lambda_1$ be the first eigenvalue of the single-well operator (6).

**Theorem 1.** *Under the assumption Hypothesis (3a), we have that there exist* $\epsilon^\star > 0$ *and a positive constant* $C$ *independent of* $\epsilon$ *such that for any* $0 < \epsilon < \epsilon^\star$ *then*

$$\left\| \psi(\tau, \cdot) - \sum_{n \in \mathbb{Z}} g_n(\tau) \mathrm{e}^{i\Lambda_1 \tau / h} u_n(\cdot) \right\|_{L^2} \leq C h^{1/2},$$

*for any* $\tau \in [0, C h^{-1/2}]$.

**Theorem 2.** *Under the assumption Hypothesis (3b), we have that there exists* $\epsilon^\star > 0$ *and two positive constants* $C$ *and* $\zeta$ *independent of* $\epsilon$ *such that for any* $0 < \epsilon < \epsilon^\star$ *then*

$$\left\| \psi(\tau, \cdot) - \sum_{n \in \mathbb{Z}} g_n(\tau) \mathrm{e}^{i\Lambda_1 \tau / h} u_n(\cdot) \right\|_{L^2} \leq C \mathrm{e}^{-\zeta / h}$$

*for any* $\tau \in [0, C\beta^{-1} h]$, *where* $\beta^{-1}$ *is exponentially large as* $h$ *goes to zero.*

*Remark 3.* In [17], the estimate of the error was given in the energy norm, and even in [23], we used the $H^1$-norm. If one wants to extend the result of Theorem 1 to the $H^1$-norm, it is clear that one has to pay a price; indeed, in the proof of Theorem 6, the term $\|u_0\|_{H^1} \sim h^{-1/2}$ would appear instead of the term $\|u_0\|_{L^2} = 1$, and therefore, the estimate of the error became meaningless. On the other hand, this argument is not critical in the case of the extension of Theorem 2 to the $H^1$-norm because the term $\|u_0\|_{H^1}$ is controlled by means of the exponentially small term $\mathrm{e}^{-\zeta/h}$. In fact, we expect that Theorem 2 still hold true with the $H^1$-norm even if we do not dwell here with the detailed proof.

### 2.3. Notation and Some Functional Inequalities

Hereafter, we denote by $\| \cdot \|_{L^p}$, $p \in [+1, +\infty]$, the usual norm of the Banach space $L^p(\mathbb{R}, \mathrm{d}x)$; we denote by $\| \cdot \|_{\ell^p}$, $p \in [+1, +\infty]$, the usual norm of the Banach space $\ell^p(\mathbb{Z})$.

Hereafter, we omit the dependence on $\tau$ in the wavefunctions $\psi$ and in the vectors $\mathbf{c}$ when this fact does not cause misunderstanding.

By $C$, we denote a generic positive constant independent of $h$ [and then, because of (2), by $\epsilon$] whose value may change from line to line.

If $f$ and $g$ are two given quantities depending on the semiclassical parameter $h$, then by $f \sim g$ we mean that

$$\lim_{h \to 0^+} \frac{f}{g} \in \mathbb{R} \backslash \{0\}.$$

Furthermore, we recall some well known results for reader's convenience:

- **One-dimensional Gagliardo–Nirenberg inequality** by §B.5 [16]:

$$\|f\|_{L^p} \le C \|\nabla f\|_{L^2}^{\delta} \|f\|_{L^2}^{1-\delta}, \ \delta = \frac{1}{2} - \frac{1}{p} = \frac{p-2}{2p}, \ p \in [2, +\infty],$$

- **Gronwall's Lemma** by Theorem 1.3.1 [15]: let $u(\tau)$ be a non-negative and continuous function such that

$$u(\tau) \le \alpha(\tau) + \int_0^\tau \delta(q) u(q) \mathrm{d}q, \ \forall \tau \ge 0,$$

where $\alpha(\tau)$ and $\delta(\tau)$ are non-negative and monotone not decreasing functions, then

$$u(\tau) \le \alpha(\tau) \mathrm{e}^{\int_0^\tau \delta(q) \mathrm{d}q}, \forall \tau \ge 0.$$

- **Agmon distance** let $E$ be a given energy and $V(x)$ be a potential function, let $[z]_+ = z$ if $z \ge 0$ and $[z]_+ = 0$ if $z < 0$; then the Agmon distance $d_A(x, y)$ between two points $x, y \in \mathbb{R}^d$ is induced by the Agmon metric $[V(x) - E]_+ \mathrm{d}x^2$ where $\mathrm{d}x^2$ is the standard metric on $L^2(\mathbb{R}^d)$:

$$d_A(x, y) = \inf_{\gamma \in \mathcal{C}} \int_0^1 \sqrt{[V(\gamma(t)) - E]_+} |\gamma'(t)| \mathrm{d}t$$

where $\mathcal{C}$ is the set of piecewise paths $\gamma$ in $\mathbb{R}^d$ connecting $\gamma(0) = x$ and $\gamma(1) = y$ (see [12] for a resume). In particular, in dimension $d = 1$ and for energy $E = V_{\min}$ we denote by $S_0 = \int_{x_n}^{x_{n+1}} \sqrt{V(x) - V_{\min}} \mathrm{d}x$ the Agmon distance between the bottoms $x_n$ and $x_{n+1}$ of two adjacent wells; by the periodicity of $V(x)$ then $S_0$ does not depend on the index $n$.

## 3. Preliminary Results

We recall here some results by [6–8] concerning the solution to the time-dependent nonlinear Schrödinger equation with initial wavefunction $\psi_0$. The linear operator $H$, formally defined as

$$H := H_B + FW$$

on the Hilbert space $L^2(\mathbb{R}, \mathrm{d}x)$, admits a self-adjoint extension on the domain $H^2(\mathbb{R})$, still denoted by $H$. In order to discuss the local and global existence of solutions to (4), we apply Theorem 4.2 by [8]: if $\psi_0 \in H^1(\mathbb{R})$ there is a unique solution $\psi \in C([-T,T], H^1(\mathbb{R}))$ to (4) with initial datum $\psi_0$, such that

$$\psi, \psi\frac{\partial(V+FW)}{\partial x}, \frac{\partial \psi}{\partial x} \in L^8([-T,T]; L^4(\mathbb{R})),$$

for some $T>0$ depending on $\|\psi_0\|_{H^1}$.

In fact (see [7]), this solution is global in time for any $\eta \in \mathbb{R}$ (because in the case of one-dimensional nonlinear Schrödinger equations the cubic nonlinearity in sub-critical) and (4) enjoys the conservation of the mass

$$\|\psi(\cdot,\tau)\|_{L^2} = \|\psi_0(\cdot)\|_{L^2}$$

and of the energy

$$\mathcal{E}\left[\psi(\cdot,\tau)\right] = \mathcal{E}\left[\psi_0(\cdot)\right]$$

where

$$\begin{aligned}\mathcal{E}(\psi) &:= \langle H\psi,\psi\rangle + \frac{\eta}{2}\|\psi\|_{L^4}^4 \\ &= h^2\left\|\frac{\partial\psi}{\partial x}\right\|_{L^2}^2 + \langle V\psi,\psi\rangle + F\langle W\psi,\psi\rangle + \frac{\eta}{2}\|\psi\|_{L^4}^4\end{aligned}$$

Here, we prove some useful preliminary a priori estimates.

**Theorem 3.** *The following a priori estimates hold true for any $\tau \in \mathbb{R}$:*

$$\begin{aligned}&\|\psi\|_{L^2} = \|\psi_0\|_{L^2} = 1 \quad \text{and} \quad \|\nabla\psi\|_{L^2} \le Ch^{-1/2}, \\ &\|\psi_1\|_{L^2} \le \|\psi_0\|_{L^2} = 1 \quad \text{and} \quad \|\nabla\psi_1\|_{L^2} \le Ch^{-1/2}, \\ &\|\psi_\perp\|_{L^2} \le \|\psi_0\|_{L^2} = 1 \quad \text{and} \quad \|\nabla\psi_\perp\|_{L^2} \le Ch^{-1/2};\end{aligned}$$

*for some positive constant $C$.*

*Proof.* From the conservation of the norm, we have that

$$\|\psi_0\|_{L^2}^2 = \|\psi\|_{L^2}^2 = \|\psi_\perp\|_{L^2}^2 + \|\psi_1\|_{L^2}^2;$$

hence,

$$\|\psi_\perp\|_{L^2} \le \|\psi_0\|_{L^2} = 1 \quad \text{and} \quad \|\psi_1\|_{L^2} \le \|\psi_0\|_{L^2} = 1.$$

From the conservation of the energy, we may obtain a priori estimate of the gradient of the wavefunction. Let

$$\mathcal{E}(\psi_0) = \langle H_B\psi_0,\psi_0\rangle + F\langle W\psi_0,\psi_0\rangle + \frac{1}{2}\eta\|\psi_0\|_{L^4}^4,$$

where $\langle H_B\psi_0,\psi_0\rangle \sim h$ since $\psi_0$ is restricted to the eigenspace associated to the first band. Recalling that $V \ge 0$ then we have that

$$h^2\|\nabla\psi_0\|_{L^2}^2 \le \langle H_B\psi_0,\psi_0\rangle \sim h,$$

which implies $\|\nabla\psi_0\|_{L^2} \le Ch^{-1/2}$. From this fact, using the fact that $W$ is a bounded potential and by the Gagliardo–Nirenberg inequality we have that

$$\|\psi_0\|_{L^4}^4 \le C\|\nabla\psi_0\|_{L^2}\|\psi_0\|_{L^2}^3 \le C\|\nabla\psi_0\|_{L^2} \le Ch^{-1/2}.$$

Hence, $\mathcal{E}(\psi_0) \sim h$ since $F \le Ch^2$ and $|\eta| \le Ch^2$ (see Remark 2). Thus, the conservation of the energy implies the following inequality:

$$\begin{aligned} h^2\|\nabla\psi\|_{L^2}^2 &= \mathcal{E}(\psi_0) - \langle V\psi,\psi\rangle - F\langle W\psi,\psi\rangle - \frac{1}{2}\eta\|\psi\|_{L^4}^4 \\ &\le \mathcal{E}(\psi_0) - V_{\min}\|\psi\|_{L^2}^2 - FW_{\min}\|\psi\|_{L^2}^2 - \frac{1}{2}\eta\|\psi\|_{L^4}^4 \\ &\le \mathcal{E}(\psi_0) - FW_{\min} - \frac{1}{2}\eta\|\psi\|_{L^4}^4 \end{aligned}$$

since $V_{\min} = 0$ and by the conservation of the norm. Let us set

$$\Lambda = \frac{\mathcal{E}(\psi_0) - FW_{\min}}{h^2} \quad \text{and} \quad \Gamma = \frac{1}{2}\frac{\eta}{h^2} = \frac{m\alpha_2}{\hbar^2},$$

then $|\Gamma| \le C$ and $\Lambda \sim h^{-1}$ as $h$ goes to zero. The previous inequality becomes

$$\|\nabla\psi\|_{L^2}^2 \le |\Lambda| + |\Gamma|\,\|\psi\|_{L^4}^4.$$

Again, the Gagliardo–Nirenberg inequality implies that

$$\|\psi\|_{L^4}^4 \le C\|\nabla\psi\|_{L^2}\|\psi\|_{L^2}^3 = C\|\nabla\psi\|_{L^2},$$

and thus, we get

$$\|\nabla\psi\|_{L^2}^2 \le |\Lambda| + |\Gamma|C\|\nabla\psi\|_{L^2}$$

from which it follows that

$$\|\nabla\psi\|_{L^2} \le \frac{1}{2}\left[|\Gamma|C + \sqrt{\Gamma^2C^2 + 4|\Lambda|}\right] \le C|\Lambda|^{1/2} \le Ch^{-1/2}$$

for some positive constant $C$.

Since $\Pi H_B = H_B\Pi$, we have that

$$\begin{aligned} \mathcal{E}(\psi_0) - F\langle W\psi,\psi\rangle - \frac{1}{2}\eta\|\psi\|_{L^4}^4 &= \langle H_B\psi,\psi\rangle = \langle H_B\psi_1,\psi_1\rangle + \langle H_B\psi_\perp,\psi_\perp\rangle \\ &= h^2\|\nabla\psi_1\|_{L^2}^2 + h^2\|\nabla\psi_\perp\|_{L^2}^2 + \langle V\psi_1,\psi_1\rangle + \langle V\psi_\perp,\psi_\perp\rangle \ge h^2\|\nabla\psi_1\|_{L^2}^2 \end{aligned}$$

since $V_{\min} \ge 0$. Then,

$$h^2\|\nabla\psi_1\|_{L^2}^2 \le Ch + \frac{1}{2}|\eta|\,\|\psi\|_{L^4}^4 \le Ch + C|\eta|\|\nabla\psi\|_{L^2} \le Ch;$$

hence,

$$\|\nabla\psi_1\|_{L^2} \le Ch^{-1/2}.$$

Similarly we get

$$\|\nabla\psi_\perp\|_{L^2} \le Ch^{-1/2},$$

and thus, the proof of the Theorem is so completed. □

**Corollary 1.** *We have the following estimates:*

$$\|\psi\|_{L^\infty} \le Ch^{-1/4},\ \|\psi_1\|_{L^\infty} \le Ch^{-1/4},\ \|\psi_\perp\|_{L^\infty} \le Ch^{-1/4},\ \forall\tau \ge 0.$$

*Proof.* They immediately follow from the one-dimensional Gagliardo–Nirenberg inequality (where $p = +\infty$ and $\delta = \frac{1}{2}$) and from the previous result. □

## 4. Construction of the Discrete Time-Dependent Nonlinear Schrödinger Equation

By the Carlsson's construction [9] resumed and expanded in Appendix A by [11] (see also §3 [23] for a short review of the main results) we may write $\psi_1$ by means of a linear combination of a suitable orthonormal base $\{u_n\}_{n\in\mathbb{Z}}$ of the space $\Pi\left[L^2(\mathbb{R})\right]$, that is

$$\psi_1(x) = \sum_{n\in\mathbb{Z}} c_n u_n(x), \tag{10}$$

where $u_n \in H^1(\mathbb{R})$ and $\mathbf{c} = \{c_n\}_{n\in\mathbb{Z}} \in \ell^2(\mathbb{Z})$ and where we omit, for simplicity's sake, the dependence on $\tau$ in the wavefunctions $\psi$, $\psi_1$, $\psi_\perp$ as well as in the vector $\mathbf{c}$.

By inserting (9) and (10) in Eq. (4), it takes the form (where $\dot{} = \frac{\partial}{\partial\tau}$)

$$\begin{cases} ih\dot{c}_n &= \langle u_n, H_B\psi\rangle + F\langle u_n, W\psi\rangle + \eta\langle u_n, |\psi|^2\psi\rangle,\ n\in\mathbb{Z} \\ ih\dot{\psi}_\perp &= \Pi_\perp H_B\psi + F\Pi_\perp W\psi + \eta\Pi_\perp|\psi|^2\psi \end{cases}, \tag{11}$$

where $\mathbf{c}\in\ell^2$ and $\psi_\perp$ are such that for any $\tau\in\mathbb{R}$

$$\|\psi_\perp\|_{L^2} \le \|\psi_0\|_{L^2} = 1 \ \text{ and } \ \sum_{n\in\mathbb{Z}} |c_n|^2 = \|\mathbf{c}\|^2_{\ell^2} = \|\psi_1\|^2_{L^2} \le \|\psi_0\|^2_{L^2} = 1.$$

By mean of the gauge choice $\psi(x,\tau)\to \mathrm{e}^{i\Lambda_1\tau/h}\psi(x,\tau)$, and then $\psi_\perp(x,\tau) \to \mathrm{e}^{i\Lambda_1\tau/h}\psi_\perp(x,\tau)$ and $c_n(\tau)\to\mathrm{e}^{i\Lambda_1\tau/h}c_n(\tau)$, (11) takes the form

$$\begin{cases} ih\dot{c}_n &= \langle u_n, H_B\psi\rangle - \Lambda_1 c_n + F\langle u_n, W\psi\rangle + \eta\langle u_n, |\psi|^2\psi\rangle,\ n\in\mathbb{Z} \\ ih\dot{\psi}_\perp &= \Pi_\perp (H_B-\Lambda_1)\psi + F\Pi_\perp W\psi + \eta\Pi_\perp|\psi|^2\psi \end{cases}, \tag{12}$$

where $\Lambda_1$ is the energy associated to the ground state of the Schrödinger operator $-h^2\frac{\partial^2}{\partial x^2}+V_n$, with single-well potential $V_n$ obtained by filling all the wells of the periodic potential $V$, but the $n$th one; since $V_n(x) = V_m(x-x_n+x_m)$ by construction (see [11,23] for details) then the spectrum of this linear operator is independent on the index $n$ and the eigenvetor $\psi_n$ associated to the ground state $\Lambda_1$ is such that $\psi_m(x) = \psi_n(x-x_m+x_n)$ .

We have that

$$\langle u_n, H_B\psi\rangle = \Lambda_1 c_n - \beta(c_{n+1}+c_{n-1}) + r_{1,n},$$

where $\Lambda_1$ and $\beta$ are independent of the index $n$ and $\beta$ is such that for any $0<\rho<S_0$ there is $C := C_\rho$ such that

$$\frac{1}{C}\mathrm{e}^{-(S_0+\rho)/h} < \beta < C\mathrm{e}^{-(S_0-\rho)/h}; \tag{13}$$

the remainder term $r_{1,n}$ is defined as

$$r_{1,n} := \sum_{m\in\mathbb{Z}} \tilde{D}_{n,m}c_m$$

where $\tilde{D}_{n,m}$ satisfies Lemma 1 in [23]. Furthermore,

$$\langle u_n, W\psi\rangle = \xi_n c_n + r_{2,n} + r_{3,n},$$

where we set

$$\xi_n = \langle u_n, W u_n \rangle, \ r_{2,n} = \sum_{m\in\mathbb{Z}\,:\,m\neq n} \langle u_n, W u_m \rangle c_m \text{ and } r_{3,n} = \langle u_n, W\psi_\perp \rangle.$$

Finally,

$$\langle u_n, |\psi|^2\psi \rangle = C_1 |c_n|^2 c_n + r_{4,n}, \ C_1 = \|u_n\|_{L^4}^4,$$

where we set

$$r_{4,n} = \langle u_n, |\psi|^2\psi \rangle - C_1 |c_n|^2 c_n$$

and where by Lemma 1.vi [23] it follows that

$$C_1 = \|u_n\|_{L^4}^4 \equiv \|u_0\|_{L^4}^4 \sim h^{-1/2} \text{ as } h \text{ goes to zero.} \tag{14}$$

Therefore, (12) may be written

$$\begin{cases} ih\dot{c}_n &= -\beta(c_{n+1}+c_{n-1}) + F\xi_n c_n + \eta C_1 |c_n|^2 c_n + r_n \\ ih\dot{\psi}_\perp &= \Pi_\perp (H_B - \Lambda_1)\psi + F\Pi_\perp W\psi + \eta \Pi_\perp |\psi|^2\psi \end{cases}, \tag{15}$$

where we set

$$r_n = r_{1,n} + F r_{2,n} + F r_{3,n} + \eta r_{4,n}.$$

Tight-binding approximation (5) is obtained by putting $\psi_\perp \equiv 0$ and by neglecting the coupling term $r_n$ in (15).

We have the following estimates.

**Lemma 1.**

$$\|\mathbf{r}_1\|_{\ell^2} \le C e^{-(S_0+\zeta)/h} \|\mathbf{c}\|_{\ell^2}$$

*for some positive constants $C$ and $\zeta$ independent of $h$.*

*Proof.* Such an estimate directly comes from Lemma 1 by [23]. □

**Lemma 2.** *For any $0<\rho<S_0$, there is a positive constant $C := C_\rho$ such that*

$$\|\mathbf{r}_2\|_{\ell^2} \le C e^{(S_0-\rho)/h} \|\mathbf{c}\|_{\ell^2}.$$

*Proof.* We set

$$W_{n,m} = \begin{cases} \langle u_n, W u_m \rangle & \text{if } n \neq m \\ 0 & \text{if } n = m \end{cases};$$

then $r_{2,n} = \sum_{m\in\mathbb{Z}} W_{n,m} c_m$. By Example 2.3 §III.2 [13], it follows that

$$\|\mathbf{r}_2\|_{\ell^2} \le \max[M', M''] \|\mathbf{c}\|_{\ell^2}$$

where $M'$ and $M''$ are such that $\sum_{m\in\mathbb{Z}} |W_{n,m}| \le M'$ and $\sum_{n\in\mathbb{Z}} |W_{n,m}| \le M''$ for any $n\in\mathbb{Z}$; then $M' = M''$ because $|W_{n,m}| = |W_{m,n}|$. Since $W$ is a bounded operator and by Lemma 1.iv [23] it immediately follows that $M' = C e^{(S_0-\rho)/h}$ for any $0<\rho<S_0$ and for some positive constant $C := C_\rho$. Hence, Lemma 2 is so proved. □

**Lemma 3.**

$$\|\mathbf{r}_3\|_{\ell^2} \le C \|\psi_\perp\|_{L^2}.$$

*Proof.* Since $r_{3,n} = \langle u_n, W\psi_\perp\rangle_{L^2}$ where $\{u_n\}_{n\in\mathbb{Z}}$ is an orthonormal base of the space $\Pi\left[L^2(\mathbb{R})\right]$; then, from the Parseval's identity it follows that

$$\|\mathbf{r}_3\|_{\ell^2} = \|\Pi W \Pi_\perp \psi\|_{L^2} = \|\Pi W \Pi_\perp \psi_\perp\|_{L^2} \leq \|\Pi W \Pi_\perp\| \, \|\psi_\perp\|_{L^2} \leq C\|\psi_\perp\|_{L^2}$$

because $\Pi W \Pi_\perp$ is a bounded potential. □

For what concerns the vector $\mathbf{r}_4$, let

$$r_{4,n} = \langle u_n, |\psi|^2\psi\rangle - C_1|c_n|^2 c_n = A_n + B_n$$

where we set

$$A_n = \langle u_n, |\psi|^2\psi\rangle - \langle u_n, |\psi_1|^2\psi_1\rangle$$

and

$$B_n = \langle u_n, |\psi_1|^2\psi_1\rangle - C_1|c_n|^2 c_n = \sum_{j,\ell,m\in\mathbb{Z}}^{\star} \langle u_n, \bar{u}_m u_\ell u_j\rangle \bar{c}_m c_\ell c_j \tag{16}$$

where $\sum_{j,m,\ell\in\mathbb{Z}}^{\star}$ means that at least one of three indexes $j$, $\ell$ and $m$ is different from the index $n$.

**Lemma 4.** *Let* $\mathbf{B} = \{B_n\}_{n\in\mathbb{Z}}$*, then for any* $0 < \rho < S_0$ *there is a positive constant* $C$ *such that*

$$\|\mathbf{B}\|_{\ell^2} \leq C\mathrm{e}^{-(S_0-\rho)/h}.$$

*Proof.* For argument's sake, let us assume that $m$ is the index different from the index $n$ in sum (16); then we have to check the term

$$\sum_{m,\ell,j\in\mathbb{Z},\, m\neq n} \langle u_m u_n, u_\ell u_j\rangle \bar{c}_m c_\ell c_j = B_{1,n} + B_{2,n} + B_{3,n}$$

where

$$\begin{aligned} B_{1,n} &= \sum_{j,m,\ell\in\mathbb{Z}}^{\star 1} \langle u_m u_n, u_\ell u_j\rangle \bar{c}_m c_\ell c_j \\ &:= \sum_{m\in\mathbb{Z}\setminus\{n\}} \sum_{\ell\in\mathbb{Z}\setminus\{m,n\}} \sum_{j\in\mathbb{Z}\setminus\{\ell,m,n\}} \langle u_m u_n, u_\ell u_j\rangle \bar{c}_m c_\ell c_j \\ B_{2,n} &= \sum_{j,m,\ell\in\mathbb{Z}}^{\star 2} \langle u_m u_n, u_\ell^2\rangle \bar{c}_m c_\ell^2 := \sum_{m\in\mathbb{Z}\setminus\{n\}} \sum_{\ell\in\mathbb{Z}\setminus\{m,n\}} \langle u_m u_n, u_\ell^2\rangle \bar{c}_m c_\ell^2 \\ B_{3,n} &= \sum_{j,m,\ell\in\mathbb{Z}}^{\star 3} \langle u_m u_n, u_m^2\rangle \bar{c}_m c_m^2 := \sum_{m\in\mathbb{Z},\, m\neq n} \langle u_n u_m, u_m^2\rangle \bar{c}_m c_m^2 \end{aligned}$$

Let $0 < \rho < S_0$ be fixed; from Lemma 1.iv [23], it follows that for any $\rho', \rho'' > 0$ such that $\rho' + \rho'' < \rho$ then there exists a positive constant $C > 0$, independent of the indexes $n$ and $m$ and of the semiclassical parameter $h$, such that

$$\|u_n u_m\|_{L^1(\mathbb{R})} \leq C\mathrm{e}^{\left[(S_0-\rho')|m-n|-\rho''\right]/h}. \tag{17}$$

Now, observing that $|c_m| \le 1$ since $\|\mathbf{c}\|_{\ell^2} \le 1$, then

$$
\begin{aligned}
|B_{3,n}| &\le \sum_{m\in\mathbb{Z},\, m\neq n} |\langle u_n u_m, u_m^2\rangle|\, |c_m|^3 \\
&\le \sum_{m\in\mathbb{Z},\, m\neq n} \|u_n u_m\|_{L^1} \|u_m\|_{L^\infty}^2\, |c_m|^2 \\
&\le \sum_{m\in\mathbb{Z},\, m\neq n} C h^{-1/2} \mathrm{e}^{-[(S_0-\rho')|n-m|-\rho'']/h}\, |c_m|^2
\end{aligned}
$$

where we make use of estimate (17) and where $\rho', \rho'' > 0$ are such that $\rho'+\rho'' < \rho$. Hence,

$$
\begin{aligned}
\|\mathbf{B}_3\|_{\ell^2} \le \|\mathbf{B}_3\|_{\ell^1} &\le \sum_{n,m\in\mathbb{Z},\ m\neq n} C h^{-1/2} \mathrm{e}^{-[(S_0-\rho')|n-m|-\rho'']/h} |c_m|^2 \\
&\le C\mathrm{e}^{-(S_0-\rho)/h} \sum_{m\in\mathbb{Z}} |c_m|^2 = C\mathrm{e}^{-(S_0-\rho)/h} \|\mathbf{c}\|_{\ell^2}^2 \\
&\le C\mathrm{e}^{-(S_0-\rho)/h}.
\end{aligned}
$$

for some positive constant $C$. For what concerns the term $B_{2,n}$, we have that

$$
\begin{aligned}
|B_{2,n}| &= \left| \sum_{m,\ell\in\mathbb{Z}}^{\star 2} \langle u_m u_n, u_\ell^2\rangle \bar{c}_m c_\ell^2 \right| \le \sum_{m,\ell\in\mathbb{Z}}^{\star 2} \langle |u_m|\,|u_n|, |u_\ell|^2\rangle\, |c_m|\, |c_\ell|^2 \\
&\le \sum_{\ell\in\mathbb{Z},\, \ell\neq n} \left\langle |u_n| \sum_{m\in\mathbb{Z}} |u_m|, |u_\ell|^2 \right\rangle |c_\ell|^2 \\
&\le \max_{\ell\in\mathbb{Z}} \|u_\ell\|_{L^\infty} \left\| \sum_{m\in\mathbb{Z}} |u_m| \right\|_{L^\infty} \sum_{\ell\in\mathbb{Z},\, \ell\neq n} \langle |u_n|, |u_\ell|\rangle\, |c_\ell|^2 \\
&\le \max_{\ell\in\mathbb{Z}} \|u_\ell\|_{L^\infty} \left\| \sum_{m\in\mathbb{Z}} |u_m| \right\|_{L^\infty} \sum_{\ell\in\mathbb{Z},\, \ell\neq n} C\mathrm{e}^{-[(S_0-\rho')|n-\ell|-\rho'']/h} |c_\ell|^2 \\
&\le C\|u_0\|_{L^\infty} \left\| \sum_{m\in\mathbb{Z}} |u_m| \right\|_{L^\infty} \sum_{\ell\in\mathbb{Z},\, \ell\neq n} \mathrm{e}^{-[(S_0-\rho')|n-\ell|-\rho'']/h} |c_\ell|^2 \\
&\le C h^{-3/4} \sum_{\ell\in\mathbb{Z},\, \ell\neq n} \mathrm{e}^{-[(S_0-\rho')|n-\ell|-\rho'']/h} |c_\ell|^2
\end{aligned}
$$

since $\|u_\ell\|_{L^\infty} = \|u_0\|_{L^\infty} \le C h^{-1/4}$ and $\left\|\sum_{m\in\mathbb{Z}} |u_m|\right\|_{L^\infty} \le C h^{-1/2}$ (see Lemma 1 [23]), from which it follows that

$$
\begin{aligned}
\|\mathbf{B}_2\|_{\ell^2} \le \|\mathbf{B}_2\|_{\ell^1} = \sum_{n\in\mathbb{Z}} |B_{2,n}| &\le C h^{-3/4} \sum_{n,\ell\in\mathbb{Z}\ \ n\neq \ell} C\mathrm{e}^{-[(S_0-\rho')|n-\ell|-\rho'']/h} |c_\ell|^2 \\
&\le C\mathrm{e}^{-(S_0-\rho)/h} \|\mathbf{c}\|_{\ell^2} \le C\mathrm{e}^{-(S_0-\rho)/h},
\end{aligned}
$$

where $\rho', \rho'' > 0$ are such that $\rho' + \rho'' < \rho < S_0$. Finally,

$$
\begin{aligned}
|B_{1,n}| &\le \sum_{m,\ell,j\in\mathbb{Z}}^{\star 1} \langle |u_m|\,|u_n|, |u_\ell|\,|u_j|\rangle |c_m|\,|c_\ell|\,|c_j| \\
&\le \frac{1}{2}\sum_{m,\ell,j\in\mathbb{Z}}^{\star 1} \langle |u_m|\,|u_n|, |u_\ell|\,|u_j|\rangle |c_m|\,[|c_\ell|^2 + |c_j|^2] \\
&\le \sum_{m,\ell,j\in\mathbb{Z}}^{\star 1} \langle |u_m|\,|u_n|, |u_\ell|\,|u_j|\rangle |c_m|\,|c_j|^2 \\
&\le \sum_{m\in\mathbb{Z}\setminus\{n\}, j\in\mathbb{Z}\setminus\{m,n\}} \left\langle |u_m|\,|u_n|, |u_j|\sum_{\ell\in\mathbb{Z}}|u_\ell| \right\rangle |c_m|\,|c_j|^2 \\
&\le \left\|\sum_{\ell\in\mathbb{Z}}|u_\ell|\right\|_{L^\infty} \sum_{m\in\mathbb{Z}\setminus\{n\}, j\in\mathbb{Z}\setminus\{m,n\}} \langle |u_m|\,|u_n|, |u_j|\rangle |c_m|\,|c_j|^2 \\
&\le \left\|\sum_{\ell\in\mathbb{Z}}|u_\ell|\right\|_{L^\infty} \sum_{j\in\mathbb{Z},\, j\ne n} \left\langle |u_n|\sum_{m\in\mathbb{Z}}|u_m|, |u_j| \right\rangle |c_j|^2 \\
&\le \left\|\sum_{\ell\in\mathbb{Z}}|u_\ell|\right\|_{L^\infty}^2 \sum_{j\in\mathbb{Z},\, j\ne n} \langle |u_n|, |u_j|\rangle |c_j|^2 \\
&\le Ch^{-1} \sum_{j\in\mathbb{Z},\, j\ne n} \mathrm{e}^{-\left[(S_0-\rho')|n-j|-\rho''\right]/h} |c_j|^2
\end{aligned}
$$

since $|c_m| \le 1$. Hence,

$$
\begin{aligned}
\|\mathbf{B}_1\|_{\ell^2} \le \|\mathbf{B}_1\|_{\ell^1} \le Ch^{-1} &\sum_{n,j\in\mathbb{Z},\; j\ne n} C\mathrm{e}^{-\left[(S_0-\rho')|n-j|-\rho''\right]/h}|c_j|^2 \\
&\le C\mathrm{e}^{-(S_0-\rho)/h}\sum_{j\in\mathbb{Z}}|c_j|^2 = C\mathrm{e}^{-(S_0-\rho)/h}\|\mathbf{c}\|_{\ell^2} \\
&\le C\mathrm{e}^{-(S_0-\rho)/h}.
\end{aligned}
$$

From these estimates, it follows that

$$
\|\mathbf{B}\|_{\ell^2} \le C\left[\|\mathbf{B}_1\|_{\ell^2} + \|\mathbf{B}_2\|_{\ell^2} + \|\mathbf{B}_3\|_{\ell^2}\right] \le C\mathrm{e}^{-(S_0-\rho)/h}
$$

and Lemma 4 is so proved. □

Now, we deal with the vector $\mathbf{A}$ with elements

$$
A_n = \langle u_n, g\rangle
$$

where

$$
g := |\psi|^2\psi - |\psi_1|^2\psi_1 = \bar{\psi}_1\psi_\perp^2 + 2|\psi_1|^2\psi_\perp + \psi_1^2\bar{\psi}_\perp + |\psi_\perp|^2\psi_\perp + 2\psi_1|\psi_\perp|^2
$$

**Lemma 5.**

$$
\|\mathbf{A}\|_{\ell^2} \le Ch^{-1/2}\|\psi_\perp\|_{L^2}
$$

*Proof.* Indeed, since $\{u_n\}_{n\in\mathbb{Z}}$ is an orthonormal base of $\Pi\left[L^2(\mathbb{R})\right]$ from the Parseval's identity it follows that

$$\begin{aligned}\|\mathbf{A}\|_{\ell^2} &= \|\Pi g\|_{L^2} \le \|g\|_{L^2} \le C\left[\|\psi_\perp^3\|_{L^2} + \|\psi_\perp^2\psi_1\|_{L^2} + \|\psi_\perp\psi_1^2\|_{L^2}\right]\\ &\le C\max\left(\|\psi_\perp\|_{L^\infty}^2, \|\psi_1\|_{L^\infty}^2\right)\|\psi_\perp\|_{L^2} \le Ch^{-1/2}\|\psi_\perp\|_{L^2}\end{aligned}$$

from Corollary 1. □

In conclusion, we have proved the following Lemma;

**Lemma 6.**

$$\|\mathbf{r}_4\|_{\ell^2} \le C\mathrm{e}^{-(S_0-\rho)/h} + Ch^{-1/2}\|\psi_\perp\|_{L^2}.$$

## 5. Validity of the Tight-Binding Approximation

First of all we need of the following estimate:

**Lemma 7.** *Let us set*

$$\lambda := Fh^{-1} + |\eta|h^{-3/2}$$

*and let* $\mathbf{c}$ *and* $\psi_\perp$ *be the solutions to* (15)*; then*

$$\|\dot{\mathbf{c}}\|_{\ell^2} \le \frac{C}{h}\max\left[\beta, h\lambda, \|\mathbf{r}\|_{\ell^2}\right]. \tag{18}$$

*Proof.* Indeed, from (15) it immediately follows that

$$\begin{aligned}\|\dot{\mathbf{c}}\|_{\ell^2}^2 &= \frac{1}{h^2}\sum_{n\in\mathbb{Z}}\left|-\beta(c_{n+1}+c_{n-1}) + F\xi_n c_n + \eta C_1|c_n|^2 c_n + r_n\right|^2\\ &\le \frac{C}{h^2}\left[\beta^2\sum_{n\in\mathbb{Z}}|c_{n+1}|^2 + \beta^2\sum_{n\in\mathbb{Z}}|c_{n-1}|^2 + F^2\max_{n\in\mathbb{Z}}|\xi_n|^2\sum_{n\in\mathbb{Z}}|c_n|^2\right.\\ &\quad\left. + \eta^2 C_1^2\sum_{n\in\mathbb{Z}}|c_n|^6 + \sum_{n\in\mathbb{Z}}|r_n|^2\right]\\ &\le \frac{C}{h^2}\left[(\beta^2 + F^2 + \eta^2 C_1^2)\|\mathbf{c}\|_{\ell^2}^2 + \|\mathbf{r}\|_{\ell^2}^2\right]\end{aligned}$$

from which estimate (18) follows since $\|\mathbf{c}\|_{\ell^2} \le 1$ and $|c_n| \le 1$, $|\xi_n| \le C$ because $W$ is a bounded potential and $C_1 \sim h^{-1/2}$. □

Hereafter, we denote by $\omega$ a quantity, whose value may change from line to line, such that

$$|\omega| \le C\mathrm{e}^{-(S_0+\zeta)/h}$$

for some $\zeta > 0$ and some $C > 0$ independent of $h$.

**Theorem 4.**

$$\|\mathbf{r}\|_{\ell^2} \le \omega + C\lambda\mathrm{e}^{-(S_0-\rho)/h} + Ch\lambda\|\psi_\perp\|_{L^2} \tag{19}$$

*Proof.* Indeed, collecting the results from Lemmata 2, 3 and 6 and from Remark 2, we have that

$$\begin{aligned}\|\mathbf{r}\|_{\ell^2} &\le \|\mathbf{r_1}\|_{\ell^2} + F\,\|\mathbf{r_2}\|_{\ell^2} + F\,\|\mathbf{r_3}\|_{\ell^2} + |\eta|\,\|\mathbf{r_4}\|_{\ell^2} \\ &\le C\mathrm{e}^{-(S_0+\zeta)/h} + CF\mathrm{e}^{-(S_0-\rho)/h} + CF\|\psi_\perp\|_{L^2} \\ &\quad + C|\eta|\mathrm{e}^{-(S_0-\rho)/h} + C|\eta|h^{-1/2}\|\psi_\perp\|_{L^2}\end{aligned}$$

from which the statement immediately follows. □

Since $\psi_\perp(x,0) = \Pi_\perp\psi_0 = 0$, then the second differential equation of the system (15) may be written as an integral equation of the Duhamel's form

$$\psi_\perp(\tau) = -i\int_0^\tau \mathrm{e}^{-i(H_B-\Lambda_1)(\tau-q)/h}\left[\frac{F}{h}\Pi_\perp W\psi + \frac{\eta}{h}\Pi_\perp|\psi^2|\psi\right]\mathrm{d}q \tag{20}$$

**Theorem 5.** *We have the following estimate*

$$\|\psi_\perp\|_{L^2} \le \left\{C\lambda + \tau Ch^{-1}\lambda\max\left[\beta, h\lambda\right]\right\}\mathrm{e}^{C\lambda\tau},\ \forall\tau\in\mathbb{R}. \tag{21}$$

*Proof.* Let

$$\begin{aligned}U_1 &:= U_1(\psi_1) = \left[\frac{F}{h}\Pi_\perp W\psi_1 + \frac{\eta}{h}\Pi_\perp|\psi_1^2|\psi_1\right] \\ U_2 &:= U_2(\psi_1,\psi_\perp) = \left[\frac{F}{h}\Pi_\perp W\psi_\perp + \frac{\eta}{h}\Pi_\perp\left(|\psi^2|\psi - |\psi_1^2|\psi_1\right)\right]\end{aligned}$$

then Eq. (20) becomes

$$\psi_\perp(\tau) = f_1(\tau) + f_2(\tau)$$

where

$$f_j(\tau) = -i\int_0^\tau \mathrm{e}^{-i(H_B-\Lambda_1)(\tau-q)/h}U_j\mathrm{d}q,\ j=1,2,$$

are such that

**Lemma 8.** *The following estimates hold true:*

$$\|f_1\|_{L^2} \le C\lambda + \tau Ch^{-1}\lambda\max\left[\beta, h\lambda\right] \tag{22}$$

*and*

$$\|f_2\|_{L^2} \le C\lambda\int_0^\tau \|\psi_\perp(q)\|_{L^2}\mathrm{d}q. \tag{23}$$

*Proof.* In order to prove estimates (22) and (23), we remark that $\mathrm{e}^{-i(H_B-\Lambda_1)(\tau-s)/h}$ is an unitary operator; hence,

$$\left\|\mathrm{e}^{-i(H_B-\Lambda_1)(\tau-s)/h}U_j\right\|_{L^2} = \|U_j\|_{L^2},\ j=1,2.$$

Now,

$$\begin{aligned}\|U_2\|_{L^2} &\le \frac{F}{h}\|\Pi_\perp W\psi_\perp\|_{L^2} + \frac{|\eta|}{h}\left\|\Pi_\perp\left(|\psi|^2\psi - |\psi_1|^2\psi_1\right)\right\|_{L^2} \\ &\le Ch^{-1}F\|\psi_\perp\|_{L^2} + Ch^{-1}|\eta|\left[\|\psi_1\psi_\perp^2\|_{L^2} + \|\psi_1^2\psi_\perp\|_{L^2} + \|\psi_\perp^3\|_{L^2}\right] \\ &\le Ch^{-1}F\|\psi_\perp\|_{L^2} + Ch^{-1}|\eta|\left[\|\psi_1\|_{L^\infty}\|\psi_\perp\|_{L^\infty} + \|\psi_1\|_{L^\infty}^2\right.\end{aligned}$$

$$
\begin{aligned}
&+ \|\psi_\perp\|_{L^\infty}^2 \big] \, \|\psi_\perp\|_{L^2} \\
&\le C \left( h^{-1} F + h^{-3/2} |\eta| \right) \|\psi_\perp\|_{L^2} = C\lambda \|\psi_\perp\|_{L^2}
\end{aligned}
$$

from Theorem 3 and Corollary 1; hence, (23) follows. In order to prove (22), we make use of an integration by parts:

$$
\begin{aligned}
f_1(\tau) &= -i \int_0^\tau \mathrm{e}^{-i(H_B-\Lambda_1)(\tau-q)/h} U_1 \mathrm{d}q \\
&= \Big[ - h \mathrm{e}^{-i(H_B-\Lambda_1)(\tau-q)/h} [H_B - \Lambda_1]^{-1} U_1 \Big]_0^\tau \\
&\quad + h \int_0^\tau \mathrm{e}^{-i(H_B-\Lambda_1)(\tau-q)/h} [H_B - \Lambda_1]^{-1} \frac{\mathrm{d}U_1}{\mathrm{d}q} \mathrm{d}q
\end{aligned}
$$

From this fact and since $\|[H_B - \Lambda_1]^{-1} \Pi_\perp\| = \left[ \mathrm{dist}(\Lambda_1, E_2^b) \right]^{-1} \sim h^{-1}$ then it follows that

$$
\begin{aligned}
\|f_1\|_{L^2} &\le \max \left[ \|U_1(\tau)\|_{L^2}, \|U_1(0)\|_{L^2} \right] + \tau \max_{s\in[0,\tau]} \left\| \frac{\mathrm{d}U_1}{\mathrm{d}\tau} \right\|_{L^2} \\
&\le C\lambda + \tau C h^{-1} \lambda \max \left[ \beta, h\lambda, \|\mathbf{r}\|_{\ell^2} \right] \\
&\le C\lambda + \tau C h^{-1} \lambda \max \left[ \beta, h\lambda \right]
\end{aligned}
$$

since

$$
\begin{aligned}
\|U_1\|_{L^2} &\le F h^{-1} \|\Pi_\perp W \psi_1\|_{L^2} + |\eta| h^{-1} \|\Pi_\perp |\psi_1|^2 \psi_1\|_{L^2} \\
&\le C F h^{-1} \|\psi_1\|_{L^2} + |\eta| h^{-1} \|\psi_1\|_{L^\infty}^2 \|\psi_1\|_{L^2} \\
&\le C\lambda
\end{aligned}
$$

and

$$
\begin{aligned}
\left\| \frac{\mathrm{d}U_1}{\mathrm{d}\tau} \right\|_{L^2} &\le C\lambda \|\dot{\psi}_1\|_{L^2} \le C\lambda \|\dot{\mathbf{c}}\|_{\ell^2} \\
&\le C h^{-1} \lambda \max \left[ \beta, h\lambda, \|\mathbf{r}\|_{\ell^2} \right]
\end{aligned}
$$

by Lemma 7, Theorem 4, and from the draft estimate $\|\psi_\perp\|_{L^2} \le 1$. □

Hence, we have the following integral inequality

$$
\|\psi_\perp\|_{L^2} \le \left\{ C\lambda + \tau C h^{-1} \lambda \max \left[ \beta, h\lambda \right] \right\} + C\lambda \int_0^\tau \|\psi_\perp\|_{L^2} \mathrm{d}q
$$

and then the Gronwall's Lemma implies that

$$
\|\psi_\perp\|_{L^2} \le \left\{ C\lambda + \tau C h^{-1} \lambda \max \left[ \beta, h\lambda \right] \right\} \mathrm{e}^{C\lambda\tau}, \ \forall \tau \in \mathbb{R} ;
$$

Theorem 5 is so proved. □

Now, we deal with the first differential equation of the system (15)

$$
\begin{cases}
i h \dot{c}_n = G_n(\mathbf{c}) + r_n, \\
c_n(0) = \langle u_n, \psi_0 \rangle,
\end{cases}
$$

where

$$
G_n(\mathbf{c}) = -\beta (c_{n+1} + c_{n-1}) + F \xi_n c_n + \eta C_1 |c_n|^2 c_n.
$$

We compare it with the equation

$$\begin{cases} ih\dot{g}_n = G_n(\mathbf{g}) \\ g_n(0) = c_n(0) \end{cases} \tag{24}$$

which represents the tight-binding approximation of (4), up to a phase factor $e^{-i\Lambda_1\tau/h}$ depending on time.

The Cauchy problem (24) is globally well-posed, that is there exists a unique solution $\mathbf{g} \in C(\mathbb{R}, \ell^2(\mathbb{Z}))$ that depends continuously on the initial data (see, e.g., Theorem 1.3 [16]). We must underline that we have the following a priori estimate $\|\mathbf{c}\|_{\ell^2} \le 1$ and the conservation of the norm of $\mathbf{g}$

$$\|\mathbf{g}\|_{\ell^2} = \|\mathbf{g}(0)\|_{\ell^2} = \|\mathbf{c}(0)\|_{\ell^2} = 1\,;$$

indeed, an immediate calculus gives that

$$\frac{d}{d\tau} ih\|\mathbf{g}\|^2_{\ell^2} = \beta\left[\sum_{n\in\mathbb{Z}} \bar{g}_{n+1}g_n + \sum_{n\in\mathbb{Z}} \bar{g}_{n-1}g_n - \sum_{n\in\mathbb{Z}} g_{n+1}\bar{g}_n - \sum_{n\in\mathbb{Z}} g_{n-1}\bar{g}_n\right] = 0$$

because $\beta$, $F$, $\eta$, $C_1$ and $\xi_n$ are real-valued.

Then, it follows that the vector $\mathbf{c} - \mathbf{g}$ satisfies to the following integral equation

$$ih\left[c_n(\tau) - g_n(\tau)\right] = \int_0^\tau \left[G_n(\mathbf{c}) - G_n(\mathbf{g})\right] dq + \int_0^\tau r_n(q) dq,$$

from which

$$\|\mathbf{c} - \mathbf{g}\|_{\ell^2} \le \frac{1}{h}\int_0^\tau \|\mathbf{G}(\mathbf{c}) - \mathbf{G}(\mathbf{g})\|_{\ell^2} dq + \frac{1}{h}\int_0^\tau \|\mathbf{r}\|_{\ell^2} dq.$$

**Lemma 9.** $\mathbf{G}$ *is a Lipschitz function such that*

$$\|\mathbf{G}(\mathbf{c}) - \mathbf{G}(\mathbf{g})\|_{\ell^2} \le C \max[\beta, h\lambda]\|\mathbf{c} - \mathbf{g}\|_{\ell^2}. \tag{25}$$

*Proof.* Indeed

$$\begin{aligned}
\|\mathbf{G}(\mathbf{c}) - \mathbf{G}(\mathbf{g})\|^2_{\ell^2} &= \sum_{n\in\mathbb{Z}} |G_n(\mathbf{c}) - G_n(\mathbf{g})|^2 \\
&= \sum_{n\in\mathbb{Z}} \big|-\beta\left[(c_{n+1} - g_{n+1}) + (c_{n-1} - g_{n-1})\right] + F\xi_n(c_n - g_n) \\
&\quad + \eta C_1\left[|c_n|^2 c_n - |g_n|^2 g_n\right]\big|^2 \\
&\le C\Bigg\{\beta^2 \sum_{n\in\mathbb{Z}} |c_{n+1} - g_{n+1}|^2 + \beta^2 \sum_{n\in\mathbb{Z}} |c_{n-1} - g_{n-1}|^2 + \sum_{n\in\mathbb{Z}} F^2\xi_n^2 |c_n - g_n|^2 \\
&\quad + \sum_{n\in\mathbb{Z}} \eta^2 C_1^2 \left||c_n|^2 c_n - |g_n|^2 g_n\right|\Bigg\} \\
&\le C\left\{2\beta^2 \|\mathbf{c} - \mathbf{g}\|^2_{\ell^2} + \left[\max_{n\in\mathbb{Z}} \xi_n^2\right] F^2 \|\mathbf{c} - \mathbf{g}\|^2_{\ell^2}\right.
\end{aligned}$$

$$+ \eta^2 C_1^2 \sum_{n\in\mathbb{Z}} \left| |c_n|^2 (c_n - g_n) + \left(|c_n|^2 - |g_n|^2\right) |g_n| \right| \Bigg\}$$

$$\leq C \left[\beta^2 + F^2 + \eta^2 C_1^2\right] \|\mathbf{c} - \mathbf{g}\|_{\ell^2}^2 \leq C \max[\beta^2, h^2\lambda^2] \|\mathbf{c} - \mathbf{g}\|_{\ell^2}^2$$

since $|c_n|^2 - |g_n|^2 = c_n \left[\bar{c}_n - \bar{g}_n\right] + \bar{g}_n \left[c_n - g_n\right]$ and (14). □

By Theorems 4 and 5, it turns out that the vector $\mathbf{r}$ is norm bounded by

$$\|\mathbf{r}\|_{\ell^2} \leq a + b\mathrm{e}^{C\lambda\tau} + c\tau\mathrm{e}^{C\lambda\tau} \tag{26}$$

for some positive constant $C$ independent of $h$ and where

$$a = \omega + C\lambda\mathrm{e}^{-(S_0-\rho)/h}, \tag{27}$$

$$b = Ch\lambda^2, \tag{28}$$

$$c = C\lambda^2 \max\left[\beta, h\lambda\right]. \tag{29}$$

Then, we get the integral inequality

$$\|\mathbf{c} - \mathbf{g}\|_{\ell^2} \leq \alpha(\tau) + \int_0^\tau \delta(q) \|\mathbf{c} - \mathbf{g}\|_{\ell^2} \mathrm{d}q \tag{30}$$

where

$$\alpha(\tau) \leq \frac{1}{h} \int_0^\tau \|\mathbf{r}\|_{\ell^2} \mathrm{d}q \leq C \left[\frac{a\tau}{h} + \frac{Cb\lambda + c}{C^2\lambda^2 h} \left(\mathrm{e}^{C\lambda\tau} - 1\right) + \frac{c\tau}{C\lambda h} \mathrm{e}^{C\lambda\tau}\right]$$

and

$$\delta(\tau) \leq C \max[h^{-1}\beta, \lambda]$$

By the Gronwall's Lemma, we finally get the estimate

$$\|\mathbf{c} - \mathbf{g}\|_{\ell^2} \leq \alpha(\tau) \mathrm{e}^{\int_0^\tau \delta(q)\mathrm{d}q} = \alpha(\tau) \mathrm{e}^{C \max[h^{-1}\beta, \lambda]\tau}$$

Therefore, we have proved that

**Lemma 10.** *Let $a$, $b$ and $c$ defined by (27)–(29), then*

$$\|\mathbf{c} - \mathbf{g}\|_{\ell^2} \leq C \left\{\frac{a\tau}{h} + \frac{Cb\lambda + c}{C^2\lambda^2 h} \left(\mathrm{e}^{C\lambda\tau} - 1\right) + \frac{c\tau}{C\lambda h} \mathrm{e}^{C\lambda\tau}\right\} \mathrm{e}^{C \max[h^{-1}\beta, \lambda]\tau} \tag{31}$$

*for some positive constant $C$ independent of $h$.*

In conclusion, recalling (2), we can state that

**Theorem 6.** *Let $\mathbf{g} \in C(\mathbb{R}, \ell^2(\mathbb{Z}))$ be the solution to the discrete nonlinear Schrödinger Eq. (24); let $\psi(\tau, x) \in C(\mathbb{R}, H^1(\mathbb{R}))$ be the solution to the nonlinear Schrödinger Eq. (4) with initial condition $\psi_0(x) = \sum g_n(0) u_n(x)$; let $a$, $b$ and $c$ defined by Lemma 10; let $\lambda$ be defined by Lemma 7. Then, there exist $\epsilon^\star > 0$ and a positive constant $C$ independent of $\epsilon$ such that for any $0 < \epsilon < \epsilon^\star$ then*

$$\left\| \psi(\tau, \cdot) - \sum_{n\in\mathbb{Z}} g_n(\tau) \mathrm{e}^{i\Lambda_1\tau/h} u_n(\cdot) \right\|_{L^2} \leq \left\{C\lambda + \tau C h^{-1} \lambda \max\left[\beta, h\lambda\right]\right\} \mathrm{e}^{C\lambda\tau} \tag{32}$$

$$+C\left\{\frac{a\tau}{h}+\frac{Cb\lambda+c}{C^2\lambda^2 h}\left(e^{C\lambda\tau}-1\right)+\frac{c\tau}{C\lambda h}e^{C\lambda\tau}\right\}e^{C\max[h^{-1}\beta,\lambda]\tau},\ \forall\tau\in\mathbb{R}^+. \tag{33}$$

*Proof.* Indeed, recalling that we made use of the gauge choice $\psi\to e^{i\Lambda_1\tau/h}\psi$, we have that

$$\left\|\psi-\sum_{n\in\mathbb{Z}}g_n e^{i\Lambda_1\tau/h}u_n\right\|_{L^2}^2=\left\|e^{-i\Lambda_1\tau/h}\psi-\sum_{n\in\mathbb{Z}}g_n u_n\right\|_{L^2}^2 = \|\psi_\perp\|_{L^2}^2+\left\|\sum_{n\in\mathbb{Z}}(c_n-g_n)\,u_n\right\|_{L^2}^2$$

where

$$\left\|\sum_{n\in\mathbb{Z}}(c_n-g_n)\,u_n\right\|_{L^2}^2=\sum_{n\in Z}|c_n-g_n|^2\|u_n\|_{L^2}^2=\|\mathbf{c}-\mathbf{g}\|_{\ell^2}^2$$

because $\{u_n\}$ is an orthonormal set of vectors. □

### 5.1. Proof of Theorem 1

Here, we assume, according with Hypothesis (3a), that the real-valued parameters $\alpha_1$ and $\alpha_2$ are fixed; in such a case we have that

$$F\sim\eta\sim h^2. \tag{34}$$

Therefore:

$$\lambda\sim h^{1/2},\ |a|,\beta\le Ce^{-(S_0-\rho)/h},\ b\sim h^2,\ c\sim h^{5/2}.$$

Then, estimate (33) makes sense for times of order $\tau\in[0,Ch^{-\gamma}]$ for some fixed $\gamma\le\frac{1}{2}$. In such an interval we have that

$$C\lambda+\tau Ch^{-1}\lambda\max[\beta,h\lambda]\sim h^{1/2}+h^{1-\gamma}$$
$$\frac{a\tau}{h}+\frac{Cb\lambda+c}{C^2\lambda^2h}\left(e^{C\lambda\tau}-1\right)+\frac{c\tau}{C\lambda h}e^{C\lambda\tau}\sim h^{1/2}+h^{1-\gamma}.$$

In particular, for $\gamma=\frac{1}{2}$ then Theorem 1 follows.

### 5.2. Proof of Theorem 2

Here, we assume, according with Hypothesis (3b), that the real-valued parameters $\alpha_1$ and $\alpha_2$ are not fixed, but both go to zero when $\epsilon$ goes to zero; in particular we have that

$$F=\mathcal{O}(\beta)\ \text{ and }\ h^{-1/2}\eta=\mathcal{O}(\beta).$$

In such a case, we have that

$$\lambda=\mathcal{O}(h^{-1}\beta),\ a=\mathcal{O}(\omega),\ b=\mathcal{O}(h^{-1}\beta^2),\ c=\mathcal{O}(h^{-2}\beta^3).$$

Estimate (33) makes sense for times of order $\tau\in[0,\beta^{-1}h]$. In such an interval we have that

$$\|\psi_\perp\|_{L^2}\le Ce^{-(S_0-\rho)/h}$$

and

$$\|\mathbf{c} - \mathbf{g}\|_{\ell^2} \leq C\mathrm{e}^{-\zeta/h}$$

for some $\zeta > 0$. Hence, Theorem 2 is proved.

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