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 local 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.

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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 $W$

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

in the limit of large periodic potential, i.e. $0 < \epsilon \ll 1$; $\alpha_1$ represents the strength of theperturbation 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.

In the physical literature a standard way to study equation (1) consists in reducing it to a discrete Schrödinger equation taking into account only nearest neighbor interactions, the so called tight-binding model [1]. 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 [2] [3] [7]. 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 [2] proved the validity of the reduction to discrete nonlinear Schrödinger equations for large times when $V$ is multiple-well trapped potential; while [14] were able to obtain a similar result for a periodic potential $V$ by assuming a specific technical condition on the initial wavefunction.

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 don’t need of special technical assumptions on the shape of

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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, let us say the first one for argument’s sake, of the Bloch operator.

By introducing the new semiclassical parameter
\[ h = \hbar \sqrt{\varepsilon/2m}, \]
the new time variable
\[ \tau = \frac{\hbar}{h} t \]
and the effective perturbation and nonlinearity strengths
\[ F = \alpha_1 \frac{2m\hbar^2}{\hbar^2} \quad \text{and} \quad \eta = \alpha_2 \frac{2m\hbar^2}{\hbar^2}, \]
then the above equation (1) takes the semiclassical form
\[ i\hbar \frac{\partial \psi}{\partial \tau} = -\hbar^2 \frac{\partial^2 \psi}{\partial x^2} + V\psi + FW\psi + \eta|\psi|^2 \psi \]
with \( h \ll 1 \).

In the tight-binding approximation solutions to (4) are approximated by solutions to the time-dependent discrete nonlinear Schrödinger equation
\[ i\hbar \dot{g}_n = -\beta(g_{n+1} - g_{n-1}) + F\xi(n)g_n + \eta C_1|g_n|^2g_n, \quad n \in \mathbb{Z}, \]
where \( \beta \) is an exponentially small positive constant in the semiclassical limit \( h \ll 1 \). Furthermore, \( \xi(n) = \langle u_n, Wu_n \rangle \) and \( C_1 = \|u_n\|_L^4 \), where, roughly speaking (a precise definition for \( u_n \) is given by \([6, 7, 17]\)), \( \{u_n\}_{n \in \mathbb{Z}} \) 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 of the Schrödinger equation with a single well potential obtained by filling all the wells, but the \( n \)-th one, of the periodic potential \( V \).

We must underline that usually the tight-binding approximation is constructed by making use of the Wannier’s functions instead of the vectors \( u_n \) \([1, 12]\). In fact, 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 \([10]\).

The analysis of the discrete nonlinear Schrödinger equations (4) 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 \( \varepsilon \). In such a case we have that \( \beta \ll |F| \) and \( \beta \ll C_1|\eta| \) and then the analysis of (4) 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 \([16, 17]\). 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. One may extend the validity of such an approximation to larger intervals of time by assuming some further conditions of the initial wavefunction or on the potential \(V\) as done by [2, 14].

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

\[ F \sim C_1 \eta \sim \beta. \]

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.

In §2 we state the assumptions on equation (3). In §3 we prove a priori estimate of the wavefunction \(\psi\) and of its gradient \(\nabla \psi\). In §4 we formally construct the discrete nonlinear Schrödinger equations; in this Section we make use of some ideas already developed by [7, 17] and we refer to these papers as much as possible. We must underline that in [7, 17] 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 Section 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 §4 we finally prove the validity of the tight-binding approximation with a precise estimate of the error, the method used is based on an idea already used by [15] for a double-well model and now applied to a periodic potential; in particular, in §5.1 we consider the case where \(\alpha_1\) and \(\alpha_2\) are fixed, i.e. model 1, and in §5.2 we consider the case where \(\alpha_1\) and \(\alpha_2\) go to zero as \(\epsilon\) goes to zero in a suitable way, i.e. model 2.

2. DESCRIPTION OF THE MODEL

2.1. Assumptions. Here, we consider the nonlinear Schrödinger equation (3) where \(F\) and \(\eta\) are defined in (2) and 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 \([-\frac{1}{2}a, \frac{1}{2}a]\).

**Hypothesis 2.** The perturbation \(W(x)\) is a smooth real-valued function. We assume that: \(W \in L^\infty(\mathbb{R})\) and there are \(C > 0\) and \(s \geq \frac{1}{3}\) such that \(|W(x)| \leq C(x)^{-s}, \forall x \in \mathbb{R}\), where \(\langle x \rangle := \sqrt{1 + x^2}\).

Concerning the parameters \(m, h, \alpha_1, \alpha_2\) and \(\epsilon\) we assume that

**Hypothesis 3.** We assume the 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

\[
\lim_{\epsilon \to 0^+} \frac{F}{\beta} \in \mathbb{R} \setminus \{0\} \quad \text{and} \quad \lim_{\epsilon \to 0^+} \frac{C_1 \eta}{\beta} \in \mathbb{R} \setminus \{0\},
\]

where the parameters \( \beta \) and \( C_1 \) depend on \( \epsilon \) (by means of \( h \)) and they are defined by (11) and (12).

Remark 2. In both cases we have that \( |F| \leq Ch^2 \) and \( |\eta| \leq Ch^2 \). 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 \( L^2(\mathbb{R}, dx) \) as

\[
H_B := -\hbar^2 \frac{d^2}{dx^2} + V.
\]  

(5)

It is well known that this operator admits self-adjoint extension, still denoted by \( H_B \), and its spectrum is given by bands:

\[
\sigma(H_B) = \bigcup_{\ell=1}^\infty [E^\ell_1, E^\ell_t], \quad \text{where} \quad E^\ell_t \leq E^\ell_{t+1} < E^\ell_{t+1}.
\]

The intervals \( (E^\ell_t, E^\ell_{t+1}) \) are named gaps; a gap may be empty, that is \( E^\ell_{t+1} = E^\ell_t \), 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. In particular, when \( h \) is small enough then the following asymptotic behaviors \( [18, 19] \)

\[
\frac{1}{C} h \leq E^\ell_t \leq Ch \quad \text{and} \quad \frac{1}{C} h \leq E^\ell_2 - E^\ell_1 \leq Ch
\]  

(6)

hold true for some \( C > 0 \); hence, the first gap between \( E^\ell_1 \) and \( E^\ell_2 \) is not empty in the semiclassical limit.

Let \( \Pi \) the projection operator associated to the first band \( [E^\ell_1, E^\ell_t] \) of \( H_B \) and let \( \Pi_\perp = 1 - \Pi \). Let

\[
\psi = \psi_1 + \psi_\perp \quad \text{where} \quad \psi_1 = \Pi \psi \quad \text{and} \quad \psi_\perp = \Pi_\perp \psi.
\]  

(7)

We assume that

**Hypothesis 4.** \( \Pi_\perp \psi_0 = 0 \); 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. Notation and some functional inequalities. Hereafter, we denote by \( \| \cdot \|_{L^p}, p \in [1, +\infty] \), the usual norm of the Banach space \( L^p(\mathbb{R}, dx) \); we denote by \( \| \cdot \|_{\ell^p}, p \in [1, +\infty] \), the usual norm of the Banach space \( \ell^p(\mathbb{Z}) \). In particular, if \( \psi = \psi(x, \tau) \) is a wavefunction then by \( \|\psi\|_{L^p} \) we mean

\[
\|\psi(\cdot, \tau)\|_{L^p(\mathbb{R}, dx)} = \left\{ \int_\mathbb{R} |\psi(x, \tau)|^p dx \right\}^{1/p}.
\]
and, similarly, if \( c = c(\tau) = \{ c_n(\tau) \}_{n \in \mathbb{Z}} \in \ell^2(\mathbb{Z}) \) then by \( \| c \|_{\ell^p} \) we mean

\[
\| c(\tau) \|_{\ell^p(\mathbb{Z})} := \left\{ \sum_{n \in \mathbb{Z}} |c_n(\tau)|^p \right\}^{1/p}.
\]

Hereafter, we omit the dependence on \( \tau \) in the wavefunctions \( \psi \) and in the vector \( c \) when this fact does not cause misunderstanding.

By \( C \) we denote a generic positive constant independent of \( h \) 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

\[
\lim_{h \to 0^+} \frac{f}{g} \in \mathbb{R} \setminus \{0\}.
\]

Let \( d_A(x, y) \) be the Agmon distance between two points \( x, y \in \mathbb{R} \) (for a definition of the Agmon distance see [8]) and let \( S_0 := d_A(x_n, x_{n+1}) \), \( n \in \mathbb{Z} \) and \( x_n := x_0 + na \), be the Agmon distance between the bottom points \( x_n \) and \( x_{n+1} \) of two adjacent wells of the periodic potential \( V \); by periodicity \( S_0 \) does not depend on the index \( n \).

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

- **One-dimensional Gagliardo-Nirenberg inequality** by §B.5 [12]:
  \[ \| f \|_{L^p} \leq C \| \nabla f \|_{L^2}^{\delta} \| f \|_{L^2}^{1-\delta}, \quad \delta = \frac{1}{2} - \frac{1}{p} = \frac{p-2}{2p}, \quad p \in [2, +\infty], \]

- **Gronwall’s Lemma** by Theorem 1.3.1 [11]: let \( u(\tau) \) be a non negative and continuous function such that
  \[ u(\tau) \leq \alpha(\tau) + \int_0^\tau \delta(q)u(q)\,dq, \quad \forall \tau \geq 0, \]
  where \( \alpha(\tau) \) and \( \delta(\tau) \) are monotone not decreasing functions, then
  \[ u(\tau) \leq \alpha(\tau)e^{\int_0^\tau \delta(q)\,dq}, \quad \forall \tau \geq 0. \]

3. **Preliminary results**

We recall here some results by [3] [4] [5] 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 \( L^2(\mathbb{R}, dx) \), admits a self-adjoint extension, still denoted by \( H \). In order to discuss the local and global existence of solutions to [4] we apply Theorem 4.2 by [4]: if \( \psi_0 \in H^1(\mathbb{R}) \) there is a unique solution \( \psi \in C([-T, T]) \) to [3] with initial datum \( \psi_0 \), such that

\[ \psi, \psi\partial_x(V + FW), \partial_x\psi \in L^6([-T, T]; L^4(\mathbb{R})), \]

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

In fact (see [4]), this solution is global in time for any \( \eta \in \mathbb{R} \) (because \( 1 < 2/d \), where \( d = 1 \) is the spatial dimension) and [3] enjoys the conservation of the mass

\[ \| \psi(\cdot, \tau) \|_{L^2} = \| \psi_0(\cdot) \|_{L^2}. \]
Theorem 1. The following a priori estimates hold true for any \( \tau \in \mathbb{R} \):

\[
\| \psi \|_{L^2} = \| \psi_0 \|_{L^2} = 1 \quad \text{and} \quad \| \nabla \psi \|_{L^2} \leq C h^{-1/2},
\]
\[
\| \psi_1 \|_{L^2} \leq \| \psi_0 \|_{L^2} = 1 \quad \text{and} \quad \| \nabla \psi_1 \|_{L^2} \leq C h^{-1/2},
\]
\[
\| \psi_\perp \|_{L^2} \leq \| \psi_0 \|_{L^2} = 1 \quad \text{and} \quad \| \nabla \psi_\perp \|_{L^2} \leq C h^{-1/2};
\]

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

\[
\| \psi_\perp \|_{L^2} \leq \| \psi_0 \|_{L^2} = 1 \quad \text{and} \quad \| \psi_1 \|_{L^2} \leq \| \psi_0 \|_{L^2} = 1 .
\]

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 \( V \geq 0 \) then we have that

\[
h^2 \| \nabla \psi_0 \|_{L^2} \leq \langle H_B \psi_0, \psi_0 \rangle \sim h ,
\]

which implies \( \| \nabla \psi_0 \|_{L^2} \leq C h^{-1/2} \). From this fact, by Remark 2 using the fact that \( W \) is a bounded potential and by the Gagliardo-Nirenberg inequality we have that

\[
\| \psi_0 \|_{L^4}^4 \leq C \| \nabla \psi_0 \|_{L^2} \| \psi_0 \|_{L^2}^2 \leq C \| \nabla \psi_0 \|_{L^2} \leq C h^{-1/2}.
\]

Thus, the conservation of the energy implies the following inequality:

\[
h^2 \| \nabla \psi \|_{L^2}^2 = \mathcal{E}(\psi_0) - \langle V \psi, \psi \rangle - F \langle W \psi, \psi \rangle - \frac{1}{2} | \eta \| \psi \|_{L^4}^4 \\
\leq \mathcal{E}(\psi_0) - V_{\min} \| \psi \|_{L^2}^2 - FW_{\min} \| \psi \|_{L^2}^2 - \frac{1}{2} | \eta \| \psi \|_{L^4}^4 \\
\leq \mathcal{E}(\psi_0) - FW_{\min} - \frac{1}{2} | \eta \| \psi \|_{L^4}^4 ,
\]

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

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

then \( | \Gamma | \leq C \) as \( h \) goes to zero, and \( \Lambda \sim h^{-1} \) since \( |F| \leq C h^2 \) and \( \mathcal{E}(\psi_0) \sim h \). The previous inequality becomes

\[
\| \nabla \psi \|_{L^2}^2 \leq | \Lambda | + | \Gamma | \| \psi \|_{L^4}^4 .
\]
Again, the Gagliardo-Nirenberg inequality implies that
\[ \|\psi\|_{L^4} \leq C\|\nabla \psi\|_{L^2}^{\frac{1}{2}}\|\psi\|_{L^2}^{\frac{3}{2}} = C\|\nabla \psi\|_{L^2}^{\frac{2}{3}} \]
and thus we get
\[ \|\nabla \psi\|_{L^2} \leq |\Lambda| + |\Gamma|C^4\|\nabla \psi\|_{L^2} \]
from which it follows that
\[ \|\nabla \psi\|_{L^2} \leq 4\left( |\Gamma|C^4 + \sqrt{\Gamma^2 C^8 + 4|\Lambda|}\right) \leq C|\Lambda|^{1/2} \leq Ch^{-1/2} \]
for some positive constant C.

Since \( \Pi H_B = H_B \Pi \), we have that
\[ \mathcal{E}(\psi) - F(W\psi, \psi) - \frac{1}{2}\eta\|\psi\|_{L^4}^4 = \langle H_B\psi, \psi \rangle = \langle H_B\psi_1, \psi_1 \rangle + \langle H_B\psi_\perp, \psi_\perp \rangle \]
\[ = h^2\|\nabla \psi_1\|_{L^2}^2 + h^2\|\nabla \psi_\perp\|_{L^2}^2 + \langle V\psi_1, \psi_1 \rangle + \langle V\psi_\perp, \psi_\perp \rangle \geq h^2\|\nabla \psi_1\|_{L^2}^2 \]
since \( V_{min} \geq 0 \). Then,
\[ h^2\|\nabla \psi_1\|_{L^2}^2 \leq \mathcal{E}(\psi) - F(W\psi, \psi) - \frac{1}{2}\eta\|\psi\|_{L^4}^4 \leq Ch + \frac{1}{2}\eta\|\psi\|_{L^4}^4 \]
\[ \leq Ch + \frac{1}{2}\eta|\Lambda|C^4\|\nabla \psi\|_{L^2}\|\psi\|_{L^2}^3 \leq Ch \]
Hence
\[ \|\nabla \psi_1\|_{L^2} \leq Ch^{-1/2} \]
Similarly we get
\[ \|\nabla \psi_\perp\|_{L^2} \leq Ch^{-1/2} \]
and thus the proof of the Theorem is so completed. \( \square \)

**Corollary 1.** We have the following estimates:
\[ \|\psi\|_{L^\infty} \leq Ch^{-1/4} \quad \|\psi_1\|_{L^\infty} \leq Ch^{-1/4} \quad \|\psi_\perp\|_{L^\infty} \leq Ch^{-1/4} \quad \forall \tau \geq 0 \]

**Proof.** They immediately follow from the one-dimensional Gagliardo-Nirenberg inequality and from the previous result. \( \square \)

4. Construction of the discrete time-dependent nonlinear Schrödinger equation

By the Carlsson’s construction \( \mathcal{C} \) resumed and expanded by \( \mathcal{C} \) (see also §3 \( \mathcal{C} \) 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 \( \Pi [L^2(\mathbb{R})] \), that is
\[ \psi_1(x) = \sum_{n \in \mathbb{Z}} c_n u_n(x), \quad (8) \]
where \( u_n \in H^1(\mathbb{R}) \) and \( c = \{c_n\}_{n \in \mathbb{Z}} \in \ell^2(\mathbb{Z}) \) 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 \( c \).

By inserting \( \mathcal{C} \) and \( \mathcal{C} \) in equation \( \mathcal{C} \) then it takes the form (where \( a = \frac{\partial}{\partial \tau} \))
\[ \begin{cases} 
  i\hbar \dot{c}_n &= \langle u_n, H_B\psi \rangle + F(u_n, W\psi) + \eta (u_n, |\psi|^2 \psi), \quad n \in \mathbb{Z} \\
  i\hbar \dot{\psi}_\perp &= \Pi_\perp H_B \psi + F\Pi_\perp W\psi + \eta \Pi_\perp |\psi|^2 \psi 
\end{cases} \quad (9) \]
where \( c \in \ell^2 \) and \( \psi_\perp \) are such that for any \( \tau \in \mathbb{R} \)
\[
\| \psi_\perp \|_{L^2} \leq \| \psi_0 \|_{L^2} = 1 \quad \text{and} \quad \sum_{n \in \mathbb{Z}} |c_n|^2 = \| c \|_{L^2}^2 = \| \psi_1 \|_{L^2}^2 \leq \| \psi_0 \|_{L^2}^2 = 1.
\]

By mean of the gauge choice \( \psi(x, \tau) = e^{i \Lambda_1 \tau / h} \psi(x, \tau) \), and then \( \psi_\perp(x, \tau) \rightarrow \psi_\perp(x, \tau) \) and \( c_n(\tau) \rightarrow e^{i \Lambda_1 \tau / h} c_n(\tau) \), (9) takes the form
\[
\begin{align*}
  &\begin{cases}
    i h \dot{c}_n = \langle u_n, H_B \psi \rangle - \Lambda_1 c_n + F \langle u_n, W \psi \rangle + \eta \langle u_n, |\psi|^2 \psi \rangle, \\
    i h \dot{\psi}_\perp = \Pi_\perp (H_B - \Lambda_1) \psi + F \Pi_\perp W \psi + \eta |\psi|^2 \psi
  \end{cases},
\end{align*}
\]

where \( \Lambda_1 \) is the energy associated to the ground state of the Schrödinger operator 
\(-h^2 \partial_{xx} + V\), with single well potential \( \tilde{V} \) obtained by filling all the wells of the periodic potential \( V \), but one (see [7, 17] for details).

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
\[
\frac{1}{C} e^{-(S_0 - \rho)/h} < \beta < C e^{-(S_0 - \rho)/h};
\]
the remainder term \( r_{1,n} \) is defined as
\[
r_{1,n} := \sum_{m \in \mathbb{Z}} \hat{D}_{n,m} c_m
\]
where \( \hat{D}_{n,m} \) satisfies Lemma 1 in [17]. Furthermore,
\[
\langle u_n, W \psi \rangle = \xi(n) c_n + r_{2,n} + r_{3,n},
\]
where we set
\[
\xi(n) = \langle u_n, W u_n \rangle, \quad r_{2,n} = \sum_{m \in \mathbb{Z} : m \neq n} \langle u_n, W u_m \rangle c_m \text{ and } r_{3,n} = \langle u_n, W \psi_\perp \rangle.
\]

Finally
\[
\langle u_n, |\psi|^2 \psi \rangle = C_1 |c_n|^2 c_n + r_{4,n}, \quad C_1 = \| u_n \|_{L^4}^4,
\]
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 [17] it follows that
\[
C_1 = \| u_n \|_{L^1}^1 \equiv \| u_0 \|_{L^1}^1 \sim h^{-1/2} \quad \text{as } h \text{ goes to zero.}
\]

Therefore, (10) may be written
\[
\begin{align*}
  &\begin{cases}
    i h c_n = -\beta (c_{n+1} + c_{n-1}) + F \xi(n) c_n + \eta C_1 |c_n|^2 c_n + r_n \\
    i h \psi_\perp = \Pi_\perp (H_B - \Lambda_1) \psi + F \Pi_\perp W \psi + \eta |\psi|^2 \psi
  \end{cases},
\end{align*}
\]

where we set
\[
r_n = r_{1,n} + Fr_{2,n} + Fr_{3,n} + \eta r_{4,n}.
\]

Tight-binding approximation (Pi) is obtained by putting \( \psi_\perp \equiv 0 \) and by neglecting the coupling term \( r_n \) in (13).

We have the following estimates.
Lemma 1.

\[ \|r_1\|_{L^2} \leq C e^{-(S_0 + \zeta)/h} \|c\|_{L^2} \]

for some positive constants \(C\) and \(\zeta\) independent of \(h\).

**Proof.** Such an estimate directly comes from Lemma 1 by [17]. \(\square\)

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

\[ \|r_2\|_{L^2} \leq C e^{(S_0 - \rho)/h} \|c\|_{L^2}. \]

**Proof.** We set

\[ W_{n,m} = \begin{cases} \langle u_n, W_{n,m} \rangle & \text{if } n \neq m \\ 0 & \text{if } n = m \end{cases} \]

then \(r_{2,n} = \sum_{m \in \mathbb{Z}} W_{n,m} e_m\). By Example 2.3 §III.2 [9] it follows that

\[ \|r_2\|_{L^2} \leq \max\{M', M''\} \|c\|_{L^2} \]

where \(M'\) and \(M''\) are such that \(\sum_{m \in \mathbb{Z}} |W_{n,m}| \leq M'\) and \(\sum_{m \in \mathbb{Z}} |W_{n,m}| \leq M''\) 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 [17] 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. \(\square\)

**Lemma 3.** Let \(s\) be defined by Hypothesis 2; then, the following estimate holds true:

\[ \|r_3\|_{L^2} \leq C h^{-1/4} \|\psi_\perp\|_{L^2}. \]

**Proof.** Since \(\sum_{n \in \mathbb{N}} |a_n|^2 \leq \left[ \sum_{n \in \mathbb{N}} |a_n| \right]^2\) then

\[
\|r_3\|_{L^2}^2 = \sum_{n \in \mathbb{Z}} |\langle u_n, W \psi_\perp \rangle|^2 \leq \left[ \sum_{n \in \mathbb{Z}} |W| |u_n|, |\psi_\perp| \right]^2 \\
\leq \left[ \sum_{n \in \mathbb{Z}} |W| |u_n| \right]_{L^2}^2 \|\psi_\perp\|_{L^2}^2
\]

Now, we are going to estimate the term \(\|\sum_{n \in \mathbb{Z}} |W| |u_n| \|_{L^2}\); to this end let us set \(A = [-R, +R]\) and \(B = \mathbb{R} \setminus A\), where \(R = (\frac{1}{2} + N) a\) and \(N > 0\) is a large enough positive number which will be defined later. Then

\[
\left\| \sum_{n \in \mathbb{Z}} |u_n| \right\|_{L^2}^2 = \int_A |W|^2 \left[ \sum_{n \in \mathbb{Z}} |u_n|^2 \right] dx + \int_B |W|^2 \left[ \sum_{n \in \mathbb{Z}} |u_n|^2 \right] dx = \\
= \int_A |W|^2 \left[ \sum_{n \in \mathbb{Z}, x_n \in A} |u_n| + \sum_{n \in \mathbb{Z}, x_n \notin A} |u_n|^2 \right] dx + \int_B |W|^2 \left[ \sum_{n \in \mathbb{Z}} |u_n|^2 \right] dx \\
\leq 2 \left\{ \int_A |W|^2 \left[ \sum_{n \in \mathbb{Z}, x_n \in A} |u_n|^2 \right] dx + \int_A |W|^2 \left[ \sum_{n \in \mathbb{Z}, x_n \notin A} |u_n|^2 \right] dx \right\} + \int_B |W|^2 \left[ \sum_{n \in \mathbb{Z}} |u_n|^2 \right] dx.
\]
We note that
\[
\int_A |W|^2 \left[ \sum_{n \in \mathbb{Z}; x_n \in A} |u_n| \right]^2 \ dx = \int_A |W|^2 \sum_{n \in \mathbb{Z}; x_n \in A} |u_n|^2 \ dx + \int_A |W|^2 \sum_{n,m \in \mathbb{Z}; x_n \in A, \ n \neq m} |u_n| |u_m| \ dx \\
\leq \|W\|_{L^\infty}^2 \sum_{n \in \mathbb{Z}; x_n \in A} \|u_n\|^2_{L^2} + \|W\|_{L^\infty}^2 \sum_{n,m \in \mathbb{Z}; x_n \in A, \ n \neq m} \|u_n u_m\|_{L^1} \\
\leq \ CN + CN e^{-(S_0 - \rho)/h},
\]
since \(\|u_n\|_{L^2} = 1\) and Lemma 1.iv [17]. For what concerns the other term let \(\chi_A\) be the characteristic function on the set \(A\), we have that
\[
\int_A |W|^2 \left[ \sum_{n \in \mathbb{Z}; x_n \notin A} |u_n| \right]^2 \ dx \leq \max_{n \in \mathbb{Z}} \|u_n\|_{L^\infty} \sum_{n \in \mathbb{Z}; x_n \neq A} \langle |W|^2, \chi_A |u_n| \rangle \\
\leq \|u_0\|_{L^\infty} \|W^2\|_{L^2} \sum_{n \in \mathbb{Z}; x_n \neq A} \|\chi_A u_n\|_{L^2} \leq C e^{-(S_0 - \rho)/2h}
\]
since \(W^2 \in L^2\) because of Hypothesis 2 and because for any \(\rho' > 0\) and \(\rho'' > 0\) there is a positive constant \(C\) such that
\[
\|\chi_A u_n\|_{L^2} \leq C e^{-\left(\langle d_A(x_n, A) - \rho'\rangle + \rho''\right)}
\]
as one can see by means of the same arguments used in the proof of Lemma 2 [7], and where the Agmon distance between \(x_n \notin A\) and \(A\) is given by
\[
d_A(x_n, A) \geq \left(\langle |n| - N \rangle + \frac{1}{2}\right) S_0.
\]
Finally
\[
\int_B |W|^2 \left[ \sum_{n \in \mathbb{Z}} |u_n| \right]^2 \ dx \leq C \left\| \sum_{n \in \mathbb{Z}} |u_n| \right\|_{L^\infty}^2 \int_B (x)^{-2s} \ dx \leq C h^{-1} N^{1-2s}.
\]
Then, we have obtained that
\[
\left\| |W| \sum_{n \in \mathbb{Z}} |u_n| \right\|_{L^2}^2 \leq CN + Ch^{-1} N^{1-2s}.
\]
If we set \(N = \lfloor h^{-\alpha} \rfloor + 1\) (where \(\lfloor x \rfloor\) is the integer part of a real number \(x\)) for \(\alpha > 0\) such that \(-\alpha = -1 - \alpha(1 - 2s)\), that is \(\alpha = 1/2s\), then we finally gets
\[
\left\| |W| \sum_{n \in \mathbb{Z}} |u_n| \right\|_{L^2}^2 \leq Ch^{-1/2s}.
\]
By collecting all these results then Lemma 3 follows.

**Remark 3.** We remark that if \(W\) has compact support then
\[
\|\tau_3\|_{L^2} \leq C \|\psi_\perp\|_{L^2}.
\]
Indeed, it immediately follows by means of a simple fact:
\[
\left\| |W| \sum_{n \in \mathbb{Z}} |u_n| \right\|_{L^2}^2 = \int_A |W|^2 \left[ \sum_{n \in \mathbb{Z}} |u_n| \right]^2 \ dx \leq CN + CN e^{-(S_0 - \rho)h} \leq C
\]
where \( N \) is a fixed positive and integer number such that the set \( A = \left[-\left(N + \frac{1}{2}\right)a, \left(N + \frac{1}{2}\right)a\right] \) contains the support set of \( W \).

For what concerns the vector \( r_4 \) let

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

where we set

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

and

\[
B_n = \langle u_n, |\psi|^2 \psi_1 \rangle - C_1|c_n|^2c_n = \sum_{j,\ell,m \in \mathbb{Z}} \langle u_n, \bar{u}_m u_{\ell,j} \rangle \bar{c}_m c_{\ell} c_j \tag{14}
\]

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

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

\[
\|B\|_{l^2} \leq Ce^{-(S_0 - \rho)/h}.
\]

**Proof.** For argument’s sake let us assume that \( m \) is the index different from the index \( n \) in the sum (14); then we have to check the term

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

where

\[
B_{1,n} = \sum_{j,\ell,m \in \mathbb{Z}}^1 \langle u_m u_n, u_{\ell,j} \rangle \bar{c}_m c_{\ell} c_j := \sum_{m \in \mathbb{Z} \setminus \{n\}} \sum_{\ell \in \mathbb{Z} \setminus \{m,n\}} \sum_{j \in \mathbb{Z} \setminus \{\ell,m,n\}} \langle u_m u_n, u_{\ell,j} \rangle \bar{c}_m c_{\ell} c_j
\]

\[
B_{2,n} = \sum_{j,\ell,m \in \mathbb{Z}}^2 \langle u_m u_n, u_{\ell,j}^2 \rangle \bar{c}_m c_{\ell}^2 := \sum_{m \in \mathbb{Z} \setminus \{n\}} \sum_{\ell \in \mathbb{Z} \setminus \{m,n\}} \langle u_m u_n, u_{\ell,j}^2 \rangle \bar{c}_m c_{\ell}^2
\]

\[
B_{3,n} = \sum_{j,\ell,m \in \mathbb{Z}}^3 \langle u_m u_n, u_{m}^2 \rangle \bar{c}_m c_m^2 := \sum_{m \in \mathbb{Z}, m \neq n} \langle u_n u_m, u_m^2 \rangle \bar{c}_m c_m^2
\]

Observing that \( |c_m| \leq 1 \) since \( \|c\|_{l^2} \leq 1 \), then

\[
|B_{3,n}| \leq \sum_{m \in \mathbb{Z}, m \neq n} |\langle u_n u_m, u_m^2 \rangle| |c_m|^2
\]

\[
\leq \sum_{m \in \mathbb{Z}, m \neq n} \|u_n u_m\|_{L^1} \|u_m\|_{L^\infty}^2 |c_m|^2
\]

\[
\leq \sum_{m \in \mathbb{Z}, m \neq n} C h^{-1/2} e^{-|\langle S_0 - \rho'\rangle n - n' - \rho''|/h} |c_m|^2
\]

where we make use of the following property (see Lemma 1.iv by [17]): for any \( \rho', \rho'' \in (0, S_0) \) there is a positive constant \( C > 0 \) independent of the indexes \( n \) and \( m \) such that

\[
\|u_n u_m\|_{L^1} \leq Ce^{-|\langle S_0 - \rho'\rangle n - n' - \rho''|/h}.
\]
Hence

\[
\|B_3\|_{\ell^2} \leq \|B_3\|_{\ell^1} \leq \sum_{n,m\in\mathbb{Z}, \ m\neq n} Ch^{-1/2} e^{-[(S_0-\rho)'|n-m| - \rho'']/h} |c_m|^2
\]

\[
\leq Ce^{-(S_0-\rho)/h} \sum_{m\in\mathbb{Z}} |c_m|^2 = Ce^{-(S_0-\rho)/h} \|c\|_{\ell^2}^2
\]

\[
\leq Ce^{-(S_0-\rho)/h}.
\]

For what concerns the term $B_{2,n}$ we have that

\[
|B_{2,n}| = \left| \sum_{m, \ell \in \mathbb{Z}} (u_m u_n, u_{\ell}^2) c_m c_{\ell}^2 \right| \leq \sum_{m, \ell \in \mathbb{Z}} \left( |u_m| |u_n|, |u_{\ell}|^2 \right) |c_m| |c_{\ell}|^2
\]

\[
\leq \max_{\ell \in \mathbb{Z}} \|u_{\ell}\|_{L^\infty} \left( \sum_{m \in \mathbb{Z}} |u_m| \right) \sum_{\ell \in \mathbb{Z}, \ \ell \neq n} \left( |u_n|, |u_{\ell}| \right) |c_{\ell}|^2
\]

\[
\leq \max_{\ell \in \mathbb{Z}} \|u_{\ell}\|_{L^\infty} \left( \sum_{m \in \mathbb{Z}} |u_m| \right) \sum_{\ell \in \mathbb{Z}, \ \ell \neq n} Ce^{-(S_0-\rho')|n-\ell| - \rho'']/h} |c_{\ell}|^2
\]

\[
\leq C \|u_0\|_{L^\infty} \left( \sum_{m \in \mathbb{Z}} |u_m| \right) \sum_{\ell \in \mathbb{Z}, \ \ell \neq n} e^{-(S_0-\rho')|n-\ell| - \rho'']/h} |c_{\ell}|^2
\]

\[
\leq Ch^{-3/4} \sum_{\ell \in \mathbb{Z}, \ \ell \neq n} e^{-(S_0-\rho')|n-\ell| - \rho'']/h} |c_{\ell}|^2
\]

since $\|u_{\ell}\|_{L^\infty} = \|u_0\|_{L^\infty} \leq Ch^{-1/4}$ and $\sum_{m \in \mathbb{Z}} |u_m| \|_{L^\infty} \leq Ch^{-1/2}$ (see Lemma 1 [17]), from which it follows that

\[
\|B_2\|_{\ell^2} \leq \|B_2\|_{\ell^1} = \sum_{n \in \mathbb{Z}} |B_{2,n}| \leq Ch^{-3/4} \sum_{n, \ell \in \mathbb{Z}, n \neq \ell} Ce^{-(S_0-\rho')|n-\ell| - \rho'']/h} |c_{\ell}|^2
\]

\[
\leq Ce^{-(S_0-\rho)/h} \|c\|_{\ell^2} \leq Ce^{-(S_0-\rho)/h}.
\]
Finally,

\[
|B_{1,n}| \leq \sum_{m,\ell,j \in \mathbb{Z}}^{*1} \langle |u_m|, |u_n|, |u_\ell|, |u_j| \rangle \langle c_m, c_\ell, c_j \rangle \\
\leq \frac{1}{2} \sum_{m,\ell,j \in \mathbb{Z}}^{*1} \langle |u_m|, |u_n|, |u_\ell|, |u_j| \rangle |c_m| |c_\ell|^2 + |c_j|^2 \\
\leq \sum_{m,\ell,j \in \mathbb{Z}}^{*1} \langle |u_m|, |u_n|, |u_\ell|, |u_j| \rangle |c_m| |c_j|^2 \\
\leq \sum_{m \in \mathbb{Z}\setminus\{n\}, j \in \mathbb{Z}\setminus\{m,n\}} \left( \sum_{\ell \in \mathbb{Z}} |u_\ell| \right) \left( \sum_{j \in \mathbb{Z}, j \neq n} \langle |u_n|, |u_j| \rangle |c_m| |c_j|^2 \right) \\
\leq \left\| \sum_{\ell \in \mathbb{Z}} |u_\ell| \right\|_{L^\infty} \sum_{j \in \mathbb{Z}, j \neq n} \langle |u_n|, |u_j| \rangle |c_j|^2 \\
\leq C h^{-1} \sum_{j \in \mathbb{Z}, j \neq n} e^{-[(S_0 - \rho') |n-j| - \rho'']/h} |c_j|^2
\]

since \(|c_m| \leq 1\). Hence,

\[
\|B_1\|_{\ell^2} \leq \|B_1\|_{\ell^2} \leq C h^{-1} \sum_{n,j \in \mathbb{Z}, j \neq n} C e^{-[(S_0 - \rho') |n-j| - \rho'']/h} |c_j|^2 \\
\leq C e^{-(S_0 - \rho)/h} \sum_{j \in \mathbb{Z}} |c_j|^2 = C e^{-(S_0 - \rho)/h} \|c\|_{\ell^2} \\
\leq C e^{-(S_0 - \rho)/h}.
\]

From these estimates it follows that

\[
\|B\|_{\ell^2} \leq C \left[ \|B_1\|_{\ell^2} + \|B_2\|_{\ell^2} + \|B_3\|_{\ell^2} \right] \leq C e^{-(S_0 - \rho)/h}
\]

and Lemma 4 is so proved. \(\square\)

Now we deal with the vector \(A\) with elements

\[
A_n = \langle u_n, g \rangle
\]

where

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

Lemma 5.

\[
\|A\|_{\ell^2} \leq C h^{-3/4} \|\psi_\perp\|_{L^2}
\]
Proof. Indeed,
\[\|A\|_{\ell^2}^2 = \sum_{n\in\mathbb{Z}} |\langle u_n, g \rangle|^2 \leq \left( \sum_{n\in\mathbb{Z}} |u_n| \right)^2 \leq \sum_{n\in\mathbb{Z}} |u_n| \leq \frac{\|g\|_{L^1}}{\|g\|_{L^1}^2} \leq C h^{-1} \|g\|_{L^1}^2,\]
where
\[\|g\|_{L^1} \leq C \left[ \|\psi\|_{L^1}^3 + \|\psi_{\perp}\|_{L^1}^2 + \|\psi_{\perp}\|_{L^2}^2 \right] \leq C \left[ \|\psi\|_{L^2} \|\psi\|_{L^\infty} + \|\psi_{\perp}\|_{L^2} \|\psi_{\perp}\|_{L^\infty} \right] \|\psi_{\perp}\|_{L^2} \leq C h^{-\frac{1}{4}} \|\psi_{\perp}\|_{L^2},\]
from Theorem 2 and Corollary 1.

In conclusion we have proved the following Lemma:

**Lemma 6.**
\[\|r_4\|_{\ell^2} \leq C e^{-(S_0-\rho)/h} + C h^{-\frac{3}{4}} \|\psi_{\perp}\|_{L^2}.\]

5. **Validity of the tight-binding approximation**

First of all we need of the following estimate:

**Lemma 7.** Let us set
\[\lambda := |F|h^{-1} + |\eta|h^{-\frac{3}{2}}\]
and let \(c\) and \(\psi_{\perp}\) be the solutions to (13); then
\[\|\dot{c}\|_{\ell^2} \leq \frac{C}{h} \max [\beta, |h\lambda|, h \|r\|_{\ell^2}] .\]  

**Proof.** Indeed, from (13) it immediately follows that
\[\|\dot{c}\|_{\ell^2}^2 = \frac{1}{h^2} \sum_{n\in\mathbb{Z}} \left[ -\beta (c_{n+1} + c_{n-1}) + F \xi(n) c_n + \eta C_1 |c_n|^2 + r_n \right]^2 \leq \frac{C}{h^2} \left[ (\beta^2 + F^2 + \eta^2 C_1^2) \|c\|_{\ell^2}^2 + \|r\|_{\ell^2}^2 \right] \]
from which the estimate (15) follows since \(\|c\|_{\ell^2} \leq 1\) and \(|c_n| \leq 1\).

Hereafter, we denote by \(\omega\) a quantity, whose value may change from line to line, such that
\[|\omega| \leq C e^{-(S_0+\zeta)/h}\]
for some \(\zeta > 0\) and some \(C > 0\) independent of \(h\).

**Theorem 2.**
\[\|r\|_{\ell^2} \leq \omega + C |F| e^{-(S_0-\rho)/h} + C (|F|h^{-1/4}s + |\eta|h^{-3/4}) \|\psi_{\perp}\|_{L^2} \]

**Proof.** Indeed, collecting the results from Lemmata 2, 3, and 6 and from Remark 2 we have that
\[\|r\|_{\ell^2} \leq \|r_1\|_{\ell^2} + |F| \|r_2\|_{\ell^2} + |F| \|r_3\|_{\ell^2} + |\eta| \|r_4\|_{\ell^2} \leq C e^{-(S_0+\zeta)/h} + C |F| e^{-(S_0-\rho)/h} + C |F| h^{-1/4} \|\psi_{\perp}\|_{L^2} + C |\eta| e^{-(S_0-\rho)/h} + C |\eta|h^{-3/4} \|\psi_{\perp}\|_{L^2} \]
from which the statement immediately follows.
Now, is an unitary operator; hence, \( f \) from Theorem 1 and Corollary 1; hence, (20) follows. In order to prove (19) we remark that

\[
F \psi = F \psi_0 = 0,
\]

then the previous equation (17) becomes

\[
\psi_\perp(\tau) = -i \int_0^\tau e^{-i(H_B - \Lambda_1)(\tau - q)/h} \left[ \frac{F}{h} F \psi + \frac{\eta}{h} \psi_\perp |\psi|^2 \psi \right] dq
\]

Theorem 3. We have the following estimate

\[
\|\psi_\perp\|_{L^2} \leq \left\{ CL + \tau Ch^{-1} \max \left[ \beta, \left( |F|h^{-1/4s} + |\eta|h^{-3/4} \right) \right] \right\} e^{C\lambda \tau}, \quad \forall \tau \in \mathbb{R}.
\]

Proof. Let

\[
U_1 := U_1(\psi_1) = \left[ \frac{F}{h} F \psi_1 + \frac{\eta}{h} \psi_\perp |\psi_1|^2 \psi_1 \right]
\]

\[
U_2 := U_2(\psi_1, \psi_\perp) = \left[ \frac{F}{h} F \psi_\perp + \frac{\eta}{h} \psi_\perp (|\psi|^2 \psi - |\psi_1|^2 \psi_1) \right]
\]

then the previous equation (17) becomes

\[
\psi_\perp(\tau) = f_1(\tau) + f_2(\tau)
\]

where

\[
f_j(\tau) = -i \int_0^\tau e^{-i(H_B - \Lambda_1)(\tau - q)/h} U_j dq, \quad j = 1, 2,
\]

is such that

Lemma 8. The following estimates hold true:

\[
\|f_1\|_{L^2} \leq CL + \tau Ch^{-1} \max \left[ \beta, \left( |F|h^{-1/4s} + |\eta|h^{-3/4} \right) \right]
\]

and

\[
\|f_2\|_{L^2} \leq CL \int_0^\tau \|\psi_\perp(q)\|_{L^2} dq.
\]

Proof. In order to prove the estimates (19) and (20) we remark that \( e^{-i(H_B - \Lambda_1)(\tau - s)/h} \) is an unitary operator; hence,

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

Now,

\[
\|U_2\|_{L^2} \leq \left\| \frac{F}{h} F \psi_\perp \right\|_{L^2} + \left\| \frac{\eta}{h} \psi_\perp |\psi|^2 \psi - |\psi_1|^2 \psi_1 \right\|_{L^2}
\]

\[
\leq Ch^{-1} |F| \|\psi_\perp\|_{L^2} + Ch^{-1} |\eta| \left[ \|\psi_\perp^2 \|_{L^2} + \|\psi_\perp^2 \|_{L^2} + \|\psi_\perp^2 \|_{L^2} \right]
\]

\[
\leq Ch^{-1} |F| \|\psi_\perp\|_{L^2} + Ch^{-1} |\eta| \left[ \|\psi_\perp\|_{L^\infty} \|\psi_\perp\|_{L^\infty} + \|\psi_\perp^2 \|_{L^\infty} + \|\psi_\perp^2 \|_{L^\infty} \right] \|\psi_\perp\|_{L^2}
\]

from Theorem 1 and Corollary 1 hence, (20) follows. In order to prove (19) we make use of an integration by parts:

\[
f_1(\tau) = -i \int_0^\tau e^{-i(H_B - \Lambda_1)(\tau - q)/h} U_1 dq
\]

\[
= \left[ -he^{-i(H_B - \Lambda_1)(\tau - q)/h} [H_B - \Lambda_1]^{-1} U_1 \right]_0^\tau + h \int_0^\tau e^{-i(H_B - \Lambda_1)(\tau - q)/h} [H_B - \Lambda_1]^{-1} \frac{dU_1}{dq} dq
\]

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From this fact and since \( \| [H_B - \Lambda_1]^{-1} \Pi_\perp \| = \| \text{dist}(\Lambda_1, E_2^0) \|^{-1} \sim h^{-1} \) then it follows that
\[
\| f_1 \|_{L^2} \leq \max \left\{ \| U_1(\tau) \|_{L^2}, \| U_1(0) \|_{L^2} \right\} + \tau \max_{s \in [0, \tau]} \left\| \frac{dU_1}{d\tau} \right\|_{L^2} \\
\leq C\lambda + \tau C h^{-1} \lambda \max \left\{ \beta, h\lambda, \| r \|_{\ell^2} \right\} \\
\leq C\lambda + \tau C h^{-1} \lambda \max \left[ \beta, \left( |F|h^{-1/4s} + |\eta|h^{-3/4} \right) \right]
\]
since
\[
\| U_1 \|_{L^2} \leq |F|h^{-1} \| \Pi_\perp W \psi_1 \|_{L^2} + |\eta|h^{-1} \| \Pi_\perp |\psi_1|^2 \psi_1 \|_{L^2} \\
\leq C|F|h^{-1} \| \psi_1 \|_{L^2} + |\eta|h^{-1} \| \psi_1 \|_{L^2}^2 \\
\leq C\lambda
\]
and
\[
\left\| \frac{dU_1}{d\tau} \right\|_{L^2} \leq C\lambda \| \psi_1 \|_{L^2} \leq C\lambda \| \psi \|_{\ell^2} \\
\leq C h^{-1} \lambda \max \left\{ \beta, h\lambda, \| r \|_{\ell^2} \right\}
\]
by Lemma 7 and Theorem 2.

Hence, we have the following integral inequality
\[
\| \psi_\perp \|_{L^2} \leq \left\{ C\lambda + \tau C h^{-1} \lambda \max \left[ \beta, \left( |F|h^{-1/4s} + |\eta|h^{-3/4} \right) \right] \right\} + C\lambda \int_0^\tau \| \psi_\perp \|_{L^2} d\tau
\]
and then the Gronwall’s Lemma implies that
\[
\| \psi_\perp \|_{L^2} \leq \left\{ C\lambda + \tau C h^{-1} \lambda \max \left[ \beta, \left( |F|h^{-1/4s} + |\eta|h^{-3/4} \right) \right] \right\} e^{C\lambda \tau}, \forall \tau \in \mathbb{R};
\]
Theorem 3 is so proved.

Now, we deal with the first differential equation of the system (13)
\[
\begin{cases}
  i\hbar \dot{c}_n = G_n(c) + r_n, \\
  c_n(0) = (u_n, \psi_0),
\end{cases}
\]
where
\[
G_n(c) = -\beta (c_{n+1} + c_{n-1}) + F\xi(n)c_n + \eta C_1 |c_n|^2 c_n.
\]
We compare it with the equation
\[
\begin{cases}
  i\hbar \dot{g}_n = G_n(g) \\
  g_n(0) = c_n(0)
\end{cases}
\]
which represents the tight-binding approximation of (13), up to a phase factor \( e^{-i\Lambda_1 \tau/\hbar} \) depending on time. We must underline that we have the following a priori estimate \( \| c \|_{\ell^2} \leq 1 \) and the conservation of the norm of \( g \)
\[
\| g \|_{\ell^2} = \| g(0) \|_{\ell^2} = \| c(0) \|_{\ell^2} = 1;
\]
indeed, an immediate calculus gives that
\[
\frac{d}{d\tau} \| \hbar g \|_{\ell^2}^2 = \beta \left[ \sum_{n \in \mathbb{Z}} \bar{g}_{n+1} g_n + \sum_{n \in \mathbb{Z}} \bar{g}_{n-1} g_n - \sum_{n \in \mathbb{Z}} \bar{g}_{n+1} \bar{g}_n - \sum_{n \in \mathbb{Z}} \bar{g}_{n-1} \bar{g}_n \right] = 0
\]
because \( \beta, F, \eta, C_1 \) and \( \xi(n) \) are real-valued.
Hence,
\[ i\hbar [c_n(\tau) - g_n(\tau)] = \int_0^\tau [G_n(c) - G_n(g)] \, dq + \int_0^\tau r_n(q) \, dq \]
from which
\[ \|c - g\|_{\ell^2} \leq \frac{1}{\hbar} \int_0^\tau \|G(c) - G(g)\|_{\ell^2} \, dq + \frac{1}{\hbar} \int_0^\tau \|r\|_{\ell^2} \, dq. \]

**Lemma 9.** \(G\) is a Lipschitz function such that
\[ \|G(c) - G(g)\|_{\ell^2} \leq C \max[\beta, h\lambda] \|c - g\|_{\ell^2}. \] (22)

**Proof.** Indeed
\[
\begin{align*}
\|G(c) - G(g)\|_{\ell^2}^2 &= \sum_{n \in \mathbb{Z}} |G_n(c) - G_n(g)|^2 \\
&= \sum_{n \in \mathbb{Z}} \left| (-\beta [(c_{n+1} - g_{n+1}) + (c_{n-1} - g_{n-1})]) + F\xi(n)(c_n - g_n) + \eta C \left| |c_n|^2 c_n - |g_n|^2 g_n \right| \right|^2 \\
&\leq C \left\{ \beta^2 \sum_{n \in \mathbb{Z}} |c_{n+1} - g_{n+1}|^2 + \beta^2 \sum_{n \in \mathbb{Z}} |c_{n-1} - g_{n-1}|^2 + \sum_{n \in \mathbb{Z}} F^2 \xi^2(n) |c_n - g_n|^2 + \right. \\
&\quad \left. + \sum_{n \in \mathbb{Z}} \eta^2 C^2 |c_n|^2 c_n - |g_n|^2 g_n \right\} \\
&\leq C \left\{ 2\beta^2 \|c - g\|_{\ell^2}^2 + \left[ \max_{n \in \mathbb{Z}} \xi^2(n) \right] F^2 \|c - g\|_{\ell^2}^2 + \eta^2 C^2 \sum_{n \in \mathbb{Z}} |c_n|^2 (c_n - g_n) + \left| (|c_n|^2 - |g_n|^2) |g_n| \right| \right\} \\
&\leq C \left[ \beta^2 + F^2 + \eta^2 C^2 \right] \|c - g\|_{\ell^2}^2 \leq C \max[\beta^2, h^2\lambda^2] \|c - g\|_{\ell^2}^2
\end{align*}
\]
since \( |c_n|^2 - |g_n|^2 = c_n |\tilde{c}_n - \tilde{g}_n| + \tilde{g}_n (c_n - g_n) \) and \([12].\)

By Theorems [2] and [3], it turns out that the vector \(r\) is norm bounded by
\[
\|r\|_{\ell^2} \leq a + be^{d\lambda\tau} + ce^{d\lambda\tau} \quad (23)
\]
for some positive constant \(d\) independent of \(h\) and where
\[
\begin{align*}
a &= \omega + C\lambda e^{-(S_0 - \rho)/h} \\
b &= C\lambda \left[ |F|h^{-1/4}s + |\eta|h^{-3/4} \right] \\
c &= Ch^{-1}\lambda \left[ |F|h^{-1/4}s + |\eta|h^{-3/4} \right] \max \left[ \beta, \left( |F|h^{-1/4}s + |\eta|h^{-3/4} \right) \right].
\end{align*}
\]
Then, we get the integral inequality
\[
\|c - g\|_{\ell^2} \leq \alpha(\tau) + \int_0^\tau \delta(q) \|c - g\|_{\ell^2} \, dq \quad (24)
\]
where
\[
\alpha(\tau) \leq \frac{1}{h} \int_0^\tau \|r\|_{\ell^2} \, dq \leq \frac{\alpha\tau}{h} + \frac{bd\lambda - c}{d^2\lambda^2 h} \left( e^{d\lambda\tau} - 1 \right) + \frac{c\tau}{d\lambda h} e^{d\lambda\tau}
\]
and
\[
\delta(\tau) \leq C \max[h^{-1}\beta, |\lambda|]
\]
By the Gronwall’s Lemma we finally get the estimate
\[
\|c - g\|_{\ell^2} \leq \alpha(\tau) e^{\int_0^\tau \delta(q) \, dq} = \alpha(\tau) e^{C \max[h^{-1}\beta, |\lambda|] \tau}
\]
Therefore, we have proved that

**Lemma 10.** Let
\[
\begin{align*}
    a &= \omega + C\lambda e^{-(S_0-\rho)/\hbar} \\
    b &= C\lambda \left(|F|\hbar^{-1/4s} + |\eta|\hbar^{-3/4}\right) \\
    c &= Ch^{-1}\lambda \left(|F|\hbar^{-1/4s} + |\eta|\hbar^{-3/4}\right) \max \left[\beta, \left(|F|\hbar^{-1/4s} + |\eta|\hbar^{-3/4}\right) \right]
\end{align*}
\]
then
\[
\|c - g\|_{L^2} \leq \left\{\frac{a\tau}{h} + \frac{bd\lambda - c}{d^2\lambda^2h} (e^{d\lambda\tau} - 1) + \frac{ct}{d\lambda h} e^{d\lambda\tau}\right\} e^{C\max[|h^{-1}\beta|,|\lambda|] \tau} \tag{25}
\]
for some positive constants \(d\) and \(C\) independent of \(h\).

In conclusion

**Theorem 4.** Let \(\psi(\tau, x)\) be the solution to the nonlinear Schrödinger equation \(\Box\) with initial condition \(\psi_0(x)\); let \(g\) be the solution to the discrete nonlinear Schrödinger equation \(\Box\); let \(a, b, c\) and \(d\) defined by Lemma 10; let \(\lambda\) be defined by Lemma 7. Then
\[
\left\|\psi(\tau, \cdot) - \sum_{n \in \mathbb{Z}} g_n(\tau) e^{iA_1\tau/h} u_n(\cdot)\right\|_{L^2} \leq \left\{C\lambda + \tau Ch^{-1}\lambda \max \left[\beta, \left(|F|\hbar^{-1/4s} + |\eta|\hbar^{-3/4}\right) \right]\right\} e^{C\lambda\tau} + \left\{\frac{a\tau}{h} + \frac{bd\lambda - c}{d^2\lambda^2h} (e^{d\lambda\tau} - 1) + \frac{ct}{d\lambda h} e^{d\lambda\tau}\right\} e^{C\max[|h^{-1}\beta|,|\lambda|] \tau}, \quad \forall \tau \in \mathbb{R}. \tag{26}
\]

**Proof.** Indeed, recalling that we made use of the gauge choice \(\psi \rightarrow e^{iA_1\tau/h} \psi\), we have that
\[
\begin{align*}
\left\|\psi - \sum_{n \in \mathbb{Z}} g_n e^{iA_1\tau/h} u_n\right\|_{L^2} &= \left\|e^{-iA_1\tau/h} \psi - \sum_{n \in \mathbb{Z}} g_n u_n\right\|_{L^2} = \left\|\psi_\perp\right\|_{L^2} + \left\|\sum_{n \in \mathbb{Z}} (c_n - g_n) u_n\right\|_{L^2} \\
&= \left\|\psi_\perp\right\|_{L^2} + \left\|\sum_{n \in \mathbb{Z}} (c_n - g_n) u_n\right\|_{L^2}
\end{align*}
\]
where
\[
\left\|\sum_{n \in \mathbb{Z}} (c_n - g_n) u_n\right\|_{L^2}^2 = \sum_{n \in \mathbb{Z}} |c_n - g_n|^2 \|u_n\|_{L^2}^2 = \|c - g\|_{L^2}^2
\]
because \(\{u_n\}\) is an orthonormal set of vectors. \(\square\)

5.1. **Model 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
\[
F \sim \eta \sim \hbar^2. \tag{27}
\]
Therefore:
\[
\lambda \sim \hbar^{1/2}, \quad |a|, \beta \leq Ce^{-(S_0-\rho)/\hbar}, \quad b \sim \hbar^{7/4}, \quad c \sim \hbar^2.
\]
Then the estimate (26) makes sense for times of order $\tau \in [0, Ch^{-\gamma}]$ for some fixed $\gamma < \frac{1}{2}$. In such an interval we have that

$$C \lambda + \tau Ch^{-1} \lambda \max \beta, \left( |F| h^{-1/4} s + |\eta| h^{-3/4} \right) \sim h^{1/2} + h^{3/4 - \gamma}$$

$$\frac{a \tau}{h} + \frac{bd \lambda - c}{h \lambda^2} \left( e^{d \lambda \tau} - 1 \right) + \frac{c \tau}{h} e^{d \lambda \tau} \sim h^{3/4 - \gamma} + h^{1 - 2 \gamma}.$$ 

In particular, for $\gamma = \frac{1}{4}$ we have the following result:

**Corollary 2.** Let $\psi(\tau, x)$ be the solution to the nonlinear Schrödinger equation (3) with initial condition $\psi_0(x)$ under the assumption Hypothesis 3a); let $g$ be the solution to the discrete nonlinear Schrödinger equation (27). Then for any $\tau \in [0, Ch^{-1/4}]

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

5.2. **Model 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

$$F \sim h^{-1/2} \eta \sim \beta.$$ 

In such a case we have that

$$\lambda \sim h^{-1} \beta, \ a \sim \omega, \ b \sim h^{-5/4} \beta^2, \ c \sim h^{-5/2} \beta^3.$$ 

The estimate (26) makes sense for times of order $\tau \in [0, \beta^{-1} h]$. In such an interval we have that

$$\|\psi\|_{L^2} \leq C e^{-(S_0 - \rho) / h}$$

and

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

for some $\zeta > 0$.

In conclusion we have that

**Corollary 3.** Let $\psi(\tau, x)$ be the solution to the nonlinear Schrödinger equation (3) with initial condition $\psi_0(x)$ under the assumption Hypothesis 3b); let $g$ be the solution to the discrete nonlinear Schrödinger equation (27). Then for any $\tau \in [0, C \beta^{-1} h]$, where $\beta^{-1}$ is exponentially large as $h$ goes to zero, we have that

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

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

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