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Nonlinear Schrödinger equations with a multiple-well potential and a Stark-type perturbation

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HIGHLIGHTS

- Model of accelerated ultracold condensate in optical lattices.
- Numerical computation of wavefunction of condensates.
- Numerical computation of the oscillating period of the center of mass of condensates.

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ABSTRACT

A Bose–Einstein condensate (BEC) confined in a one-dimensional lattice under the effect of an external homogeneous field is described by the Gross–Pitaevskii equation. Here we prove that such an equation can be reduced, in the semiclassical limit and in the case of a lattice with a finite number of wells, to a finite-dimensional discrete nonlinear Schrödinger equation. Then, by means of numerical experiments we show that the BEC's center of mass exhibits an oscillating behavior with modulated amplitude; in particular, we show that the oscillating period actually depends on the shape of the initial wavefunction of the condensate as well as on the strength of the nonlinear term. This fact opens a question concerning the validity of a method proposed for the determination of the gravitational constant by means of the measurement of the oscillating period.

1. Introduction

Laser-cooled atoms have drawn a lot of attention as for potential applications to interferometry and high-precision measurements, from the determination of gravitational constants to geophysical applications [1–4], see also [5,6] for a recent review. The idea of using ultracold atoms moving in an accelerated optical lattice [7–11] has opened the field to multiple applications. In particular, by means of the method proposed by Cladé et al. [12], a value for the constant g has been measured using ultracold Strontium atoms confined in a vertical optical lattice [13]; such a result has been improved by using a larger number of atoms and reducing the initial temperature of the sample [14]. Determination of g has been obtained by measuring the period T of the Bloch oscillations of the atoms in the vertical optical lattice; recalling that

$$T = \frac{2\pi\hbar}{mgb}, \tag{1}$$

where m is the mass of the Strontium atom, $\hbar$ is the Planck constant and b is the lattice period, then a precise value of the constant g has been obtained by means of the experimental measurements of the oscillating period. Since Bloch oscillations with period (1) have been predicted by the Bloch Theorem [15] only for a one-body particle in a periodic field and under the effect of a Stark potential then it has been chosen, in the experiments above, a particular Strontium's isotope ^{88}Sr; in fact, the scattering length a_s of atoms ^{88}Sr is very small and thus it has been assumed by [13,14] that the effects of the atomic binary interactions are negligible. The obtained value for the constant g was consistent with the one obtained by classical gravimeters; but it was affected by a relative uncertainty of order 6×10^{-6} because of a larger scattering in repeated measurements, mainly due to the initial position instability of the trap. Such a technique is also proposed to measure surface forces [16], too.

The critical point of this experimental procedure concerns the validity of the Bloch Theorem and the estimate of the effect of the atomic binary interactions on the oscillating period of the BEC. In order to discuss this point here we are inspired by a realistic model of a one-dimensional cloud of cold atoms in a periodical optical lattice under the effect of the gravitational force. The periodic

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potential has the shape

$$V_{per}(x) = V_0 \sin^2(k_L x) \tag{2}$$

where $b = \frac{1}{2}\lambda_L$ is the period, and $\lambda_L = \frac{2\pi}{k_L}$. The one-dimensional BEC is governed by the time-dependent Gross–Pitaevskii equation with a periodic potential and a Stark potential

$$i\hbar\partial_t \psi = H_B\psi + fx\psi + \gamma|\psi|^2\psi, \quad f = mg, \tag{3}$$

where the wavefunction $\psi(\cdot, t) \in L^2(R, dx)$ is normalized to one:

$$\|\psi(\cdot,t)\|_{L^2} = \|\psi_0(\cdot)\|_{L^2} = 1,$$

and where

$$H_B = -\frac{\hbar^2}{2m}\partial^2_{xx} + V_{per}(x)$$

is the Bloch operator with periodic potential $V_{per}(x)$. By γ we denote the effective one-dimensional nonlinearity strength.

It is a well known fact (see Section 6.1 by [15]) that when the wavefunction ψ is prepared on the first band of the Bloch operator and if the nonlinear term is absent, i.e. $\gamma = 0$, then the dominant term of the wavefunction ψ exhibits a periodic behavior with Bloch period T within an interval with amplitude $\frac{B_1}{|f|}$, where B_1 is the width of the first band and where $f \in \mathbb{R}$ is the strength of the external homogeneous field (in the case of $f = mg$ then f takes only positive values, obviously). Therefore, for times of the order of the Bloch period T we may assume that the motion of the BEC occurs in a finite interval. Hence, we can restrict ourselves to the analysis of Eq. (3) in a suitable finite interval and then we may assume to consider a multiple-well potential $V_N(x)$ (with a fixed number N of wells) and that the Stark potential x is replaced by a Stark-type potential $W_N(x)$ due to a homogeneous external field which acts only in a bounded region containing the N wells (see Fig. 1). That is, instead of (3) we consider, as a model for a BEC in an optical lattice under an external homogeneous field, the time-dependent non-linear Schrödinger equation (NLS)

$$\begin{cases} i\epsilon\partial_t\psi = H_N\psi + fW_N(x)\psi + \gamma|\psi|^2\psi, \\ \quad H_N = -\epsilon^2\partial^2_{xx} + V_N \\ \psi(x,0) = \psi_0(x) \end{cases} \tag{4}$$

where $\epsilon > 0$ plays the role of the semiclassical parameter (we prefer to denote here the small semiclassical parameter by ϵ instead of the usual notation $\hbar$ because in a subsequent section we will discuss a real physical model where $\hbar$ will assume its *fixed* physical value; with such a notation it turns out that the Bloch period is given by $T = \frac{2\pi\epsilon}{|f|b}$). We assume that the N wells have all the same shape and we denote by $b > 0$ the distance between the adjacent absolute minima points.

The study of the dynamics of the wavefunction ψ, solution of (4), is then achieved by means of a discrete nonlinear Schrödinger equation (DNLS). The idea is basically simple and it consists in assuming that the wavefunction ψ may be written as a superposition of vectors $u_\ell(x)$ localized on the ℓth cell of the lattice; that is

$$\psi(x,t) \sim \sum_{\ell=1}^{N} c_\ell(t)u_\ell(x).$$

Such an approach has been successfully used in the cases of semiclassical NLS with multiple-well potentials [17–19] or with periodic potentials (see [20–22]), without the external field with potential W_N. Eventually, $u_\ell(x)$ may coincide with the Wannier function $\mathcal{W}_1(x - x_\ell)$ associated to the first band of the Bloch operator H_B or with the semiclassical single well ground state eigenfunction $u_\ell^{sc}(x)$. By means of such an approach the unknown

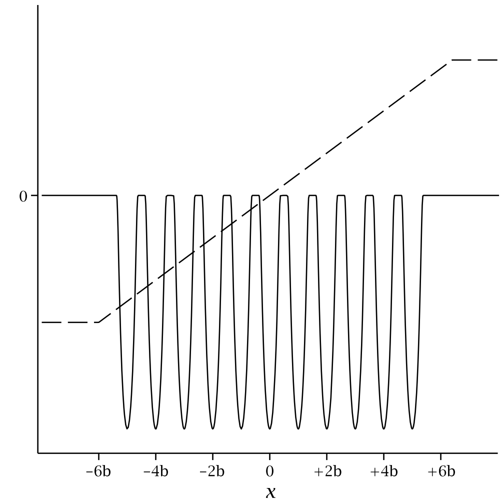

Fig. 1. Plot of the multiple-wells potential V_N (full line) and of the Stark-type potential W_N (broken line), where $N = 11$. By $b > 0$ we denote the distance between the adjacent absolute minima points.

functions $c_\ell(t)$ turn out to be the solutions of a system of time-dependent equations in which dominant terms are given by (here we denote $\dot{} = \frac{d}{dt}$)

$$\begin{aligned} i\epsilon\dot{c}_\ell &= -\lambda_D c_\ell - \beta(c_{\ell+1} + c_{\ell-1}) + \gamma\|u_\ell\|^4_{L^4}|c_\ell|^2 c_\ell \\ &\quad + fb\ell c_\ell, \quad \ell = 1,\ldots,N \end{aligned} \tag{5}$$

where λ_D is the ground state of a single cell potential and where β is the hopping matrix element between neighboring sites. In fact, the parameter β is expected to be such that 4β is equal to the amplitude B_1 of the first band [23]. In (5) we will fix $c_0 \equiv c_{N+1} \equiv 0$. Eq. (5) represents a discrete nonlinear Schrödinger equation (DNLS).

Our approach is both semiclassical and perturbative. It is semiclassical in the sense that it holds true in the semiclassical regime of ϵ small enough; and it is perturbative in the sense that the external field f and the nonlinearity power strength γ must be small when ϵ goes to zero (see Hypothesis 3 for details). Under these conditions we prove the validity of the N-mode approximation (5) with a rigorous estimate of the remainder term *for times of the order of the Bloch period*. Then, we numerically solve the N-mode approximation (5), and we compute the oscillating period taking into account the nonlinear interaction. In fact, the behavior of the wavefunction is not simply periodic in time; it turns out that the center of mass $\langle x\rangle^t = \langle\psi, x\psi\rangle$ shows an oscillating motion with modulated amplitude. The oscillating period turns out to be depending on the nonlinearity parameter strength γ and we see that it also depends on the distribution of the initial wavefunction ψ_0. In particular, when ψ_0 is a symmetric wavefunction then the oscillating period is almost constant for small γ and it practically coincides with the Bloch period T; on the other hand when ψ_0 is an asymmetrical function the oscillating period actually depends on γ. This fact is in contradiction with the Bloch Theorem (which holds true when $\gamma = 0$), which implies that the Bloch period T does not depend on the shape of the initial wavefunction, and it may explain the relatively large uncertainty observed by [14] in their experiments, as discussed in the Conclusions.

The paper is organized as follows. In Section 2 we derive the DNLS (5) from the NLS (4) in the semiclassical limit $\epsilon \to 0$ for times of the order of the Bloch period T with a rigorous estimate of the remainder term. In particular: in Section 2.1 we introduce the assumptions and we recall some preparatory results; in Section 2.2 we derive the DNLS by making use of some ideas, previously given by [18], adapted to the case of multiple-well potential with an external Stark-type perturbation. In Section 3 we consider a realistic experiment and we compute the wavefunction dynamics by making use of the DNLS. In particular: in Section 3.1 we discuss the validity of the N-mode approximation for different values of the parameters; in Section 3.2 we numerically compute the wavefunction for times of the order of the Bloch period. In the Appendix we write the Wannier functions in terms of the Mathieu functions.

Notation. Let g be a quantity depending on the semiclassical parameter ϵ. In the following

$$g = \tilde{\mathcal{O}}\left(e^{-S_0/\epsilon}\right)$$

means that for any $\epsilon^\star > 0$ and any $\rho \in (0, S_0)$ there exists $C := C_{\rho,\epsilon^\star} > 0$ such that

$$|g| \leq Ce^{-(S_0-\rho)/\epsilon}, \quad \forall \epsilon \in (0, \epsilon^\star).$$

By

$$g = \left(\epsilon^{+\infty}\right)$$

means that for any $\epsilon^\star > 0$ and any $M \in \mathbb{N}$ there exists $C := C_{M,\epsilon^\star} > 0$ such that

$$|g| \leq C\epsilon^M, \quad \forall \epsilon \in (0, \epsilon^\star).$$

Hereafter, by C we denote a generic positive constant independent of ϵ.

Let $N \in \mathbb{N}$, then by $\mathbb{N}_N := \{1, 2, \ldots, N\}$ we denote the set of first N positive integer numbers.

By $\|\cdot\|_{L^p}$ we denote the norm of the Banach space $L^p(\mathbb{R})$, by $\langle\cdot,\cdot\rangle$ we denote the scalar product of the Hilbert space $L^2(\mathbb{R})$.

2. Derivation of the DNLS (5)

2.1. Assumptions and preliminary results

We consider the time-dependent non-linear Schrödinger equation (4) where V_N is a multiple-well potential and $W_N(x)$ is a bounded Stark-type potential. In particular we assume that

Hypothesis 1. Let $V(x) \in C_0^\infty(\mathbb{R})$ be an even (i.e. $V(-x) = V(x)$) smooth function with compact support with a non degenerate minimum value at $x = 0$:

$$V(x) > V_{\min} = V(0), \quad \forall x \in \mathbb{R},\ x \neq 0.$$

The multiple-well potential is defined as

$$V_N(x) = \sum_{\ell=1}^{N} V(x - x_\ell)$$

for some fixed $N > 1$, where $x_\ell = \left(\ell - \frac{N+1}{2}\right) b$ and where $b > 0$ is such that $\operatorname{supp} V \subset \left(-\frac{b}{2}, +\frac{b}{2}\right)$.

Hence, by construction the potential $V_N(x)$ has exactly N wells with not degenerate minima at $x = x_\ell$, $\ell \in \mathbb{N}_N$.

Remark 1. We assume that $V(x)$ is an even function just for argument's sake. As discussed in Remark 6 this assumption may be removed. Furthermore, we assume that v is a smooth function as usual; in fact, a lesser regularity (e.g. C^2) would be enough.

Hypothesis 2. Let $W_N(x) \in C(\mathbb{R})$ be the monotone not decreasing function defined as

$$W_N(x) = \begin{cases} -L & \text{if } x < -L \\ x & \text{if } x \in [-L, L] \\ L & \text{if } x > L \end{cases}$$

for some $L > \frac{N+1}{2}b$.

That is the Stark-type potential W_N is linear in the region containing the wells and it is a constant function outside this region (see Fig. 1). In the "limit" where N goes to infinity the potential V_N becomes a periodic potential with period b and the external potential W_N becomes the Stark potential x.

Remark 2. We restrict ourselves to a multiple-well potential V_N with a finite number of wells only for sake of simplicity; one could consider the case of a periodic potential by making use of the tools developed by [20]. On the other side, the assumption on W_N is not merely for the sake of simplicity; actually, the Stark-type potential W_N is a bounded operator while the Stark potential x is not a bounded operator and this fact is a source of several technical problems. In fact, in real experiments the BEC is trapped in a finite spatial region.

Hypothesis 3. We assume to be in the **semiclassical limit**, that is we look for the solution of (4) in the limit of ϵ that goes to zero. We assume also that the other two parameters γ and f are small for ϵ small. That is we assume that there exists $\epsilon^\star > 0$ such that

$$Ce^{-(S_0-\rho)/\epsilon} \leq |f| \leq C\epsilon^s, \quad \forall \epsilon \in (0, \epsilon^\star),$$

for some $s > 2$, $C > 0$ and $\rho \in (0, S_0)$ independent of ϵ; furthermore, we assume also that

$$\frac{|\gamma|\epsilon^{-1/2}}{|f|} \leq C \tag{6}$$

for some positive constant C and for any $\epsilon \in (0, \epsilon^\star)$.

The self-adjoint extension of the linear Schrödinger operator formally defined on $L^2(\mathbb{R})$ as

$$H_N = -\epsilon^2 \partial_{xx}^2 + V_N$$

has an almost degenerate ground state with dimension N. More precisely, let $\{\lambda\}_{\ell\in\mathbb{N}_N}$ be the collection of the N lowest eigenvalues of H_N with each λ_ℓ associated normalized eigenvectors v_ℓ. In particular we have that (see Lemma 2 [23])

$$\lambda_\ell = \lambda_D - 2\beta \cos\left(\ell \frac{\pi}{N+1}\right) + O(\epsilon^\infty) e^{-S_0/\epsilon}, \quad \ell \in \mathbb{N}_N,$$

where

$$S_0 = \int_{x_0}^{x_1} \sqrt{V_N(x) - V_{\min}}\, dx > 0$$

is the Agmon distance between two wells. By λ_D we denote the ground state of the single well operator with associated eigenvector w;

$$\left[-\epsilon^2 \partial_{xx}^2 + V\right] w = \lambda_D w, \tag{7}$$

where the single well potential V has been introduced by Hypothesis 1. By w^{sc} we denote the semiclassical approximation of the eigenvector w. Since V is an even function then

$$w(-x) = w(x) \quad \text{and} \quad w^{sc}(-x) = w^{sc}(x).$$

The numerical pre-factor β is the hopping matrix element between neighboring wells, and it is such that 4β is asymptotic to the amplitude of the first band of the periodic Bloch operator H_B; i.e. $4\beta \sim B_1 := E_1^t - E_1^b$ where E_1^b and E_1^t are, respectively, the bottom and the top of the first band. Such a numerical pre-factor is going to be exponentially small, i.e.

$$\beta = \tilde{\mathcal{O}}(e^{-S_0/\epsilon}) \quad \text{as } \epsilon \to 0^+.$$

Remark 3. Hypothesis 3 means that, from a practical point of view, the parameter f cannot be arbitrarily small, but it has a lower bound of order β. On the other hand, the parameter γ may be arbitrarily small.

The associated normalized eigenvectors are given by [23]

$$v_\ell = \sum_{j=1}^N \alpha_{\ell,j} u_j^{sc} + O(\epsilon^\infty) e^{-S_0/\epsilon}$$

where

$$\alpha_{j,\ell} = \alpha_{\ell,j} = \sqrt{\frac{2}{N+1}} \sin\left(j\ell \frac{\pi}{N+1} \right)$$

and where $u_j^{sc}(x)$ is the semiclassical single well ground state eigenfunction localized on the jth cell; by construction

$$u_j^{sc}(x) = w^{sc}(x - x_j). \tag{8}$$

Now, let Π be the projection operator associated with the N eigenvalues λ_ℓ, i.e.

$$\Pi = \sum_{\ell=1}^N \langle v_\ell, \cdot \rangle v_\ell$$

and let

$$\Pi_c = 1 - \Pi.$$

Let $F = \Pi(L^2(\mathbb{R}))$ be the N-dimensional space spanned by the N eigenvectors v_ℓ, $\ell \in \mathbb{N}_N$.

Remark 4. Let $\sigma(H_N)$ be the spectrum of H_N; then it is a well known semiclassical result that

$$C^{-1}\epsilon \leq \operatorname{dist}\left(\{\lambda_\ell\}_{\ell=1}^N, \sigma(H_N) \setminus \{\lambda_\ell\}_{\ell=1}^N \right) \leq C\epsilon$$

for some positive constant $C > 0$. Hence, since H_N is a self-adjoint operator then (see formula 3.16 in Ch.V by [24]).

$$\left\| [H_N - \lambda_D]^{-1} \Pi_c \right\|_{\mathcal{L}(L^2 \to L^2)} \leq C\epsilon^{-1}$$

for some $C > 0$.

Remark 5. By [20] it has been proved that there exists a suitable orthonormal base u_ℓ, $\ell \in \mathbb{N}_N$, of the space F. The functions u_ℓ are practically localized on the ℓth well. More precisely, they are such that

i. $\|u_\ell - u_\ell^{sc}\|_{L^p} = \tilde{\mathcal{O}}\left(e^{-S_0/\epsilon}\right)$ for any $p \in [2, +\infty]$ and any $\ell \in \mathbb{N}_N$;
ii. $\|u_\ell u_j\|_{L^1} = \tilde{\mathcal{O}}\left(e^{-S_0|j-\ell|/\epsilon}\right)$ for any $j, \ell \in \mathbb{N}_N$;
iii. $\|u_\ell\|_{L^p} \leq C\epsilon^{-\frac{p-2}{4p}}$, $p \in [2, +\infty]$, and $\|\partial_x u_\ell\|_{L^2} \leq C\epsilon^{-1/2}$ for any $\ell \in \mathbb{N}_N$;
iv. The matrix with elements $\langle u_\ell, H_N u_j \rangle$ can be written as

$$\left(\langle u_\ell, H_N u_j \rangle \right) = \lambda_D 1_N - \beta \mathcal{T} + D_N$$

where $\mathcal{T}$ is the tridiagonal Toeplitz matrix such that

$$\mathcal{T}_{j,\ell} = \begin{cases} 0 & \text{if } |j-\ell| \neq 1 \\ 1 & \text{if } |j-\ell| = 1 \end{cases}$$

and where the remainder term D_N is a bounded linear operator from $\ell^p(\mathbb{N}_N)$ to $\ell^p(\mathbb{N}_N)$ with bound

$$\|D_N\|_{\mathcal{L}(\ell^p(\mathbb{N}_N) \to \ell^p(\mathbb{N}_N))} = \tilde{\mathcal{O}}\left(e^{-(S_0+\alpha)/\epsilon}\right), \quad p \in [1, +\infty],$$

for some $\alpha > 0$.

We finally assume that the initial state is prepared on the first N "ground states". That is

Hypothesis 4. $\Pi_c \psi_0 = 0$.

It is well known that under the assumptions above the NLS (4) is locally well posed, and the conservation of the norm and of the energy [25,26]

$$\mathcal{E}(\psi) = \langle \psi, H_N \psi \rangle + \frac{1}{2}\gamma \|\psi\|_{L^4}^4 + f\langle \psi, W_N \psi \rangle$$

easily follow:

$$\|\psi(\cdot, t)\|_{L^2} = \|\psi_0(\cdot)\|_{L^2} \quad \text{and} \quad \mathcal{E}(\psi(\cdot, t)) = \mathcal{E}(\psi_0(\cdot)).$$

Furthermore the following *a priori* estimate follows, too.

Lemma 1. *There exists a positive constant $C > 0$ such that*

$$\|\psi\|_{H^1} \leq C\epsilon^{-1/2} \quad \text{and} \quad \|\psi\|_{L^p}^p \leq C\epsilon^{-\frac{p-2}{4}}, \quad \forall p \in [2, +\infty].$$

Proof. Indeed, from Theorem 2 by [18] and its remarks it follows that

$$\|\nabla\psi\|_{L^2} \leq C\sqrt{\Lambda} \quad \text{and} \quad \|\psi\|_{L^p} \leq C\Lambda^{\frac{p-2}{4p}}$$

for some $C > 0$ and ϵ small enough, where

$$\Lambda = \frac{\mathcal{E}(\psi_0) - V_{\min}^f}{\epsilon^2}$$

and where $V_{\min}^f = \min_x[V_N(x) + fW_N(x)]$. In particular, since $fW_N(x) \geq -fL = O(\epsilon^s)$ for some $s > 2$, because L is fixed, and since $\Pi_c\psi_0 = 0$ then $\Lambda \sim \epsilon^{-1}$; therefore

$$\|\nabla\psi\|_{L^2} \leq C\epsilon^{-1/2} \quad \text{and} \quad \|\psi\|_{L^p} \leq C\epsilon^{-\frac{p-2}{4p}}. \quad \square$$

Hence, the global well-posedness of the NLS follows [25,26].

2.2. N-mode approximation

Let ψ be the normalized solution of the NLS equation written in the formula

$$\psi = \psi_1 + \psi_c, \quad \psi_1 = \Pi\psi = \sum_{\ell=1}^N c_\ell u_\ell \quad \text{and} \quad \psi_c = \Pi_c\psi, \tag{9}$$

for some complex-valued functions $c_\ell(t)$. By substituting (9) into the NLS (4) then it takes the formula

$$\begin{cases} i\epsilon\partial_t c_\ell = \langle u_\ell, H_N\psi_1 \rangle + \gamma\langle u_\ell, |\psi(\cdot,\tau)|^2\psi(\cdot,\tau)\rangle \\ \qquad + f\langle u_\ell, W_N\psi(\cdot,\tau)\rangle \\ i\epsilon\partial_t\psi_c = H_N\psi_c + \gamma\Pi_c|\psi(\cdot,\tau)|^2\psi(\cdot,\tau) \\ \qquad + f\Pi_c W_N\psi(\cdot,\tau). \end{cases} \tag{10}$$

We are going now to get an *a priori* estimate of the remainder term ψ_c. First of all we rescale the time $t \to \tau = \frac{\beta}{\epsilon}t$ and we redefine the wavefunction up to a gauge factor $\psi(x,t) \to \psi(x,\tau) := e^{-i\lambda_D t/\epsilon}\psi(x,t)$ (with abuse of notation let us denote by ψ both the former wavefunction $\psi(x,t)$ as well as the new wavefunction $\psi(x,\tau)$ depending on the slow time τ and obtained by the former one up to a phase factor). The Bloch period becomes

$$\tau_B = \frac{\beta}{\epsilon}T = \frac{2\pi\beta}{|f|b}.$$

Hence, (10) becomes (where $'$ denotes the derivative with respect to τ)

$$\begin{cases} i\beta c_\ell' = \langle u_\ell, (H_N - \lambda_D)\psi_1\rangle + \gamma\langle u_\ell, |\psi(\cdot,t)|^2\psi(\cdot,t)\rangle \\ \qquad + f\langle u_\ell, W_N\psi(\cdot,t)\rangle \\ i\beta\psi_c' = (H_N - \lambda_D)\psi_c + \gamma\Pi_c|\psi(\cdot,t)|^2\psi(\cdot,t) \\ \qquad + f\Pi_c W_N\psi(\cdot,t). \end{cases} \tag{11}$$

Theorem 1. *Suppose Hypotheses 1–4 be satisfied. Then the remainder ψ_c can be estimated in the time interval with size of order of the Bloch period. That is for any fixed $M \in \mathbb{N}$ it follows that*

$$\max_{\tau\in[0,M\tau_B]} \|\psi_c(\cdot,\tau)\|_{L^2} \le C\frac{|f|}{\epsilon}$$

for some positive constant $C > 0$.

Proof. From the first equation of (11) and recalling that

$$\sum_{\ell=1}^N |c_\ell(\tau)|^2 = \|\psi_1\|_{L^2}^2 = 1 - \|\psi_c\|_{L^2}^2 \le 1$$

then *a priori* estimate follows

$$\begin{aligned} |c_\ell'| &\le \frac{\langle u_\ell, (H_N-\lambda_D)\psi_1\rangle}{\beta} + \frac{|\gamma|}{\beta}\|\psi\|_{L^\infty}^2 + \frac{|f|}{\beta}\|W_N\|_{L^\infty} \\ &\le C + \frac{|\gamma|\epsilon^{-1/2}}{\beta} + \frac{|f|}{\beta}L \end{aligned} \tag{12}$$

because $\|u_\ell\|_{L^2} = 1$ and $\|\psi\|_{L^2} = 1$, and from Remark 5iv. and Lemma 1.

Concerning ψ_c it satisfies to the following integral equation

$$\psi_c = I + II$$

where we set

$$I := -\frac{i}{\beta}\int_0^\tau e^{-i(H_N-\lambda_D)(\tau-s)/\beta}\Pi_c A ds$$

$$II := -\frac{i}{\beta}\int_0^\tau e^{-i(H_N-\lambda_D)(\tau-s)/\beta}\Pi_c B ds$$

and where A and B are defined as

$$A := \gamma|\psi_1|^2\psi_1 + fW_N\psi_1$$

$$B := \gamma\left[\bar\psi_1\psi_c^2 + |\psi_c|^2\psi_c + 2|\psi_1|^2\psi_c + 2|\psi_c|^2\psi_1 + \psi_1^2\bar\psi_c\right] + fW_N\psi_c$$

such that

$$A + B = \gamma|\psi|^2\psi + fW_N\psi.$$

By means of standard arguments [18] and making use of the fact that the operator W_N is bounded then it follows that

Lemma 2. *Let*

$$\Gamma = |\gamma|\epsilon^{-1/2} + |f|.$$

Then the functions A and B are such that

$$\|A\|_{L^2} \le C\Gamma, \qquad \|B\|_{L^2} \le C\Gamma\|\psi_c\|_{L^2} \quad \text{and}$$

$$\left\|\frac{\partial A}{\partial\tau}\right\|_{L^2} \le C\Gamma^2\beta^{-1}.$$

Proof. Indeed,

$$\begin{aligned} \|A\|_{L^2} &\le |\gamma|\,\|\psi_1\|_{L^\infty}^2\|\psi_1\|_{L^2} + |f|\,\|W_N\|_{L^\infty}\|\psi_1\|_{L^2} \\ &\le C\left[|\gamma|\epsilon^{-1/2} + |f|\right] \end{aligned}$$

since $\|\psi_1\|_{L^\infty} \le C\max_\ell \|u_\ell\|_{L^\infty} \le C\epsilon^{-1/4}$. Similarly, the estimate of the function B follows recalling that $\|\psi_c\|_{L^\infty} \le C\epsilon^{-1/4}$ from Lemma 1. Finally, the estimate concerning $\frac{\partial A}{\partial \tau}$ immediately follows from (12). □

Hence, the estimates of the integrals I and II follow; in particular, integral II can be simply estimated as

$$\|II\|_{L^2} \le C\Gamma\beta^{-1}\int_0^\tau \|\psi_c(\cdot,s)\|_{L^2}ds$$

since

$$\left\|e^{-i(H_N-\lambda_D)(\tau-s)/\beta}\right\|_{\mathcal{L}(L^2\to L^2)} = 1.$$

On the other hand, before to get the estimate of integral I we perform an integration by parts in order to gain a pre-factor β:

$$\begin{aligned} I &= \left[-ie^{-i(H_N-\lambda_D)(\tau-s)/\beta}[H_N-\lambda_D]^{-1}\Pi_c A\right]_0^\tau \\ &\quad + i\int_0^\tau e^{-i(H_N-\lambda_D)(\tau-s)/\beta}[H_N-\lambda_D]^{-1}\Pi_c\frac{\partial A}{\partial s}ds. \end{aligned}$$

From this fact and recalling that (Remark 4)

$$\|[H_N-\lambda_D]^{-1}\Pi_c\|_{\mathcal{L}(L^2\to L^2)} \le C\epsilon^{-1}$$

then

$$\begin{aligned} \|I\|_{L^2} &\le C\epsilon^{-1}\max_{s\in[0,\tau]}\left[\|A\|_{L^2} + \tau\left\|\frac{\partial A}{\partial s}\right\|_{L^2}\right] \\ &\le C\epsilon^{-1}\Gamma[1+\Gamma\beta^{-1}\tau]. \end{aligned}$$

Therefore, we have that

$$\|\psi_c\|_{L^2} \le C\Gamma\beta^{-1}\int_0^\tau \|\psi_c(\cdot,s)\|_{L^2}ds + C\epsilon^{-1}\Gamma(1+\Gamma\beta^{-1}\tau).$$

From the Gronwall's lemma it follows that

$$\|\psi_c(\cdot,\tau)\|_{L^2} \le C\epsilon^{-1}\Gamma(1+\Gamma\beta^{-1}\tau)e^{C\Gamma\beta^{-1}\tau}.$$

In particular we observe that

$$\begin{aligned} \max_{\tau\in[0,M\tau_B]}\|\psi_c(\cdot,\tau)\|_{L^2} &\le C\epsilon^{-1}\Gamma(1+\beta^{-1}\Gamma M\tau_B)e^{C\Gamma\beta^{-1}M\tau_B} \\ &\le C\Gamma\epsilon^{-1} \le C\frac{|f|}{\epsilon} \end{aligned}$$

proving the Theorem since $\Gamma \le C|f|$ from Hypothesis 3 and since $\tau_B = \frac{2\pi}{b}\frac{\beta}{|f|}$. □

We are going now to estimate the solutions c_ℓ of the first equation of (11) which can be written as

$$i\beta c_\ell' = \langle u_\ell, (H_N-\lambda_D)\psi_1\rangle + \langle u_\ell, A\rangle + \langle u_\ell, B\rangle$$

where the term $\langle u_\ell, (H_N-\lambda_D)\psi_1\rangle$ can be represented by property iv. of Remark 5. Concerning the term $\langle u_\ell, B\rangle$ the following estimate uniformly holds with respect to the index ℓ

$$|\langle u_\ell, B\rangle| \le \|B\|_{L^2} \le C\Gamma\|\psi_c\|_{L^2}.$$

Furthermore

$$\begin{aligned} \langle u_\ell, A\rangle &= \gamma\sum_{j,k,m=1}^N \bar c_j c_k c_m\langle u_\ell, \bar u_j u_k u_m\rangle + f\sum_{j=1}^N c_j\langle u_\ell, W_N u_j\rangle \\ &= \gamma|c_\ell|^2 c_\ell\|u_\ell\|_{L^4}^4 + fc_\ell\langle u_\ell, W_N u_\ell\rangle + \gamma r_\ell^a + fr_\ell^b \end{aligned}$$

where

$$r_\ell^a = \sum_{j,k,m\in\mathbb{N}_N : |j-\ell|+|m-\ell|+|k-\ell|>0} \bar c_j c_k c_m\langle u_\ell, \bar u_j u_k u_m\rangle$$

and

$$r_\ell^b = \sum_{j,\ell\in\mathbb{N}_N,\, j\ne\ell} c_j\langle u_\ell, W_N u_j\rangle$$

are remainder terms.

We have that

Lemma 3. *The following estimates uniformly hold with respect to the indexes ℓ, j, m and k:*

i. $\langle u_\ell, W_N u_\ell\rangle = \ell b - \frac{N+1}{2}b + \tilde{\mathcal{O}}\left(e^{-S_0/\epsilon}\right)$;
ii. $\langle u_\ell, W_N u_j\rangle = \tilde{\mathcal{O}}\left(e^{-S_0|j-\ell|/\epsilon}\right)$;

iii. $\langle u_\ell, \bar{u}_j u_m u_k\rangle = \tilde{\mathcal{O}}\left(e^{-S_0 r/\epsilon}\right)$ *where*

$$r = \max\left[|j-\ell|, |m-\ell|, |k-\ell|, |j-m|, |j-k|, |k-m|\right].$$

Proof. Indeed, let $I_\ell = [x_\ell - b, x_\ell + b]$, $\ell = 1, 2, \ldots, N$, then

$$\langle u_\ell, W_N u_\ell\rangle = \int_{I_\ell} |u_\ell(x)|^2 x dx + \int_{\mathbb{R}\setminus I_\ell} |u_\ell(x)|^2 W_N(x) dx$$

where $u_\ell(x) = w(x - x_\ell) + \tilde{\mathcal{O}}\left(e^{-S_0/\epsilon}\right)$ from (8) and Remark 4. Therefore

$$\int_{I_\ell} |u_\ell(x)|^2 x dx = x_\ell \int_{I_0} |w(x)|^2 dx + \int_{I_0} |w(x)|^2 x dx + \tilde{\mathcal{O}}\left(e^{-S_0/\epsilon}\right)$$
$$= x_\ell \left[\|w\|^2_{L^2} - \|w\|^2_{L^2(\mathbb{R}\setminus I_0)}\right] + \tilde{\mathcal{O}}\left(e^{-S_0/\epsilon}\right)$$

where w is normalized and $\int_{I_0} |w(x)|^2 x dx = 0$ because $w(x) = w(-x)$. From this fact and since $\|u_\ell\|_{L^2(\mathbb{R}\setminus I_\ell)} = \tilde{\mathcal{O}}(e^{-S_0/\hbar})$ (see Lemma 4iii. and Lemma 5 by [20]) then the asymptotic behavior i. follows. The other two asymptotic behaviors ii. and iii. similarly follow from property ii. by Remark 5; indeed

$$|\langle u_\ell, W_N u_j\rangle| \leq \|W_N\|_{L^\infty} \|u_\ell u_j\|_{L^1} = \tilde{\mathcal{O}}\left(e^{-S_0|j-\ell|/\epsilon}\right)$$

and, where we assume that $r = |j - \ell|$,

$$|\langle u_\ell, \bar{u}_j u_m u_k\rangle| \leq \|u_m\|_{L^\infty} \|u\|_{L^\infty} \|u_\ell u_j\|_{L^1} = \tilde{\mathcal{O}}\left(e^{-S_0 r/\epsilon}\right)$$

proving so the estimates ii. and iii. □

From this lemma, from the previous computation and from the gauge transformation ($c_\ell \to c_\ell e^{-i\frac{N+1}{2\beta}b\tau}$) it follows that the first equation of (11) becomes a DNLS of the form

$$i\beta c'_\ell = -\beta \sum_{m=1}^N \mathcal{T}_{\ell,m} c_m + \gamma \|u_\ell\|^4_{L^4} |c_\ell|^2 c_\ell + f\ell b c_\ell + \tilde{\mathcal{O}}\left(e^{-S_0/\epsilon}\right) \quad (13)$$

where

$$\|u_\ell\|^4_{L^4} = \|w\|^4_{L^4} + \tilde{\mathcal{O}}\left(e^{-S_0/\epsilon}\right)$$

and where the remainder terms $\tilde{\mathcal{O}}\left(e^{-S_0/\epsilon}\right)$ are uniform with respect to the index ℓ.

Remark 6. In fact, if $V(x)$ is not an even function then by means of standard semiclassical arguments it follows that property Lemma 3i. becomes

$$\langle u_\ell, W_N u_\ell\rangle = \ell b + c + \tilde{\mathcal{O}}\left(e^{-S_0/\epsilon}\right)$$

for some constant c independent of the index ℓ. In such a case we must add the term fcc_ℓ to the right hand side of the DNLS above and, by means of a gauge choice $c_\ell \to c_\ell e^{-i\frac{fc}{\beta}\tau}$, we can remove this term obtaining again Eq. (13).

Now, we are able to prove that

Theorem 2. *Let $d_\ell(\tau)$ be the solutions of the DNLS*

$$i\beta d'_\ell = -\beta \sum_{m=1}^N \mathcal{T}_{\ell,m} d_m + \gamma \|w^{sc}\|^4_{L^4} |d_\ell|^2 d_\ell + f\ell b d_\ell \quad (14)$$

satisfying the initial conditions $d_\ell(0) = c_\ell(0)$, where $c_\ell(\tau)$ and ψ_c are the solutions of (11). Then, for any fixed $M \in \mathbb{N}$ it follows that

$$\max_{\tau\in[0,M\tau_B],\ \ell=1,2,\ldots,N} |c_\ell(\tau) - d_\ell(\tau)| = \tilde{\mathcal{O}}\left(e^{-S_0/\epsilon}\right) \quad \text{as } \epsilon \to 0.$$

Proof. The proof is a simply consequence of Eq. (13) and from the fact that $\tau_B = \frac{2\pi}{b}\frac{\beta}{f}$ and Hypothesis 3. □

3. Numerical analysis of a real model

We consider the experiment where a cloud of ultracold Strontium atoms ^{88}Sr are trapped in a one-dimensional optical lattice with potential (2). Realistic data for the experiment are [14]:

- Lattice period: $b = \lambda_L/2 = 266$ nm, $\lambda_L = 532$ nm;
- Lattice potential depth: $V_0 = \Lambda_0 \cdot E_R$ where E_R is the photon recoil energy $E_R = \frac{2\pi^2\hbar^2}{m\lambda_L^2} = 50.38$ kHz $\cdot\, \hbar$ and where Λ_0 is between 3 and 10;
- Mass of the Strontium 88 isotope: $m = 87.91$ a.u. $= 1.46 \cdot 10^{-22}$ gr;
- Effective one-dimensional nonlinearity strength: let $\gamma_{3D} = \frac{4\mathcal{N}\pi a_s \hbar^2}{m}$ be the effective nonlinearity strength for the three-dimensional Gross–Pitaevskii equation, then it is expected that the effective one-dimensional nonlinearity strength γ is of the order [27]

  $$\gamma \approx \frac{\gamma_{3D}}{2\pi d_\perp^2}$$

  where $d_\perp$ is the oscillator length of the transverse confinement; here a_s denotes the scattering length of the Strontium 88 isotope: $a_s = -a_0 \div 13a_0$, where a_0 is the Bohr radius; $\mathcal{N}$ is the number of atoms of the condensate; in typical experiments $d_\perp \approx 180 \cdot 10^{-6}$ m and $\mathcal{N} = 10^5 \div 10^6$;
- Acceleration constant $g = 9.807$ m/s^2.

The confined BEC is governed by Eq. (4) and here we make use of the N-mode approximation (14), that is the wavefunction ψ has the form $\psi \sim \sum_\ell c_\ell u_\ell$ where c_ℓ are the solutions of (14) and where u_ℓ are functions localized on the ℓth lattice site. In order to justify the validity of such an approximation we will check if the model is in the *semiclassical regime*, that is if the first band is almost flat and if semi-classical approximation u_ℓ^{sc} agrees or not with the Wannier function $\mathcal{W}_1(x - x_\ell)$. Such a qualitative criterion has been also adopted by other authors [28–30] and we will see that our results agree with the results contained in these papers. In particular, in [30] has been computed the hopping matrix elements $\langle u_\ell, H_N u_j\rangle$ too, where it has been numerically verified that these coefficients are negligible when $|j - \ell| > 1$ for $\Lambda_0 \geq 10$; thus, for such values of Λ_0 it is admitted that the N-mode approximation, consisting to describe (4) in terms of a nearest-neighbor model (14), works.

3.1. Validity of the semiclassical approximation

The semiclassical approximation $w^{sc}(x)$ of the wavefunction has dominant behavior

$$w^{sc}(x) = \frac{(m\mu)^{1/8}}{(\pi\hbar)^{1/4}} e^{-\sqrt{m\mu}x^2/2\hbar} \quad (15)$$

in the semiclassical limit, where $\mu = \frac{d^2 V_{per}(0)}{dx^2} = 2V_0 k_L^2$, $V_0 = \Lambda_0 E_R$; it is normalized $\|w^{sc}\|_{L^2} = 1$. We may remark that the effective semiclassical parameter in adimensional units is given by

$$\frac{1}{\sqrt{\Lambda_0}} = \frac{2\pi^2\hbar}{b^2\sqrt{m\mu}},$$

and then the semiclassical approximation may be written as

$$w^{sc}(x) = \left[\frac{2\pi\sqrt{\Lambda_0}}{b^2}\right]^{1/4} e^{-x^2\pi^2\sqrt{\Lambda_0}/b^2}.$$

Hence

$$\|w^{sc}\|^4_{L^4} = \left[\frac{m\mu}{(\pi\hbar)^2}\right]^{1/4} \sqrt{\frac{\pi}{2}} = \frac{\pi\Lambda_0^{1/4}}{b}.$$

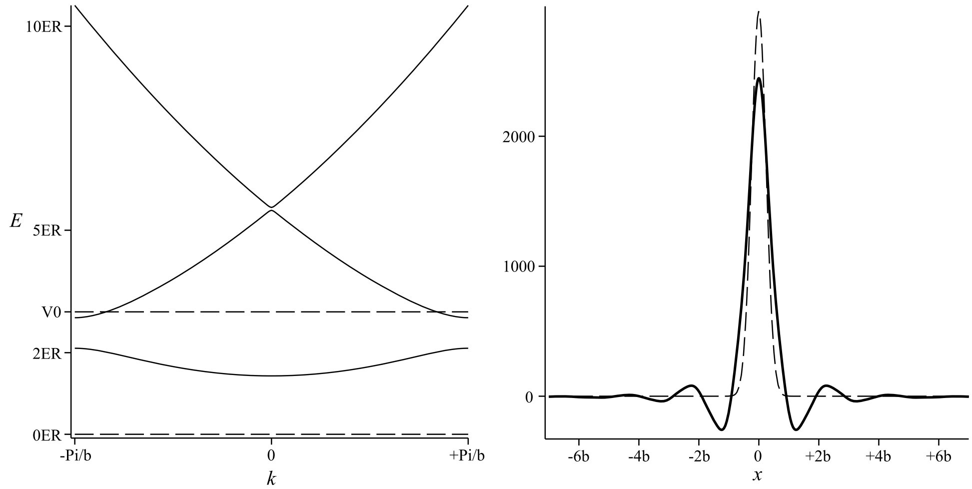

Fig. 2. Here we plot in the left hand side panel the first three band functions $E_n(k)$, $n=1,2,3$ and $k \in \left[-\frac{\pi}{b}, +\frac{\pi}{b}\right]$, for the Bloch operator H_B where $\Lambda_0 = 3$. It turns out that the width of the first gap is of the same order of the width of the first band. In the right hand side panel we plot the graph of the functions w^{sc} (broken line) and $\mathcal{W}_1$ (full line).

We will see that for Λ_0 "large enough" (i.e. $\Lambda_0 \geq 10$) then the first band is almost flat and the semiclassical function w^{sc} well approximates the Wannier function $\mathcal{W}_1$, as we expect to observe in the semiclassical limit $\Lambda_0 \to \infty$ (see, e.g., [31]).

Remark 7. By the scaling

$$x \to 2k_L x, \quad t \to E_R t/\hbar, \qquad \psi(x) \to \frac{1}{\sqrt{2k_L}} \psi\left(\frac{x}{2k_L}\right)$$

and setting

$$F = \frac{mg}{2E_R k_L}, \qquad \zeta = \frac{\gamma}{2E_R k_L}, \qquad \epsilon = \frac{1}{\sqrt{\Lambda_0}}$$

then (3) takes the form

$$\begin{aligned} &i\partial_t \psi = -\partial^2_{xx}\psi + \frac{1}{\epsilon^2}\sin^2(x/2) + Fx\psi + \zeta|\psi|^2\psi, \\ &\|\psi\|_{L^2} = 1. \end{aligned} \tag{16}$$

Eq. (16) is equivalent, up to a change of scale of the time, to the equation

$$i\epsilon\partial_t\psi = -\epsilon^2\partial^2_{xx}\psi + \sin^2\left(\frac{x}{2}\right)\psi + fx\psi + \gamma|\psi|^2\psi$$

where we set

$$t \to t/\sqrt{\epsilon}, \qquad f = F\epsilon^2, \qquad \gamma = \epsilon^2\zeta$$

and where $\epsilon = \Lambda_0^{-1/2}$ plays the role of the semiclassical parameter.

We compute now the band functions and the Wannier functions for different values of Λ_0. The semiclassical wavefunction w^{sc} is computed by (15), while the Wannier function $\mathcal{W}_1(x)$ may be computed by means of the Mathieu functions (see Appendix).

3.1.1. Model $\Lambda_0 = 3$

The first bands of the Bloch operator $H_B = -\frac{\hbar^2}{2m}\partial^2_{xx} + \Lambda_0 E_R \sin^2(k_L x)$ have endpoints

$(n=1)$ $E_1^b = 1.43 \cdot E_R$ and $E_1^t = 2.11 \cdot E_R$;
$(n=2)$ $E_2^b = 2.86 \cdot E_R$ and $E_2^t = 5.49 \cdot E_R$;
$(n=3)$ $E_3^b = 5.56 \cdot E_R$ and $E_3^t = 10.51 \cdot E_R$.

Hence, the values of the width of the first two bands are given by

$$B_1 := E_1^t - E_1^b = 0.68 \cdot E_R \quad \text{and} \quad B_2 := E_2^b - E_1^t = 2.63 \cdot E_R.$$

Furthermore it follows that the first gap has amplitude $g_1 = E_2^b - E_1^t = 0.77 \cdot E_R$ of the order of the first band amplitude, while the width of the other gaps is very small (see Fig. 2, left hand side panel). If we compare the first Wannier function $\mathcal{W}_1(x)$ and the semiclassical approximation $w^{sc}(x)$ it turns out that (see also Fig. 2, right hand side panel)

$$\|\mathcal{W}_1 - w^{sc}\|^2_{L^2} = 0.091.$$

3.1.2. Model $\Lambda_0 = 10$

The first bands of the Bloch operator H_B have endpoints

$(n=1)$ $E_1^b = 4.32 \cdot E_R$ and $E_1^t = 4.58 \cdot E_R$;
$(n=2)$ $E_2^b = 7.02 \cdot E_R$ and $E_2^t = 8.87 \cdot E_R$;
$(n=3)$ $E_3^b = 9.54 \cdot E_R$ and $E_3^t = 14.07 \cdot E_R$.

Hence, the values of the width of the first two bands are given by

$$B_1 := E_1^t - E_1^b = 0.26 \cdot E_R \quad \text{and} \quad B_2 := E_2^b - E_1^t = 1.85 \cdot E_R.$$

Furthermore it also follows that the first gap has amplitude $g_1 = E_2^b - E_1^t = 2.44 \cdot E_R$ is much larger than the amplitude of the first band and that the width of the other gaps is very small (see Fig. 3, left hand side panel). If we compare the first Wannier function $\mathcal{W}_1(x)$ and the semiclassical approximation $w^{sc}(x)$ it turns out that (see also Fig. 3, right hand side panel)

$$\|\mathcal{W}_1 - w^{sc}\|^2_{L^2} = 0.055.$$

Hence, we may conclude that for $\Lambda_0 = 10$ the N-mode approximation properly works.

3.2. Numerical analysis of the model for $\Lambda_0 = 10$

We have seen that for $\Lambda_0 \geq 10$ the N-mode approximation is justified. For $\Lambda_0 = 10$ we have that

$$\beta \sim \frac{1}{4}B_1 = 0.065 \cdot E_R.$$

Eq. (14) takes the form

$$id'_\ell = -\sum_{m=1}^N \mathcal{T}_{\ell,m} d_m + \eta|d_\ell|^2 d_\ell + \ell\delta d_\ell, \quad \ell \in \mathbb{N}_N,$$

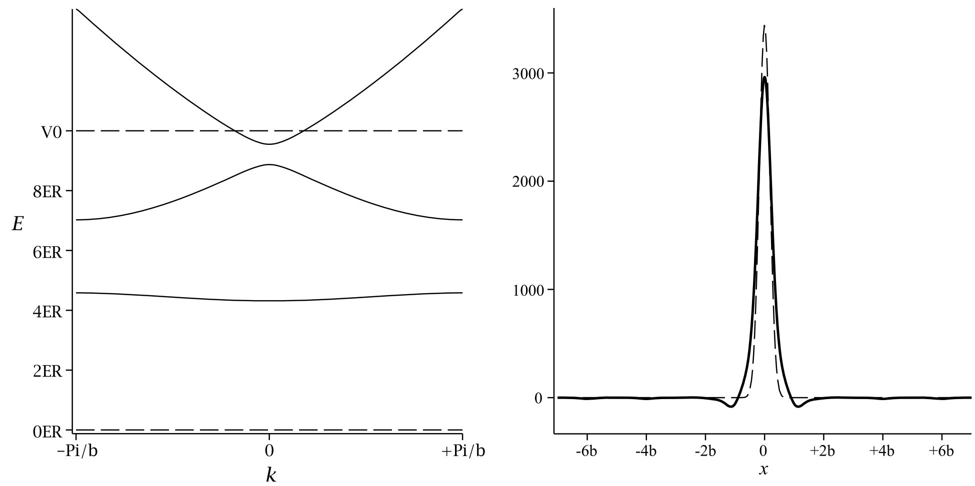

Fig. 3. Here we plot in the left hand side panel the first three band functions $E_n(k)$, $n = 1, 2, 3$ and $k \in \left[-\frac{\pi}{b}, +\frac{\pi}{b}\right]$, for the Bloch operator H_B where $\Lambda_0 = 10$. It turns out that the first band is almost flat, in fact its width is 1/10th of the width of the first gap. In the right hand side panel we plot the graph of the functions w^{sc} (broken line) and $\mathcal{W}_1$ (full line).

where we set

$$\eta = \frac{\gamma \|w^{sc}\|_{L^4}^4}{\beta} \approx \frac{4\mathcal{N}\pi a_s \hbar^2}{m} \frac{\pi \Lambda_0^{1/4}}{b} \frac{1}{2\pi d_\perp^2} \frac{1}{\beta}$$
$$= -0.151 \cdot 10^{-1} \div 0.197$$

and

$$\delta = \frac{fb}{\beta} = \frac{mgb}{\beta} = 1.103.$$

The Bloch period is given by

$$T = \frac{2\pi\hbar}{mgb} = 1.740 \text{ ms}.$$

Hence, the parameters f, γ and β are in a suitable range as discussed in Remark 3. Furthermore, the motion of the Bloch oscillator occurs in an interval with width

$$\frac{B_1}{|f|} = \frac{0.26 \cdot E_R}{mg} = 9.65 \cdot 10^{-7} \text{ m} \approx 3.6 \cdot b. \tag{17}$$

Hence, the N-mode approximation with $N = 40$ properly works.

We consider three different situations. In the first one we assume that the state is initially prepared on a single lattice site, that is ψ_0 is a Wannier type function. In the other two cases we assume that the initial wavefunction ψ_0 is a symmetric or asymmetrical wavefunction initially prepared on different lattice sites.

3.2.1. *ψ_0 is initially prepared on a single lattice cell*

We consider a numerical experiment where $\psi_0(x) = u_{N/2}(x)$, that is $c_\ell(0) = 0$, for $\ell \neq N/2$, and $c_{N/2}(0) = 1$ (where $N = 40$). In fact, in such a case we observe a *breathing motion* for the wavefunction; that is, the wavefunction, initially prepared in a Wannier state localized on a single site of the optical lattice, symmetrically spreads in space and it periodically returns to its initial shape (Fig. 4, top panel, obtained for $\eta = 0.2$). Then the expected value of the center of mass

$$\langle x \rangle^t = \langle \psi(\cdot, t), x\psi(\cdot, t)\rangle$$

is practical constant $\langle x \rangle^t \approx 0$ up to small fluctuations.

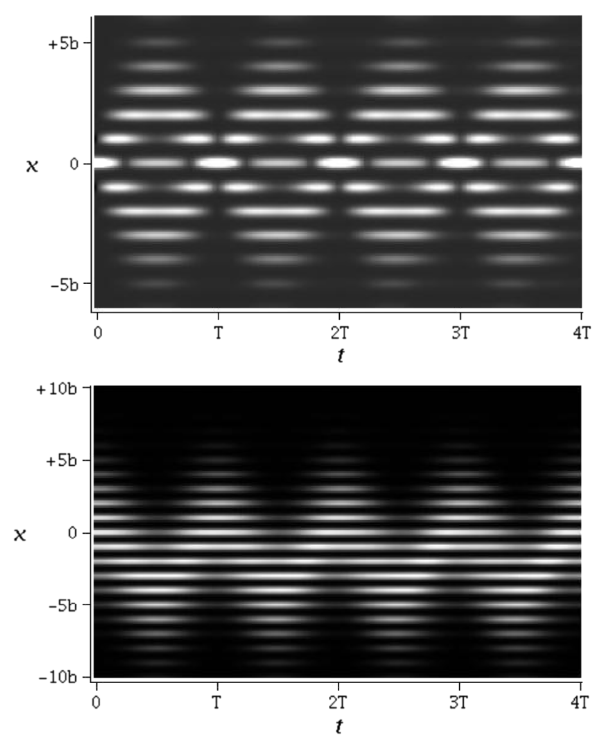

Fig. 4. In the top panel we plot the absolute value of the wavefunction $\psi(x, t)$ initially prepared on a single Wannier state for $\eta = 0.2$, it turns out that it symmetrically spreads in space and periodically returns to its initial shape without motion of the center of mass. In the bottom panel we plot the absolute value of the wavefunction initially prepared on several lattice sites for $\eta = 0.2$; it turns out that the center of mass oscillates with no marked changes of the shape of the wavefunction. Here T denotes the Bloch period and b is the distance between two adjacent wells. Dark regions mean that $|\psi(x, t)|$ is practically zero there, white regions mean that $|\psi(x, t)|$ has its maximum value there.

3.2.2. *ψ_0 is a symmetric wavefunction initially prepared on different lattice cells*

We consider a numerical experiment where $N = 40$ and $\psi_0(x) = \sum_{\ell=0}^{40} c_\ell u_\ell(x)$, where c_ℓ have a symmetric Gaussian-type distribution around $\ell = N/2$. That is the initial value of the coefficients $c_\ell(t)$ is given in Table 1, the initial wavefunction ψ_0 is plotted in Fig. 5, left hand side panel. In such a case the center of mass $\langle x \rangle^t$ oscillates in space and the wavefunction moves with no marked changes in shape (see Fig. 4, bottom panel). In particular,

Table 1
Initial values of the coefficients $c_\ell := c_\ell(0)$ of the wavefunction. The initial wavefunction ψ_0 has a symmetric shape and its width is of order of several lattice periods.

$c_0 = 0$	$c_{10} = 0.396 \cdot 10^{-3}$	$c_{21} = 0.429$	$c_{31} = 0.898 \cdot 10^{-4}$
$c_1 = 0$	$c_{11} = 0.151 \cdot 10^{-2}$	$c_{22} = 0.347$	$c_{32} = 0.177 \cdot 10^{-4}$
$c_2 = 0$	$c_{12} = 0.502 \cdot 10^{-2}$	$c_{23} = 0.244$	$c_{33} = 0.303 \cdot 10^{-5}$
$c_3 = 0$	$c_{13} = 0.149 \cdot 10^{-1}$	$c_{24} = 0.149$	$c_{34} = 0$
$c_4 = 0$	$c_{14} = 0.363 \cdot 10^{-1}$	$c_{25} = 0.788 \cdot 10^{-1}$	$c_{35} = 0$
$c_5 = 0$	$c_{15} = 0.788 \cdot 10^{-1}$	$c_{26} = 0.363 \cdot 10^{-1}$	$c_{36} = 0$
$c_6 = 0$	$c_{16} = 0.149$	$c_{27} = 0.149 \cdot 10^{-1}$	$c_{37} = 0$
$c_7 = 0.303 \cdot 10^{-5}$	$c_{17} = 0.244$	$c_{28} = 0.502 \cdot 10^{-2}$	$c_{38} = 0$
$c_8 = 0.177 \cdot 10^{-4}$	$c_{18} = 0.347$	$c_{29} = 0.151 \cdot 10^{-2}$	$c_{39} = 0$
$c_9 = 0.898 \cdot 10^{-4}$	$c_{19} = 0.429$	$c_{30} = 0.396 \cdot 10^{-3}$	$c_{40} = 0$
	$c_{20} = 0.460$		

Table 2
Initial values of the coefficients $c_\ell := c_\ell(0)$ of the wavefunction. The initial wavefunction ψ_0 has an asymmetrical shape and its width is of order of several lattice periods.

$c_0 = 0$	$c_{10} = 0.180 \cdot 10^{-3}$	$c_{21} = 0.252$	$c_{31} = 0.175 \cdot 10^{-4}$
$c_1 = 0$	$c_{11} = 0.814 \cdot 10^{-3}$	$c_{22} = 0.170$	$c_{32} = 0.323 \cdot 10^{-5}$
$c_2 = 0$	$c_{12} = 0.330 \cdot 10^{-2}$	$c_{23} = 0.103$	$c_{33} = 0$
$c_3 = 0$	$c_{13} = 0.121 \cdot 10^{-1}$	$c_{24} = 0.546 \cdot 10^{-1}$	$c_{34} = 0$
$c_4 = 0$	$c_{14} = 0.414 \cdot 10^{-1}$	$c_{25} = 0.257 \cdot 10^{-1}$	$c_{35} = 0$
$c_5 = 0$	$c_{15} = 0.133$	$c_{26} = 0.106 \cdot 10^{-1}$	$c_{36} = 0$
$c_6 = 0$	$c_{16} = 0.351$	$c_{27} = 0.386 \cdot 10^{-2}$	$c_{37} = 0$
$c_7 = 0$	$c_{17} = 0.496$	$c_{28} = 0.123 \cdot 10^{-2}$	$c_{38} = 0$
$c_8 = 0.614 \cdot 10^{-5}$	$c_{18} = 0.471$	$c_{29} = 0.340 \cdot 10^{-3}$	$c_{39} = 0$
$c_9 = 0.354 \cdot 10^{-4}$	$c_{19} = 0.411$	$c_{30} = 0.826 \cdot 10^{-4}$	$c_{40} = 0$
	$c_{20} = 0.336$		

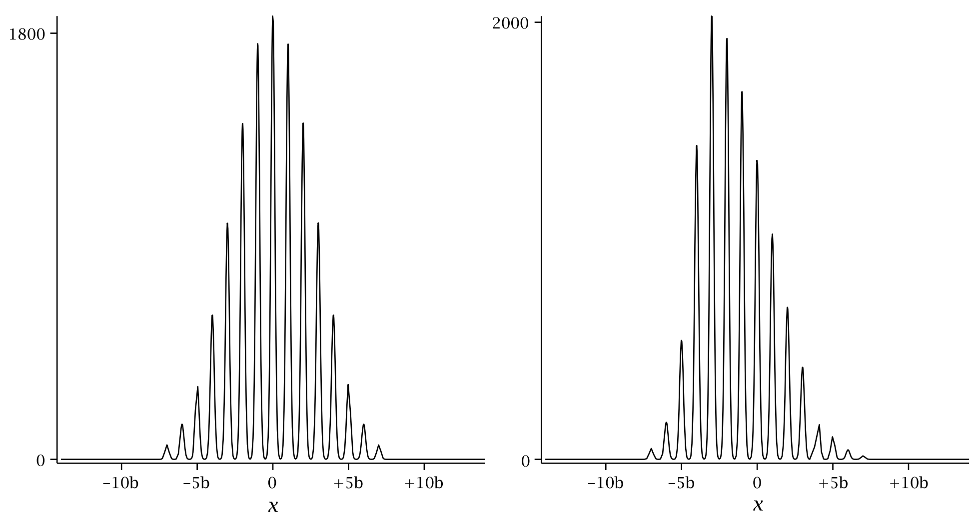

Fig. 5. Here we plot the absolute value of the initial wavefunction ψ_0 prepared on several lattice sites; the left hand side panel corresponds to the symmetric initial wavefunction, the right hand side panel corresponds to the asymmetrical one.

the function $\langle x \rangle^t$ exhibits, for $\eta \neq 0$, an oscillating motion where the wavefunction amplitude is modulated (see Fig. 6) and where the oscillating (pseudo-)period (that is the time interval between two consecutive minima or maxima points) depends on η. In Fig. 7 we plot the mean value of the oscillating period of the motion of the center of mass after 14 oscillations for η in the range $[-0.1, +0.2]$; it turns out that the relative uncertainty with respect to the Bloch period is of order $2.4 \cdot 10^{-5}$.

3.2.3. ψ_0 is an asymmetrical wavefunction initially prepared on different lattice cells

We consider a numerical experiment where $N = 40$ and $\psi_0(x) = \sum_{\ell=0}^{40} c_\ell u_\ell(x)$, where c_ℓ have an asymmetrical Gaussian-type distribution. That is the initial value of the coefficients $c_\ell(t)$ is given in Table 2, the initial wavefunction is plotted in Fig. 5, right hand side panel. As in the symmetric case the center of mass $\langle x \rangle^t$ oscillates in space and the wavefunction moves with no marked changes in shape. Even in such a case the function $\langle x \rangle^t$ exhibits, for $\eta \neq 0$, an oscillating motion where the wavefunction amplitude is modulated (see Fig. 8). In contrast with the symmetric case the oscillating (pseudo-)period (that is the time interval between two consecutive minima or maxima points) actually depends on η; in Fig. 7 we plot the mean value of the oscillating period of the center of mass after 14 oscillations for η in the range $[-0.1, +0.2]$ and it is not almost constant like in the previous case, in particular it turns out that the relative uncertainty with respect to the Bloch period is of order $4.6 \cdot 10^{-4}$, which is 20 times the relative uncertainty observed in the symmetrical case.

4. Conclusion

In this paper we have proved that in the semiclassical limit the N-mode approximation (14), corresponding to a discrete nonlinear

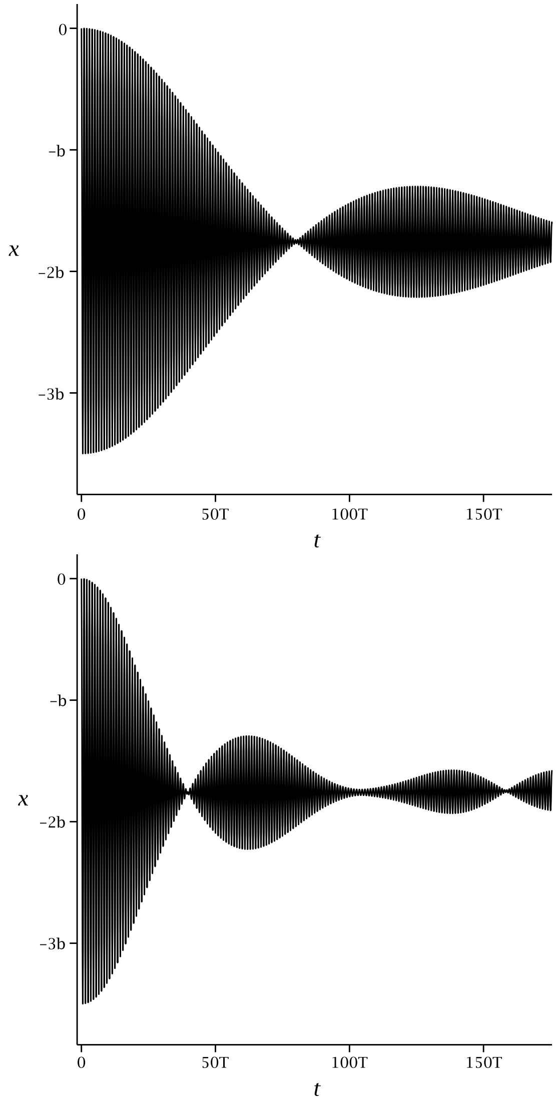

Fig. 6. Here we plot the motion of the center of mass of the wavefunction initially prepared on several lattice sites. The initial wavefunction is a symmetric function. Top panel corresponds to the case of $\eta = 0.1$, bottom panel corresponds to the case of $\eta = 0.2$. The center of mass rapidly oscillates with modulation of the amplitude. The width of the oscillations is in a range lesser or equal to $3b$ in agreement with (17).

Schrödinger equation with a finite number of modes, gives the solution of the Gross–Pitaevskii equation (4) for a BEC in a multiple-well lattice in a Stark-type external field. Furthermore, we have numerically solved the N-mode approximation considering a real model, where for some values of the physical parameters the validity of the N-mode approximation (14) seems to be justified. In particular, we have seen that a state initially prepared on several wells has an oscillating behavior with modulated amplitude, the oscillating (pseudo-)period is computed for different values of the nonlinear strength and it turns out that such a period is practically constant when the initial state is a symmetric one; on the other side, such a period actually depends on the nonlinear strength when the initial state is an asymmetrical one. This observation opens a question about the validity of the method proposed by Cladé et al. [12] for the determination of the gravitational constant g by means of the measurement of the oscillating period [13,14], where it has been assumed that the oscillating period coincides with the Bloch period T independently from the shape of the initial wavefunction and of the value of the nonlinearity strength parameter.

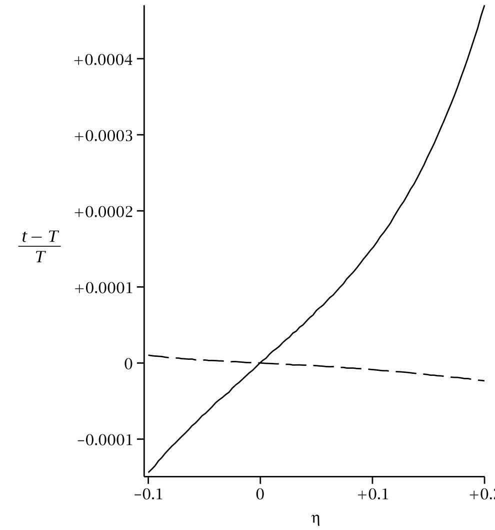

Fig. 7. Here we plot the mean value of the pseudo-period of the oscillating motion of the center of mass after 14 oscillations, as function of the effective nonlinearity parameter η. Broken line corresponds to the case of a symmetric wavefunction prepared on several lattice sites; it turns out that in such a case the oscillating period is almost constant. Full line corresponds to the case of an asymmetrical wavefunction prepared on several lattice sites; it turns out that it actually depends on η. Here T denotes the Bloch period, while t denotes the oscillating period.

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Appendix. Band functions and Wannier functions

For a generic one-dimensional Bloch operator H_B the spectrum is given by a sequence of infinitely many closed intervals named bands. These intervals are the image of functions named band functions. The band functions of H_B are denoted by $E_n(k)$, where the quasimomentum k runs in the Brillouin zone $\left[-\frac{\pi}{b}, +\frac{\pi}{b}\right]$. The spectrum of the Bloch operator H_B is given by the bands $\sigma(H_B) = \cup_{n=1}^{\infty}[E_n^b, E_n^t]$ where

$$E_n^b = \begin{cases} E_n(0) & \text{if } n \text{ is even} \\ E_n(\pi/b) & \text{if } n \text{ is odd} \end{cases},$$

$$E_n^t = \begin{cases} E_n(\pi/b) & \text{if } n \text{ is even} \\ E_n(0) & \text{if } n \text{ is odd.} \end{cases}$$

In the case of potential (2) the band functions may be explicitly computed. In particular let us look for the Bloch functions of the equation

$$H_B\psi = E\psi, \quad H_B = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_0\sin^2(k_L x).$$

If we set

$$\mathcal{E} = \left(E - \frac{1}{2}V_0\right)\frac{2m}{\hbar^2}, \qquad q = 2k_L,$$

$$\tilde{V}_0 = \frac{V_0 m}{\hbar^2} = \frac{m\Lambda_0 E_r}{\hbar^2} = \frac{1}{2}\Lambda_0 k_L^2$$

and recalling that $\sin^2(\theta) = \frac{1}{2}[1 - \cos(2\theta)]$ then the Mathieu equation takes the form

$$\left[\tilde{H}_B - \mathcal{E}\right]\psi = 0 \quad \text{where } \tilde{H}_B = -\frac{d^2}{dx^2} - \tilde{V}_0\cos(qx). \tag{18}$$

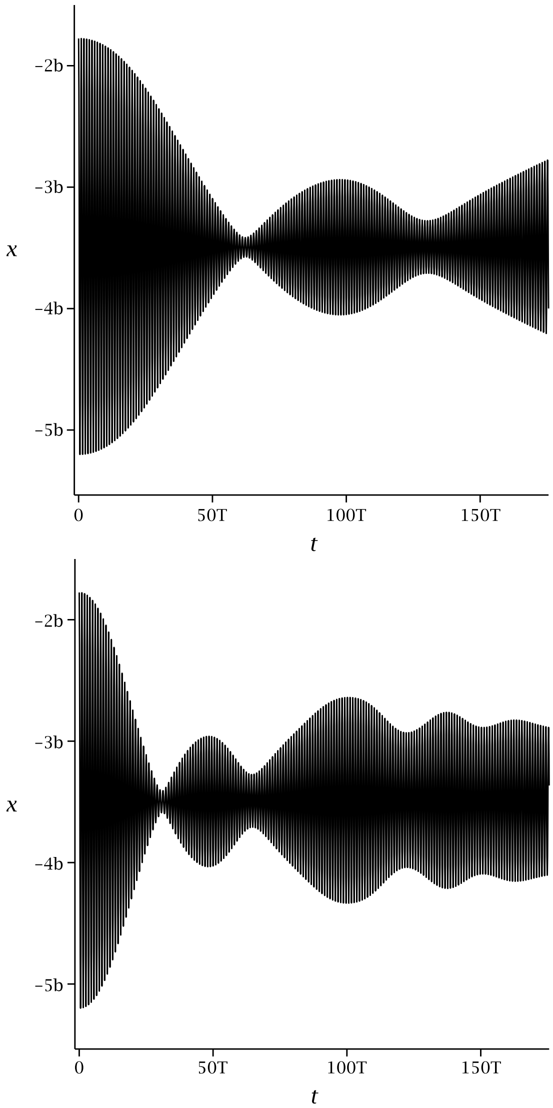

Fig. 8. Here we plot the motion of the center of mass of the wavefunction initially prepared on several lattice sites. The initial wavefunction is an asymmetrical function. Top panel corresponds to the case of $\eta = 0.1$, bottom panel corresponds to the case of $\eta = 0.2$. The center of mass rapidly oscillates with modulation of the amplitude. The width of oscillation is in a range lesser or equal to $3b$ in agreement with (17).

It has a fundamental set of solutions [32]

$$\phi_1(x, \mathcal{E}) = C\left[\frac{4\mathcal{E}}{q^2}, -\frac{\tilde{V}_0}{q^2}, \frac{1}{2}qx\right] \quad \text{and}$$
$$\phi_2(x, \mathcal{E}) = \frac{2}{q}S\left[\frac{4\mathcal{E}}{q^2}, -\frac{\tilde{V}_0}{q^2}, \frac{1}{2}qx\right]$$

where S and C denote the two Mathieu's functions, satisfying the conditions

$$\phi_1(0, \mathcal{E}) = 1, \qquad \frac{\partial \phi_1(0, \mathcal{E})}{\partial y} = 0 \quad \text{and}$$
$$\phi_2(0, \mathcal{E}) = 0, \qquad \frac{\partial \phi_2(0, \mathcal{E})}{\partial y} = 1.$$

Hence, the band functions $\mathcal{E}_n(k)$ associated to the spectral problem (18) are the solutions of the equation $\mu(\mathcal{E}) = \cos(kb)$ where

$$\mu(\mathcal{E}) = \phi_1(b, \mathcal{E}) = C\left[\frac{4\mathcal{E}}{q^2}, -\frac{\tilde{V}_0}{q^2}, \pi\right].$$

Let $\lambda = e^{ikb}$, then the equation $\mu(\mathcal{E}) = \cos(kb)$ can be written as $\mu(\mathcal{E}) = \frac{1}{2}(\lambda + \lambda^{-1})$. We observe that for $k \in \left[0, \frac{\pi}{b}\right]$ then $\sin(kb) = \sqrt{1 - \mu^2(\mathcal{E})}$. The Bloch function is given by [33]

$$\psi(x, \mathcal{E}) = \frac{\chi(x, \mathcal{E})}{\sqrt{N(\mathcal{E})}}$$

where

$$\begin{aligned}\chi(x, \mathcal{E}) &= \phi_2(b, \mathcal{E})\phi_1(x, \mathcal{E}) + \frac{1}{2}[\lambda(\mathcal{E}) - \lambda^{-1}(\mathcal{E})]\phi_2(x, \mathcal{E}) \\ &= \phi_2(b, \mathcal{E})\phi_1(x, \mathcal{E}) + i\sqrt{1 - \mu(\mathcal{E})^2}\phi_2(x, \mathcal{E})\end{aligned}$$

and

$$N(\mathcal{E}) = -\frac{4\pi}{b}\phi_2(b, \mathcal{E})\frac{d\mu}{d\mathcal{E}}.$$

We recall that the Bloch function $\psi_n(x, k) = \psi(x, \mathcal{E}_n(k))$, where $\mathcal{E}_n$ is the band function associated to $\tilde{H}_B$, is normalized to one:

$$\frac{2\pi}{b}\int_0^b |\psi_n(x, k)|^2 dx = 1$$

and furthermore it is such that

$$\psi_n(x, -k) = \overline{\psi_n(x, k)}.$$

Finally, the Wannier function on the zero-th cell associated to the nth band is given by

$$\begin{aligned}\mathcal{W}_n(x) &= \left(\frac{b}{2\pi}\right)^{1/2}\int_{-\pi/b}^{+\pi/b} \psi_n(x, k)dk \\ &= 2\left(\frac{b}{2\pi}\right)^{1/2}\int_0^{+\pi/b} \Re\psi_n(x, k)dk \\ &= 2\left(\frac{b}{2\pi}\right)^{1/2}\int_0^{\pi/b} \frac{\phi_2(b, \mathcal{E}_n(k))\phi_1(x, \mathcal{E}_n(k))}{\sqrt{N(\mathcal{E}_n(k))}}dk \\ &= \frac{b}{\sqrt{2\pi}}\int_0^{\pi/b} \frac{\sqrt{\phi_2(b, \mathcal{E}_n(k))}\phi_1(x, \mathcal{E}_n(k))}{\sqrt{-\frac{d\mu(\mathcal{E}_n(k))}{d\mathcal{E}}}}dk \\ &= \frac{1}{\sqrt{2\pi}}\int_{\mathcal{E}_n(0)}^{\mathcal{E}_n(\pi/b)} \frac{\sqrt{\phi_2(b, \mathcal{E})}\phi_1(x, \mathcal{E})\sqrt{-\frac{d\mu(\mathcal{E})}{d\mathcal{E}}}}{\sqrt{1 - \mu^2(\mathcal{E})}}d\mathcal{E}\end{aligned}$$

since the Mathieu functions are real valued when their arguments are real numbers. In particular,

$$\mathcal{W}_1(x) = \frac{1}{\sqrt{2\pi}}\int_{\mathcal{E}_1^b}^{\mathcal{E}_1^t} \frac{\sqrt{\phi_2(b, \mathcal{E})}\phi_1(x, \mathcal{E})\sqrt{-\frac{d\mu(\mathcal{E})}{d\mathcal{E}}}}{\sqrt{1 - \mu^2(\mathcal{E})}}d\mathcal{E}.$$

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