An effective mass model
for the simulation of ultra-scaled confined devices

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Abstract

In this paper, we present the derivation and the simulation of an effective mass model, describing the quantum motion of electrons in an ultra-scaled confined nanostucture. Due to the strong confinement, the crystal lattice is considered periodic only in the one dimensional transport direction and an atomistic description of the entire cross-section is given. Using an envelope function decomposition, an effective mass approximation is obtained. It consists of a sequence of one dimensional device dependent Schrödinger equations, one for each energy band, in which quantities retaining the effects of the confinement and of the transversal crystal structure are inserted. In order to model a gate-all-around Field Effect Transistor, self-consistent computations include the resolution, in the whole domain, of a Poisson equation describing a slowly varying macroscopic potential. Simulations of the electron transport in a simplified one wall carbon nanotube are presented.

Keywords: strong confinement, effective mass approximation, envelope function decomposition, Schrödinger-Poisson system, nanotransistors, carbon nanotube.

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1 Introduction

The extreme miniaturization reached by the electronic devices brings the necessity of using new models to describe the electron transport and to design the device architecture. To a reduced channel length it corresponds also a strong reduced lateral dimension, which induces quantization effects that cannot be captured by classical models. Ultra–scaled

\textsuperscript{*}Naoufel Ben Abdallah tragically passed away in July 2010 when this work was not yet completed. We remember him as a talented researcher, an enthusiastic supervisor and a generous person.
strongly confined structures (like nanowires [11, 13] and nanotubes [27, 2]) are becoming promising component in the future nanoelectronics. The numerical modeling of such devices is very important in order to predict their behavior, to access their performance limits and to design new configurations. When the cross–section diameter is below $3 \text{ nm}$, the strong confinement affects the energy band structure and bulk material properties cannot be used in the simulations (see [15] e.g., and references therein). Atomistic ab-initio computations give accurate description of the transport in these innovative devices (see [28] e.g.), but they are computationally too demanding, and cannot be used in a device design framework. The aim of this paper is to present a new model, that allows for computationally efficient simulations, for describing the transport in ultra–scaled confined devices. The model amounts to a set of one dimensional effective mass Schrödinger equations in the longitudinal direction, one for each energy band, coupled with a 3D Poisson equation for the self–consistent electrostatic potential. The novelty of the paper lies in the derivation of a new effective mass approximation for nanowires/nanotubes (both in the non–degenerate case and in the degenerate case), and in definition of the 3D electron density needed for self-consistent computations.

Effective mass approximation is a well known approximation in solid state physics (see [3, 34] e.g.) and it received recent attention in the mathematical literature. We recall results for 3D periodic crystals obtained by means of Wigner function techniques [30], two-scale homogenization arguments [1] or envelope function decompositions [6]. We also mention [32] where effective mass results are given for nonlinear Schrödinger equations related to Bose–Einstein condensates on optical lattices, and [12] where the effective mass approximation is performed for a Schrödinger equation singularly perturbed by a confinement potential and a strong magnetic field. For the strongly confined devices considered here, the assumption of infinite periodic structure, which allows to derive the commonly used effective mass approximation, is not valid anymore, and a new setting is required. Indeed, in the case of nanowires or nanotubes, the potential generated by the crystal structure, that fast oscillates in the scale defined by the crystal spacing, can be considered periodic only in the longitudinal direction, since the cross–section comprises only few ions. Therefore, thanks to lateral dimensions comparable to the lattice spacing, the longitudinal effective mass equations are found averaging out not only the lattice potential, but also the lateral dimension.

In the first part of the paper, the formal derivation of the new effective mass model is given for a wire of infinite extension in the longitudinal direction, where the electrons are subject to a lattice potential and to a slowly varying external potential. The key tool to find the asymptotic model is the use of an envelope function decomposition. The approach follows the work of [6] where the effective mass approximation in the case of 3D periodic potentials is obtained expanding the wave function on a modified Bloch basis that has the form introduced by [24]. In the case of nanowire/nanotubes, the elements of the modified
Bloch basis, that are constructed taking into account the confinement, are “localized” in the transverse direction (see Section 2), so that the Brillouin zone in one dimensional, and one dimensional transport problems are obtained when letting the lattice spacing to zero.

As an intermediate step of the asymptotics, the so-called $k \cdot p$ model is derived. Then, perturbation theory allows to diagonalize the differential part of the $k \cdot p$ Hamiltonian, and filtering the fast oscillations in time gives the final system. In the non-degenerate case (the eigenvalue of the Bloch type problem are all simple), each envelope function has a fast oscillating scale in time related to the corresponding eigenvalue of the Bloch type problem, so that adiabatic decoupling occurs, as it is common for fast oscillating system (see [33] e.g., and references therein). An infinite set of decoupled one dimensional effective mass Schrödinger equations, one for each energy band, is obtained (see Proposition 3.1). In the degenerate case, the final system is not decoupled anymore. A system of coupled Schrödinger equations with dimension equal to the multiplicity of the eigenvalue is obtained in correspondence to each multiple eigenvalue. The kinetic part of the limiting effective mass Hamiltonian is diagonal and the coupling occurs through the potential (see Proposition 3.2).

In the second part of the paper the effective mass model, obtained for an infinite wire, in used to compute the 1D scattering states of electrons moving in a bounded nanodevice under the action of an external applied potential and of the self-consistent potential generated by the electrons in the 3D structure. The 3D Poisson equation for the electrostatic potential requires the definition of the 3D macroscopic charge density, that is obtained combining the 1D transport densities with the atomistic information of the strongly confined cross-section. To summarize, the model used in the simulations consists of two steps. The first step requires the solution (to be done once, for a given device) of a Bloch type problem (on a 3D cell) to provide, in particular, the effective mass for each band. The second step is the resolution of the coupled stationary 1D Schrödinger – 3D Poisson system, where the physical quantities computed in the previous step are incorporated. We refer to [19] for a non ballistic classical transport model that is adapted to the peculiarities of nanowires, where the device dependent physical quantities are defined as in the present paper. Finally, we point out that our approach differs from the subband decomposition method [29, 9] where the confinement is taken into account during the Schrödinger-Poisson iterative algorithm, solving at each iteration an eigenvalue problem on slices perpendicular to the transport direction.

In order to assess the capability of the model to describe the transport in a strongly confined structure, numerical experiments are performed for a very simplified one wall carbon nanotube. The model is able to incorporate relevant physical features, such as band effects, providing qualitatively accurate current–voltage characteristics. Moreover, the dimension reduction for the transport problem allows for computationally efficient simulations. A similar approach, that amounts to 1D transport problems in each band...
and 3D electrostatic computations, has been used in [25] where simulation of transport in a silicon nanowire are given in the non degenerate case. We also mention that in [15] and [16] the band effects are taken into account using a high order approximation of the dispersion relation in a subband decomposition framework.

The paper is organized as follows. The first part considers the wire with infinite extension. In Section 2 the envelope function decomposition for confined structure is obtained. Section 3 is devoted to the formal derivation of the effective mass model, in the non-degenerate case, as well as in the degenerate case. In the second part, the electron transport is considered in a bounded device. A self-consistent Schrödinger–Poisson model is presented in Section 4. Section 5 collects the equations actually used in the simulation of transport in a nanotube and describes the iterative algorithm. Finally, the numerical experiments are presented in Section 6.

2 Envelope function decomposition

In the first part of the paper, we consider a confined nanostructure with infinite longitudinal extension. The structure is characterized by a finite cross-section composed of few ions, so that the lateral dimension is comparable to the typical spacing between lattice sites. The electrons in this nanostructure are subjected to an external potential $V$ and to a bounded potential $W_L$ generated by the crystal lattice, fast oscillating in the scale defined by the crystal spacing. Since the cross-section comprises few ions, $W_L$ is considered periodic only in the longitudinal $x$-direction. Denoting by $\epsilon$ the (scaled) lattice spacing and by $\omega_{\epsilon}$ the cross-section, we consider the following Schrödinger equation in the homogenization scaling

$$
\begin{cases}
  i\partial_t \psi^\epsilon = -\frac{1}{2} \Delta \psi^\epsilon + \frac{1}{2\epsilon^2} W_L(x_{\epsilon}, z_{\epsilon}) \psi^\epsilon + V(x, z_{\epsilon}) \psi^\epsilon, & (x, z) \in \mathbb{R} \times \omega_{\epsilon}, \\
  \psi^\epsilon = 0 \text{ for } z \in \partial \omega_{\epsilon}, \\
  \psi^\epsilon(t = 0) = \psi^{in,\epsilon},
\end{cases}
$$

(2.1)

where $\psi^{in,\epsilon}$ is a given initial value. Since the diameter of $\omega_{\epsilon}$ is comparable to $\epsilon$, the variable $z$ varying in the transverse section can be considered as fast variable, and it can be rescaled as $z' = z/\epsilon$ giving

$$
\begin{cases}
  i\partial_t \psi^\epsilon = -\frac{1}{2} \partial_{xx} \psi^\epsilon - \frac{1}{2\epsilon^2} \Delta_{z'} \psi^\epsilon + \frac{1}{\epsilon^2} W_L(x_{\epsilon}, z_{\epsilon}') \psi^\epsilon + V(x, z_{\epsilon}') \psi^\epsilon, & (x, z') \in \mathbb{R} \times \omega, \\
  \psi^\epsilon = 0 \text{ for } z' \in \partial \omega, \\
  \psi^\epsilon(t = 0) = \psi^{in,\epsilon},
\end{cases}
$$

(2.2)

where $\omega$ denotes the scaled cross-section. We point out that the external potential $V$ is acting both on the macroscopic scale $x$ and on the microscopic scale $z/\epsilon$. We assume that $V$ is slowly varying in $x$. 

4
The key tool to find the asymptotic model is the use of an envelope function decomposition, which allows to separate the fast and the slow variables. The orthonormal basis for the decomposition is made of eigenfunctions of the following problem in the unit cell $U = (-1/2, 1/2) \times \omega$.

$$\begin{align*}
-\frac{1}{2} \Delta \chi_n + W_L(y, z') \chi_n &= E_n \chi_n, \\
\chi_n(y, z') &= 0 \quad \text{on } \partial \omega, \quad \chi_n \text{ 1-periodic in } y, \\
\int_U |\chi_n|^2 dydz' &= 1.
\end{align*}$$

We point out that the operator $\Delta$ here denotes the full 3D Laplace operator in the variables $y$ and $z'$. Physically relevant potential $W_L$ are real-valued and bounded. Therefore, the eigenfunctions $\chi_n$ are real-valued and form a complete orthonormal basis of $L^2(U)$. The sequence of the eigenvalues $E_n \in \mathbb{R}$ is not decreasing with $E_n \to +\infty$. Because of the periodic conditions, they are not necessarily distinct.

**Remark 2.1.** The peculiarity of the strongly confined structure is reflected in the choice of the unit cell problem (2.3). We point out that this unit cell $U$ comprises the entire cross-section of the wire. Therefore, the eigenvectors depend on the device under consideration, for instance on the device geometry and on the growing orientation of the wire. Moreover, the homogeneous Dirichlet condition imposes confinement in the transverse directions, while periodicity is considered only in the transport direction.

**Remark 2.2.** We point out that problem (2.3) is a Bloch type problem. Indeed, analogously to the 3D crystal case, we can consider the eigenvalue problem for the fibered Hamiltonian, depending on the wave vector $k$,

$$H_L(k) = \frac{1}{2} k^2 - ik \partial_y - \frac{1}{2} \Delta + W_L(y, z').$$

Since $W_L$ is periodic only in the 1D transport direction, the dual variable $k$ varies in a 1D Brillouin zone (see also Remark 2.3). More precisely, let us consider, in the unit cell $U$,

$$H_L(k) \chi_{n,k} = E_n(k) \chi_{n,k},$$

with the same boundary conditions as in (2.3). The eigenvalues $E_n(k)$ are the energy bands of the confined nanostructure and the associated eigenvectors $\chi_{n,k}$ are the so-called Bloch functions. We notice that the operator in problem (2.3) is nothing but $H_L(0)$, that $\chi_n = \chi_{n,0}$ and $E_n = E_n(0)$. In particular, $E_n$ is the energy of the $n^{th}$ band at $k = 0$. Consequently, with a slight abuse of notation, we follow the denomination of [6] and throughout the paper we shall refer to the 1-periodic functions $\chi_n(y, z')$, eigenvectors of (2.3), as Bloch functions whereas the quasi-periodic functions $e^{iky} \chi_n(y, z')$ will be called Bloch waves.
**Definition 2.1.** For each pair of Bloch functions \( (\chi_n(y, z'), \chi_n'(y, z')) \), we define averaged quantities on the periodic direction as the functions

\[
g_{nn'}(z') = \int_{-1/2}^{1/2} \chi_n(y, z') \chi_n'(y, z') dy. \tag{2.6}
\]

These quantities will be used throughout the paper to reconstruct 3D functions from 1D wave functions (subject to the transport), and to project a 3D potential to the 1D transport direction.

**Notation.** We shall use the symbol \( \hat{\cdot} \) for the Fourier transform in \( L^2(\mathbb{R}) \) and, with an abuse of notation, we shall keep the same notation for the Fourier transform in the variable \( x \) of a function \( \psi(x, z') \in L^2(\mathbb{R} \times \omega) \)

\[
\hat{\psi}(k, z') = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \psi(x, z') e^{-ikx} dx. \tag{2.7}
\]

Moreover, the scalar product in \( L^2(U) \) will be denoted by \( <f, g> = \int_U f(y, z')g(y, z')dydz' \).

We also use the notation \( 1_A \) to denote the indicator function of the set \( A \).

The following Theorem is an extension to the nanowire case of the result given in [6] for 3D periodic crystals, considering the variable \( z' \in \omega \) as a parameter.

**Theorem 2.1.** Let \( \{\chi_n(x, z')\} \) be the set of orthonormal eigenfunctions given by (2.3). For every function \( \psi \in L^2(\mathbb{R} \times \omega) \) there exists a unique sequence \( \{f_n(x)|n \in \mathbb{N}\} \), with \( f_n \in L^2(\mathbb{R}) \) and \( supp \ \hat{f}_n \subset (-\pi, \pi) \), such that

\[
\psi(x, z') = \sum_{n \in \mathbb{N}} f_n(x) \chi_n(x, z'). \tag{2.8}
\]

Moreover, the Parseval identity holds

\[
\|\psi(x, z')\|^2_{L^2(\mathbb{R} \times \omega)} = \sum_{n \in \mathbb{N}} \|f_n(x)\|^2_{L^2(\mathbb{R})}. \tag{2.9}
\]

Finally, the Fourier transform of \( f_n \) is given by

\[
\hat{f}_n(k) = \int_{\mathbb{R} \times \omega} u_{n,k}(x, z') \psi(x, z') dx dz', \tag{2.10}
\]

where, for \( x \in \mathbb{R}, z' \in \omega, k \in \mathbb{R}, n \in \mathbb{N}, \)

\[
u_{n,k}(x, z') = \frac{1}{\sqrt{2\pi}} 1_{(-\pi, \pi)}(k)e^{ikx} \chi_n(x, z'). \tag{2.11}
\]

**Proof.** ✷ Fourier basis decomposition in the transport direction : Let us first consider a regular function \( \psi \in \mathcal{S}(\mathbb{R}_x; L^2(\omega)) \). We can write

\[
\psi(x, z') = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}_k} \hat{\psi}(k, z') e^{ikx} dk = \frac{1}{\sqrt{2\pi}} \sum_{l \in \mathbb{Z}} \int_{-\pi+2\pi l}^{\pi+2\pi l} \hat{\psi}(k, z') e^{ikx} dk
\]

\[
= \frac{1}{\sqrt{2\pi}} \sum_{l \in \mathbb{Z}} e^{i2\pi lx} \int_{-\pi}^{\pi} \hat{\psi}(\xi + 2\pi l, z') e^{i\xi x} d\xi.
\]
Consequently, we obtain the following decomposition

\[ \psi(x, z') = \sum_{l \in \mathbb{Z}} G_l(x, z') e^{2\pi ilx}, \quad (2.12) \]

where \( G_l \) is defined as

\[ G_l(x, z') = \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} \hat{\psi}(\xi + 2\pi l, z') e^{i\xi x} d\xi. \quad (2.13) \]

Clearly the Fourier transform (in the first variable) of \( G_l \) has support in \((-\pi, \pi)\). Uniqueness of the decomposition can be easily checked, assuming that (2.12) holds for some \( \hat{G}_l \) with \( \text{supp} \hat{G}_l(\xi, .) \subset (-\pi, \pi) \). In this case, we get

\[ \hat{\psi}(k, z') = \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} \hat{\psi}(\xi) e^{-i(k - 2\pi l)x} dx = \sum_{l \in \mathbb{Z}} \hat{G}_l(k - 2\pi l, z') = \mathbf{1}_{(-\pi + 2\pi l, \pi + 2\pi l)}(k) \hat{G}_l(k - 2\pi l, z'), \quad (2.14) \]

Finally, for a fixed \( z' \),

\[ \sum_{l \in \mathbb{Z}} \|G_l(x, z')\|_{L^2(\mathbb{R}_x)}^2 = \sum_{l \in \mathbb{Z}} \|\hat{G}_l(\xi, z')\|_{L^2(\mathbb{R}_\xi)}^2 \]

\[ = \sum_{l \in \mathbb{Z}} \int_{-\pi}^{\pi} |\hat{\psi}(\xi + 2\pi l, z')\mathbf{1}_{(-\pi, \pi)}(\xi)|^2 d\xi \]

\[ = \sum_{l \in \mathbb{Z}} \int_{-\pi}^{\pi} |\hat{\psi}(k, z')|^2 dk \]

\[ = \|\hat{\psi}(k, z')\|_{L^2(\mathbb{R}_k)}^2 = \|\psi(x, z')\|_{L^2(\mathbb{R}_x)}^2. \quad (2.15) \]

Hence, we obtain

\[ \sum_{l \in \mathbb{Z}} \|G_l(x, z')\|_{L^2(\mathbb{R}_x \times \omega)^2} = \|\psi(x, z')\|_{L^2(\mathbb{R}_x \times \omega)}^2. \quad (2.16) \]

**Bloch function decomposition**: For \( x \in \mathbb{R}, y \in (-1/2, 1/2), z' \in \omega \), let us define

\[ F(x, y, z') = \sum_{l \in \mathbb{Z}} G_l(x, z') e^{i2\pi ly}. \quad (2.17) \]

On the one hand, since the sequence \( \{e^{i2\pi ly} | l \in \mathbb{Z}\} \) forms an orthonormal basis of \( L^2(-1/2, 1/2) \), we have

\[ \int_{-1/2}^{1/2} |F(x, y, z')|^2 dy = \sum_{l \in \mathbb{Z}} |G_l(x, z')|^2, \]

\[ = \|F(x, y, z')\|_{L^2(\mathbb{R}_y)}^2. \]
and consequently

\[
\|F(x, y, z')\|_{L^2(\mathbb{R}_r \times U)}^2 = \sum_{l \in \mathbb{Z}} \|G_l(x, z')\|_{L^2(\mathbb{R}_r \times \omega)}^2. \tag{2.18}
\]

On the other hand, for fixed \(x\), \(F(x, y, z')\) is a 1-periodic function in \(y\), so it can be expanded in terms of \(\{\chi_n(y, z')\}\). We get

\[
F(x, y, z') = \sum_{n \in \mathbb{N}} f_n(x)\chi_n(y, z'), \tag{2.19}
\]

where \(f_n(x)\) is the Fourier coefficient with respect to \(\chi_n(y, z')\), defined by

\[
f_n(x) = \langle F(x, y, z'), \chi_n(y, z') \rangle, \tag{2.20}
\]

and the Parseval identity holds:

\[
\|F(x, y, z')\|_{L^2(U)}^2 = \sum_{n \in \mathbb{N}} |f_n(x)|^2.
\]

Integration over \(\mathbb{R}_r\) gives

\[
\|F(x, y, z')\|_{L^2(\mathbb{R}_r \times U)}^2 = \sum_{n \in \mathbb{N}} \|f_n(x)\|_{L^2(\mathbb{R}_r)}^2. \tag{2.21}
\]

For \(y = x\), due to (2.12), (2.17) reads \(\psi(x, z') = F(x, x, z')\). Therefore, (2.19) gives the decomposition (2.8), and (2.21) gives the isometry property (2.9). In order to extend the theorem to functions of \(L^2(\mathbb{R}_x \times \omega)\) we check the uniqueness.

**Uniqueness of \(\{f_n| n \in \mathbb{N}\}\):** We assume that (2.19) holds for some sequence \(\{\tilde{f}_n| n \in \mathbb{N}\}\).

For fixed \(z'\), we expand \(\chi_n(y, z')\) in terms of the Fourier basis of \(L^2(-1/2, 1/2)\), denoting by

\[
c_{n,l}(z') = \int_{-1/2}^{1/2} \chi_n(y, z') e^{-i2\pi ly} dy \tag{2.22}
\]

the Fourier coefficients of \(\chi_n\). We obtain

\[
F(x, y, z') = \sum_{l \in \mathbb{Z}} \tilde{G}_l(x, z') e^{i2\pi ly},
\]

with

\[
\tilde{G}_l(x, z') = \sum_{n \in \mathbb{N}} \tilde{f}_n(x)c_{n,l}(z'). \tag{2.23}
\]

Using the quantities \(g_{nn'}\)'s defined in (2.6), we have

\[
\sum_{l \in \mathbb{Z}} \tilde{G}_l(x, z') c_{n', l}(z') = \sum_{l \in \mathbb{Z}} \sum_{n \in \mathbb{N}} \tilde{f}_n(x)c_{n,l}(z')c_{n',l}(z') = \sum_{n \in \mathbb{N}} \tilde{f}_n(x)g_{nn'}(z').
\]
Finally, integrating over $\omega$ and exploiting the orthonormality of the $\chi_n$'s on $\mathcal{U}$, we have

$$\tilde{f}_n(x) = \sum_{l \in \mathbb{Z}} \int_{\omega} \tilde{G}_l(x, z') c_{n,l}(z') dz' .$$  \hspace{1cm} (2.24)

Because of the uniqueness of decomposition (2.12) (and in turns of (2.17)) $\tilde{G}_l = G_l$ and thus (2.24) coincides with (2.20).

- **Fourier transform**: The Fourier transform $\hat{f}_n$ can be easily computed, using the fact that the sequence $\{e^{-i2\pi l y}| l \in \mathbb{Z}\}$ forms an orthonormal basis of $L^2(-1/2, 1/2)$. Indeed, from definition (2.20), with (2.17), we write

$$f_n(x) = \sum_{l \in \mathbb{Z}} \int_{\omega} G_l(x, z') c_{n,l}(z') dz' ,$$  \hspace{1cm} (2.25)

where the notation (2.22) for the Fourier coefficients of $\chi_n$ is used. Therefore, taking into account (2.14), we have

$$\hat{f}_n(k) = \frac{1}{\sqrt{2\pi}} \sum_{l \in \mathbb{Z}} \int_{\omega} \mathbb{I}_{(-\pi, \pi)}(k) \left( \int_{\mathbb{R}_x} \psi(x, z') e^{-i(k+2\pi l)x} dx \right) c_{n,l}(z') dz'.$$

Noticing that $\chi_n(x, z') = \sum_{l \in \mathbb{Z}} c_{n,l}(z') e^{-i2\pi lx}$, we finally obtain

$$\hat{f}_n(k) = \frac{1}{\sqrt{2\pi}} \mathbb{I}_{(-\pi, \pi)}(k) \int_{\mathbb{R}_x \times \omega} \psi(x, z') e^{-ikx} \chi_n(x, z') dxdz'.$$

\[ \square \]

**Definition 2.2.** The functions $f_n$ of Theorem 2.1 will be called the envelope functions of $\psi$ with respect to the basis $\{\chi_n| n \in \mathbb{N}\}$.

It is immediate to write expressions (2.8) and (2.9) of Theorem 2.1 in terms of the Fourier transform $\hat{f}_n$. It gives the following Corollary.

**Corollary 2.2.** Let $\{f_n| n \in \mathbb{N}\}$ be the envelope functions of $\psi \in L^2(\mathbb{R} \times \omega)$ with respect to the basis $\{\chi_n| n \in \mathbb{N}\}$. Then

$$\psi(x, z') = \sum_{n \in \mathbb{N}} \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} \hat{f}_n(k) e^{ikx} \chi_n(x, z') dk .$$  \hspace{1cm} (2.26)

And, the following identity holds

$$\|\psi(x, z')\|_{L^2(\mathbb{R} \times \omega)}^2 = \sum_{n \in \mathbb{N}} \|\hat{f}_n(k)\|_{L^2(-\pi, \pi)}^2 .$$  \hspace{1cm} (2.27)
Remark 2.3. The functions (2.11) are generalized Bloch waves, in the form introduced by Kohn and Luttinger [24] (used in [6] for obtaining in a rigorous way the effective mass for 3D periodic crystals). As we shall see in the next section, they do not allow to completely diagonalize the periodic part of the Hamiltonian. However, since the wave vector $k$ only appears in the plane wave and not in the periodic part $\chi_n$, they have the advantage of completely separating the oscillating part of the wave function from its slowly varying one. In nanowires/nanotubes, confinement plays an important role and it is reflected in the form of the Bloch waves (2.11), which are “localized” in the $z'$ variable, so that scattering is allowed only in the one dimensional longitudinal direction. Indeed, as already pointed out, the wave vector $k$ varies in the 1D domain $(-\pi, \pi)$. It turns out that $(-\pi, \pi)$ is the fundamental domain of the reciprocal lattice, usually called Brillouin zone in solid state physics.

Remark 2.4. The Parseval identity (2.9) tells that the wave function density can be obtained as superposition of envelope function densities, which depend only on the $x$ variable, the dependence on the variable $z'$ being averaged out. However, in self–consistent computations the external electrostatic potential is acting on the entire 3D structure, so that explicit dependence on $z'$ has to be kept. A straightforward computation, based on (2.17) and (2.19), shows that

$$
\sum_{l \in \mathbb{Z}} |G_l(x, z')|^2 = \int_{-1/2}^{1/2} \left[ \sum_{n \in \mathbb{N}} f_n(x) \chi_n(y, z') \right]^2 dy = \sum_{n, n'} f_n(x) \overline{f_{n'}(x)} g_{nn'}(z'),
$$

with $g_{nn'}$ defined in (2.6). Therefore, recalling (2.15), we obtain, for a fixed $z'$

$$
\int_{\mathbb{R}} |\psi(x, z')|^2 dx = \int_{\mathbb{R}} \left( \sum_{n, n'} f_n(x) \overline{f_{n'}(x)} g_{nn'}(z') \right) dx.
$$

We emphasize the presence of the $g_{nn'}$’s that carry the contribution of the confinement.

For any $0 < \epsilon << 1$, the scaled version of the envelope function decomposition is obtained with the same computation as in Theorem 2.1 using the fact that to the primitive cell $C_\epsilon := (-\epsilon/2, \epsilon/2)$ it corresponds the primitive cell of the reciprocal lattice $B_\epsilon := (-\pi/\epsilon, \pi/\epsilon)$, with $|C_\epsilon| |B_\epsilon| = 2\pi$. We get

$$
\psi(x, z') = \sum_{n \in \mathbb{N}} f_n^\epsilon(x) \chi_n(x, z'),
$$

and the Parseval identity holds

$$
\|\psi(x, z')\|_{L^2(\mathbb{R} \times \omega)}^2 = \sum_{n \in \mathbb{N}} \|f_n^\epsilon(x)\|_{L^2(\mathbb{R})}^2,
$$

together with

$$
\int_{\mathbb{R}} |\psi(x, z')|^2 dx = \int_{\mathbb{R}} \left( \sum_{n, n'} f_n^\epsilon(x) \overline{f_{n'}^\epsilon(x)} g_{nn'}(z') \right) dx.
$$

Moreover, the Fourier transform \( \hat{f}_n^{\epsilon} \) has a support in \( \mathcal{B}_\epsilon \) and it is defined by

\[
\hat{f}_n^{\epsilon}(k) = \int_{\mathbb{R} \times \omega} \overline{u_{n,k}^{\epsilon}(x,z')} \psi(x,z') dx dz',
\]

where the (generalized) scaled Bloch waves are given by

\[
u_{n,k}^{\epsilon}(x,z') = \frac{1}{\sqrt{2\pi}} e^{ikx} \chi_n(\frac{x}{\epsilon}, z').
\]

The functions \( f_n^{\epsilon} \) will be called the \( \epsilon \)-scaled envelope functions relative to the basis \( \{ \chi_n \}_{n \in \mathbb{N}} \). The decomposition of \( \psi \) in terms of the Fourier transform \( \hat{f}_n^{\epsilon} \) is given by

\[
\psi(x,z') = \sum_{n \in \mathbb{N}} \frac{1}{\sqrt{2\pi}} \int_{\mathcal{B}_\epsilon} \hat{f}_n^{\epsilon}(k) e^{ikx} \chi_n(\frac{x}{\epsilon}, z') dk.
\]

### 3 Effective mass model derivation

In this section, we shall present the formal derivation of the limiting effective mass approximation used in the next sections of the paper. Intermediate models, corresponding to different approximation levels, will be introduced and discussed. This approach has in particular the advantage of deriving the well known \( k \cdot p \) model as an intermediate model between the original Schrödinger equation and its limiting effective mass approximation. The rigorous derivation and the related error estimates which allow to compare the respective dynamics are subject of a forthcoming paper. The ideas will be largely based on the ones developed in [6] for 3D crystals.

To perform the asymptotic process, we start from the exact dynamics of the sequence of envelope functions \( f^\epsilon = (f_1^\epsilon, f_2^\epsilon, \ldots) \) (Section 3.1). The first approximation level is obtained averaging the slowly varying external potential \( V \) on the unit cell in the longitudinal direction. Inserting this approximation in the exact dynamics of envelope functions, we obtain the dynamics of a sequence that will be denoted by \( f_{kp}^\epsilon = (f_{kp,1}^\epsilon, f_{kp,2}^\epsilon, \ldots) \). The notation \( f_{kp}^\epsilon \) is used to emphasize that the obtained model is nothing but the well known \( k \cdot p \) model in the case of ultra-scaled confined nanostructures, as we will describe in Section 3.2. A second approximation is obtained diagonalizing the free \( k \cdot p \) Hamiltonian, expanding the corresponding eigenvalues with perturbation techniques. At this approximation level, we construct an effective mass operator (Section 3.3) and we obtain a second intermediate model called effective mass dynamics for the sequence denoted by \( f_{em}^\epsilon = (f_{em,1}^\epsilon, f_{em,2}^\epsilon, \ldots) \). Finally, since the equations of the effective mass dynamics still contain fast oscillations in time with a frequency related to the energy band, the last approximation level consists in considering long time averages. Starting from the effective mass dynamics, we filter oscillations by setting \( f_{em,n}^\epsilon(t,x) = h_{em,n}^\epsilon(t,x) e^{-iEn t/\hbar} \) and by passing to the limit (Section 3.4). The obtained model is called limiting effective mass approximation, and the corresponding
solution will be denoted by \( h_{em} = (h_{em,1}, h_{em,2}, \ldots) \). Notations wise, we also introduce the definitions

\[
g'_n(t, k) = \hat{f}'_n(t, k), \quad g'_{kp,n}(t, k) = \hat{f}'_{kp,n}(t, k) \quad \text{and} \quad g'_{em,n}(t, k) = \hat{f}'_{em,n}(t, k),
\]

for the Fourier transforms of the respective functions.

In the non-degenerate case, the final model, that intends to approximate, in a suitable sense (see also Remark 3.4), \( \psi^e(x, z') \) by means of \( \sum_{n \in \mathbb{N}} h_{em,n}(x)e^{-iE_n t} \chi_n(x, z') \) and that will be used for the numerical simulation, is summarized in the following Proposition.

**Proposition 3.1.** Assume that all the eigenvalues \( E_n \) of the problem (2.3) are simple. Then, the limiting effective mass approximation is given by an infinite set of 1D Schrödinger equations that in the \( n^{th} \) band have the form

\[
i \partial_t h_{em,n}(t, x) = -\frac{1}{2m^*_n} \partial_{xx} h_{em,n}(t, x) + V_{nn}(x) h_{em,n}(t, x).
\]

\( m^*_n \) denotes the \( n^{th} \) band effective mass and it is defined by

\[
\frac{1}{m^*_n} = 1 - 2 \sum_{n' \neq n} \frac{P_{nn'} P_{n'n}}{E_n - E_n'},
\]

where

\[
P_{nn'} = \langle \partial_y \chi_{n'}(y, z'), \chi_n(y, z') \rangle
\]

are the matrix elements of the first order derivative operator between Bloch functions. Moreover, \( V_{nn'} \) is an effective potential given by

\[
V_{nn'}(x) = \int_{\omega} V(x, z') g_{nn'}(z') dz',
\]

constructed by projecting the 3D potential \( V \) in the transport direction through the \( g_{nn'} \)'s defined in (2.6).

**Remark 3.1.** We point out that the effective mass and the effective potential in the limiting model depend on the device structure since they are computed by means of the Bloch functions (2.3). This is an important feature of the model, since, as already mentioned in the introduction, simulations with bulk material quantities fail to reproduce the physical experiments \([15]\).

Moreover, we shall see in Section 3.5 that, since the wave vector \( k \) is a scalar, the use of the asymptotic expansion for the perturbed eigenvalues (in order to diagonalize the free \( k \cdot p \) Hamiltonian) is justified not only in the non-degenerate case, but also in the degenerate one (see [21]). However, the presence of multiple eigenvalues does not allow to completely separate the time scales and the long time averaging process leads to a coupling in the potential term. Consequently, in the degenerate case, the final set of equations is not decoupled anymore, but in connection to each multiple eigenvalue \( E_n \), a system of dimension equal to the multiplicity of \( E_n \) is obtained, as stated in the next Proposition.
Proposition 3.2. Assume that each eigenvalue $E_n$ of the problem (2.3) has multiplicity $\alpha_n \geq 1$ and denote by $\chi_{n,\alpha}$, with $1 \leq \alpha \leq \alpha_n$, the $\alpha_n$ eigenvectors associated with $E_n$. To simplify notations, we say that $\chi_{n,\alpha}$ is the $(n-\alpha)^{th}$ eigenvector (where $n-\alpha = \sum_{n'=n}^{\alpha_n} \alpha_{n'} + \alpha$).

Let

$$P_{(n,\alpha',n')}(t,x,z') = \langle \partial_y \chi_{n',\alpha'}(y,z'), \chi_{n,\alpha}(y,z') \rangle$$

be defined analogously to (3.4). Then, the degenerate limiting effective mass approximation is described by a set of $\alpha_n \times \alpha_n$ system, where the generic $n-\alpha$th equation has the form

$$i\partial_t h_{\text{em},n,\alpha}(t,x) = -\frac{1}{2m_{n,\alpha}^*} \partial_{xx} h_{\text{em},n,\alpha}(t,x) + \sum_{\alpha'=1}^{\alpha_n} V_{(n,\alpha,\alpha')(x)} h_{\text{em},n,\alpha'}(t,x),$$

where the effective mass $m_{n,\alpha}^*$ is now defined by

$$\frac{1}{m_{n,\alpha}^*} = 1 - 2 \sum_{n' \neq n}^{n} \frac{P_{(n,\alpha',n')(n',\alpha)} P_{(n',\alpha,n)}}{E_n - E_{n'}}$$

and the effective potential $V_{(n,\alpha',\alpha')}$ is defined analogously to (3.5).

Remark 3.2. The evolution equations (3.2) and (3.7) need to be supplemented by initial conditions. Let $\psi_{\text{in},\epsilon} \in L^2(\mathbb{R}; H^1_0(\omega))$ be an initial datum for (2.2) and let $f_{\text{in},\epsilon}$ its scaled envelope function relative to the basis $\chi_n$ (see (2.29)). In the same spirit of [6], we may assume that the sequence $f_{\text{in},\epsilon}$ is uniformly smooth and it converges to an initial datum $f_{\text{in}}$ in $L^2(\mathbb{N}, L^2(\mathbb{R}))$ as $\epsilon$ tends to zero. Then, we can take $h_{\text{em},\text{in}} := f_{\text{in}}$ as initial condition for (3.2) and $h_{\text{em},n,\alpha} := f_{n,\alpha}$ as initial condition for (3.7).

Moreover, for the different intermediate models ((3.18), (3.33), (3.34), (3.47) and (3.48)), that will be obtained in the next sections, the initial condition will be intended to be $f_{\text{in},\epsilon}$.

In the following, we give some formal ideas in order to understand the different levels of approximation and thus to present the different intermediate models with their respective dynamics.

3.1 Envelope function dynamics

We first derive the exact dynamics of the envelope functions of $\psi(\epsilon, t, x, z')$, solution of Schrödinger equation (2.2). We consider that

$$\psi(\epsilon, t, x, z') = \sum_{n \in \mathbb{N}} f_n^\epsilon(t, x) \chi_n(\frac{x}{\epsilon}, z')$$

is its $\epsilon$-scaled envelope function decomposition relative to the basis $\{\chi_n| n \in \mathbb{N}\}$ defined in (2.3). Then, after some computations that we present in the appendix, we obtain that the exact dynamics of the envelope function Fourier transform is given, component wise, by

$$i\partial_t g^\epsilon_n(t, k) = \frac{1}{2} k^2 g^\epsilon_n(t, k) + \frac{1}{\epsilon^2} E_n g^\epsilon_n(t, k)$$

$$-i \sum_{n' \in \mathbb{N}} P_{n'n} g^\epsilon_{n'}(t, k) + (U g^\epsilon_n)(t, k),$$

(3.10)
where the $P_{nn'}$'s are defined in (3.4) and $\mathcal{U}^e$ is the operator defined component wise, for any element $g = (g_1, g_2, \ldots)$, by

$$(\mathcal{U}^e g)_n(t, k) = \sum_{n' \in \mathbb{N}} \int_{\mathbb{R}^k} U_{nn'}^e(k, k') g_{n'}(t, k') dk'. \tag{3.11}$$

The kernel $U_{nn'}^e(k, k')$ is given explicitly by

$$U_{nn'}^e(k, k') = \frac{1}{2\pi} k_B^e(k') k_B^e(k) \int_{\mathbb{R}^x \times \omega} e^{i(k'-k)x} \chi_{n'}(\frac{x}{\epsilon}, z') V(x, z') \chi_n(\frac{x}{\epsilon}, z') dx dz'. \tag{3.12}$$

Finally, in position variables, (3.10) reads as follows

$$i\partial_t f^e_n(t, x) = -\frac{1}{2} \partial_{xx} f^e_n(t, x) + \frac{1}{\epsilon^2} E_n f^e_n(t, x) - \frac{1}{\epsilon} \sum_{n' \in \mathbb{N}} P_{nn'} \partial_x f^e_{n'}(t, x) + (\mathcal{V}^e f^e)_n(t, x), \tag{3.13}$$

where, the non local operator $\mathcal{V}^e$ is defined, component wise, by

$$(\mathcal{V}^e f^e)_n(t, k) = \sum_{n' \in \mathbb{N}} \int_{\mathbb{R}^k} U_{nn'}^e(k, k') g_{n'}(t, k') dk'. \tag{3.14}$$

### 3.2 $k \cdot p$ model

The first approximation level consists in averaging on the unit cell the operator $\mathcal{U}^e$ defined in (3.11). Since the $\chi_n$'s are 1-periodic in the first variable, we have

$$\lim_{\epsilon \to 0} \int_{\mathbb{R}^x} e^{i(k'-k)x} \chi_{n'}(\frac{x}{\epsilon}, z') V(x, z') \chi_n(\frac{x}{\epsilon}, z') dx = \int_{\mathbb{R}^x} V(x, z') e^{i(k'-k)x} dx \int_{-1/2}^{1/2} \chi_n(y, z') \chi_{n'}(y, z') dy.$$  

Thus, using definition (2.6) for $g_{nn'}(z')$, the formal limit of (3.12) is given by

$$U_{nn'}(k, k') = \frac{1}{2\pi} \int_{\omega} \left( \int_{\mathbb{R}^x} e^{i(k'-k)x} V(x, z') dx \right) g_{nn'}(z') dz'$$

$$= \frac{1}{\sqrt{2\pi}} \int_{\omega} \hat{V}(k - k', z') g_{nn'}(z') dz', \tag{3.15}$$

and the formal limit of $\mathcal{U}^e$ is the operator $\mathcal{U}^0$ defined component wise, for any element $g = (g_1, g_2, \ldots)$, by

$$(\mathcal{U}^0 g)_n(t, k) = \sum_{n' \in \mathbb{N}} \int_{\mathbb{R}^k} U_{nn'}(k, k') g_{n'}(t, k') dk'. \tag{3.16}$$

$$= \sum_{n' \in \mathbb{N}} \int_{\mathbb{R}^k} \left( \frac{1}{\sqrt{2\pi}} \int_{\omega} \hat{V}(k - k', z') g_{nn'}(z') dz' \right) g_{n'}(t, k') dk'. $$
In the physical literature, the model obtained substituting in the exact dynamics (3.10) \( U^\varepsilon \) with \( U^0 \) is usually referred to as \( k \cdot p \) model. In Fourier space, the \( k \cdot p \) dynamics is given, component wise, by the equation

\[
i \partial_t g_{kp,n}(t,k) = \left\{ \begin{array}{ll} \frac{1}{2} k^2 g_{kp,n}(t,k) + \frac{1}{\varepsilon^2} E_n g_{kp,n}(t,k) & \\
 - \frac{i}{\varepsilon} k \sum_{n' \in \mathbb{N}} P_{nn'} g_{kp,n'}(t,k) + (U^0 g_{kp})_n(t,k), \end{array} \right.
\]

(3.17)

where \( U^0 \) is given by (3.16). A back Fourier transform gives that \( f_{kp}^\varepsilon \) is solution, component wise, of

\[
i \partial_t f_{kp,n}(t,x) = \left\{ \begin{array}{ll} \frac{1}{2} \partial_{xx} f_{kp,n}(t,x) + \frac{1}{\varepsilon^2} E_n f_{kp,n}(t,x) & \\
 - \frac{i}{\varepsilon} \sum_{n' \in \mathbb{N}} P_{nn'} \partial_x f_{kp,n'}(t,x) + (V^0 f_{kp})_n(t,x), \end{array} \right.
\]

(3.18)

where the operator \( V^0 \) is defined, component wise, by

\[
(V^0 f_{kp})_n(t,x) = \sum_{n' \in \mathbb{N}} V_{nn'}(x) f_{kp,n'}(t,x),
\]

(3.19)

with \( V_{nn'} \) defined in (3.5). The non local operator \( V^\varepsilon \) converges to the non-diagonal multiplication operator \( V^0 \). We emphasize that the differential part of (3.18) is the same as the one of the exact dynamics of the envelope functions (3.13). Notice also that the effect of confinement is incorporated in the energy band value \( E_n \), in the derivative operator between Bloch functions \( P_{nn'} \), and in the effective potential matrix \( V_{nn'} \).

### 3.3 Diagonalization of the \( k \cdot p \) Hamiltonian

The second approximation level is obtained ignoring the effects of the potential \( V \) and diagonalizing the free \( k \cdot p \) Hamiltonian. In this section, we make the assumption that all the eigenvalues \( E_n \) of the (Bloch type) problem (2.3) are simple, and that they are numbered in increasing order, i.e.

\[
E_1 < E_2 < ... \tag{3.20}
\]

Therefore, the diagonalization of the free \( k \cdot p \) Hamiltonian relies on non-degenerate perturbation theory and it leads to the construction of an effective mass operator.

In order to proceed to this approximation, we multiply this operator by \( \varepsilon^2 \), we choose \( \xi = \varepsilon k \) as small parameter and we study the corresponding operator that is defined by

\[
(A(\xi))_{nn'} = E_n \delta_{nn'} - i \xi P_{nn'} + \frac{1}{2} \xi^2 \delta_{nn'},
\]

(3.21)

where \( \delta_{nn'} \) denotes the Kronecker symbol. A non-degenerate perturbation technique is applied to approximate the eigenvalues \( \lambda_n(\xi) \) of \( A(\xi) \):

\[
A(\xi) v_n(\xi) = \lambda_n(\xi) v_n(\xi).
\]

(3.22)
Remark 3.3. We point out that the operator $A(\xi)$ is nothing but the expression of the fibered Hamiltonian (2.4) in the basis $\{\chi_n | n \in \mathbb{N}\}$. More precisely, we have $(A(\xi))_{mn} = \langle H_C(\xi) \chi_n(y, z'), \chi_m(y, z') \rangle$. Therefore, it is easy to see that $\lambda_n(\xi) = E_n(\xi)$ and $v_n(\xi) = \langle \chi_n(y, z'), \chi_n(y, z') \rangle$, where $\chi_n(\xi)$ denotes the eigenvector of the fibered Hamiltonian $H_C(\xi)$ as defined in Remark 2.2.

Defining the following operators

$$
(A^0)_{nn'} = E_n \delta_{nn'}, \quad (A^1)_{nn'} = -iP_{nn'} \quad \text{and} \quad (A^2)_{nn'} = \frac{1}{2} \delta_{nn'},
$$

(3.23)

we notice that $A(\xi) = A^0 + \xi A^1 + \xi^2 A^2$. For simplicity, in the following, we consider those operators acting on $l^2 = \{a_n \in \mathbb{C} | (\sum_{n \in \mathbb{N}} |a_n|^2)^{1/2} < +\infty\}$. We expand $v_n(\xi)$ and $\lambda_n(\xi)$ as

$$
v_n(\xi) = v^0_n + \xi v^1_n + \xi^2 v^2_n + \ldots \quad \lambda_n(\xi) = \lambda^0_n + \xi \lambda^1_n + \xi^2 \lambda^2_n + \ldots
$$

(3.24)

Inserting this expression into (3.22) and collecting terms with the same order of $\xi$ yields

$$
A^0 v^0_n = \lambda^0_n v^0_n,
$$

(3.25)

$$
A^0 v^1_n + A^1 v^0_n = \lambda^0_n v^1_n + \lambda^1_n v^0_n,
$$

(3.26)

$$
A^0 v^2_n + A^1 v^1_n + A^2 v^0_n = \lambda^0_n v^2_n + \lambda^1_n v^1_n + \lambda^2_n v^0_n.
$$

(3.27)

The system (3.25) gives directly $\lambda^0_n = E_n$ and $v^0_n = e_n$, where $e_n$ is the $n^{th}$ vector of the canonical basis in $l^2$. Next, we project (3.26) on $e_n$ and we obtain

$$
E_n v^1_{n,n} - iP_{nn} = E_n v^1_{n,n} + \lambda^1_n,
$$

where $v^1_{n,n'}$ is the $(n')^{th}$ component of $v^1_n$. Integration by parts in (3.4) gives $P_{nn'} = -P_{n'n}$ and thus $P_{nn} = 0$. We conclude that $\lambda^1_n = 0$.

Projecting (3.26) on $e_{n'} (n' \neq n)$ gives

$$
v^1_{n,n'} = -i \frac{P_{n'n}}{E_n - E_{n'}}.
$$

(3.28)

Finally, we project (3.27) on $e_n$ to get

$$
E_n v^2_{n,n} - i \sum_{n'} P_{nn'} v^1_{n,n'} + \frac{1}{2} = E_n v^2_{n,n} + \lambda^2_n.
$$

Using (3.28) and the fact that $P_{nn} = 0$, we obtain

$$
\lambda^2_n = \frac{1}{2} \left(1 - 2 \sum_{n' \neq n} \frac{P_{nn'} P_{n'n}}{E_n - E_{n'}}\right).
$$

(3.29)

Then, defining $m^*_n$ as in (3.3), we conclude saying that

$$
\lambda_n \simeq \lambda^0_n + \xi^2 \lambda^2_n = E_n + \frac{1}{2} \frac{\xi^2}{m^*_n}.
$$

(3.30)
Consequently, at a second approximation level, the differential part of the $k \cdot p$ Hamiltonian of the equation (3.17) can be diagonalized and it leads to the dynamics of the sequence $g_{\text{em}}^\epsilon = (g_{\text{em},1}^\epsilon, g_{\text{em},2}^\epsilon, \ldots)$, solution, component wise, of the equation

$$i \partial_t g_{\text{em},n}^\epsilon(t, k) = (A_{\text{em}}^\epsilon g_{\text{em}}^\epsilon)_n(t, k) + (H_{\text{em}}^\epsilon g_{\text{em}}^\epsilon)_n(t, k).$$

(3.31)

The operator $A_{\text{em}}^\epsilon$ is defined by

$$(A_{\text{em}}^\epsilon g_{\text{em}}^\epsilon)_n(t, k) = \left( \frac{E_n}{\epsilon^2} + \frac{1}{2} \frac{k^2}{m_n^*} \right) g_{\text{em},n}^\epsilon(t, k),$$

(3.32)

where $m_n^*$ is the $n^{th}$ band effective mass given by (3.3). Finally, a back Fourier transform gives that $f_{\text{em}}^\epsilon$ is solution, component wise, of

$$i \partial_t f_{\text{em},n}^\epsilon(t, x) = - \frac{1}{2m_n^*} \partial_{xx} f_{\text{em},n}^\epsilon(t, x) + \frac{1}{\epsilon^2} E_n f_{\text{em},n}^\epsilon(t, x) + \sum_{n' \in \mathbb{N}} V_{nn'}(x) f_{\text{em},n'}^\epsilon(t, x).$$

(3.33)

### 3.4 Limiting effective mass dynamics

The equation (3.33) involves fast oscillations in time. Therefore, the last approximation level consists in considering long time averages. The fast oscillations can be filtered out by setting $f_{\text{em},n}^\epsilon(t, x) = h_{\text{em},n}^\epsilon(t, x) e^{-iE_n^\epsilon t}$. Then, the sequence $h_{\text{em}}^\epsilon$ is solution, component wise, of

$$i \partial_t h_{\text{em},n}^\epsilon(t, x) = - \frac{1}{2m_n^*} \partial_{xx} h_{\text{em},n}^\epsilon(t, x) + \sum_{n' \in \mathbb{N}} e^{-i(E_{n'}^\epsilon - E_n^\epsilon) t} V_{nn'}(x) h_{\text{em},n'}^\epsilon(t, x).$$

(3.34)

We separate the diagonal part of the Hamiltonian of (3.34)

$$(H_0 h)_n = - \frac{1}{2m_n^*} \partial_{xx} h_n(x) + V_{nn}(x) h_n(x),$$

(3.35)

and the off–diagonal part given by the operator

$$(R^\epsilon (t) h)_n = \sum_{n' \neq n} e^{-i(E_{n'}^\epsilon - E_n^\epsilon) \frac{t}{\epsilon^2}} V_{nn'}(x) h_{n'}(x).$$

(3.36)

Formally, we have that

$$R^\epsilon(t) = \epsilon^2 \frac{d}{dt} \tilde{R}^\epsilon(t),$$

(3.37)

where

$$(\tilde{R}^\epsilon(t) h)_n = \sum_{n' \neq n} \frac{i}{(E_{n'}^\epsilon - E_n^\epsilon)} e^{-i(E_{n'}^\epsilon - E_n^\epsilon) t} V_{nn'}(x) h_{n'}(x).$$

(3.38)
Since $H_0$ is the complete Hamiltonian of (3.2) of Proposition 3.1, using a generalized Duhamel formula for the evolution of $h_{em}^\epsilon$ we can formally write
\[
 h_{em}^\epsilon(t) - h_{em}(t) = \int_0^t S(t-s) R^\epsilon(s) h_{em}^\epsilon(s) ds,
\]
where $S(t) = e^{-itH_0}$ is the (diagonal) unitary group generated by $H_0$. Therefore, thanks to (3.37), integration by parts shows that the action of the evolution operator (3.36) vanishes in the limit $\epsilon \to 0$ and $h_{em}^\epsilon$ formally converges to the solution of the averaged system (3.2). Consequently, we formally obtain the limiting effective mass approximation presented in Proposition 3.1.

**Remark 3.4.** In view of self–consistent computations, we are now interested in the formal limit $\epsilon \to 0$ of (2.31). The transformation $f_n^\epsilon(t,x) = h_n^\epsilon(t,x)e^{-iE_n^\epsilon t}$, that allows to filter oscillations in time, conserves the modulus $|f_n^\epsilon(t,x)|$. Consequently, we can write
\[
 \sum_{n,n'} f_n^\epsilon(t,x)f_{n'}^\epsilon(t,x)g_{nn'}(z') = \sum_{n\in\mathbb{N}} |f_n^\epsilon(t,x)|^2 g_{nn}(z') + \sum_{n\in\mathbb{N}} h_n^\epsilon(t,x) \left( \sum_{n'\neq n} h_{n'}^\epsilon(t,x)e^{-i(E_n^\epsilon - E_{n'}) \frac{t}{\epsilon^2}} g_{nn'}(z') \right).
\]

Because of the vanishing average over long time periods of $e^{-i(E_{n'} - E_n) \frac{t}{\epsilon^2}}$, we can say that the second term (corresponding to the off–diagonal part) vanishes in the limit $\epsilon \to 0$. Moreover, we previously saw that a formal limiting process allows to pass from the dynamics of $f_n^\epsilon$ to the effective mass dynamics of $h_{em,n}$. Therefore, $\int_{\mathbb{R}} |\psi^\epsilon(t,x,z')|^2 dx$ converges formally to the averaged term
\[
 \int_{\mathbb{R}} \left( \sum_{n\in\mathbb{N}} |h_{em,n}(t,x)|^2 g_{nn}(z') \right) dx,
\]
where, in the superposition of the densities, the multiplication by $g_{nn}$'s allows to take into account the effects of the cross-section confinement.

### 3.5 Approximate dynamics in the degenerate case

We now discuss the degenerate case and consider each eigenvalue $E_n$ with its multiplicity $\alpha_n \geq 1$. As we shall see, the differences, compared to the non-degenerate case, take place mainly in two instances : during the diagonalization of the free $k \cdot p$ Hamiltonian and at the level of the long time averaging process.

In Section 3.3, the unperturbed eigenvalues, as well as the perturbed ones, have been numbered in increasing order. In the degenerate case, crossing of the modes may lead to a loss of regularity of the perturbed eigenvalues. However, as already mentioned at the beginning of section 3, one peculiarity of nanowires (with respect to 3D crystals) is that the
perturbation parameter $\xi$ is scalar, and Kato’s results [21] say that in the neighborhood of $\xi = 0$ there are $\alpha_n$ (not necessarily distinct) eigenvalues which are analytic, together with the corresponding eigenvectors. We denote the perturbed regular eigencouple of (3.22) by $(\lambda_{n,\alpha}(\xi), v_{n,\alpha}(\xi))$. Then, in view of Remark 3.3 the same numbering is inherited by the eigenvectors $\chi_{n,\alpha}$. Moreover, as defined in Proposition 3.2, we use the notation $n-\alpha = \sum_{n' < n} \alpha_{n'} + \alpha$.

Expanding the eigenvectors $v_{n,\alpha}(\xi)$ and the eigenvalue $\lambda_{n,\alpha}(\xi)$ of $A(\xi)$ and collecting the terms with the same order of $\xi$ as in the non-degenerate case, we still can write

$$A^0 v_{n,\alpha} = \lambda^0_{n,\alpha} v_{n,\alpha},$$

$$A^1 v_{n,\alpha} + A^0 v_{n,\alpha} = \lambda^1_{n,\alpha} v_{n,\alpha} + \lambda^0_{n,\alpha} v_{n,\alpha},$$

$$A^2 v_{n,\alpha} + A^1 v_{n,\alpha} + A^0 v_{n,\alpha} = \lambda^2_{n,\alpha} v_{n,\alpha} + \lambda^1_{n,\alpha} v_{n,\alpha} + \lambda^0_{n,\alpha} v_{n,\alpha}.$$

The system (3.40) gives directly $\lambda^0_{n,\alpha} = E_n$ and $v^0_{n,\alpha} = e_{n,\alpha}$ where $e_{n,\alpha}$ is the $n-\alpha$th vector of the canonical basis in $l^2$.

The projection of (3.41) on $e_{n,\alpha}$ implies $\lambda^1_{n,\alpha} = 0$, because integration by parts still implies $P_{(n,\alpha n,\alpha)} = 0$. Then, projecting (3.41) on $e_{n,\alpha'} (\alpha' \neq \alpha)$ gives

$$P_{(n,\alpha' n,\alpha)} = 0. \tag{3.43}$$

Also, projecting (3.41) on $e_{n',\alpha'} (n' \neq n)$, we obtain

$$-iP_{(n',\alpha' n,\alpha)} + E_{n'} v^1_{n',\alpha' n,\alpha} = E_n v^1_{n,\alpha' n',\alpha'}$$

where $v^1_{n,\alpha' n',\alpha'}$ is the $(n'-\alpha')$th component of $v^1_{n,\alpha'}$. It gives

$$v^1_{n,\alpha' n',\alpha'} = -iP_{(n',\alpha' n,\alpha)} E_n - E_{n'}. \tag{3.44}$$

Finally, using $P_{(n,\alpha n,\alpha)} = 0$ and (3.43), the projection of (3.42) on $e_{n,\alpha}$ simplifies to

$$E_n v^2_{n,\alpha n,\alpha} - i \sum_{n' \neq n} \sum_{\alpha' = 1}^{\alpha_{n'}} P_{(n,\alpha n',\alpha')} v^1_{n,\alpha' n',\alpha'} + \frac{1}{2} = E_n v^2_{n,\alpha n,\alpha} + \lambda^2_{n,\alpha}.$$

Using (3.44), we obtain

$$\lambda^2_{n,\alpha} = \frac{1}{2} \left(1 - 2 \sum_{n' \neq n} \sum_{\alpha' = 1}^{\alpha_{n'}} \frac{P_{(n,\alpha n',\alpha')} P_{(n',\alpha' n,\alpha)}}{E_n - E_{n'}}\right). \tag{3.45}$$

We conclude saying that

$$\lambda_{n,\alpha} \simeq \lambda^0_{n,\alpha} + \xi^2 \lambda^2_{n,\alpha} = E_n + \frac{1}{2} \frac{\xi^2}{m^*_{n,\alpha}}, \tag{3.46}$$

where the effective mass $m^*_{n,\alpha}$ is defined in (3.8).
Consequently, in the degenerate case, the inverse Fourier transform of the sequence \( g_{\epsilon m} = (g_{\epsilon m,1}, \ldots, g_{\epsilon m,1,\alpha_1}, g_{\epsilon m,2,1}, \ldots) \), which is denoted by \( f_{\epsilon m} = (f_{\epsilon m,1,1}, \ldots, f_{\epsilon m,1,\alpha_1}, f_{\epsilon m,2,1}, \ldots) \), is solution, component wise, of

\[
i\partial_t f_{\epsilon m,n,\alpha}(t, x) = -\frac{1}{2m^*_{n,\alpha}} \partial_{xx} f_{\epsilon m,n,\alpha}(t, x) + \frac{1}{\epsilon^2} E_n f_{\epsilon m,n,\alpha}(t, x) + \sum_{n' \neq n} \sum_{\alpha' = 1}^{\alpha'} V_{n,\alpha, n',\alpha'}(x) f_{\epsilon m,n',\alpha'}(t, x).
\]

(3.47)

**Remark 3.5.** In the above computations we obtained (3.43) thanks to the analyticity of the perturbed eigenvalues and of the corresponding eigenvectors, that allowed to write (3.40)–(3.42), so that no drift term appears in the approximate equation (3.47). Moreover, we can project (3.42) on \( e_{n,\alpha'} \), with \( \alpha' \neq \alpha \) to obtain

\[
\sum_{n''} \sum_{\alpha'' = 1}^{\alpha''} \frac{P_{n,\alpha', n''} P_{n'',\alpha'' n,\alpha}}{E_n - E_{n''}} = 0.
\]

Therefore, in the case of nanowires, the effective mass equations have a simpler structure than in the case of 3D crystals reported, e.g., in [34, 20].

Again, the last level of approximation consists in filtering fast oscillations in time of (3.47) by setting \( f_{\epsilon m,n,\alpha}(t, x) = h_{\epsilon m,n,\alpha}(t, x) e^{-iE_n \frac{t}{\epsilon}} \). Then, \( h_{\epsilon m,n,\alpha} \) is solution of

\[
i\partial_t h_{\epsilon m,n,\alpha}(t, x) = -\frac{1}{2m^*_{n,\alpha}} \partial_{xx} h_{\epsilon m,n,\alpha}(t, x) + \sum_{n' \in \mathbb{N}} \sum_{\alpha' = 1}^{\alpha'} e^{-i(E_{n'} - E_n) \frac{t}{\epsilon}} V_{n,\alpha, n',\alpha'}(x) h_{\epsilon m,n',\alpha'}(t, x).
\]

(3.48)

As for the non–degenerate case, we can still define a remainder operator in the form

\[
(R'(t)h)_{n,\alpha} = \sum_{n' \neq n} \sum_{\alpha' = 1}^{\alpha'} e^{-i(E_{n'} - E_n) \frac{t}{\epsilon}} V_{n,\alpha, n',\alpha'}(x) h_{n',\alpha'}(x).
\]

(3.49)

But, in this case, the \( H_0 \) operator is not diagonal anymore

\[
(H_0 h)_{n,\alpha} = -\frac{1}{2m^*_{n,\alpha}} \partial_{xx} h_{n,\alpha}(x) + \sum_{\alpha' = 1}^{\alpha} V_{n,\alpha, n',\alpha'}(x) h_{n',\alpha'}(x).
\]

(3.50)

We still can formally pass to the limit when \( \epsilon \to 0 \) to obtain Proposition 3.2. We emphasize that the important difference with the non-degenerate case is that a complete separation of the oscillating time scales is not possible and the final system retains a coupling through the potential.
Remark 3.6. Also the formal limit of (2.31) as \( \epsilon \to 0 \) is different than in the non-degenerate case. In the degenerate case, the first member of (3.39) can be restated emphasizing the multiplicity of the eigenvalues as

\[
\sum_{n \in \mathbb{N}} \sum_{\alpha=1}^{\alpha_n} \sum_{n' \in \mathbb{N}} \sum_{\alpha'=1}^{\alpha_{n'}} f_{n,\alpha}^{\epsilon}(t, x) \overline{f_{n',\alpha'}^{\epsilon}(t, x)} g(n, \alpha, n', \alpha') (z').
\]

Clearly, in this case, the transformation \( f_{n,\alpha}^{\epsilon}(t, x) = h_{n,\alpha}^{\epsilon}(t, x) e^{-iE_n^{\epsilon} t/\hbar} \), for \( \alpha = 1, \ldots, \alpha_n \), does not allow to obtain a diagonal density in the \( \epsilon \to 0 \) limit. Indeed, \( \int_{\mathbb{R}} |\psi_{\epsilon}(t, x, z')|^2 dx \) converges formally to the averaged term

\[
\int_{\mathbb{R}} \left( \sum_{n \in \mathbb{N}} \sum_{\alpha=1}^{\alpha_n} h_{\text{em},n,\alpha}(t, x) \overline{h_{\text{em},n,\alpha'}(t, x)} g(n, \alpha, n', \alpha') (z') \right) dx,
\]

where a coupling among bands corresponding to the same eigenvalue is present. Instead, the coupling disappears if we integrate in the variable \( z' \), because of the orthogonality of the \( \chi_{n,\alpha} \)'s. Therefore, \( \int_{\mathbb{R} \times \Omega} |\psi^{\epsilon}(t, x, z')|^2 dx dz \) converges formally to the averaged term

\[
\int_{\mathbb{R}} \left( \sum_{n \in \mathbb{N}} \alpha_n |h_{\text{em},n,\alpha}(t, x)|^2 \right) dx.
\]

4 The stationary 1D Schrödinger - 3D Poisson problem

A FET (Field Effect Transistor) based on a nanowire or a nanotube is described by a bounded 3D domain defined as \( \Omega = (x_L, x_R) \times \omega, \) where \((x_L, x_R)\) denotes the bounded longitudinal section and \( \omega \) denotes the 2D cross-section. The transport in the longitudinal direction of the FET is described by a sequence of 1D Schrödinger equations of the form (3.2) on \((x_L, x_R)\). The system is considered as an open quantum system: electrons are injected from the leads considered as reservoirs, they travel through the channel (active region) and they leave the device through another reservoir. Transparent Boundary Conditions TBCs [14, 23, 7] are used to complete the system. More precisely, TBCs are computed assuming that in the leads the potential \( V_{nn} \) is constant, equal to \( V_{nn}(x_L) \) in the left lead (Source contact) and equal to \( V_{nn}(x_R) \) in the right lead (Drain contact). Then, the plane waves, solutions in the leads, are linked to the solution inside \((x_L, x_R)\) via continuity conditions (for the wave function and its derivative).

For each \( n^{th} \) band and for each wave vector \( k \), we consider the stationary Schrödinger equation

\[
-\frac{1}{2m_n^*} \partial_{xx} \psi_n^k(x) + V_{nn}(x) \psi_n^k(x) = \mathcal{E}_n^k \psi_n^k(x), \quad x \in (x_L, x_R),
\]

with \( \mathcal{E}_n^k = \frac{k^2}{2m_n^*} + V_{nn}(x_L) \) if \( k > 0 \) and with \( \mathcal{E}_n^k = \frac{k^2}{2m_n^*} + V_{nn}(x_R) \) if \( k < 0 \). The TBCs take the form

\[
\partial_x \psi_n^k(x_L) + ik \psi_n^k(x_L) = 2ik \quad \text{and} \quad \partial_x \psi_n^k(x_R) = ip_+(k) \psi_n^k(x_R) \quad \text{for} \quad k > 0,
\]

\[21\]
\[ \partial_x \psi_n^k(x_R) + ik \psi_n^k(x_R) = 2ik \quad \text{and} \quad \partial_x \psi_n^k(x_L) = -ip_+(k) \psi_n^k(x_L) \quad \text{for } k < 0, \tag{4.3} \]

where
\[ p_\pm(k) = \sqrt{k^2 \mp 2m^*_n(V_{nn}(x_R) - V_{nn}(x_L))} \]

We point out, once again, that the “memory” of the cross-section is encoded in the effective mass \( m^*_n \) given by (3.3) and in the effective potential \( V_{nn}(x) \) defined in (3.5).

In the degenerate case, if \( E_n \) has multiplicity \( \alpha_n \), a system of dimension \( \alpha_n \), in the form (3.7) has to be considered. Accordingly, TBC’s for systems must be introduced. As in the scalar case, plane wave solutions in the leads are computed, assuming constant potential. From the dispersion relation the group velocity is obtained and comparison of the sign of the group velocities with those of the wave vectors allows to identify the ingoing and the outgoing waves. Finally, the TBC’s are derived, as in the single Schrödinger equation case, by eliminating the reflection and the transmission coefficients, giving a system of dimension \( \alpha_n \), which turns out to be a matrix form of equations (4.2) or (4.3). This derivation requires to distinguish various cases and it is far from the scope of this paper. We refer to [18] for the explicit computation in this context and to [8] for the derivation of TBC’s in the case of a two-band Schrödinger model.

Next, in an open system electrons are considered in mixed states and the 1D density carried by the \( n^{th} \) band \( N_{1D}^n \) is given superimposing the densities of states injected from the reservoirs, that is
\[ N_{1D}^n(x) = \int \phi_n(k) |\psi_n^k(x)|^2 \, dk, \tag{4.4} \]

where \( \phi_n(k) \) characterizes the electron injection from the reservoirs. In the subsequent simulation, the Boltzmann statistics is used (see Section 5.4).

The electrostatic behavior of the device is described by the self-consistent electrostatic potential solution of a Poisson equation in the 3D device. In view of Remarks 2.4 and 3.4, the 3D macroscopic charge density \( \rho(x, z) \) (entering in the second member of the Poisson equation) is computed as superposition of densities in each band by means of the relation
\[ \rho(x, z) = \sum_{n \in \mathbb{N}} N_{1D}^n(x) g_{nn}(\frac{z}{\epsilon}) \quad (x, z) \in \Omega, \tag{4.5} \]

where the \( g_{nn}(z) \), defined in (2.6), takes into account the confinement part of the wave function and \( N_{1D}^n(x) \) is the 1D density carried by \( n^{th} \) band given by (4.4). In the degenerate case, the 3D charge density is computed by
\[ \rho(x, z) = \sum_{n \in \mathbb{N}} \sum_{\alpha=1}^{\alpha_n} \sum_{\alpha'=1}^{\alpha_n} N_{1D}^{(n,\alpha \ n',\alpha')}(x) g_{(n,\alpha \ n',\alpha')}(\frac{z}{\epsilon}) \quad (x, z) \in \Omega, \tag{4.6} \]

where \( g_{(n,\alpha \ n',\alpha')} \) and \( N_{1D}^{(n,\alpha \ n',\alpha')} \) are respectively defined analogously to (2.6) and (4.4). In this case, a coupling occurs between the energy bands corresponding to the same eigenvalue (see Remark 3.6).
Finally, the total current density is given by

$$J(x) = \sum_{n \in \mathbb{N}} J_n(x), \quad x \in (x_L, x_R),$$

(4.7)

where the current density in the \(n^{th}\) band is expressed by

$$J_n(x) = \frac{1}{m_n^*} \int_{\mathbb{R}} \phi_n(k) \mathcal{I} \left( \overline{\psi_n^k(x)} \partial_x \psi_n^k(x) \right) dk,$$

(4.8)

where \(\mathcal{I}\) denotes the imaginary part. Due to the TBCs, multiplying the 1D stationary Schrödinger equation (4.1) by \(\psi_n^k\) and taking the imaginary part give immediately that the current density \(J_n\) is constant in space. In the degenerate case, since the system (3.8) has a diagonal kinetic part, the conserved quantity in correspondence to the multiple eigenvalue \(E_n\) is \(\sum_{\alpha=1}^{\alpha_n} J_{n,\alpha}(x)\), where the current density \(J_{n,\alpha}\) is analogous to (4.8). Therefore, the total current density is defined by

$$J(x) = \sum_{n \in \mathbb{N}} \sum_{\alpha=1}^{\alpha_n} \sum_{\alpha=1}^{\alpha_n} J_{n,\alpha}(x), \quad x \in (x_L, x_R).$$

(4.9)

To summarize, the model consists of two steps. The first step requires the resolution of the Bloch type problem (2.3) in the primitive cell, and it provides the energies, the effective masses and the functions (2.6). This computation is done only once for a given device. We point out that these quantities depend not only on the material, but also on the given device, e.g. on the geometrical structure and on the growing orientation of the wire. We also emphasize that the model relies on an atomistic computation in the primitive cell and not in the entire structure. Then, the second step consists of the resolution of the coupled Schrödinger-Poisson system, where the physical quantities computed in the previous step are included. The 1D Schrödinger equations with open boundary conditions describe the electron transport along the wire, whereas the 3D Poisson equation models the electrostatic potential in the entire structure. The reduced dimensionality of the Schrödinger equations greatly decreases the computational time in the simulations.

5 Numerical implementation for a nanotube

5.1 Modeled device

The numerical simulations that will be presented in Section 6 aim at testing the capability of the model to describe the electron transport in an ultra-scaled confined structure and they will be carried out in a very simplified case, a one–wall carbon nanotube with a cross-section made of 12 atoms disposed on a squared frame, surrounded by one atom layer of dielectric acting like an insulator.

The transport problem is solved for a gate-all-around FET (Field Effect Transistor) with channel length equal to 10 nm doped with a donor concentration equal to \(N_D^{-} = 10^{21}\). 
m$^{-3}$, with Source and Drain regions 10 nm long, largely doped ($N_D^+ = 10^{26}$ m$^{-3}$). A schematic representation of the device is given in Fig.1. The $x$ variable corresponds to the transport direction, whereas $(z_1, z_2)$ describes the 2D cross-section. The lattice spacing $\epsilon$ is equal to $3.57\,\text{Å}$ for carbon. Therefore, the wire cross-section edge $l$ (equal to $6\epsilon \approx 2\text{nm}$) is tiny compared to the longitudinal length $L$ equals to 30 nm.

### 5.2 Pseudo-potential

The potential $W_L$ generated by the crystal lattice and used to compute the Bloch functions (2.3) is visualized in Fig.2. It is a pseudo-potential used by [35] for *ab-initio* atomistic-based electronic density calculations for carbon nanotubes. In correspondence of each nucleus, we take $W_L(r) = \sum_{i=1}^{3} A_i \exp(-a_ri)$, where $r$ is the distance to the nucleus and the coefficients $A_i$ and $a_i$ have been defined in [26] to reproduce the band structure of the carbon nanotube. A large potential barrier (we chose 15 eV) is used at the boundaries of the nanotube to take in account the dielectric layer.

### 5.3 Implemented equations

For the sake of completeness, we recall the equations which are used in the simulations, writing them in unscaled form. First, the Bloch functions $\chi_n^\epsilon(x, z')$ are the normalized eigenfunctions of the following problem in the cell $\mathcal{U}_\epsilon = (-\epsilon/2, \epsilon/2) \times \omega$,

$$
\begin{cases}
    -\frac{\hbar^2}{2m_e} \Delta \chi_n^\epsilon + W_L(x, z') \chi_n^\epsilon = E_n \chi_n^\epsilon, \\
    \chi_n^\epsilon(x, z') = 0 \text{ on } \partial\omega, \quad \chi_n^\epsilon \epsilon\text{-periodic in } x,
\end{cases}
$$

(5.1)
where $\epsilon$ is the lattice spacing, $\hbar$ is the reduced Planck constant and $m_e$ is the electron mass.

Although not all the eigenvalues of (5.1) are simple in the present case, still a decoupled system can be considered. Actually, it turns out that, for the problem under consideration with the gate-all-around, the off-diagonal terms in the potential matrix ($V_{n,\alpha n,\alpha'}$ with $\alpha \neq \alpha'$) are negligible. Then, the transport is described by a set of 1D Schrödinger equations with TBCs, which can be expressed, for a positive wave vector $k > 0$ (see (4.1) with (4.2)), as follows

$$
\begin{align*}
-\frac{\hbar^2}{2m^*_n} \partial_{xx} \psi^k_n(x) + V_{nn}(x) \psi^k_n(x) &= \left(\frac{\hbar^2 k^2}{2m^*_n} + V_{nn}(x_L)\right) \psi^k_n(x), \quad x \in (x_L, x_R), \\
\partial_x \psi^k_n(x_L) + ik \psi^k_n(x_L) &= 2ik, \\
h \partial_x \psi^k_n(x_R) &= i\sqrt{\hbar^2 k^2 - 2m^*_n (V_{nn}(x_R) - V_{nn}(x_L))} \psi^k_n(x_R),
\end{align*}
$$

(5.2)

where

$$
m_e/m^*_n = 1 - \frac{2\hbar^2}{m_e} \sum_{q \neq n} \frac{P_{mn} P_{qn}}{E_n - E_q}
$$

and

$$
V_{nn}(x) = \int_\omega V(x, \epsilon z') g_{nn}(z') \, dz' \quad \text{with} \quad g_{nn}(z') = \int_{-\epsilon/2}^{\epsilon/2} |\chi^R_n(x, z')|^2 \, dx.
$$

(5.3)

(5.4)

For negative wave vector $k < 0$, the equations are similar (see (4.1) with (4.3)).

Next, we compute the 1D charge densities (4.4) for each band $n$ and then the macroscopic 3D charge density $\rho$ (4.5). Finally, the electrostatic potential $V_P$ is solution of the following 3D Poisson equation

$$
-\nabla \left(\epsilon_r(z) \nabla V_P(x, z)\right) = \frac{q}{\epsilon_0} (N_D(x, z) - \rho(x, z)), \quad (x, z) \in \Omega.
$$

(5.5)

$q$ is the elementary charge, $\epsilon_0$ the permittivity in vacuum, $\epsilon_r$ the relative permittivity and $N_D$ the prescribed doping density (null in the oxide and the air regions, and given as in

Figure 2: Pseudo-potential energy (eV) : 1D $W_L(r)$ (left) and $W_L(x = 0, z)$ (right).
Section 5.1 in the carbon region). Equation (5.5) is supplemented by boundary conditions that will be made explicit in Section 5.5. Notice that this equation gives the potential \( V_P \) (expressed in Volts), instead the Schrödinger equation (5.2) is written in terms of an energy \( V \) (expressed in Joules). They are linked by the relation \( V = -qV_P \).

Finally, the current density in physical variables is given by

\[
J(x) = \sum_{n \in \mathbb{N}} \frac{q\hbar}{m^*_n} \int_{\mathbb{R}} \phi_n(k) \text{Im} \frac{\psi_n^*(x) \partial_x \psi_n(x)}{\psi_n^*(x) \partial_x \psi_n(x)} \, dk, \quad x \in (x_L, x_R). \tag{5.6}
\]

5.4 Distribution function and Fermi level

In this work, we choose the Boltzmann statistic to describe the distribution \( \phi_n \) used to compute the 1D charge densities (4.4). It is typically defined by

\[
\phi_n(k) = \frac{C}{\sqrt{m^*_n}} e^{-\left(\frac{\hbar^2 k^2}{2m^*_n} + E_n - \mu_{eq}\right) / (k_B T)} \tag{5.7}
\]

where \( C \) is a physical constant independent of the band index, \( k_B \) the Boltzmann constant, \( T \) the lattice temperature and \( \mu_{eq} \) the Fermi level at thermal equilibrium. We notice that \( \phi_n(k) \) does not depend on the contact lead under consideration, and it is the same in the non-equilibrium case. Indeed, a cancellation occurs in the exponent, since both the energy \( E_n \) and the Fermi level \( \mu_{eq} \) are shifted by the same potential energy \( V_{nn} \).

Next, we have to determine the Fermi level at thermal equilibrium. More precisely, we compute directly the constant term \( C e^{\mu_{eq}/(k_B T)} \). It is obtained under the hypothesis of quasi-neutrality at the boundaries

\[
\int_{\omega_e} \left( \rho(x_c, z) - N_D(x_c, z) \right) \, dz = 0, \tag{5.8}
\]

where \( x_c = x_L \) or \( x_c = x_R \). We suppose that the potential \( V \) is constant along the transport direction and consequently all the wave functions \( \psi_n^k \) contributing to \( \rho \) have unitary modulus. After calculations, we obtain the explicit formula

\[
C e^{\mu_{eq}/(k_B T)} = \frac{\int_{\omega_e} N_D(x_c, z) \, dz}{\sum_n \int_{\mathbb{R}} \frac{1}{\sqrt{m^*_n}} e^{-\left(\frac{\hbar^2 k^2}{2m^*_n} + E_n\right) / (k_B T)} \, dk}. \tag{5.9}
\]

5.5 Poisson boundary conditions

In this subsection, we discuss the choice of boundary conditions for the 3D Poisson equation (5.5). The boundary \( \partial \Omega \) of the computational domain is split in three parts: \( \partial \Omega = \Gamma_C \cup \Gamma_G \cup \Gamma_N \).

\( \Gamma_C \) corresponds to the ohmic Source and Drain contacts i.e. \( \Gamma_C = \{(x, z) \in \partial \Omega \text{ such that } x = x_c\} \). On \( \Gamma_C \), we impose a Robin boundary condition

\[
\partial_x V_P + \alpha_c \left(V_P - (V_{Applied} + V_b)\right) = 0
\]
in order to control at the same time the value and the slope of the potential. The sign of \( \alpha \) is chosen to have coercivity of the bilinear form and the value of \( \alpha \) is of order of \( \frac{1}{L} \). \( V_{Applied} \) corresponds to the applied potential at ohmic contacts. Finally, \( V_b \) is the built-in potential defined, solving at the contacts, a 2D Poisson equation

\[
\begin{cases}
-\nabla(\varepsilon_r \nabla V_b(z)) = \frac{\varepsilon_0}{\varepsilon_r} N_D(x_c, z) - \frac{q}{\varepsilon_0} \rho_{2D}(z), & z \in \omega, \\
\partial_v V_b = 0, & \int_{\omega} V_b(z) dz = 0.
\end{cases}
\]

We notice that \( V_b \) is the same at Source and Drain contact because of the same doping density. Moreover, the density \( \rho_{2D} \) does not depend on the potential. Indeed, we make the same assumption than for the Fermi level calculation (i.e. \( V \) constant in the transport direction) and thus the density can be expressed explicitly (using (4.5), (4.4), (5.7) and (5.9)). Fig.3 displays the shape of the 2D built-in potential for our nanotube device.

![Figure 3: Shape of the 2D built-in potential energy \( V_b \) (eV).](image)

Next, \( \Gamma_G \) corresponds to the gate, that is chosen here all-around (see Fig.1), and a gate potential \( V_G \) is applied on \( \Gamma_G \) to modulate the number of free electrons. Finally, we impose homogeneous Neumann boundary conditions in the remain boundary domain \( \Gamma_N = \partial \Omega \setminus (\Gamma_C \cup \Gamma_G) \). To sum up, we supplement the Poisson equation (5.5) with the following boundary conditions

\[
\begin{cases}
\partial_x V_P + \alpha_c \left( V_P - (V_{Applied} + V_b) \right) = 0 & \text{on } \Gamma_C, \\
V_P = V_G & \text{on } \Gamma_G, \\
\partial_v V_P = 0 & \text{on } \Gamma_N.
\end{cases}
\]
5.6 Algorithm

We now discuss the implementation of the entire problem (5.1)-(5.5) emphasizing the delicate numerical points.

5.6.1 First block : to solve the eigenvalue problem in the primitive cell

The starting point is to solve the eigenvalue problem (5.1). It is discretized with \( Q_1 \) finite elements on parallelepipeds. This choice is motivated by the fact that the mesh should preserve the symmetries of the structure. Moreover, due to the fine pattern of the pseudo-potential (see Fig.2), a fine mesh is necessary. The 1D lattice spacing (of length \( \epsilon \)) must be decomposed by a minimum of 20 discretization points, which gives, for a 3D uniform mesh, about 250 000 degrees of freedom for the finite element space. The problem (5.1) is reduced to a generalized eigenvalue problem of the form \( Au = \lambda Bu \), solved using the library Arpack [22]. This software is based upon an algorithmic variant of the Arnoldi process called the Implicitly Restarted Arnoldi Method [31]. We compute the smallest eigenvalues (corresponding to the bands with the lowest energies).

5.6.2 Second block : to solve the Schrödinger-Poisson problem

The previous block, done only once for the given device, provides the energies \( E_n \), the effective masses \( m^*_n \) and the functions \( g_{nn} \)'s. These quantities are inserted in the Schrödinger-Poisson problem (5.2)-(5.5). The first step is to compute the solution of (5.10) to get the built-in potential \( V_b \) at the ohmic contacts. The procedure is then initialized by taking \( V(.,z) = V_b(z) \). Next, we consider the whole system (5.2)-(5.5) at thermal equilibrium (for zero applied Drain–Source voltage). Finally, we consider the resolution of the Schrödinger-Poisson system when a Drain-Source voltage \( V_{DS} \) is applied. We start from the obtained potential at thermal equilibrium and we increment the voltage by steps of 0.02 V. At each outer iteration, the computed potential is used to initialize the inner iteration algorithm. To conclude, all this procedure (initialization, thermal equilibrium solution and Drain–Source voltage continuation) is repeated for different gate voltage \( V_G \).

Here we detail the discretization schemes and the iterative algorithm for the inner solution of the Schrödinger–Poisson problem (5.2)-(5.5). Because of the highly nonlinear coupling between the density and the potential equations, the inner iteration procedure is done by an iterative method of Gummel type. It is described in the following steps :

(i) For a given 3D potential \( V_{P}^{old} \), we compute a 1D potential \( V_{nn} \) for each \( n^{th} \) band using (5.4).

(ii) The 1D Schrödinger equation with TBCs is solved for each \( n^{th} \) band and each wave
vector \( k \). For \( k > 0 \), equation (5.2) is transformed into an initial value problem
\[
\begin{align*}
-\frac{\hbar^2}{2m^*_n} \partial_{xx} \varphi^k_n(x) + V_{nn}(x) \varphi^k_n(x) &= \left(\frac{\hbar^2 k^2}{2m^*_n} + V_{nn}(x_L)\right) \varphi^k_n(x), \\
\varphi^k_n(x_R) &= 1, \\
\partial_x \varphi^k_n(x_R) &= i \sqrt{\frac{\hbar^2 k^2}{2m^*_n} - 2m^*_n (V_{nn}(x_R) - V_{nn}(x_L))}.
\end{align*}
\]
(5.12)

It suffices to normalize \( \varphi^k_n(x) \) by \( 2i k/\left[ \partial_x \varphi^k_n(x_L) + 2i k \varphi^k_n(x_L) \right] \) to recover \( \psi^k_n(x) \). The ODE is then discretized with a Crank-Nicolson scheme, which is a conservative scheme and it avoids numerical dissipation for large \( k \)'s. The negative wave vector case is treated analogously.

(iii) We can compute the 1D charge density \( N^n_{1D} \) (4.4) for each \( n \)th band and, afterwards, the 3D charge density \( \rho \) (4.5).

(iv) We solve the 3D Poisson equation (5.5) with the boundary conditions (5.11) using \( Q_1 \) finite elements on parallelepipeds and we obtain a new potential \( V^\text{new}_{P} \). The high nonlinearity of the coupled Schrödinger–Poisson system is the most delicate step of the procedure. A simple-minded iterative algorithm fails to converge and a Newton-Raphson method is computationally expensive. We use an iterative method of Gummel type, which amounts to substitute the Poisson equation (5.5) with
\[
-\nabla \left( \epsilon_r \nabla V^\text{new}_{P}(x,z) \right) = \frac{q}{\epsilon_0} N_D(x,z) - \frac{q}{\epsilon_0} \rho \left[ V^\text{old}_{P}(x,z) \right] \left(1 + \frac{q}{k_B T} (V^\text{new}_{P} - V^\text{old}_{P}) \right). \tag{5.13}
\]

The algorithm has been introduced in [17] for the Drift-Diffusion model and it has been extended to the present form for a Schrödinger-Poisson system [10]. We also refer to [29] where this method is used in the simulation of a 2D ballistic Schrödinger-Poisson system.

(v) We repeat the four previous steps until the difference \( \|V^\text{new}_{P} - V^\text{old}_{P}\|_{L^\infty} \) becomes sufficiently small.

This entire procedure gives computationally efficient simulations upon condition that the choice of meshes is judicious. Since the high energy wave functions are strongly oscillating, a fine mesh size is needed to solve the 1D Schrödinger equations. On the contrary, the Poisson equation is solved in the whole domain and a larger mesh size is allowed in the transport direction. Therefore, in the simulations performed in Section 6, we solve the Schrödinger equations with 400 discretization points, whereas the mesh used for the Poisson equation contains only 50 points in the transport direction. Concerning the 2D cross section, the computed quantities have always a fine pattern (see Fig.3, e.g.) and we
use for the Poisson equation the same 2D mesh used to solve the eigenvalue problem (see Section 5.6.1). It gives a 3D finite element method for the Poisson equation with about 660,000 degrees of freedom.

We conclude this section pointing out that parallelization can be used in several instances of the procedure in order to decrease the overall computational cost. For example, in the transport part, we solve a large number of Schrödinger equations for different wave vectors $k$. All these equations are independent from each other and can be treated simultaneously, using the MPI standard. Finally, the most expensive part is the resolution of the linear system associated with the 3D Poisson equation. It is parallelized by using the library PETSc [4, 5].

6 Numerical results

Figure 4: $g_{nn}(z)$ for 41$^{th}$ mode (top), 42$^{th}$ and 43$^{th}$ mode (bottom, from left to right).

We present in this part some results obtained for the simplified one-wall carbon nan-
tube described in Section 5.1, aiming at reproducing the qualitative behavior of the device. Therefore, the Schrödinger-Poisson system is solved only in the first three “conduction” bands. Looking at the energies $E_n$, the most significant gap is observed between the 40th and the 41st band. Consequently, we choose to consider the 41st, 42nd and the 43rd bands.

In the present simulation, mode 42th and mode 43th coincide. Nevertheless, as already pointed out in Section 5.3, the computed off-diagonal potential term $V_{42,43}$ is virtually zero and the coupling of these two bands can be neglected.

In Fig.4 the 2D quantities $g_{nn}(z)$’s are presented. We notice that the 12 ion cores of the cross-section clearly appear, showing that the $g_{nn}$’s retain information of the confinement and of the cross-section structure. Moreover, we point out that the two bottom pictures, corresponding to the multiple eigenvalue, coincide up to a rotation.

Figure 5: 1D potential energies (eV) (left) and 1D densities ($m^{-3}$)(right) for different $V_{DS}$, with $V_G = -0.1$ V.

These $g_{nn}$’s (as well as effective masses $m_n^*$ and energies $E_n$) are included in the transport problem solved for a gate-all-around FET. We start to compute the thermal equilibrium. Then, we apply a Drain–Source voltage $V_{DS}$. To visualize the results, we first present 1D curves instead of 3D plots. 1D profiles of the density and of the potential are presented for a fixed gate voltage $V_G = -0.1$ V in Fig.5. These 1D curves are results of an integration of 3D quantities over the 2D wire section. In the left figure, variations at $x = 5$ nm and $x = 25$ nm are due to the gate, instead variations at $x = 10$ nm and $x = 20$ nm are consequences of the doping. We remark that the 1D potential in the channel has a value close to $V_G$, confirming that the transport is mainly controlled by the gate.

In order to show the changes due to the voltage, that are not clearly visible from the 1D density pictures, it is interesting to plot the average velocity, defined as $v(x) = J/[q \sum_n N_{1D}^n(x)]$. Fig.6 illustrates how the average velocity increases with the applied Drain–Source voltage $V_{DS}$. It is also apparent that, for larger values of the Drain–Source voltage, velocities tend to a saturation regime (see also Fig.11).
Figure 6: Average velocity \(\text{(ms}^{-1}\text{)}\) for \(V_G = -0.1\) V.

Figure 7: 3D potential energy (eV) (left) and 3D density \(\text{(m}^{-3}\text{)}\) (right) at thermal equilibrium for \(V_G = -0.1\) V.

The description of the entire 3D device is visualized in Fig.7, where the 3D potential energy (left) and the 3D density (right) are plotted at thermal equilibrium for \(V_G = -0.1\) V. In the left picture of Fig.7 the structure of the FET is apparent, with the Source, Drain and channel regions and a clear influence of the gate. Fig.7 does not allow to appreciate the fine structure of the potential, that seems to be constant in the cross-section. Only at the logarithmic scale, that is used in Fig.8 to represent the 2D potential in the central slice \((x = 15\) nm), we can recognize the cross-section influence. The fine pattern exhibited by the plot confirm the need of the 660 000 dof’s, used for the Poisson computation.

The right picture of Fig.7 allows to visualize the formation of a channel for each nucleus. The transport from Source to Drain is illustrated by Figs.9 and 10, that represent the density, in logarithmic scale, in a 2D slice along the transport direction \((x\text{-axis in the})\)
Figure 8: 2D cross-section at $x = 15$ nm of the potential energy in logarithmic scale at equilibrium for $V_G = -0.1$ V.

Figure 9: 2D slice (crossing 2 nuclei) of density in logarithmic scale at equilibrium (left) and for $V_{DS} = 0.2$ V (right), with $V_G = -0.1$ V. $x$-axis is the transport direction.

Figure 10: 2D slice (crossing 4 nuclei) of density in logarithmic scale at equilibrium (left) and for $V_{DS} = 0.2$ V (right), with $V_G = -0.1$ V. $x$-axis is the transport direction.
pictures). Fig.9 shows a slice that crosses two ions and Fig.10 corresponds to a slice that
crosses four ions. Comparing the thermal equilibrium pictures (left) with the ones for
$V_{DS} = 0.2$ V (right), we clearly observe the electron motion from the left to the right. Moreover, the different sharpness of the density around the ion cores in Fig.9 and in Fig.10 shows the influence of the neighboring ions.

Finally, in Fig.11, the output current–voltage characteristics of our simulated device
(for the fixed gate voltage $V_G = -0.1$ V) are presented, plotting the total current, as well
as the partial current carried by each band. As expected, the current in the first band
is larger than the one in the other two bands. The second band and the third band,
which correspond to the same eigenvalue, carry virtually the same current. We notice that
the qualitative behavior of these curves is similar to that of the conventional MOSFETs
with two typical regimes: an ohmic regime for small values of Drain-Source voltage and a
quasi-saturation regime for $V_{DS} > 0.12V$.

![Figure 11: Current-voltage characteristics for $V_G = -0.1$ V.](image)

We conclude saying that, even for this simplified problem, the model is able to capture
the qualitative behavior of the most relevant physical quantities, well describing the electron
transport in an ultra-scaled confined structure.

**Appendix A. Derivation of the exact dynamics (3.10)**

The solution $\psi^\varepsilon(t, x, z')$ of Schrödinger equation (2.2) can be decomposed according to
(2.34), where the Fourier transform $g^\varepsilon_n(t, k)$ of the $\varepsilon$-scaled envelope function is given by
formula (2.32) and the Bloch waves are defined in (2.33).
So, multiplying the Schrödinger equation (2.2) by \( u^\epsilon_{n,k}(x, z') \) and integration over \( \mathbb{R}_x \times \omega \) leads to the following expression

\[
\int_{\mathbb{R}_x \times \omega} i \partial_t \psi^\epsilon_{n,k} dx dz' = \int_{\mathbb{R}_x \times \omega} \left( -\frac{1}{2} \partial_{xx} \psi^\epsilon + \frac{1}{\epsilon^2} W(x, z') \psi^\epsilon + V(x, z') \psi^\epsilon \right) u^\epsilon_{n,k} dx dz'.
\]  

We treat each term separately. Concerning the first term, formula (2.32) gives immediately

\[
\int_{\mathbb{R}_x \times \omega} i \partial_t \psi(t, x, z') u^\epsilon_{n,k}(x, z') dx dz' = i \partial_t g^\epsilon_n(t, k).
\]  

In the same way, the last term can be treated easily. We obtain

\[
\int_{\mathbb{R}_x \times \omega} V(x, z') \psi(t, x, z') u^\epsilon_{n,k}(x, z') dx dz' = \sum_{n' \in \mathbb{N}} \int_{\mathbb{R}_k} U^\epsilon_{nn'}(k, k') g^\epsilon_n(t, k') dk',
\]  

where \( U^\epsilon_{nn'}(k, k') \) is defined in (3.12).

Differentiation with respect to \( x \) of the scaled Bloch wave (2.33) gives

\[
\partial_x u^\epsilon_{n,k}(x, z') = ik u^\epsilon_{n,k}(x, z') + \frac{1}{\epsilon} \frac{1}{\sqrt{2\pi}} I_{B_\epsilon}(k) e^{ikx} \partial_y \chi_n(x, z'),
\]  

and

\[
\partial_{xx} u^\epsilon_{n,k}(x, z') = -k^2 u^\epsilon_{n,k}(x, z')
\]

\[
+ \frac{1}{\sqrt{2\pi}} I_{B_\epsilon}(k) e^{ikx} \left( \frac{2ik}{\epsilon} \partial_y \chi_n(x, z') + \frac{1}{\epsilon^2} \partial_{yy} \chi_n(x, z') \right),
\]

where \( \partial_y \chi_n(x, \frac{z}{\epsilon}, z') \) denotes the derivative of \( \chi_n \) with respect to the first argument.

The second term in (A.1) can be rewritten integrating by parts twice and using the above differentiation formulas, obtaining

\[
\frac{k^2}{2} \int_{\mathbb{R}_x \times \omega} \psi(t, x, z') u^\epsilon_{n,k}(x, z') dx dz'
\]

\[
+ \frac{ik}{\epsilon} \frac{1}{\sqrt{2\pi}} I_{B_\epsilon}(k) \int_{\mathbb{R}_x \times \omega} \psi(t, x, z') e^{-ikx} \partial_y \chi_n(x, z') dx dz'
\]

\[
- \frac{1}{2\epsilon^2} \frac{1}{\sqrt{2\pi}} I_{B_\epsilon}(k) \int_{\mathbb{R}_x \times \omega} \psi(t, x, z') e^{-ikx} \partial_{yy} \chi_n(x, z') dx dz'.
\]

The third term in (A.1) becomes

\[
- \frac{1}{2\epsilon^2} \frac{1}{\sqrt{2\pi}} I_{B_\epsilon}(k) \int_{\mathbb{R}_x \times \omega} \psi(t, x, z') e^{-ikx} \Delta \chi_n(x, z') dx dz',
\]
and the fourth term is written as
\[
\frac{1}{\epsilon^2} \frac{1}{\sqrt{2\pi}} \mathbb{I}_B(k) \int_{\mathbb{R}_x \times \omega} \psi^\epsilon(t, x, z') e^{-ikx} W_L(\frac{x}{\epsilon}, z') \chi_n(\frac{x}{\epsilon}, z') dx dz'. \tag{A.8}
\]

Now, we group (A.6), (A.7) and (A.8). It gives
\[
\frac{1}{\epsilon^2} \frac{1}{\sqrt{2\pi}} \mathbb{I}_B(k) \int_{\mathbb{R}_x \times \omega} \psi^\epsilon(t, x, z') e^{-ikx} \left( -\frac{1}{2} \partial_{yy} + \Delta_{\omega} \right) + W_L \right) \chi_n(\frac{x}{\epsilon}, z') dx dz'. \tag{A.9}
\]

Recalling the eigenvalue problem (2.3) and the definition of Bloch waves (2.33), (A.9) becomes
\[
\frac{1}{\epsilon^2} \int_{\mathbb{R}_x \times \omega} \psi^\epsilon(t, x, z') E_n u^\epsilon_{n,k}(x, z') dx dz' = \frac{1}{\epsilon^2} E_n g^\epsilon_{n,k}(t, k). \tag{A.10}
\]

To conclude, we need to treat the term (A.5). Using (2.34), we have
\[
\frac{ik}{\epsilon} \frac{1}{\sqrt{2\pi}} \mathbb{I}_B(k) \int_{\mathbb{R}_x \times \omega} \psi^\epsilon(t, x, z') e^{-ikx} \partial_y \chi_n(\frac{x}{\epsilon}, z') dx dz' = \frac{i}{\epsilon} \frac{1}{\sqrt{2\pi}} \mathbb{I}_B(k') \mathbb{I}_B(k)
\sum \int_{\mathbb{R}_x \times \omega} \int_{\mathbb{R}_x \times \omega} e^{i(k'-k)x} \partial_y \chi_n(\frac{x}{\epsilon}, z') \chi_n(\frac{x}{\epsilon}, z') dx dz' \tag{A.11}
\]
and
\[
\int_{\mathbb{R}_x \times \omega} e^{i(k'-k)x} \partial_y \chi_n(\frac{x}{\epsilon}, z') \chi_n(\frac{x}{\epsilon}, z') dx dz'
= \sum_{l \in \mathbb{Z}} \int_{-\epsilon/2}^{\epsilon/2} \int_{\omega} e^{i(k'-k)x} \partial_y \chi_n(\frac{x}{\epsilon}, z') \chi_n(\frac{x}{\epsilon}, z') dz' dx
= \sum_{l \in \mathbb{Z}} e^{i(k'-k)x} \int_{-\epsilon/2}^{\epsilon/2} \int_{\omega} e^{i(k'-k)x} \partial_y \chi_n(\frac{s}{\epsilon}, z') \chi_n(\frac{s}{\epsilon}, z') dz' ds, \tag{A.12}
\]
with \(k, k' \in \mathbb{B}_\epsilon\). We recall that the function
\[
\Delta_T(t) = \sum_{r \in \mathbb{Z}} \delta(t - rT)
\]
for a given \(T\), usually referred to as the Dirac comb function, is periodic of period \(T\), and it can be represented as a Fourier series, with all Fourier coefficients \(1/T\). It holds
\[
\Delta_T(t) = \frac{1}{T} \sum_{l \in \mathbb{Z}} e^{i2\pi lt/T}.
\]

Therefore, we have
\[
\frac{1}{2\pi} \sum_{l \in \mathbb{Z}} e^{i(k-k')tx} = \epsilon^{-1} \sum_{r \in \mathbb{Z}} \delta(k - k' - \frac{2\pi}{\epsilon} r). \tag{A.13}
\]

36
Since $k$ and $k'$ in (A.11) are both in the scaled Brillouin zone $B_\epsilon$, $k - k' = \frac{2\pi r}{\epsilon}$ is only possible if $r = 0$. Thus, using (A.13) with $r = 0$ in (A.12) yields

$$\epsilon^{-1} \mathbb{1}_{B_\epsilon}(k') \mathbb{1}_{B_\epsilon}(k) \delta(k - k') \int_{-\epsilon/2}^{\epsilon/2} \int_\omega \partial_y \chi_n(s, z') \chi_n'(s, z') dz' ds$$

$$= \mathbb{1}_{B_\epsilon}(k') \mathbb{1}_{B_\epsilon}(k) \delta(k - k') \int_{-1/2}^{1/2} \int_\omega \partial_y \chi_n(y, z') \chi_n'(y, z') dz' dy.$$

Defining $P_{nn'}$ as in (3.4) and noticing that $P_{n'n} = -P_{nn'}$, the term (A.11) becomes finally

$$-\frac{i}{\epsilon} k \sum_{n'} P_{nn'} g_n'(t, k).$$

Consequently, grouping each term, we obtain (3.10).

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References


