Application of the multiband $kp$-models to the quantum transport in quasi-periodic crystals
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Abstract

We consider the quantum transport of a particle in a crystal where the global three dimensional translation symmetry is lost. Our analysis concerns solid state structures where the microscopic potential of the ions is no longer periodic. This includes materials with variable chemical composition, intergrowth compounds and abrupt junctions. The application of the $kp$ multiband envelope function models to the description of the quantum mechanical motion in such a quasi-periodic structures is investigated. By using a spectral decomposition technique, we show that when the interatomic distance is asymptotically small, the particle probability density can be obtained by the envelope $kp$ model with variable coefficients.

1 Introduction

During the last century, a great interest was devoted to the study of the mathematical models that describe the motion of a quantum particle in a crystal. This effort was motivated by the practical applications of the theory to several area, in particular to the solid state physics and, in the field of the electronic engineering, to the design of nanodevices in semiconductor structures. The solid is often modeled by a perfectly periodic crystal where the ions have a fix position and are arranged at the vertices of a regular array.

At the microscopical level, a crystal is defined by the electrostatic potential of the ions in a small volume denoted as primitive atomic cell. The quantum mechanical wave function of the particle in such a structure shows a two-scale behavior. Around the atomic nuclei it oscillates at the length scale $r/\varepsilon$ that hereafter will be denoted by “microscopic” scale. Here, the small parameter $\varepsilon$ (lattice parameter) is the typical separation between the lattice sites and $r$ is the position. On the opposite limit, several important electronic properties of the system can be deduced by studying the variation of the wave function at the “marcoscpopic” scale $r$, which is independent from $\varepsilon$. This micro-macro behavior of the particle wave function makes the study of the particle motion in periodic structures particularly challenging. Various approaches have been developed in the physical literature that provide a simplified description of the particle motion. In particular, we refer to the class of models derived in the so called “$kp$-envelope function” approach. In this approach, by using a suitable spectral decomposition procedure, the particle wave function is decomposed into a set of smooth functions denoted envelope functions. They vary only at the macroscopic scale. As a final result, the microscopic periodic potential of the lattice, is substituted by a set of constant parameters that in literature are often referred to as Kane parameters [11].
However, real materials contain microscopic imperfections and unhomogeneities on the chemical composition that are not taken into account in the usual derivation of the kp models. A common practice is to adopt the kp description of the dynamics for uniform systems also in these cases. The non-uniformity of the crystal is modeled by letting, without any rigorous justification, the Kane parameters depend on the position. A vast literature is devoted to this delicate and controversial subject, and various recipes have been proposed for the generalization of the kp technique to non-periodic crystals [8]. Such approximation procedures are based on the observation that when the modification of periodic potential of the ions in a real material is sufficiently smooth at the macroscopic scale, the particle in the lattice "see" a microscopic potential that, in the first approximation, can be considered as periodic. In this way, the effects of the microscopic imperfections are taken into account in the particle evolution equation only at the macroscopic level by inserting a gentle variation of the coefficients that characterize the material [3, 14, 19].

Various authors have investigated the particle dynamics in the limit of vanishing lattice parameter (homogenization scaling). In the case of perfectly uniform crystals, the rigorous limit $\varepsilon \to 0$ has been performed by Poupaud and Ringhofer [20], Allaire and Piatnitski [1] and more recently by Barletti and Ben Abdallah [4]. They use different techniques and slightly different hypothesis. In [1], a generalized form of the kinetic energy of the particle in the crystal is considered. The Schrödinger equation is extended in order to include a periodic metric. The limit equation is obtained by eliminating the component of the solution parallel to a suitable set of periodic Bloch functions which are determined by the initial condition. This restrict the application of this technique to problems with initial data defined by a finite number of Bloch waves. In [20], the homogenization limit is investigated by using the quantum phase-space framework. In this context, the particle wave function is substituted by a pseudo-distribution function defined in the phase-space [9, 17, 18]. The mathematical analysis is performed in this framework and the limit of the evolution equation for the pseudo-distribution function is obtained. The final equation is expressed in term of the particle wave function by transforming back the result into the Schrödinger formalism.

In this paper we investigate the application of the homogenization scaling to non-periodic crystals. We focus on the quasi-periodic crystals also denoted intergrowth compounds [6]. They are crystalline compounds that do not possess three dimensional translational symmetry. They can be characterized as a collection of subsystems, each one being translational symmetric in good approximation. In analogy with the mathematical study performed in Ref. [4], we study the homogenization limit by applying the kp decomposition procedure. We extend various results derived in Ref. [4] to the quasi-periodic crystals. In particular, we discuss the convergence of the particle wave function toward the solution of a kp model with variable coefficients. However, a important difference with the aforementioned works should be mentioned. In the present work, the particle dynamics is described by the kp multiband model also in the continuous limit. This contrast with the other mathematical studies of uniform systems [1, 20, 4] where the particle motion is described by the so called single band effective mass equation. In the present paper we are interested in the rigorous justification of the use of the kp models with variable coefficients. We are motivated by the importance that the kp models have in the study of the particle motion in non-uniform crystals. The homogenization scaling provides the natural framework where this analysis can be performed. The derivation of the single band effective mass equation with variable coefficients as a limit of our kp system, will be addressed in a separate publication.
2 Envelope function approach

For sake of generality, we will consider a $d$-dimensional crystal. The geometry of the microscopical structure of the solid is specified by the so called “Wigner-Seitz cell” that we will denote by $C$. The Wigner-Seitz cell is defined to be the volume that when translated through all the vectors of the Bravais lattice $L$, fills $\mathbb{R}^d$ without overlapping. The Bravais lattice is the set
\[
L = \left\{ \sum_i^n n_i a_i | \ n_i \in \mathbb{Z} ; \ e_i \in \mathbb{R}^d \right\},
\]
where $a_i$ are $d$ independent vectors. We introduce the lattice parameter $\varepsilon$ that scales the distance among the atoms of the crystal. More precisely, we define the scaled Bravais lattice as $L^\varepsilon = \varepsilon L$ and the scaled Wigner-Seitz cell $C^\varepsilon = \left\{ \sum_i^n x_i a_i | \ x_i \in \left[ -\frac{\varepsilon}{2}, \frac{\varepsilon}{2} \right] \right\}$. Finally, the scaled First Brilluin Zone $B^\varepsilon$ is defined by the volume $B^\varepsilon = \left\{ \sum_i^n x_i b_i | \ x_i \in \left[ -\frac{1}{2}, \frac{1}{2} \right] \right\}$, where $b_i$ are $d$ independent vectors such that $b_i \cdot a_j = 2\pi \delta_{ij}$. The dot denotes the scalar product and $\delta_{ij}$ is the Kronecker’s delta. The periodic rearrangement of the basis set $b_i$ gives the scaled reciprocal lattice $L^\varepsilon = \left\{ \sum_i^n n_i b_i | \ n_i \in \mathbb{Z} ; \ b_i \in \mathbb{R}^d \right\}$. We have
\[
|B^\varepsilon| = (2\pi)^d,
\]
where the modulus indicates the volume.

According to the quantum mechanical theory, the evolution of a particle in the presence of the electrostatic potential of fix ions is given by the single particle Schrödinger equation
\[
i \frac{\partial \psi^\varepsilon(r,t)}{\partial t} = H_L^\varepsilon \psi^\varepsilon(r,t).
\]
The function $\psi^\varepsilon$ is denoted as the particle wave function. We use physical units where $\hbar = 1$ and the mass of the particle is equal to one. The Hamiltonian operator is given by
\[
H_L^\varepsilon = -\frac{1}{2} \Delta r + \frac{1}{\varepsilon^2} W_L^\varepsilon \left( \frac{r}{\varepsilon} \right).
\]
The function $W_L^\varepsilon$ in Eq. (3) is the total electrostatic potential of the ions (quasi-periodic potential). In order to model solids with variable chemical composition, we assume that $W_L^\varepsilon$ depends both on the macroscopic scale $r$ and on the microscopic scale $r/\varepsilon$. In the present contribution, we consider a particular class of quasi-periodic crystals. We assume that $W_L^\varepsilon$ has the form
\[
W_L^\varepsilon \left( \frac{r}{\varepsilon}, r \right) = |C^\varepsilon| \sum_{R_i \in L} W_i \left( \frac{r}{\varepsilon} \right) \delta^\varepsilon (R_i - r)
\]
where the sum is taken over all the lattice site $R_i$. The smooth functions $\delta^\varepsilon$ are the Fourier transform of the characteristic function of the scaled First Brillouin Zone $\mathbb{I}_{B^\varepsilon}$
\[
\delta^\varepsilon(r) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} e^{i r \cdot k} \mathbb{I}_{B^\varepsilon} (k) \, dk
\]
We denote $\delta^\varepsilon$ by “pseudo-delta” function. For future references, we note that
\[ |C^\varepsilon| \sum_{R \in \mathcal{L}^\varepsilon} \delta^\varepsilon(R) = \sum_j |C^\varepsilon| \int_{\mathbb{R}^d} e^{i R \cdot k} \delta^\varepsilon(R) \, dk = 1. \tag{6} \]

We use the following definition for the Fourier transform of a $L^2(\mathbb{R}^d)$ function
\[ f(r) = \frac{1}{(2\pi)^d/2} \int_{\mathbb{R}^d} \tilde{f}(k) e^{ik \cdot r} \, dk \tag{7} \]
and we denotes the transformed function by the tilde. The set of functions $W_i(r)$ in Eq. (4) describe the ionic potential around the lattice site $R_i$. They are $\mathcal{C}$-periodic functions:
\[ W_i \left( \frac{r + R}{\varepsilon} \right) = W_i \left( \frac{r}{\varepsilon} \right) \quad \text{for all } R \in \mathcal{L}^\varepsilon. \tag{8} \]

The expression (4) indicates that the electrostatic potential is the sum of $\mathcal{C}^\varepsilon$-periodic functions weighted by the pseudo-delta functions $\delta^\varepsilon$. From the definition (5) it is evident that the function $\delta^\varepsilon(r)$ approximates the Dirac’s delta distribution $\delta(r)$ for small $\varepsilon$. Consequently, when the distance $|R - r|$ is large, the pseudo-delta function $\delta^\varepsilon(R - r)$ goes to zero. The total electrostatic potential $W_0^\varepsilon$ can thus be approximated by $W_i(\xi)$ inside the volume $\mathcal{C}(R_i)$ that denotes the fundamental domain centered at the lattice site $R_i$. By a suitable definition of the set of potentials $W_i(\xi)$, we can describe crystals whose microscopical potential changes from an atomic cell to another located to a macroscopic distance $R$. The class of quasi-periodic electrostatic potentials given in Eq. (4) has been introduced by Foreman in Ref. [10]. Some numerical tests showed that a wide range of non-periodic structures can be modeled with this kind of non-periodic ionic potentials. As an example, we mention the the sharp junctions between two different materials in a semiconductor heterostructure. We remark that, by writing in the expansion (4) we assumed implicitly the existence of a common symmetry group for all the $W_i$. Consequently, our modelization is able to tackle only with composite materials characterized by a single fundamental Wigner-Seitz cell.

The major difficulty encountered in the analytical and numerical study of the equation of motion (2) concerns the multiscale behaviour of $\psi^\varepsilon$. The wavefunction is characterized by two different scales: it is highly oscillating in the proximity of the atomic sites while it varies gently in the interatomic space. The rapidly varying component of $\psi$ is characterized by the length $r/\varepsilon$ that goes to zero when the lattice crystal approaches to the homogeneization limit.

In order to clarify the strategy that we adopted for the study of the limit of small $\varepsilon$, we review the main results of the standard $kp$ theory for periodic crystals and for $\varepsilon = 1$. The study of the electron motion in a periodic system has been deeply investigated by physicists and mathematicians. One of the main results, the Bloch theorem, concerns the periodic systems (with our notations $W_0^\varepsilon(\xi, r) = W_0^\varepsilon(\xi) \equiv W(r)$). It states that the eigenfunctions of the crystal Hamiltonian can be obtained by the set of periodic eigenfunctions $u_{n,k}(r)$ obtained by the following eigenvalue problem
\[ \left[ \frac{k^2}{2} - ik \cdot \nabla - \frac{\Delta r}{2} + W(r) \right] u_{n,k}(r) = E_n u_{n,k}(r). \tag{9} \]
Here, $k$ is a parameter that belongs to the First Brilluin Zone $\mathcal{B}$. If $W(r)$ is a bounded periodic function, Eq. (9) admits an orthonormal set of periodic solutions $\{u_{n,k}(r)\}$ which are also a
Hilbert basis of $L^2(\mathbb{C})$. By using the completeness of the periodic Bloch functions $u_{n,k}(r)$, it is possible to extend the set $\{u_{n,k}(r)\}$ to a basis set of $L^2(\mathbb{R}^d)$. An important application of this result concerns the study of the particle motion in crystal perturbed by some non-periodic potential $U$. In this case, the evolution equation

$$i\frac{\partial \psi}{\partial t} = \left[ -\frac{\Delta_r}{2} + W(r) + U(r) \right] \psi$$  \hspace{1cm} (10)

is replaced by a set of equations for the expansion coefficients $\varphi_n = \langle \chi_n | \psi \rangle_{L^2(\mathbb{R}^d)}$ where the parenthesis denotes the $L^2$ internal product and $\{\chi_n\}$ is a basis set of $L^2(\mathbb{R}^d)$. Various choices of the $\{\chi_n\}$ are possible and a large number of models has been developed. In particular, we refer to the Luttinger-Kohn basis set defined by [13, 23]

$$\chi_n(r) = e^{i k \cdot r} u_{n,0}(r)$$  \hspace{1cm} (11)

where $k \in B$. The solution of Eq. (10) is expanded as

$$\psi(r,t) = \sum_n u_{n,0}(r) \varphi_n(r,t)$$  \hspace{1cm} (12)

where the $\varphi_n(r)$ are denoted as envelope functions. They are the solutions of the following set of equations

$$i\frac{\partial \varphi_n}{\partial t} = E_n \varphi_n - \frac{\Delta_r}{2} \varphi_n + \sum_{n'} P_{n,n'} \cdot \nabla_r \varphi_{n'} ,$$  \hspace{1cm} (13)

where the $P_{n,n'}$ are denoted Kane parameters and are the matrix elements in the Wigner-Sietz cell of the gradient operator (the overline denotes the conjugation)

$$P_{n,n'} = \int_{\mathcal{C}} \overline{u_{n,0}(r)} \nabla_r u_{n',0}(r) \, dr .$$  \hspace{1cm} (14)

The Luttinger-Kohn model has been largely applied to the study of the electronic properties of solids and in particular of semiconductor heterostructures [6, 5, 17]. The reason of the success of this and other similar approaches (that are generally denoted as $kp$ models) is that the expansion (12) factorizes the solution $\psi$ in products between a fast varying function $u$ (whose oscillations scale with the interatomic distance) and a function $\varphi$ that varies at the macroscopic scale. In particular, the envelope functions are a set of smooth functions. The regularity of the envelope functions $\varphi_n(r)$ arises from some general properties of the Hamiltonian operator (left side of Eq. (9)) and of the set $\chi_n(r)$ over which the solution is projected. It is easy to verify that the Fourier transform of $\varphi_n$ is compactly supported on the First Brillouin Zone $B$. This property guarantee that the spatial derivatives of the $\varphi_n$ are bounded. In what follows, the spaces of the functions whose Fourier transform is defined in a compact domain will play a key role in the study of the homogeneization limit $\varepsilon \to 0$.

In the standard Luttinger-Kohn approach, the potential $U$ is treated as a perturbation of the periodic Hamiltonian and it is assumed that $U$ is nearly constant inside the fundamental volume $\mathcal{C}$ [16]. Materials containing some modification of the microscopic structure of the ions, cannot be described by this approach. The reason of such a limitation of the Luttinger-Kohn theory is that the decomposition given in Eq. (12) makes use of a single set of periodic Bloch functions. As stated before, they are obtained by the eigenvalue problem (9). In this way, it is
implicitly assumed that all the crystal is well described by the periodic microscopic potential $W$. This hypothesis is no longer true for materials with variable chemical composition. Inside to a volume $\Omega_0$ containing several atomic cells, the particles "see" a microscopic potential $W_0$ that can be considerably different from that inside to a volume $\Omega_1$ containing a different type of ions and located at a distance $L \gg a_0$ ($a_0$ denotes the mean interatomic distance) from $\Omega_0$. As a first step in view to the extension of the $kp$ approach to composite materials, let's we consider the restriction of the ionic potential to the volume $C(R_i)$ (where $C(R_i)$ is the Wigner-Sietz cell displaced to the lattice site $R_i$). Denoting this restriction by $W_i(r)$, we consider the periodic prolongation of the electrostatic potential outside $C(R_i)$. This leads to the definition of a "fictitious" periodic crystal labeled by the atomic position $R_j$. In this way, we obtain a set of periodic potentials $\{W_i| i \in \mathbb{Z}^d\}$. At each $W_i$ we can associate a basis set of $L^2(\mathbb{R}^d)$. The elements of the Luttinger-Kohn-Foreman (LKF) basis set $\{\chi_{j,n}^\varepsilon, j \in \mathbb{Z}; n \in \mathbb{N}\}$ are given by

$$\chi_{j,n}^\varepsilon(r) \equiv |\varepsilon^\varepsilon| \delta^\varepsilon(r - R_j) u_{n,j}^\varepsilon(r).$$

More into details, the $u_{n,j}$ are the periodic Bloch functions for $k = 0$ of the "j-th virtual crystal". They are the eigenvalues of the following equation

$$\left[-\frac{\varepsilon^2}{2} \Delta_{\varepsilon} + W_j \left(\frac{r}{\varepsilon}\right)\right] u_{n,j}^\varepsilon \left(\frac{r}{\varepsilon}\right) = E_n^j u_{n,j}^\varepsilon \left(\frac{r}{\varepsilon}\right),$$

where we defined

$$u_{n,j}^\varepsilon \left(\frac{r}{\varepsilon}\right) \equiv \varepsilon^{d/2} u_{n,j}^\varepsilon(r).$$

The periodic functions $u_{n,j}^\varepsilon(r)$ are normalized in the usual way

$$\int_{\mathbb{C}_\varepsilon} |u_{n,j}^\varepsilon(r)|^2 \, dr = \int_{\mathbb{C}_\varepsilon} |u_{n,j}^\varepsilon(r)|^2 \, dr = 1.$$ 

The properties of othonormality and completeness of the LKF basis set are discussed in Appendix A.

3 Preliminary results

We describe the sets of functions that will be used in the study of the homogenization limit of Eq. (2). At first, we consider the "space of the discrete envelope functions", denoted by $\mathcal{E}_d$. The elements of this space are written by the sequence $\{\varphi_{j,n}| j \in \mathbb{Z}^d, n \in \mathbb{N}\}$. The first index labels the position in the lattice $\mathcal{L}$ and the second one, denoted band index, labels the energetic branch of the Hamiltonian eigenspace.

**Definition 1** The space $\mathcal{E}_d = l^2(\mathbb{N}, \mathbb{Z}^d)$ is the Hilbert space of the sequences $\{\varphi_{j,n}| j \in \mathbb{Z}^d, n \in \mathbb{N}\}$, such that $\|\varphi\|^2_{\mathcal{E}_d} = \sum_{n,j} |\varphi_{n,j}|^2 < \infty$. 

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The inner product of $\mathcal{E}_d$ is given by the canonical bilinear form $\langle \phi, \mu \rangle_{\mathcal{E}_d} = \sum_{n,j} \overline{\phi_{j,n}} \mu_{j,n}$, where the overline denotes the conjugation.

In the following, we will consider the sequences $\varphi_{j,n}$ for which $\sum_n |\varphi_{j,n}|^2$ is the probability to find the particle around the lattice site $R_j$. When $\varepsilon$ goes to zero the atomic sites became closer and closer. Under this condition, we expect that the probability density to find the particle around the lattice site $R_j$ goes to zero the atomic sites. With this in mind, we consider the set of the continuous functions $\varphi_{j,n}$ (interpolating functions), with domain $\mathbb{R}^d$, such that, in correspondence to the lattice site $R_j$, $\varphi_{n}(R_j) = \varphi_{j,n}$. For technical reasons, it is convenient to require that the $\varphi_{n}$ are smooth functions whose Fourier transform vanishes outside the First Brillouin Zone (FBZ). We define the following auxiliary space

**Definition 2** The space $L^2_\Omega$ is the subspace of the $L^2$-functions supported in $\Omega$

$$L^2_\Omega = \left\{ \mu \in L^2(\mathbb{R}^d) \mid \text{supp}(\mu) \subset \Omega \right\},$$

where $\Omega$ is a proper subset of $\mathbb{R}^d$.

In particular, the space $l^2_\Omega (\mathbb{N}, L^2_\Omega)$ contains the sequences $\{\mu_j(R)\}$ that vanish outside $\Omega$ and such that $\sum_n \|\mu_n\|^2_{L^2(\mathbb{R}^d)} < \infty$.

We define the interpolation operator $\mathcal{F}^\varepsilon$ that maps the $\varphi_{j,n}$ to a continuous function

$$\mathcal{F}^\varepsilon(\mu)(n, R) = \frac{1}{|B^\varepsilon|} \sum_j \mu_{n,j} \int_{\mathbb{R}^d} e^{-i(R-R_j)\cdot k} \mathbb{1}_{B^\varepsilon}(k) \, dk = |C^\varepsilon| \sum_j \mu_{n,j} \delta^\varepsilon(R_j - R),$$

where $\mu \in \mathcal{E}_d$, $R \in \mathbb{R}^d$ and $R_j \in \mathcal{F}^\varepsilon$. Hereafter, we will denote by the underline the elements that belong to the image of $\mathcal{F}^\varepsilon$, $\mu = \mathcal{F}^\varepsilon \mu$. From the definition (20) it is immediate to verify that $\underline{\mu}_{n,j}(R_j) = \mu_{n,j}$ (note the normalization $\delta^\varepsilon(0) = |C^\varepsilon|^{-1}$).

In the following, we will denote the Fourier transform (see Eq. (7)) by the symbol $\mathcal{F}$ and the inverse by $\mathcal{F}^{-1}$.

**Definition 3** The space $\mathcal{E}^\varepsilon_c = \mathcal{F}^{-1}l^2_\Omega$, denoted as “space of the continuous envelope functions”, contains all the sequence $\{\mu_j(R)\} \in l^2(L^2(\mathbb{R}^d))$ whose Fourier transform is compactly supported in the $\varepsilon$-scaled First Brillouin Zone $B^\varepsilon$.

Hereafter, we will denote by $\mathcal{B}(A, B)$ the space of linear bounded operators from $A$ to $B$. The first useful property of the map $\mathcal{F}^\varepsilon$ is

**Lemma 3.1** For every $\varepsilon > 0$ the operator $|C^\varepsilon|^{-1/2} \mathcal{F}^\varepsilon \in \mathcal{B}(\mathcal{E}_d, \mathcal{E}^\varepsilon_c)$ is an isometry.

**Proof:** This property is easily verified by some calculations. We have

$$\|\mathcal{F}^\varepsilon \mu\|^2_{\mathcal{E}^\varepsilon_c} = \sum_n \|\underline{\mu}_n\|^2_{L^2(\mathbb{R}^d)} = \sum_n \|\overline{\mu}_n\|^2_{L^2(\mathbb{R}^d)} = \sum_n 2\pi \int_{\mathbb{R}^d} \frac{1}{|B^\varepsilon|} \sum_j \mu_{n,j} e^{i\mathcal{R}_j \cdot k} \mathbb{1}_{B^\varepsilon}(k) \, dk$$

$$= \frac{2\pi}{|B^\varepsilon|} \sum_{n,j,j'} \frac{\mu_{n,j} \mu_{n,j'}}{|B^\varepsilon|} \int_{\mathbb{R}^d} e^{i(R_j - R_{j'})} \mathbb{1}_{B^\varepsilon}(k) \, dk = \frac{2\pi}{|B^\varepsilon|} \|\mu\|^2_{\mathcal{E}_d} = |C^\varepsilon| \|\mu\|^2_{\mathcal{E}_d},$$

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where we used
\[ \tilde{\mu}_n(k) = \mathcal{F}^{-1}_{\mathbb{R}^d} \mu_n = \frac{1}{(2\pi)^{d/2}} |B^c| \sum_j \mu_j \int_{\mathbb{R}^d} e^{i\mathbf{r} \cdot (\mathbf{k} - \mathbf{k}')} e^{i\mathbf{R}_j \mathbf{k}' \cdot (\mathbf{k}')} \, d\mathbf{k}' = (2\pi)^{d/2} |B^c| \sum_j \mu_j e^{i\mathbf{R}_j \mathbf{k}' \cdot (\mathbf{k})}. \]

The space of the continuous envelope functions \( \mathcal{E}_c^\varepsilon \) is the subspace of \( \ell^2 \left( \mathbb{N}, \mathbb{L}^2(\mathbb{R}^d) \right) \) with inner product
\[ \langle \psi | \varphi \rangle_{\mathcal{E}_c^\varepsilon} = \sum_n \int_{B^c} \overline{\psi}_n(k) \tilde{\varphi}_n(k) \, dk \]
and norm
\[ \| \psi \|_{\mathcal{E}_c^\varepsilon}^2 = \sum_n \int_{\mathbb{R}^d} |\overline{\psi}_n(k)|^2 \| \tilde{\varphi}_n(k) \|_{\mathbb{L}^2(\mathbb{R}^d)} \, dk = \sum_n \| \delta^\varepsilon \ast \psi_n \|_{\mathbb{L}^2(\mathbb{R}^d)}^2. \]  

The asterisk denotes convolution and we used the well known property of the Fourier transform \( \delta^\varepsilon \ast \psi_n = \mathcal{F} \left( \psi_n \delta_{B^c} \right) \). We remark that the \( \mathcal{E}_c^\varepsilon \) norm coincides with the \( \ell^2 \left( \mathbb{N}, \mathbb{L}^2(\mathbb{R}^d) \right) \) norm for all the functions \( \varphi \in \mathcal{E}_c^\varepsilon \) since in this case \( \delta^\varepsilon \ast \varphi_n = \varphi_n \). When \( \varepsilon \to 0 \) the space \( \mathcal{E}_c^\varepsilon \) becomes dense in \( \ell^2 \left( \mathbb{N}, \mathbb{L}^2(\mathbb{R}^d) \right) \). In the following, we will denote \( \mathcal{E}_c^0 \equiv \ell^2 \left( \mathbb{N}, \mathbb{L}^2(\mathbb{R}^d) \right) \). The interpolation operator maps the “fully discrete” space \( \mathcal{E}_d \) into \( \mathcal{E}_c^\varepsilon \). By construction, we have that the interpolating functions have a Fourier transform with support contained in \( B^c \). This condition is true for all summable sequences. In order to distinguish between “smooth” and “rapidly varying” sequences we define a class of functional spaces containing sequences whose Fourier transform is strictly contained in the FBZ \( B^c \). We have the following

**Definition 4** Let \( \varepsilon, \varepsilon' \in \mathbb{R}^+ \), \( \mathcal{E}^{\varepsilon,\varepsilon'}_d \in \ell^2 \left( \mathbb{N}, \mathbb{Z}^d \right) \) is the Hilbert space
\[ \mathcal{E}^{\varepsilon,\varepsilon'}_d = \left\{ \varphi \in \ell^2 \left( \mathbb{N}, \mathbb{Z}^d \right) \mid \exists \varphi \in \mathcal{E}_c^\varepsilon \right\}. \]

We define the space of the regular functions \( \mathcal{H}^\mu = \ell^2 \left( \mathbb{N}, \mathcal{H}^\kappa(\mathbb{R}^d) \right) \), where \( \mathcal{H}^\kappa \) is the Sobolev space of the functions with generalized \( \kappa \)-derivative in \( L^2 \). Explicitly

**Definition 5** For \( \kappa \geq 0 \), \( \mathcal{H}^\kappa \) is the subspace of \( \mathcal{E}^0_c \) containing all the sequences \( \varphi \) such that
\[ \sum_n \| \varphi_n \|_{\mathcal{H}^\kappa(\mathbb{R}^d)}^2 = \sum_n \left[ \left( 1 + |k|^2 \right)^{\kappa/2} \tilde{\varphi}_n \right]_{\mathbb{L}^2(\mathbb{R}^d)}^2 < \infty. \]  

The following Lemma provides some straightforward estimates of the gradient of the interpolating functions. It states that for \( \varepsilon > 0 \) the norm of the Sobolev space \( \mathcal{H}^\kappa \) is equivalent to the \( \mathcal{E}_c^\varepsilon \) norm: \( \| \varphi_n \|_{\mathcal{H}^\kappa(\mathbb{R}^d)} \leq C \varepsilon^{-s} \| \varphi_n \|_{\mathbb{L}^2(\mathbb{R}^d)} \) where the constant \( C \) is independent from \( \varepsilon \).

**Lemma 3.2** Let \( \mu \in \mathcal{E}_c^\varepsilon \) and \( s \in \mathbb{N} \) we have
\[ \left\| \nabla^{(s)}_{\mathbb{R}^d} \mu_n \right\|_{\mathbb{L}^2(\mathbb{R}^d)} \leq \left( \frac{\rho(B)}{\varepsilon} \right)^s \| \mu_n \|_{\mathbb{L}^2(\mathbb{R}^d)} \quad \forall n \in \mathbb{N} \]  

where \( \rho(B) \) is the diameter of the First Brillouin Zone.
The proof of this statement is easily obtained by using the Fourier representation.

In the following, we will consider operators defined on the space of the interpolated functions \( \mathcal{E}_c^\varepsilon \) or \( L^2(\mathbb{R}) \), obtained by \( \mathcal{J} \)-transposition of operators defined on \( \mathcal{E}_d \). Let \( \mathcal{A} \) be a map from \( \mathcal{E}_d \) in itself (not necessarily bounded) defined by the matrix \( \mathbf{A} \)

\[
(A\varphi)_{j,n} = \sum_{n',j'} A_{n,n';j,j'} \varphi_{n',j'} .
\]  

(25)

The Lemma 3.3 below provides a sufficient condition for which the operator defined by

\[
(\mathcal{A}\varphi) (n, R) \equiv \sum_{n'} \int_{\mathbb{R}^d} A_{n,n'} (R, R') \varphi_{n'} (R') \, dR
\]

(26)

is unitarily equivalent to \( A \). In particular, we obtain the form of the matrix \( A_{n,n'} \) such that \( \mathcal{A} \mathcal{J}^\varepsilon \varphi = \mathcal{J}^\varepsilon A \varphi \).

**Lemma 3.3** Let \( \mu \in \mathcal{E}_c^\varepsilon/\alpha \) with \( 0 < \alpha \leq 1 \) and \( \mu_{n',j'} \equiv A_{n,n';j,j'} \in \mathcal{E}_c^\varepsilon/\alpha' \) with \( 0 < \alpha' \leq 1 \) for every \( n \in \mathbb{N} \) and \( j \in \mathbb{Z}^d \). If \( \frac{1}{\alpha} + \frac{1}{\alpha'} \leq 1 \) we have

\[
\sum_{n'} \int_{\mathbb{R}^d} A_{n,n'} (R, R') \varphi_{n'} (R') \, dR = \left( \mathcal{J}^\varepsilon \sum_{n',j'} A_{n,n';j,j'} \varphi_{n',j'} \right) (R) ,
\]

(27)

where

\[
A_{n,n'} (R, R') \equiv \sum_{j,j'} \delta^\varepsilon (R_j - R) \delta^\varepsilon (R_{j'} - R') A_{n,n';j,j'} .
\]

(28)

**Proof:** From the definition of interpolating function given in Eq. (20) we note that

\[
\frac{1}{|\mathbb{C}|} \int_{\mathbb{R}^d} \varphi_{n}(R) \, dR = \sum_{j} \varphi_{n,j} \int_{\mathbb{R}^d} \delta^\varepsilon (R_j - R) \, dR = \sum_{j} \varphi_{n,j} .
\]

(29)

We define the sequence \( \mu_{n',j'} \equiv A_{n,n';j,j'} \) for each \( n, j \in \mathbb{N} \) and \( \mu_{n'} (R) \equiv \mathcal{J}^\varepsilon (\mu_{n',j'}) \). Since the Fourier transform of the product \( \mu \varphi \) is the convolution of the Fourier transform of \( \mu \) and \( \varphi \), the diameter of the support of \( \mathcal{F}(\mu \varphi) \) is smaller than \( \rho \left( \mathcal{B}^\varepsilon/\alpha' \right) \leq \rho (B^\varepsilon) \) where \( \rho \) denotes the diameter and we used \( \frac{1}{\alpha} + \frac{1}{\alpha'} \leq 1 \). This ensures that the product \( \mu_{n'}(R) \varphi_n(R) \) belongs to \( \mathcal{E}_c^\varepsilon \). Equation (29) leads to

\[
\sum_{j} \mu_{n',j'} \varphi_{n,j} = \frac{1}{|\mathbb{C}|} \int_{\mathbb{R}^d} \mu_{n'}(R) \varphi_n(R) \, dR .
\]

(30)

From the definition of \( \mu \) we have

\[
\left( \mathcal{J}^\varepsilon \sum_{n',j'} A_{n,n';j,j'} \varphi_{n',j'} \right) (R) = \frac{1}{|\mathbb{C}|} \sum_{n'} \left( \mathcal{J}^\varepsilon \int_{\mathbb{R}^d} \left( \mathcal{J}^\varepsilon A_{n,n';j,j'} \right) (R') \varphi_{n'} (R') \, dR' \right) (R) .
\]

that gives Eq. (27).
This Lemma focuses on the definition of a continuous operator with kernel \( A_{n,n'}(R,R') \) starting from the matrix \( A_{n,n',j,j'} \). With some additional assumptions on the smoothness of the coefficients, the contrary is also true. In fact, if the matrix \( A_{n,n'}(R,R') \) belongs to the space \( F^1 L^2_\Omega \) for some volume \( \Omega \subset \mathbb{R}^d \) uniformly with respect to \( n,n' \), it is always possible to find a \( \varepsilon \) sufficiently small such that \( \Omega \subset B^{\varepsilon/\alpha} \). Under this hypothesis, the continuous operator in the left side of the Eq. (27) can be replaced by the right side with \( A_{n,n',j,j'} = A_{n,n'}(R_i,R_j) \).

From the definition of the interpolated functions, it is easy to see that the derivative operator can be transposed to the space of the discrete envelope functions. Let \( h \) be a \( C^\infty(\mathbb{R}^d) \) function, we define the “discrete differential” operator \( D_{[h]:\alpha} \)

\[
[D_{[h]:\alpha}]_{j'}(\mu) = \frac{1}{|B^e|} \int_{B^e} \sum_j \mu_{j'} h(k) e^{i(R_{j'}-R_{j''})k} \, dk
\]

where \( \mu_i \) is a sequence in \( \mathcal{E}_d \) and, in order to compact the notation, we omitted the explicit indication of the band index. The operator \( D \) is denoted as the derivative operator for the following reason. The space \( \mathcal{E}_d \) contains all the sequences obtained by evaluating some \( \mu \in \mathcal{E}_c \) at the grid points \( R_j \in \mathbb{L}^e \). It is possible to calculate the \( n \)-th derivative for any functions in this class, by the following steps. We evaluate the Fourier transform of the function, we multiply it by the polynomial \((-i k)^n \) and we transform it back into the original variables. Equation (31) implements this operation by using the sequence \( j = \mu(R_j) \). For sake of compactness we will use the shorthand notations

\[
[D^n\mu]_j \equiv [D_{[-i k]^n}]:\alpha \]  

We check the link between \( D \mu \) and the gradient of the interpolating function \( \mu \)

\[
[D\mu]_{n,j} = \frac{1}{(2\pi)^{d/2}} \int_{B^e} \tilde{\mu}_n(k) (-i k) e^{-i R_j k} \, dk = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d \times \mathbb{L}^e} \left( \nabla_r \tilde{\mu}_n(r) \right) e^{i (r-R_j)k} \, dr \, dk = \nabla_r \tilde{\mu}_n(r) \big|_{r=R_j}
\]

where we used the definition of the interpolating function given in Eq. (20). In the same way,

\[
[D^2\mu]_{n,j} = \Delta_r \tilde{\mu}_n(r) \big|_{r=R_j}
\]

For future references, we list some properties of the discrete differential operator \( D \).

**Lemma 3.4** The following properties hold true

i) \( D \) is a derivative operator, namely, given \( \mu, \eta \in \mathcal{E}_d \) we have

\[
D' (\mu \eta) = \sum_{r=0}^{l} \binom{l}{r} (D^{(l-r)} \mu) (D^r \eta)
\]

ii) “Composition” rule

\[
[D_{[h]:\alpha} [D_{[h]:\alpha}] = [D_{[h]:\alpha}]_j
\]
iii) “Integration by part” rule

\[
\sum_j D^l_{[-ik];\alpha} \mu^l_{\alpha} [D^{(m-l)}_{[-ik];\alpha}]_j = (-1)^l \sum_j \mu_j [D^{(m-l)}_{[-ik];\alpha}]_j .
\]  
(37)

Proof: The statements i) – iii) follow directly from the definition of \(D\) and from spectral the properties of the functions that belong to the space \(E_\varepsilon^c\). Concerning Eq. (36), we have

\[
\left[ D_{[h \gamma];\alpha} [D_{[h \gamma];\alpha}]_j \right] = \frac{1}{|B|^2} \sum_j \int_{\mathbb{R}^d} \mu_j \ h (k) h' (k') e^{i(R_jk - R_jk')} \times
\sum_{m',l'} \epsilon^{R_j(r'k' - R_jr'k')} \sum_{j} e^{R_j(r'k' - R_jr'k')} \ dR \ dR' .
\]

For Eq. (36), we write

\[
\sum_j D_{[-ik];\alpha} \mu^l_{\alpha} [D^{(m-l)}_{[-ik];\alpha}]_j = \sum_j \int_{\mathbb{R}^d} \mu_j \ h (k) h' (k') e^{i(R_jk - R_jk')} \times
\sum_{m',l'} \epsilon^{R_j(r'k' - R_jr'k')} \ dR \ dR' .
\]

Finally, Eq. (35) is a direct consequence of the point ii).

\[\square\]

4 Description of the \(kp\) asymptotic limit and main results.

In this section, we describe briefly the procedure adopted for the study of the asymptotic limit \(\varepsilon \to 0\). In particular, we state the hypotheses and the main results. We consider the class of the quasi-periodic crystals defined by Eq. (4). We study the limit \(\varepsilon \to 0\) of the Schrödinger equation (2)

\[
\frac{\partial \psi^\varepsilon (r, t)}{\partial t} = \left[- \frac{1}{2} \Delta_r + \frac{1}{\varepsilon^2 |C| (2\pi)^d} \sum_j W_j \left(\frac{r}{\varepsilon}\right) \int_{\mathbb{R}^d} e^{-i(r-R_j)k} \psi^\varepsilon (k) \ dR \right] \psi^\varepsilon (r, t) .
\]  
(38)

When \(\varepsilon\) goes to zero, the microscopical periodic structure of the potential is lost and the crystal is described by a continuous macroscopic system. We consider the expansion of \(\psi^\varepsilon\) on the Luttinger-Kohn-Foreman basis set (15). The expansion coefficients \(\varphi^\varepsilon_{n,j}\) are defined in each point of the scaled Bravais lattice. In order to describe the crystal by a continuous medium, we interpolate the \(\varphi^\varepsilon_{n,j}\) with a set of continuous envelope functions. They are given by \(\varphi^\varepsilon (R) = J^\varepsilon \varphi^\varepsilon_{n,j}\), where the interpolation operator is defined in Eq. (20). It is possible to show that the continuous envelope functions satisfy the equation

\[
\varepsilon^2 i \frac{\partial \varphi^\varepsilon_n}{\partial t} = \mathcal{H}^\varepsilon [\varphi^\varepsilon] + \varepsilon^2 J^\varepsilon [\varphi^\varepsilon] .
\]  
(39)
where
\[
\mathcal{H}_{k'p}^\xi = E_n(R)\varphi_n^\xi(R, t) + \varepsilon \sum_{n'} \nabla_{R'} \left[ S_{n,n'}(R, R') \varphi_n^\xi(R', t) \right]_{R'=R} \\
+ \sum_{n'} \frac{\varepsilon^2}{2} \Delta_{R'} \left[ N_{n,n'}(R, R') \varphi_n^\xi(R', t) \right]_{R'=R}
\]
(40)

The explicit form of the operator \( \mathcal{F}^\xi \) is given in Eq. (79) below. Apart from \( \mathcal{F}^\xi \), the system of Eq. (39) is the straightforward extension of the \( kp \) envelope function model given in Eq. (13). The only difference is that the Kane coefficients \( S \) and \( N \) are no longer constants. Equation (13) is easily recovered as a particular case. For the periodic systems \( N \) and \( S \) are the constant-in-space matrices \( N_{n,n'} = \delta_{n,n'} \) and \( S_{n,n'}(R, R') = P_{n,n'} \).

In order to start with the analysis of the problem, in sec. 5.2 we show (Theorem 4) that the \( kp \) envelope function system (39) is well posed. After, we focus on the limit of small \( \varepsilon \). We provide two main results, the first concerns the physical meaning of the envelope functions obtained by the expansion of the wave function \( \psi^\xi \) on the local basis \( \chi_{j,n} \). We have, as expected in the framework of the \( kp \) theory, that the sum over the band index of the modulus square of the envelope functions converges to the particle density
\[
\sum_{n} |\varphi_n^\xi(r, t)|^2 - |\psi^\xi(r, t)|^2 \to 0
\]
(41)

Finally, we show that the operator \( \mathcal{F}^\xi \) can be neglected (Theorem 5).

Suitable smoothness assumptions for the quasi-periodic potential \( W_\xi \) are required. In particular, it is necessary to ensure that the variation of the microscopic potential along the Bravais lattice is sufficiently smooth. We assume that a function \( W : (\mathbb{R}^d, C) \to \mathbb{R} \) and a set \( \Omega \in \mathbb{R}^d \) exist such that
\[
W_j \left( \frac{R}{\varepsilon} \right) = W \left( R_j, \frac{R}{\varepsilon} \right),
\]
(42)

where \( j \in \mathbb{Z}^d, R_j \in \mathcal{L}^\varepsilon \) and \( r \in C \). We assume that the function \( W \) belongs to the space \( \mathcal{W}_\Omega \):
\[
\mathcal{W}_\Omega = \left\{ W \in L^2(\mathbb{R}^d \times C) \mid u(r) = W \left( R, \frac{r}{\varepsilon} \right) \in L^\infty(C^\varepsilon) \quad \forall R \in \mathbb{R}^d \right\}
\]
(43)

In particular, the gradients with respect to the macroscopic variable of the functions in \( \mathcal{W}_\Omega \) are uniformly bounded. We have that for all \( \kappa \geq 0 \) a constant \( C \) exists such that
\[
\text{ess sup}_{r \in C} \int_{\mathbb{R}^d} (1 + k^2)^{\kappa/2} \left| \widetilde{W} \left( \frac{k}{\varepsilon} \right) \right|^2 \, dk < C ,
\]
(44)

where
\[
\widetilde{W} \left( \frac{k}{\varepsilon} \right) = \frac{1}{(2\pi)^d/2} \int_{\mathbb{R}^d} W \left( R, \frac{r}{\varepsilon} \right) e^{-iR \cdot k} \, dR .
\]
(45)

In the same way, for the periodic Bloch functions we assume that a set of functions \( \{ u_n \in \mathcal{W}_\Omega \mid n \in \mathbb{N} \} \) exists such that
\[
u_{j,n} \left( \frac{R}{\varepsilon} \right) = u_n \left( R_j, \frac{R}{\varepsilon} \right) \quad j \in \mathbb{Z}^d ; R_j \in \mathcal{L}^\varepsilon ; n \in \mathbb{N} .
\]
(46)
Furthermore, we postulate some smoothness conditions for the eigenvalues of the Bloch problem. At first, we require that the eigenvalues of Eq. (16) are simple and that there exists a growing sequence \( \{ \epsilon_n \in \mathbb{R}^+ | n \in \mathbb{N} \} \) with \( \lim_{n \to \infty} \epsilon_n = +\infty \) such that for all \( n \in \mathbb{N} \) (“band gap condition”)

\[
\epsilon_n < \inf_{j \in \mathbb{Z}^d} E_n^j \leq \sup_{j \in \mathbb{Z}^d} E_n^j < \epsilon_{n+1}.
\] (47)

Finally, we assume that a function \( E \in \ell^\infty(C^1(\mathbb{R}^d)) \) exists such that

\[
E_n^j = E_n(R_j) \quad j \in \mathbb{Z}^d ; \ R_j \in \mathcal{L}^\epsilon ; \ n \in \mathbb{N} .
\] (48)

It is not difficult to verify that as a consequence of the smoothness hypothesis of the quasi-periodic potential, Bloch function and band energy functions, we have the following bounds

\[
\sup_n \sup_R \| \nabla_R u_n(R, \cdot) \|_{L^2_{\mathcal{C}^1}} < \infty
\] (49)

\[
\sup_R \left( \| \nabla_R W(R, \cdot) \|_{L^2_{\mathcal{C}^1}} + \| W(R, \cdot) \|_{L^2_{\mathcal{C}^1}} \right) < \infty
\] (50)

\[
\sup_n \sup_R \| \nabla_R E_n(R) \| < \infty .
\] (51)

We state the main result of our paper

**Theorem 1** Assume that \( W^\epsilon \in \mathfrak{W}_\Omega \), the eigenvalue of the Bloch equation are simple and such that Eqs. (47),(48) hold true. Let \( \psi^\epsilon(t) \in L^2(\mathbb{R}^d) \cap C^1(\mathbb{R}^d) \) be the unique solution of the Schrödinger equation (2), with initial conditions \( \psi_0 \in L^2(\mathbb{R}^d) \cap C^1(\mathbb{R}^d) \). Let \( \varphi_0 = \lim_{\varepsilon \to 0} \mathcal{J}^\epsilon |\mathcal{C}^\epsilon|^{-1/2} \langle \chi_{j,n} | \psi_0 \rangle \) the projection of the initial datum on the Luttinger-Kohn-Foreman basis set given by Eq. (15). Assume that \( \varphi_0 \in \mathcal{H}^\kappa \) for some \( \kappa > 2 \). Then, for almost all \( r \in \mathbb{R}^d \) we have the following convergence in time

\[
\lim_{\varepsilon \to 0} \left( \sum_n |\varphi^\epsilon_n(r,t)|^2 - |\psi^\epsilon(r,t)|^2 \right) = 0 ,
\] (52)

where \( \varphi^\epsilon \) is the unique solution of the kp system with variable coefficients

\[
\frac{\partial \varphi^\epsilon}{\partial t} = \frac{\mathcal{H}^\epsilon_{kp}}{\varepsilon^2} \varphi^\epsilon
\]

\( \varphi^\epsilon(t = 0) = \varphi_0 . \)

5 Study of the multiband “kp” model

5.1 Derivation of the model

We derive the kp multiband envelope model. The starting point is the Schrödinger evolution equation (2). We expand the wave function \( \psi \) on the LKF basis set \( \{ \chi^\epsilon_{j,n} | j \in \mathbb{Z}^d, n \in \mathbb{N} \} \) defined in Eq. (15). We have
Theorem 2 Let $u_{n,j}^\varepsilon \in L^2(C^\varepsilon)$ be a family of $L^\varepsilon$-periodic eigenfunctions of the kp-Bloch Equation (16). For every $j \in \mathbb{Z}^d$ the sequence $\{u_{n,j}^\varepsilon\}_{n \in \mathbb{N}}$ is an orthonormal basis of $L^2(C^\varepsilon)$. Then, for every $\psi \in L^2(\mathbb{R}^d)$ there exists a unique sequence $\varphi^\varepsilon \in \mathcal{E}_d$ such that
\[
\psi(r) = |C^\varepsilon|^{1/2} \sum_{n,j} \varphi_{n,j}^\varepsilon(r - R_j) u_{n,j}^\varepsilon(r) .
\] (53)
The envelope functions $\varphi_{n,j}^\varepsilon$ are obtained by the scalar product
\[
\varphi_{n,j}^\varepsilon = \frac{1}{|C^\varepsilon|^{1/2}} \int_{\mathbb{R}^d} \chi_{j,n}^\varepsilon(r) \psi^\varepsilon(r) \, dr ,
\] (54)
where
\[
\chi_{j,n}^\varepsilon(r) = |C^\varepsilon| \delta^\varepsilon(r - R_j) u_{n,j}^\varepsilon(r) .
\] (55)
The proof of this statement is postponed to the Appendix A. The modulus of the wave function is one of the most important physical quantities in the description of the particle motion. It gives the probability to find the particle around a certain position. In the kp formalism, this information can be extract directly from the envelope function representation. In particular, when $\varepsilon \to 0$, the value $\sum_n |\varphi_{j,n}^\varepsilon|^2$ converges to $|\psi(R_j)|^2$, the probability to find the particle around the lattice site $R_j$.

Theorem 3 Let $\psi \in C^0(\mathbb{R}^d) \cap L^2(\mathbb{R}^d)$. We have
\[
\lim_{\varepsilon \to 0} \sum_n |\varphi_{n}^\varepsilon(R)|^2 = |\psi(R)|^2 ,
\] (56)
for all $R \in \mathbb{R}^d$, where $\varphi_{n}^\varepsilon(R) = (\mathcal{F}^\varepsilon \varphi_{n,j}^\varepsilon)(R)$ is the function interpolating the $\varphi_{n,j}$ defined in Eq. (54).

The proof of this statement is given in Appendix A.

Equation (2) gives
\[
i \frac{\partial \varphi_{n,j}^\varepsilon(t)}{\partial t} = \sum_{n',j'} (T_{n,n',j,j'}^\varepsilon + W_{n,n',j,j'}^\varepsilon) \varphi_{n',j'}^\varepsilon(t) ,
\] (57)
where
\[
T_{n,n',j,j'}^\varepsilon \equiv -\frac{1}{2} \int_{\mathbb{R}^d} \chi_{j,n}^\varepsilon(r) \Delta_r \chi_{j',n'}^\varepsilon(r) \, dr
\] (58)
and
\[
W_{n,n',j,j'}^\varepsilon \equiv \frac{1}{\varepsilon^2} \int_{\mathbb{R}^d} \chi_{j,n}^\varepsilon(r) W_{\varepsilon}^\varepsilon \left( \frac{r}{\varepsilon} , r \right) \chi_{j',n'}^\varepsilon(r) \, dr .
\] (59)
Equation (57) gives the evolution of the system in terms of the two-indices unknown $\varphi_{n,j}$. For this reason, we will refer to Eq. (57) as the “fully discrete” kp system. In analogy with the case of the uniform systems where the kp evolution equation is given by Eq. (13), it is more convenient to express Eq. (57) in terms of the continuous functions that interpolate the $\varphi_{n,j}$. However, differing from the standard kp-envelope function approach, the derivation of the kp equation of motion for a quasi-periodic crystal encounters several technical difficulties. In order to proceed, we state here a preliminary Lemma based on the spectral decomposition technique. It is useful for the calculation of integrals containing the product of functions that vary both at the macroscopic and at microscopic scale.
Lemma 5.1 Let $\varepsilon > 0$ and $f_j \in L^2(\mathbb{R}^d \times \mathcal{C}^\varepsilon)$ with $j = 0, \ldots, N-1$ be a set of functions such that $f_j(\cdot, x) \in \mathcal{E}^{\varepsilon/\alpha_j}$ $(f_0(\cdot, x) \in \mathcal{E}^{\varepsilon})$ for almost all $x \in \mathcal{C}^\varepsilon$, $\alpha_j \in \mathbb{R}^+$ and $\sum_{j=1}^{N-1} \alpha_j^{-1} \leq 1$. Moreover, the $f_j$ are $\mathcal{L}^\varepsilon$-periodic with respect to the second variable $(f_j(r, x + \mathbf{R}) = f_j(r, x)$ for all $r \in \mathbb{R}^d$, $\mathbf{R} \in \mathcal{L}^\varepsilon$). We have

$$
\prod_{j=1}^{N-1} \int_{\mathbb{R}^d} f_0(r, r) f_j(r, r) \, dr = \frac{|\mathcal{C}^\varepsilon|^{-N/2}}{(2\pi)^{Nd/2-1}} \prod_{j=1}^{N-1} \sum_{G_j \in \mathcal{L}^\varepsilon} \int_{\mathbb{R}^d} \hat{f}_0(k_0, G_0) \hat{f}_j(k_j, G_j)
\times \delta^K_{G^\Sigma,0} \delta \left(k_0 - \sum_{j=1}^{N-1} k_j\right) \, dk_j \, dk_0 ,
$$

where $G^\Sigma = \sum_{j=1}^{N-1} G_j$ and

$$
\hat{f}_j(k, G) = \frac{1}{(2\pi)^{d/2} |\mathcal{C}^\varepsilon|^{1/2}} \int_{\mathbb{R}^d} f_j(r, x) e^{-i(r \cdot k + x \cdot G)} \, dx .
$$

Proof: Every function $g(r, x) \in L^2(\mathbb{R}^d \times \mathcal{C}^\varepsilon)$ can be Fourier transformed with respect the first variable. Furthermore, the result can be expanded by the Fourier’s series. We obtain

$$
g(r, x) = \frac{1}{(2\pi)^{d/2} |\mathcal{C}^\varepsilon|^{1/2}} \sum_{G \in \mathcal{L}^\varepsilon} \int_{\mathbb{R}^d} \hat{g}(k, G) e^{i(r \cdot k + x \cdot G)} \, dk
$$

By applying this equation to each term in the left side of Eq. (60), we have

$$
\prod_{j=1}^{N-1} \int_{\mathbb{R}^d} f_0(r, r) f_j(r, r) \, dr = \frac{|\mathcal{C}^\varepsilon|^{-N/2}}{(2\pi)^{Nd/2-1}} \prod_{j=1}^{N-1} \sum_{G_j \in \mathcal{L}^\varepsilon} \int_{\mathbb{R}^d} \hat{f}_0(k_0, G_0) \hat{f}_j(k_j, G_j)
\times e^{ir \cdot (\sum_{j=1}^{N-1} G_j + \sum_{j=1}^{N-1} k_j)} \, dk_j \, dk_0 \, dr
$$

$$
= \frac{|\mathcal{C}^\varepsilon|^{-N/2}}{(2\pi)^{Nd/2-1}} \prod_{j=1}^{N-1} \sum_{G_j \in \mathcal{L}^\varepsilon} \int_{\mathbb{R}^d} \hat{f}_0(k_0, G_0) \left(-G^\Sigma - \sum_{j=1}^{N-1} k_j, G_0\right)
\hat{f}_j(k_j, G_j) \ll_{B^\varepsilon} \left(G^\Sigma + \sum_{j=1}^{N-1} k_j\right) \ll_{B^\varepsilon/\alpha_j} (k_j) \, dk_j .
$$

We have that $\hat{f}_j \in L^2_{B^\varepsilon/\alpha_j}$ and $\sum_{j=1}^{N-1} \alpha_j \leq 1$. There are two possibilities, either the vector $\sum_{j=1}^{N-1} k_j$ belongs to the Brillouin Zone $B^\varepsilon$ or one of the functions inside the integral vanishes. In both cases we can write $\ll_{B^\varepsilon} \left(G^\Sigma + \sum_{j=1}^{N-1} k_j\right) = \delta^K_{G^\Sigma,0}$ and we obtain Eq. (60).

As a particular case of the Lemma 5.1, we have

Lemma 5.2 Assume that $f, g \in \mathcal{E}^{\varepsilon}$ and let $u, v \in L^2(\mathcal{C}^\varepsilon)$ be $\mathcal{L}^\varepsilon$-periodic functions. We have (spectral decomposition rule)

$$
\int_{\mathbb{R}^d} \tilde{f}(r) g(r) \overline{u(r)} v(r) \, dr = \frac{1}{|\mathcal{C}^\varepsilon|} \int_{\mathbb{R}^d} \tilde{f}(k) \tilde{g}(k) \ll_{B^\varepsilon}(k) \, dk \sum_{G \in \mathcal{L}^\varepsilon} \overline{\tilde{u}(G)} \tilde{v}(G)
$$

$$
= \int_{\mathbb{R}^d} \tilde{f}(r) g(r) \, dr \int_{\mathcal{C}^\varepsilon} \overline{\pi(x)} v(x) \, dx .
$$
We consider here an application of the discrete derivative operator $D$ defined in Eq. (31). We focus on a particular class of matrix operators defined in $E_d$ that can be expressed in terms of $D \varphi$. In order to proceed, we introduce a set of complex polynomial $g_s$, $h_s$ with $s = 1, \ldots, S$; $S < \infty$, and we assume that $f (k) = \sum_s g_s (k') h_s (k - k')$ for some polynomial $f$ (here $(k')$ is a dummy variable).

**Lemma 5.3** Let $f$ be a complex polynomial, $\varphi \in \ell^2$, $S \in \mathcal{B} (\ell^2)$ and

$$K_{j,j'}^{j,j} = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} f (k) e^{-i (R_j - R_{j'}) \cdot k} \delta_{B_r} (k) \, dk.$$  \hspace{1cm} (65)

We have

$$\eta_j = \sum_j S_{j,j'}^{j,j} \varphi_{j'} = \frac{|B|^d}{(2\pi)^d} \sum_{s=1}^S \left[ D_{[h_s]_\alpha} S_{j,\alpha}^{j,\alpha} \right] _j \left[ D_{[g_s]_\alpha} \varphi_{\alpha} \right] _j .$$  \hspace{1cm} (66)

**Proof:** By noting that

$$|K_{j,j'}^{j,j}| \leq \frac{|B|}{(2\pi)^d} \max_{x \in B} (f) ,$$

we have $\|\eta\|_{\ell^2} \leq C$. We express the sequence $\varphi_{j}$ in terms of the interpolating function $\varphi$ (see Eq. (20)) $\varphi_{j} = (\mathcal{I} \varphi) (R_j)$ and we take the Fourier transform. We have

$$\sum_{j'} S_{j,j'}^{j,j} \varphi_{j'} = \frac{1}{(2\pi)^d} \sum_{j',s} \left[ D_{[h_s]_\alpha} S_{j,\alpha}^{j,\alpha} \right] _j \int_{\mathbb{R}^d} e^{-i R_j \cdot k} g_s (k) \varphi_{j'} (k') \delta_{B_r} (k') \, dk' \times \int_{\mathbb{R}^d} e^{i (R_j' - R_j) \cdot k} \delta_{B_r} (k) \, dk$$

$$= \frac{1}{(2\pi)^d} \sum_{s} \left[ D_{[h_s]_\alpha} S_{j,\alpha}^{j,\alpha} \right] _j \sum_{j'} \int_{\mathbb{R}^d} g_s (k') \varphi_{j'} e^{i (R_j' - R_j) \cdot k} \delta_{B_r} (k') \, dk'$$

$$= \frac{|B|^d}{(2\pi)^d} \sum_{s} \left[ D_{[h_s]_\alpha} S_{j,\alpha}^{j,\alpha} \right] _j \left[ D_{[g_s]_\alpha} \varphi_{\alpha} \right] _j .$$

Proceeding in the same way, it is possible to verify that if we modify the definition of $K$ (Eq. (65)) by substituting the lattice coordinate $R_j$ with the generic position $r$, the right side of Eq. (66) becomes

$$|B|^d \sum_{s,j'} \delta_{B^r} (R_j' - r) \left[ D_{[h_s]_\alpha} S_{j,\alpha}^{j,\alpha} \right] _j \left[ D_{[g_s]_\alpha} \varphi_{\alpha} \right] _j .$$

As will be more clear in the following, in analogy with the integration by part technique, the Lemma 5.3 is applied whenever it is useful to displace the derivative operator among the factors of a product.

We proceed now to evaluate the matrices $T^\varepsilon$ and $W^\varepsilon$ given in Eqs. (58)-(59). At first, we consider $T^\varepsilon$. We write

$$- \frac{2}{|C|^2} T^\varepsilon = T^{kp,^\varepsilon} + T^{Tu,^\varepsilon} + T^{Tf,^\varepsilon} ,$$
where
\[ T_{n,n';j,j'}^{kp,\varepsilon} = 2 \int_{\mathbb{R}^d} \delta^2(r - R_j) \overline{w_{n,j}} \left( \nabla_r \delta^2(r - R_{j'}) \right) \cdot \left( \nabla_r u_{n';j,j'}^{\varepsilon} \right) \, dr \]
\[ T_{n,n';j,j'}^{Tu,\varepsilon} = \int_{\mathbb{R}^d} \delta^2(r - R_j) \overline{w_{n,j}} \left( \Delta_r u_{n';j,j'}^{\varepsilon} \right) \, dr \]
\[ T_{n,n';j,j'}^{Tf,\varepsilon} = \int_{\mathbb{R}^d} \delta^2(r - R_j) \left( \Delta_r \delta^2(r - R_{j'}) \right) \overline{u_{n,j}} u_{n';j,j'}^{\varepsilon} \, dr . \]

As it is customary in the $kp$ theory, we expand the gradient of the periodic function $u^\varepsilon$ on the basis set \( \{ u_{j,n}^\varepsilon | n \in \mathbb{N} \} \)
\[ \nabla_r u_{n';j,j'}^{\varepsilon} = \frac{1}{\varepsilon} \sum_{n'} u_{n',j,j'}^{\varepsilon}(r) P_{n',n}^j(r) , \]
where we defined the matrix $P^j$ as a straightforward extension of the Kane parameters given in Eq. (14)
\[ \frac{1}{\varepsilon} P_{n',n}^j = \int_{\mathbb{C}} \overline{u_{n',j,j'}^{\varepsilon}(r)} \left( \nabla_r u_{n';j,j'}^{\varepsilon}(r) \right) \, dr = \frac{1}{\varepsilon} \int_{\mathbb{C}} \overline{u_{n'}^{\varepsilon}(r)} \left( \nabla_r u_{n'}^{\varepsilon}(r) \right) \, dr . \]
We apply the Lemma 5.2 and we obtain
\[ T_{n,n';j,j'}^{kp,\varepsilon} = \frac{2}{\varepsilon |\mathbb{C}|^2} S_{n,n';j,j'} \cdot K_{j,j'}^\varepsilon , \]
where $K$ is given by Eq. (65) and we defined
\[ S_{n,n';j,j'} = \sum_{n''} N_{n,n'',j,j'} P_{n'',n}^j(n'';n) = \int_{\mathbb{C}} \overline{u_{n,j}^{\varepsilon}(r)} \left( \nabla_r u_{n';j,j'}^{\varepsilon}(r) \right) \, dr \quad (67) \]
\[ N_{n,n',j,j'} = \sum_{G \in \mathbb{C}^*} \overline{u_{n,j}^{\varepsilon}(G)} \overline{u_{n',j,j'}^{\varepsilon}(G)} = \int_{\mathbb{C}} \overline{u_{n'}^{\varepsilon}(r)} u_{n';j,j'}^{\varepsilon}(r) \, dr . \quad (68) \]
The hat denotes the coefficients of the Fourier series (see Eq. (120) in the Appendix A).
Concerning the term $T_{n,n';j,j'}^{kp,\varepsilon}$, we apply the Lemma 5.3 with $f = i\mathbf{k}$. We consider the polynomials \( \{(g_s, h_s)\} = \{(i\mathbf{k}, 1); (1, i\mathbf{k})\} \). We have
\[ \sum_{j'} T_{n,n';j,j'}^{kp,\varepsilon} \varphi_{j'} = \frac{2}{\varepsilon |\mathbb{C}|^2} \left( \mathcal{D}_{[i\mathbf{k}];\alpha} S_{n,n',j,j'} \right) \varphi_j - S_{n,n',j,j'} \cdot \nabla_r \varphi_{j'}(r) \bigg|_{r=R_j} \]
\[ = -\frac{2}{\varepsilon |\mathbb{C}|^2} \sum_{n',n''} \left[ \mathcal{D}_{[-i\mathbf{k},\alpha]} N_{n,n',j,j'} \cdot P_{n'',j,j'}^{\alpha} \right] \varphi_{j'} . \]
Where we used Eq. (33). We proceed in the same way for the term $T_{n,n';j,j'}^{Tu,\varepsilon}$. We apply the Lemma 5.3 with $f = \mathbf{k}^2$ and \( \{(g_s, h_s)\} = \{(i\mathbf{k})^2, 1\}; \sqrt{2}(i\mathbf{k}, i\mathbf{k}); (1, (i\mathbf{k})^2)\} \). We obtain
\[ |\mathbb{C}|^2 \sum_{j'} T_{n,n';j,j'}^{Tu,\varepsilon} \varphi_{j'} = \delta^K_{n,n'} \Delta_{n,n'} \varphi_{j'}(r) \bigg|_{r=R_j} - 2 \left[ \mathcal{D}_{[i\mathbf{k};\alpha]} N_{n,n',j,j'} \right] \nabla_r \varphi_{j'}(r) \bigg|_{r=R_j} \]
\[ + \left[ \mathcal{D}_{[i\mathbf{k};\alpha]} N_{n,n',j,j'} \right] \varphi_j \]
\[ = -\frac{1}{2} \sum_{n'} \left[ \mathcal{D}_{[-i\mathbf{k};\alpha]} N_{n,n',j,j'} \varphi_{n,n'} \right] . \]
After few calculations, the two remaining terms of Eq. (57) can be written as

\[
\frac{|C|^2}{2} T_{n,n',j;j'} + W_{n,n',j;j'}^{\varepsilon} = \sum_{j''} Z_{n,n',j;j''}^{\varepsilon} + \frac{E_{n''}^{j'} K_{j;j'} K_{n,n'}}{\varepsilon^2},
\]

with

\[
Z_{n,n',j;j''}^{\varepsilon} = \frac{|C|^3}{\varepsilon^2} \int_{C^2} \delta(r - R_j) \delta(r - R_{j''}) \delta(r - R_{j''}) \times \left[ W_{j''} \left( \frac{r}{\varepsilon} \right) - W_{j'} \left( \frac{r}{\varepsilon} \right) \right] \overline{u_{n,j}^{\varepsilon}}(r) u_{n',j'}^{\varepsilon}(r) \, dr.
\]

We remark that \( Z^{\varepsilon} \) is not present in the usual formulation of the \( kp \) equation of motion for uniform system. The term \( Z^{\varepsilon} \) is a consequence of the use of different periodic Bloch functions \( u_{n,j}^{\varepsilon} \) in the definition of the basis set \( \{ \chi_{j,n} \} \). It is immediate to verify that in the case of a uniform periodic lattice \( Z^{\varepsilon} \) vanishes (the periodic potential \( W_j \) in Eq. (4) does not depend anymore from the index \( j \)). Under some assumptions on the regularity of the potential \( W_j^{\varepsilon} \), the kernel of \( Z^{\varepsilon} \) includes the class of the functions that belong to \( \mathcal{E}^{\varepsilon/\alpha} \) for some \( \alpha \geq 1 \). For this reason, concerning the applications of the theory, we can neglect \( Z^{\varepsilon} \) any time we consider crystals where the variation of the chemical is sufficiently smooth. However, from a rigorous point of view, at the end of this section we will show that in the limit \( \varepsilon \to 0 \) the operator \( Z^{\varepsilon} \) vanishes. This is proven in the Theorem 5. The following Lemma characterizes more precisely the kernel of \( Z^{\varepsilon} \)

**Lemma 5.4** Let \( \varepsilon > 0 \) and \( \varphi \in \ell^2 \). Under the following assumption on the smoothness the quasi-periodic potential and the Bloch function

\[
\tilde{W}_j^{\varepsilon} (G) \in \mathcal{E}^{\varepsilon/\alpha'} \quad \text{uniformly on } G \in \mathcal{L}^{\varepsilon},
\]

\[
\tilde{u}_{n,j}^{\varepsilon} (G) \varphi_j \in \mathcal{E}^{\varepsilon/\alpha'} \quad \text{uniformly on } G \in \mathcal{L}^{\varepsilon}, n \in \mathbb{N}
\]

\[
\tilde{W}_j^{\varepsilon} (G) \tilde{u}_{n,j}^{\varepsilon} (G') \varphi_j \in \mathcal{E}^{\varepsilon/\alpha} \quad \text{uniformly on } G, G' \in \mathcal{L}^{\varepsilon}, n \in \mathbb{N},
\]

with \( \frac{1}{\alpha'} + \frac{1}{\alpha} \leq 1 \) and \( \alpha \leq 1 \) and

\[
\tilde{W}_j^{\varepsilon} (G) = \frac{1}{|C\varepsilon|^{1/2}} \int_{C^2} W_j^{\varepsilon}(r) e^{-iG \cdot r} \, dr
\]

\[
\tilde{u}_{n,j}^{\varepsilon} (G) = \frac{1}{|C\varepsilon|^{1/2}} \int_{C^2} u_{n,j}^{\varepsilon}(r) e^{-iG \cdot r} \, dr
\]

we have

\[
\sum_{j'',j'} Z_{n,n',j;j'',j''}^{\varepsilon} \varphi_j' = 0.
\]

**Proof:** Proceeding as in Lemma 5.1, we write \( Z_{n,n',j;j''}^{\varepsilon} \) in the Fourier space. After few calculations we obtain

\[
\sum_{j'',j'} Z_{n,n',j;j'',j''}^{\varepsilon} \varphi_j' = \delta_{n,n'} \delta_{j,j'} + \delta_{n,n'} \delta_{j,j'},
\]
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where

$$\delta_{n,n';j} = \frac{|C_{\epsilon}|^{3/2}}{\pi^2} \int_{\mathbb{R}^{2d}} \sum_{\mathbf{G},\mathbf{G}',\mathbf{G}'' \in \mathcal{L}^*} \frac{u_{n,j}(\mathbf{G}) S_{n,n';j}^{\epsilon}(\mathbf{k}',\mathbf{k}'',\mathbf{G}',\mathbf{G}'') I_{\mathbf{B}^r}(\mathbf{k}') I_{\mathbf{B}^r}(\mathbf{k}'')}{e^{i\mathbf{R}_j(\mathbf{G} - \mathbf{k}' - \mathbf{k}'')} I_{\mathbf{B}^r}(-\mathbf{G} + \mathbf{k}' + \mathbf{k}'')} \, dk' \, dk'' .$$

(76)

We defined $G^\Sigma \equiv G + G' + G''$, $s = a, b$ and

$$S_{n,n';j}^{\epsilon}(\mathbf{k}',\mathbf{k}'',\mathbf{G}',\mathbf{G}'') = \sum_{j''} \tilde{W}_{j''}^{\epsilon}(\mathbf{G}'') e^{i\mathbf{R}_j' k''} \sum_{j'} \bar{u}_{n',j'}^{\epsilon}(\mathbf{G}') \varphi_{j'} e^{i\mathbf{R}_j k'}$$

(77)

$$S_{n,n';j}^{be}(\mathbf{k}',\mathbf{k}'',\mathbf{G}',\mathbf{G}'') = -\frac{2\pi^d}{|C_{\epsilon}|} \sum_{\mathbf{G}'' \in \mathcal{L}^*} \delta(\mathbf{G}'' - \mathbf{k}'') \sum_{j'} \tilde{W}_{j'}^{\epsilon}(\mathbf{G}'') \bar{u}_{n',j'}^{\epsilon}(\mathbf{G}') \varphi_{j'} e^{i\mathbf{R}_j k'} .$$

(78)

In Eq. (77) we put into evidence that $S_{\epsilon}^{ae}$ is the product of two Fourier series. Equations (70)-(71) ensure that we can restrict the double integral to the set of $\mathbf{k}'$ and $\mathbf{k}''$ such that $\mathbf{k}' + \mathbf{k}'' \in \mathcal{B}^c$. Since, by definition, the vectors of the reciprocal lattice $\mathcal{L}^*$ connect the centers of two different Brillouin zones, the relationship $\mathbf{k}' + \mathbf{k}'' + \mathbf{G} \in \mathcal{B}^c$ implies $\mathbf{G} = 0$. As a consequence, Eq. (76) simplifies to

$$\delta_{n,n';j}^{ae} = \frac{1}{|C_{\epsilon}|^{1/2} \pi^2} \sum_{\mathbf{G},\mathbf{G}',\mathbf{G}'' \in \mathcal{L}^*} \frac{u_{n,j}(\mathbf{G}) \tilde{W}_{j}^{\epsilon}(\mathbf{G}'') \bar{u}_{n',j}^{\epsilon}(\mathbf{G}')}{e^{i\mathbf{R}_j(\mathbf{G} - \mathbf{k}' - \mathbf{k}'')} I_{\mathbf{B}^r}(\mathbf{k}')} \delta_{G^\Sigma,0} \varphi_j .$$

In the same way

$$\delta_{n,n';j}^{be} = -\frac{|C_{\epsilon}|^{1/2}}{\pi^2} \int_{\mathbb{R}^{2d}} \sum_{\mathbf{G},\mathbf{G}',\mathbf{G}'' \in \mathcal{L}^*} \bar{u}_{n,j}(\mathbf{G}) \tilde{W}_{j'}^{\epsilon}(\mathbf{G}'') \bar{u}_{n',j'}^{\epsilon}(\mathbf{G}') \varphi_{j'} \times e^{i\mathbf{R}_j(\mathbf{G} - \mathbf{k}' - \mathbf{k}'')} I_{\mathbf{B}^r}(-\mathbf{G} + \mathbf{k}' + \mathbf{k}'') I_{\mathbf{B}^r}(\mathbf{k}') \delta(\mathbf{G}'' - \mathbf{k}'') \, dk' \, dk'' .$$

$$= -\frac{|C_{\epsilon}|^{1/2}}{\pi^2} \int_{\mathbb{R}^{2d}} \sum_{j'} \sum_{\mathbf{G},\mathbf{G}',\mathbf{G}'' \in \mathcal{L}^*} \bar{u}_{n,j}(\mathbf{G}) \tilde{W}_{j'}^{\epsilon}(\mathbf{G}'') \bar{u}_{n',j'}^{\epsilon}(\mathbf{G}') \delta_{G^\Sigma,0} \varphi_{j'} \times e^{i\mathbf{R}_j(\mathbf{G} - \mathbf{k}' - \mathbf{k}'')} I_{\mathbf{B}^r}(\mathbf{k}') \, dk' \, dk'' .$$

$$= -\delta_{n,n';j}^{ae} ,$$

where we used $I_{\mathbf{B}^r}(\mathbf{k}') \delta(\mathbf{G}'' - \mathbf{k}'') = \delta_{G''',0} \delta(\mathbf{k}'')$, $I_{\mathbf{B}^r}(-\mathbf{G} + \mathbf{k}' + \mathbf{k}'') I_{\mathbf{B}^r}(\mathbf{k}')$.

In view to the continuous limit, it is convenient to write the operator $Z^\epsilon$ in terms of the interpolating functions. We define the map $Z^\epsilon[\varphi] : \mathcal{E}_c^0 \rightarrow \mathcal{E}_c^0$ as

$$Z^\epsilon[\varphi] = \sum_{n',j',j''} \delta_{n',j',j''} \varphi_{n'}(\mathbf{R}_{j'}) .$$

(79)

In order to obtain some bound of $Z^\epsilon$ we use the following
Lemma 5.5 Let $\varphi \in \mathcal{E}_c^0$ and $\Omega$ be a bounded set of $\mathbb{R}^d$. Assume that $\mathcal{F}^e u_{n,j}(r), \mathcal{F}^e W_j(r)$ belongs to the space $\mathcal{F}^{-1} L_{\Omega}^2$ for all $n \in \mathbb{N}$ and almost all $r \in \mathcal{C}_c$. We have

$$\mathcal{F}^e [\varphi] = \mathcal{F}^e [\varphi^*],$$

(80)

where

$$\varphi_n^*(R) = \frac{1}{(2\pi)^{d/2}} \int_{|k| > \rho^e} \hat{\varphi}_n(k) e^{i k \cdot R} \, dk$$

(81)

with $\rho^e \equiv \max \left[ 0, \frac{1}{4 \rho(B)} - \frac{1}{2 \rho(\Omega)} \right]$.

Proof: Proceeding as in Lemma 5.1, we write $Z_{n,n',j,j'}^e$ in the Fourier space. After few calculations we obtain

$$\mathcal{F}^e [\varphi] = \sum_{n'} \mathcal{F}^{C^{3/2}} e^{2(2\pi)^{d/2} \mathcal{F}^e} \int_{\mathbb{R}^{2d}} \sum_{G,G' \in \mathcal{C}_c^e} \mathcal{F}^{n,j}(G) \mathcal{F}^{n',j}(G') \mathcal{F}^{n,j'}(G'') \mathcal{F}^{n',j'}(G''') \times \left| \hat{u}_{n,j}(G) \mathcal{F}^{n,j}(G') \mathcal{F}^{n',j}(G'') \mathcal{F}^{n,j'}(G'') \mathcal{F}^{n',j'}(G''') \right| dG \, dk.$$

(82)

Here, $G^e \equiv G + G' + G''$ and

$$\mathcal{F}^{n,j}(G) \mathcal{F}^{n',j}(G') = M(k'';G'') \sum_{j'} g_{j'}(k',n',G') - \delta(k'') \sum_{j'} \mathcal{W}^{j'}(G'') g_{j'}(k',G'),$$

(83)

where we defined

$$M(k'';G'') \equiv \sum_{j'} \mathcal{W}^{j'}(G'') e^{i R_{j'} \cdot k''}$$

(84)

$$g_{j'}(k',n',G') \equiv \mathcal{F}^{n,j}(G') \varphi_{n'}(R_{j'},R_j) e^{i R_{j'} \cdot k'}. $$

(85)

Furthermore, we define the set $Y \subset \mathbb{R}^{2d} \equiv \{ (k',k'') \in \mathbb{R}^{2d} \mid k' + k'' \in B^c \}$. Proceeding as in Lemma 5.4, we obtain

$$\int_Y \sum_{G,G',G'' \in \mathcal{C}_c^e} \mathcal{F}^{n,j}(G) \mathcal{F}^{n',j}(G') \mathcal{F}^{n,j'}(G'') \mathcal{F}^{n',j'}(G''') \times \left| \hat{u}_{n,j}(G) \mathcal{F}^{n,j}(G') \mathcal{F}^{n',j}(G'') \mathcal{F}^{n,j'}(G'') \mathcal{F}^{n',j'}(G''') \right| dG \, dk = 0.$$

(86)

Consequently, we can restrict the integral on the variable $(k',k'')$ in the Eq. (76) to the region outside $Y$. We characterize this region more into details. We consider the first term of Eq. (83). Since $\mathcal{F}^e W_j(r)$ belongs to the space $\mathcal{F}^{-1} L_{\Omega}^2$, the same holds true for the coefficients of the Fourier series $\mathcal{W}_j^e(G)$. The support of $M$ stays inside $\Omega$, and the region outside $Y$ can we written as $\{ k' \in \mathbb{R}^d \mid k' + \Omega \notin B^c \}$. Furthermore, $\sum_{j'} g_{j'}(k')$ is the Fourier series of the product between $u \varphi$. Form the elementary properties of the Fourier series, we have that the support of $\sum_{j'} g_{j'}(k')$ is given by the vectorial sum of the support of $u$ and $\varphi$. Consequently, we can restrict the function $\hat{\varphi}_n(k')$ to the region $\{ k' \in \mathbb{R}^d \mid k' + 2 \Omega \notin B^c \}$. For the other values, the integral vanishes. The same considerations apply for the second term of Eq. (83). This ensures that we can substitute $\varphi$ with the cutoff on the Fourier space provided by Eq.
Collecting all the calculations, the evolution equation of the particle projected in the LKF basis, is expressed by the following system

\[
\begin{aligned}
&i\varepsilon^2 \frac{\partial \varphi_n^\varepsilon(t)}{\partial t} = E_n^\varepsilon \varphi_n^\varepsilon + \varepsilon \sum_{n'} \left( \sum_{n''} \left[ D[-i\mathbf{k}]_{\alpha} N_{n,n'';j,\alpha} P_{n''}^\alpha \psi_{a,n''} \right]_j + \frac{\varepsilon}{2} \left[ D[-i\mathbf{k}^2]_{\alpha} N_{n,n';j,\alpha} \psi_{a,n'} \right]_j \right) \\
&+ \sum_{j''} Z^\varepsilon_{n,n';j,j''} \varphi_n^\varepsilon_{j''}.
\end{aligned}
\]  

(87)

We express the equations of motion in terms of the interpolating functions. We obtain

\[
\begin{aligned}
&\varepsilon^2 \frac{\partial \varphi_n^\varepsilon(R, t)}{\partial t} = \mathcal{H}_K^\varepsilon \varphi_n^\varepsilon + \varepsilon^2 \mathcal{F}[\varphi^\varepsilon],
\end{aligned}
\]

(88)

where we defined

\[
\begin{aligned}
&\mathcal{H}_K^\varepsilon = \mathcal{E} + \varepsilon \mathcal{S} + \varepsilon^2 \mathcal{G}, \\
&\mathcal{E} \varphi = E_n(R) \varphi_n(R), \\
&\mathcal{S} \varphi = \sum_{n'} \nabla_{R'} \left[ S_{n,n'}(R, R') \varphi_{n'}(R', t) \right]_{R' = R}, \\
&\mathcal{G} \varphi = \sum_{n'} \frac{1}{2} \Delta_{R'} \left[ N_{n,n'}(R, R') \varphi_{n'}(R', t) \right]_{R' = R}.
\end{aligned}
\]  

Here, the coefficients $S_{n,n'}$ and $N_{n,n'}$ are obtained by straightforward interpolation of the discrete counterparts given in Eqs. (67)-(68). Explicitly (see also Eq. (17) for the comparison)

\[
\begin{aligned}
&S_{n,n'}(R, R') = \varepsilon \int_{C^\varepsilon} \frac{\overline{u}_n^\varepsilon(R, r)}{u_{n'}^\varepsilon(R', r)} (\nabla_r u_{n'}^\varepsilon (R', r)) \, dr, \\
&N_{n,n'}(R, R') = \int_{C^\varepsilon} \frac{\overline{u}_n^\varepsilon(R, r)}{u_{n'}^\varepsilon(R', r)} u_{n'}^\varepsilon(R', r) \, dr,
\end{aligned}
\]

(93)  

(94)

where, in order simplify the notations, we set $u_{n'}^\varepsilon(R, r) = \mathcal{F} \left( u_{n,j}^\varepsilon(r) \right) = \varphi_n^\varepsilon(R, r)$. It is easy to verify that Eq. (88) coincides with Eq. (87) in correspondence of the lattice sites. For example $E_n(R_j) \varphi_n(R_j) = E_n^\varepsilon \varphi_n(R_j) = \mathcal{F} \left( E_n \varphi_n \right)(R_j)$ and $\left( \mathcal{S} \varphi \right)(R_j) = \sum_{n'} \left[ D[-i\mathbf{k}]_{\alpha} S_{n,n';j,\alpha} \psi_{a,n'} \right]_j$, where we used Eq. (33).

### 5.2 Study of the kp dynamics

Equation (88) is well posed

**Theorem 4** The kp Hamiltonian operator $\mathcal{H}_K^\varepsilon$ is essentially self-adjoint in $\mathcal{E}_c^0$ with domain

\[
D(\mathcal{H}_K^\varepsilon) \left\{ \varphi \in \mathcal{H}^2 | \sum_n c_n^2 \| \varphi_n \|^2_{L^2(\mathbb{R}^d)} < \infty \right\}.
\]

As a preliminary for the proof, we state some bonds of the gradient of the interpolating and periodic functions.
Lemma 5.6 Let \( \{ u_{n,j}^\varepsilon \in L^2(\mathbb{C}^\delta) : j \in \mathbb{Z}^d, n \in \mathbb{N} \} \) be a sequence of \( \mathcal{L} \)-periodic Bloch eigenfunctions of Eq. (16) with unitary norm and eigenvalue \( E_{n,j}^\varepsilon \). Assume that \( u_n(R, r) \in \mathcal{F}^{-1}L^2_{\Omega} \) for all \( n \in \mathbb{N} \) and almost every \( r \in \mathbb{C}^\delta \). For some \( \varepsilon > 0 \) and for all \( R \in \mathbb{R}^d \), there exist two constants \( C_0 \) and \( C_1 \) independent of \( R \) and \( \varepsilon \), such that the following bounds hold true

\[
\frac{\varepsilon^2}{2} \| \nabla_R u_{n,j}^\varepsilon (R, r) \|_{L^2(\mathbb{C}^\delta)}^2 \leq C_0 + \varepsilon_n
\]

and

\[
\frac{\varepsilon^2}{2} \| \nabla_R \nabla_R u_{n,j}^\varepsilon (R, r) \|_{L^2(\mathbb{C}^\delta)}^2 \leq C_0 + C_1 \varepsilon_n.
\]

**Proof:** From the definition of the Bloch functions given in Eq. (16) we obtain

\[
\frac{\varepsilon^2}{2} \int_{\mathbb{C}^\delta} | \nabla_R u_{n,j}^\varepsilon (r) |^2 \, dr = E_{n,j}^\varepsilon - \int_{\mathbb{C}^\delta} W_j \left( \frac{r}{\varepsilon} \right) | u_{n,j}^\varepsilon (r) |^2 \, dr
\]

\[
\leq E_{n,j}^\varepsilon + \| W_j \|_{L^\infty} \| u_{n,j}^\varepsilon \|_{L^2(\mathbb{C}^\delta)}^2 \leq \varepsilon_n + C.
\]

We fix \( n \) and we define the sequence \( g_i = \| \nabla_R u_{n,i}^\varepsilon \|_{L^2(\mathbb{C}^\delta)}^2 \). Since the Fourier transform of \( u^\varepsilon \) belongs to \( L^2_{\Omega} \), we can choose \( \varepsilon_0 \) sufficiently small such that \( g \equiv 3^\varepsilon g_i = 3^\varepsilon g_i \). It is sufficient that \( \Omega \subset B^{\varepsilon_0} \). In this way the Fourier transform of \( g \) has support contained in \( B^{\varepsilon_0} \) and the interpolation of the sequence \( g_i \) with a finer grid gives always the same result. In particular, \( g \in C^0(\mathbb{R}^d) \) and for every \( R_j \in \mathcal{L}, g(R_j) = g_i \). For the continuity of \( g \), we have that \( \forall \varepsilon > 0 \) there exists a ball \( B^\delta_j \) centered in \( R_j \) with radius \( \delta > 0 \) such that

\[
\sup_{R \in B^\delta_j} \| g(R) - g_i \| \leq \varepsilon,
\]

and \( \sup_{R_j \in \mathcal{L}} \sup_{R \in B^\delta_j} | g(R) | \leq \varepsilon_n + C + \varepsilon \). Consequently, for \( \varepsilon < \min (\delta / \rho (\mathcal{C}), \varepsilon_0) \), where \( \rho \) denotes the diameter, a constant \( C_0 \) exists such that \( \frac{\varepsilon^2}{2} \| g \| \leq \varepsilon_n + C_0 \). Equation (95) follows from the observation that \( g = \| 3^\varepsilon \nabla_R u_{n,j}^\varepsilon \|_{L^2(\mathbb{C}^\delta)}^2 \). For Eq. (96) we apply the discrete derivative operator to Eq. (16) (throughout this proof \( n \) is a fixed index). Using the Lemma 3.4, we obtain

\[
\frac{\varepsilon^2}{2} \int_{\mathbb{C}^\delta} | \nabla \nabla_R u_{n,j}^\varepsilon (r) |^2 \, dr = \int_{\mathbb{C}^\delta} W_j \left( \frac{r}{\varepsilon} \right) - E_{n,j}^\varepsilon \| \nabla_R u_{n,j}^\varepsilon (r) \|_{L^2(\mathbb{C}^\delta)}^2 \, dr
\]

\[
+ \int_{\mathbb{C}^\delta} \left( \nabla_R u_{n,j}^\varepsilon (r) \right) u_{n,j}^\varepsilon (r) \nabla \left[ E_{n,j}^\varepsilon - W_j \left( \frac{r}{\varepsilon} \right) \right] \, dr,
\]

for the last term we have

\[
\left\| \int_{\mathbb{C}^\delta} \left( \nabla_R u_{n,j}^\varepsilon (r) \right) u_{n,j}^\varepsilon (r) \nabla \left[ E_{n,j}^\varepsilon - W_j \left( \frac{r}{\varepsilon} \right) \right] \, dr \right\|^2 \leq \| \nabla u_{n,j}^\varepsilon \|_{L^2(\mathbb{C}^\delta)}^2 \left( \| \nabla E_{n,j}^\varepsilon \|_{L^\infty} + \| \nabla W_j \|_{L^\infty} \right)^2
\]

and we obtain

\[
\frac{\varepsilon^2}{2} \int_{\mathbb{C}^\delta} | \nabla_R u_{n,j}^\varepsilon (r) |^2 \, dr \leq \| \nabla u_{n,j}^\varepsilon \|_{L^2(\mathbb{C}^\delta)}^2 \left[ \varepsilon_n + \| W_j \|_{L^\infty} \left( \| \nabla E_{n,j}^\varepsilon \|_{L^\infty} + \| \nabla W_j \|_{L^\infty} \right) \right].
\]
Proceeding in the same way as for Eq. (95), we apply the interpolation operator and the previous estimation holds true when the discrete index $j$ is replaced by the continuous variable $R$.

**Lemma 5.7** For every $\epsilon > 0$, the operator $\epsilon \mathcal{S} + \epsilon^2 \mathcal{M}$ is relatively bounded in $\mathcal{E}^\epsilon$ by $\mathcal{E}$, with $\mathcal{E}$-bound less than 1.

**Proof:** The domain of the operators are readily defined

\[
D(\mathcal{S}) = \{ \varphi \in \mathcal{H}^1 \mid \mathcal{S}\varphi \in \mathcal{E}^0 \} \\
D(\mathcal{M}) = \{ \varphi \in \mathcal{H}^2 \mid \mathcal{M}\varphi \in \mathcal{E}^0 \}.
\]

Concerning $\mathcal{E}$ it is easy to verify

\[
D(\mathcal{E}) = \left\{ \varphi \in \mathcal{E}^0 \mid \sum_n \epsilon_n^2 \|\varphi_n\|^2_{L^2(\mathbb{R}^d)} < \infty \right\}.
\]

For every $\varphi \in \mathcal{E}^\epsilon$ we have

\[
\epsilon^2 \|\mathcal{S}\varphi\|^2_{\mathcal{E}^\epsilon} = \epsilon^4 \sum_n \int_{\mathbb{R}^d} \nabla_R \varphi \nabla_R \varphi \left[ \int_{C^n} \frac{u_n^\epsilon}{\epsilon} \left( \nabla_{r'} \zeta \right)(R, r') \right] \times \left( \nabla_{r''} \zeta \right)(R', r'') \ dr' \ dr'' \int_{R'=R''=R} dR
\]

\[
= \epsilon^4 \int_{\mathbb{R}^d} \int_{C^n} \left| \nabla_R \varphi \nabla_R \varphi \right|^2 \ dr \ dR.
\]

Where we defined $\zeta(R, r) = \sum_n \varphi_n(R) u_n^\epsilon(R, r)$. Furthermore,

\[
\|\zeta\|^2_{L^2(\mathbb{R}^d \times C^n)} \leq \sum_n \int_{\mathbb{R}^d} \left| \varphi_n(R) \right|^2 \ dR \int_{C^n} \left| u_n^\epsilon(R, r) \right|^2 \ dr = \|\varphi\|^2_{\mathcal{E}^\epsilon},
\]

where we used Eq. (18). By using the Lemma 3.2 and the Lemma 5.6, Eq. (100) gives

\[
\epsilon^2 \|\mathcal{S}\varphi\|^2_{\mathcal{E}^\epsilon} \leq \sum_n (C_0 + C_1 \epsilon_n) \epsilon^2 \|\varphi_n\|^2_{H^1(\mathbb{R}^d)} \leq \sum_n (C_0 + C_1 \epsilon_n) \|\varphi_n\|^2_{L^2(\mathbb{R}^d)}.
\]

Since $\epsilon_n$ is a growing sequence that goes to infinity, there exists a value $n_0 \in \mathbb{N}$ and a constant $c \leq 1$ such that $C \epsilon_n \leq c \epsilon_n^2$. Furthermore, let $\{g_n\} \in \ell^1$ be a positive sequence, we have

\[
C \sum_{n > n_0} \epsilon_n g_n \leq c \sum_{n > n_0} \epsilon_n^2 g_n
\]

and since $\sum_{n \leq n_0} \epsilon_n g_n \leq \epsilon_{n_0} \|g\|_{\ell^1}$, we have $C \sum_n \epsilon_n g_n \leq c \sum_n \epsilon_n^2 g_n + C_1 \|g\|_{\ell^1}$. By applying this inequality to $g_n = \|\varphi_n\|^2_{L^2(\mathbb{R}^d)}$ we obtain

\[
\epsilon^2 \|\mathcal{S}\varphi\|^2_{\mathcal{E}^\epsilon} \leq \epsilon \sum_n \epsilon_n^2 \|\varphi_n\|^2_{L^2(\mathbb{R}^d)} + C \|\varphi\|^2_{\mathcal{E}^\epsilon} \leq c \|\mathcal{E}\varphi\|^2_{\mathcal{E}^\epsilon} + C \|\varphi\|^2_{\mathcal{E}^\epsilon}.
\]
Concerning the operator \( \mathcal{N} \), few calculations give
\[
\| \mathcal{N} \varphi \|_{\mathcal{E}_\varepsilon}^2 = \frac{1}{4} \int_{\mathbb{R}^d} \left| \int_{\mathcal{C}_\varepsilon} |\Delta_R \zeta(R, r)\, dr |^2 \right. .
\] (102)
We obtain
\[
4\varepsilon^4 \left\| \mathcal{N} \varphi \right\|_{\mathcal{E}_\varepsilon}^2 \leq \varepsilon^4 \sup_{n \in \mathbb{N}} \| D^2 u_{n,j} \|_{L^2(\mathcal{C}_\varepsilon)}^2 \| \varphi \|_{\mathcal{E}_\varepsilon}^2 + \varepsilon^4 \sup_{n \in \mathbb{N}} \| D u_{n,j} \|_{L^2(\mathcal{C}_\varepsilon)}^2 \| \varphi \|_{\mathcal{E}_\varepsilon}^2 + \varepsilon^4 \| \varphi \|_{\mathcal{E}_\varepsilon}^2,
\]
\[
\leq C \| \varphi \|_{\mathcal{E}_\varepsilon}^2 .
\]
\[\square\]

By using standard arguments (see e.g. Ref. [12] for the details) the Lemma 5.7 ends the proof of the Theorem 4. The Stone’s Theorem ensures the existence of the group \( e^{-i/t} \mathcal{H}_{kp} \) for any \( \varepsilon > 0 \). In order to prove that also \( \frac{i}{\varepsilon} \mathcal{H} \mathcal{E}_{kp} + i \mathcal{E} \) generates group we need one more estimate.

**Lemma 5.8** Let \( \varphi \in \mathcal{H}^\kappa \) for some \( \kappa > 2 \). Then a constant \( C > 0 \) exists such that
\[
\| \mathcal{E} \varphi \|_{\mathcal{E}_0} \leq C \| \mathcal{E} \varphi \|_{\mathcal{H}_0} \| \varphi \|_{\mathcal{H}^\kappa}
\] (103)
and for \( \kappa = 2 \)
\[
\lim_{\varepsilon \to 0} \| \mathcal{E} \varphi \|_{\mathcal{E}_0} = 0 .
\] (104)

**Proof:** From the definition of \( \mathcal{E} \) and the Lemma 5.5 we have
\[
\mathcal{E} \varphi = \frac{\mathcal{E}^\kappa}{\varepsilon^2} \sum_{n,n'_{j,j'}} u_{n,n',j,j'} \delta^\varepsilon(R_j - r) \varphi_{n'_{j,j'}}(R_{j'}) ,
\] (105)
where
\[
u_{n,n',j,j'} = \sum_{j''} \mathcal{E}^\kappa \int_{\mathcal{C}_\varepsilon} \prod_{s = j,j',j''} \delta^\varepsilon(r' - R_s) \left[ W_{j''} \left( \frac{r'}{\varepsilon} \right) - W_{j'} \left( \frac{r'}{\varepsilon} \right) \right] \mu_{n,j''}(r') u_{n',j'}(r') \, dr'.
\] (106)
The pseudo-delta function \( \delta^\varepsilon \) belongs to the space \( C^\infty(\mathbb{R}^d) \). It is easy to see that the maximum of the function is in \( r = 0 \)
\[
\| \mathcal{E} \|_{\mathcal{C}} \delta^\varepsilon(0) = 1 .
\] (107)
With this and Eq. (6) we can estimate \( u \). We obtain
\[
|u|^2 \leq 2 \| W \|_{L^\infty(\mathbb{R}^d x \mathcal{C})}^2 .
\]
We have
\[
\| \mathcal{E} \varphi \|_{\mathcal{E}_0}^2 \leq 2 \| W \|_{L^\infty(\mathbb{R}^d x \mathcal{C})}^2 \sum_{n,n',j,j'} \frac{1}{\varepsilon^4} \int_{\mathcal{C}_\varepsilon} \left| \mathcal{E}^\kappa \right| \left( \frac{2\pi}{2\pi} \right)^d \int_{B_r} \sum_j e^{(R_j - r)k} \varphi_{n'_{j,j'}}(R_{j'}) \, dk \right|^2 \, dr
\]
\[
\leq 2 \| W \|_{L^\infty(\mathbb{R}^d x \mathcal{C})}^2 \| \mathcal{E} \|_{\mathcal{E}_0}^2 \| \varphi \|_{\mathcal{E}_0}^2 .
\] (108)
and
\[ \frac{1}{\varepsilon^4} \| \varphi^* \|_{E^0_{\varepsilon}}^2 = \sum_{n} \frac{1}{\varepsilon^4} \int_{|k| > \rho^e} |\tilde{\varphi}_n(k)|^2 \, dk \leq \varepsilon^{2(\kappa-2)} \sum_{n} \int_{|k| > \rho^e} |k|^{2\kappa} |\tilde{\varphi}_n(k)|^2 \, dk \leq \varepsilon^{2(\kappa-2)} \| \varphi \|_{H^{2\kappa}}^2. \tag{109} \]

This proves Eq. (103). The case \( \kappa = 2 \) is treated similarly and the previous equation gives
\[ \frac{1}{\varepsilon^4} \| \varphi^* \|_{E^0_{\varepsilon}}^2 \leq \sum_{n} \int_{|k| > \rho^e} (1 + |k|^2) |\tilde{\varphi}_{n'}(k)|^2 \, dk, \tag{110} \]
that in the limit \( \varepsilon \to 0 \) goes to zero for every \( H^2 \) function.

\[ \square \]

5.3 Study of \( \lim_{\varepsilon \to 0} 3^\varepsilon \)

Equation (108) ensures that \( \varepsilon^2 3^\varepsilon \) is relatively bounded in \( E^\varepsilon \) by \( C \), with \( C \)-bound less than 1. We write the solution of the kp system given in Eq. (88) by \( \varphi(t) = e^{-it[\frac{1}{2} \mathcal{H}_{kp} + 3^\varepsilon]} \varphi_0 \) where \( \varphi_0 \in E^0 \) denotes the initial datum for \( t = 0 \). The following lemma concerns the bound of the \( H^\kappa \)-norm of the solution.

Lemma 5.9 Let \( \varphi_0 \in H^{\kappa} \) for some \( \kappa \geq 2 \). There exists a constant \( C(\kappa) \geq 0 \) independent of \( \varepsilon \) such that
\[ \| \varphi(t) \|_{H^{\kappa}} \leq C(\kappa) t \| \varphi_0 \|_{H^{\kappa}}, \tag{111} \]
for all \( t \geq 0 \) where \( \varphi(t) \) is the solution of Eq. (88) with initial datum \( \varphi_0 \).

Proof: It is easy to verify that for any mild solution of Eq. (88) the following equation holds true [7]
\[ \partial_t^s \varphi(t) = G(t) \partial_t^s \varphi_0 + \frac{1}{\varepsilon^2} \int_0^t G(t-t') \left[ \partial_t^s, \mathcal{H}_{kp} + \varepsilon^2 3^\varepsilon \right] \varphi(t') \, dt', \]
where we denoted the evolution group by \( G(t) = e^{-it[\frac{1}{2} \mathcal{H}_{kp} + 3^\varepsilon]} \). Furthermore, the parenthesis denotes the commutator and the symbol \( \partial_t^s \) denotes the partial derivative of order \( s \) with respect the \( i \)-th axial direction: \( \partial_t^s \varphi(R) \equiv \frac{\partial^s \varphi}{\partial R_i^s} \) with \( 1 \leq i \leq d \) and \( R_i \) is \( i \)-th coordinate of \( R \). We have
\[ \| \partial_t^s \varphi(t) \|_{E^0_{\varepsilon}} \leq \| \partial_t^s \varphi_0 \|_{E^0_{\varepsilon}} + \frac{1}{\varepsilon^2} \int_0^t \| \left[ \partial_t^s, \mathcal{H}_{kp} + \varepsilon^2 3^\varepsilon \right] \varphi(t') \|_{E^0_{\varepsilon}} \, dt'. \]
From Eq. (105) we have
\[ \partial_t^s 3^\varepsilon \varphi = -\frac{|C|}{\varepsilon^2} \sum_{n', j, j'} u_{n, n', j, j'} \frac{\partial^s}{\partial R_j^s} \delta^\varepsilon(R_j - R) \varphi^s_{n'}(R_{j'}) \]
\[ = \frac{|C|}{\varepsilon^2} \sum_{n', j, j'} \left[ D_{(i-ki), n, n', j, j'} \right] \delta^\varepsilon(R_j - R) \varphi^s_{n'}(R_{j'}) \]
and
\[ [\partial^*_\varepsilon, \mathcal{F}] \varphi = \frac{|C^\varepsilon|}{\varepsilon^2} \sum_{n',j,j'} \left( [D_{(i_k)^*}]_{j}^{[u_{n,n',\alpha,j'}]} - [D_{(i_k)^*}]_{j'}^{[u_{n,n',\alpha,j}]} \right) \delta^\varepsilon (R_j - R) \varphi_{n'} (R_{j'}), \]
where we used Eq. (37). Proceeding as in Lemma 5.8, we obtain the following estimate for the commutator
\[ \| [\partial^*_\varepsilon, \mathcal{F}] \varphi (t) \|_{\mathcal{E}_0^s} \leq 2 \| W \|_{L^2 (H^s (\mathbb{R}^d, C^s))} \sup_n \int_{\mathbb{R}^d} \| \partial^s_{\varepsilon} u_n (R, r) \|^2 \, dr \, dR \| \varphi (t) \|_{\mathcal{H}^2} \leq C \| \varphi (t) \|_{\mathcal{H}^2}. \] (112)

The estimation of the commutator containing the kp Hamiltonian proceed in a more standard way. We have three terms (see Eqs. (91)-(92)). In order to illustrate the procedure, we consider the first order term \( \partial \varphi \). After few calculations, we obtain
\[ \varepsilon^{-1} [\partial^*_\varepsilon, \mathfrak{S}] \varphi = \sum_{r=1}^{s} \sum_{n'} \left( \mathcal{D}_{\varepsilon} \left[ \mathcal{D}_{[S_{n,n',j}]_{j}} \right] \varphi_{n'} + \left[ \mathcal{D}_{[S_{n,n',j}]_{j}} \right] \varphi_{n'} + \left[ \mathcal{D}_{[S_{n,n',j}]_{j}} \right] \varphi_{n'} \right) \]
where we used Eq. (37). Proceeding as in Lemma 5.8, we obtain the following estimate for the commutator
\[ \| [\partial^*_\varepsilon, \mathfrak{S}] \varphi (t) \|_{\mathcal{E}_0^s} \leq C \| \varphi (t) \|_{\mathcal{H}^2}. \] (113)

This expression shows that \( \varepsilon^{-1} [\partial^*_\varepsilon, \mathfrak{S}] \) is bounded by the \( \mathcal{H}^s \) norm of \( \varphi \). Collecting all the results, we have
\[ \| [\partial^*_\varepsilon, \mathfrak{S}] \varphi (t) \|_{\mathcal{E}_0^s} \leq C \| \varphi_0 \|_{\mathcal{E}_0^s} + C \int_0^t \left( \| \varphi (t') \|_{\mathcal{H}^s} + \| \varphi (t') \|_{\mathcal{H}^2} \right) \, dt'. \]

The application of the Gronwall’s Lemma provides Eq. (111). \( \square \)

With the following theorem, we show that the term \( \mathcal{F} \) can be neglected in the homogenization limit

**Theorem 5** Let \( \varphi \) be solution of Eq. (88) with initial data \( \varphi_0 \in \mathcal{H}^\kappa \) for some \( \kappa > 2 \). Then for all \( t \leq T \),
\[ \lim_{\varepsilon \to 0} \| \varphi (t) - \eta (t) \|_{\mathcal{E}_0^s} = 0, \] (114)
where \( \eta \) is the solution of Eq. (88) for \( \mathcal{F} \equiv 0 \) and initial data \( \varphi_0 \).

**Proof:** We write the solution \( \varphi \) as
\[ \varphi (t) = \mathcal{G}_0 (t) \varphi_0 + \int_0^t \mathcal{G}_0 (t-s) \mathcal{F} [\varphi (s)] \, ds, \] (115)
where \( \mathcal{G}_0 (t) \) denotes unitary the group generated by \( e^{-i \frac{t}{\varepsilon} \mathcal{H}_\varphi} \). It is sufficient to show that
\[ \lim_{\varepsilon \to 0} \| \varphi (t) - \eta (t) \|_{\mathcal{E}_0^s} = \left\| \int_0^t \mathcal{G}_0 (t-s) \mathcal{F} [\varphi (s)] \, ds \right\|_{\mathcal{E}_0^s} \] (116)
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is zero. It follows directly from Lemma 5.8 and Lemma 5.9
\[
\left\| \int_0^t \mathcal{G}_0(t - s) \mathfrak{P}(s) \right\|_{L^2} \leq \int_0^t \| \mathfrak{P}(s) \|_{L^2} \, ds \leq C \varepsilon^{k-2} \int_0^t \| \mathfrak{P}(s) \|_{\mathcal{H}^n} \, ds \\
\leq C_1 (e^{Ct} - 1) \varepsilon^{k-2} \| \varphi_0 \|_{\mathcal{H}^n}.
\]

A Completeness and orthogonality of the LKF basis

Before to address the study of the completeness of the Luttinger-Kohn-Foreman basis set, we give some formal results that concern the projection procedure used in the kp approach. These results are useful for the computation and we limit ourselves to give the formal expressions without addressing to the rigorous convergence of the series (the rigorous results are the Theorems 2 and 3, whose proof is given at the end of this Appendix). We consider a class of basis sets of \(L^2(\mathbb{R}^d)\) that contains the Luttinger-Kohn-Foreman basis as a particular case. We assume that the set of functions \(\{ \phi_j^e \in \mathcal{E}_c^e \mid j \in \mathbb{Z}^d \}\) has the following properties of completeness and orthonormality in the Fourier space

\[
\sum_j \overline{\phi_j^e} (k) \phi_j^e (k') = \delta (k - k') \mathbb{1}_{B^e} (k) \tag{117}
\]

\[
|\mathcal{E}^e| \left\| \int_{B^e} \phi_j^e (k) \overline{\phi_j^e} (k') \, dk' \right\| = \delta_{j,j'}^K. \tag{118}
\]

It is easy to verify that as a particular case we have \(f_j^e (r) = \delta^e (R_j - r)\). From Eq. (117) it follows that for all \(R, R' \in \mathcal{L}^e\)

\[
\sum_j f_j^e (r - R) \overline{f_j^e} (r - R') = \sum_j \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \phi_j^e (k) \overline{\phi_j^e} (k') \mathbb{1}_{B^e} (k) e^{i (r - R' - R) \cdot k} \, dk' \, dk \\
= \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \mathbb{1}_{B^e} (k) e^{-i (R - R') \cdot k} \, dk = \delta_{R,R'}^K. \tag{119}
\]

We recall here some elementary spectral properties based on the \(\mathcal{L}\)-periodicity. Let’s \(g \in L^2(\mathcal{E}^e)\) and \(\mathcal{L}^e\)-periodic \(g (r + R) = g (r)\) for all \(R \in \mathcal{L}^e\). The Fourier expansion of \(g\) is given by

\[
g (r) = \frac{1}{|\mathcal{E}^e|^{1/2}} \sum_{G \in \mathcal{L}^*} \hat{g} (G) \, e^{i r G}, \tag{120}
\]

where the Fourier coefficients are

\[
\hat{g} (G) = \frac{1}{|\mathcal{E}^e|^{1/2}} \int_{\mathcal{E}^e} g (r) \, e^{-i r \cdot G} \, dr. \tag{121}
\]

We remind that \(\mathcal{E}^e\) is the Wigner-Seitz cell (with volume \(|\mathcal{E}^e| = \varepsilon^d |\mathcal{C}|\)) of the \(\varepsilon\)-scaled crystal and \(\mathcal{L}^*\) denotes the reciprocal lattice. Concerning the periodic function \(g\), we can also address
the Fourier transform in the distributional sense. The formal expansion gives

$$\hat{g}(k) = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} g(r) e^{-ir\cdot k} \, dr = \frac{(2\pi)^{d/2}}{|C^\varepsilon|^{1/2}} \sum_{G \in \mathbb{L}^\varepsilon^*} \hat{g}(G) \delta(G - k),$$  \hspace{1cm} (122)

where we used Eq. (120). Moreover, by taking a partition of the space $\mathbb{R}^d$ in $C^\varepsilon$ cells, we have

$$\hat{g}(k) = \frac{1}{(2\pi)^{d/2}} \sum_{R \in \mathbb{L}^\varepsilon} \int_{C^\varepsilon(R)} g(r) e^{-ir\cdot k} \, dr = \frac{|C^\varepsilon|^{1/2}}{(2\pi)^{d/2}} \sum_{R \in \mathbb{L}^\varepsilon} e^{iR\cdot k} \hat{g}(k).$$  \hspace{1cm} (123)

Together with Eq. (122) we obtain the following equation

$$|C^\varepsilon| \sum_{R \in \mathbb{L}^\varepsilon} e^{iR\cdot k} \hat{g}(k) = (2\pi)^d \sum_{G \in \mathbb{L}^\varepsilon^*} \hat{g}(G) \delta(G - k).$$  \hspace{1cm} (124)

If $g_i$ denote a set of complete orthonormal $L^2(C^\varepsilon)$-periodic functions of $L^2(C^\varepsilon)$,

$$\int_{C^\varepsilon} g_i(r) g_j(r) \, dr = \delta^K_{i,j},$$  \hspace{1cm} (125)

$$\sum_j \overline{g}_j(G) \hat{g}_j(G') = \delta^K_{G,G'}. \hspace{1cm} (126)$$

We have

$$\sum_j \overline{g}_j(r) g_j(r') = \frac{1}{|C^\varepsilon|} \sum_{G,G' \in \mathbb{L}^\varepsilon^*} e^{iG'\cdot r - iG\cdot r} \sum_j \overline{g}_j(G) \hat{g}_j(G') = \frac{1}{|C^\varepsilon|} \sum_{G \in \mathbb{L}^\varepsilon^*} e^{i(r' - r)\cdot G} = \sum_{R \in \mathbb{L}^\varepsilon} \delta(R - r' + r).$$  \hspace{1cm} (127)

In particular, concerning the Fourier coefficients of the Bloch functions $u_{n,j}(r)$ the previous equations become

$$\sum_{G \in \mathbb{L}^\varepsilon^*} \overline{u}_{n,j}^\varepsilon(G) u_{n',j}^\varepsilon(G) = \delta^K_{n,n'},$$  \hspace{1cm} (128)

$$\sum_n u_{n,j}^\varepsilon(r) u_{n,j}^\varepsilon(r') = \sum_{R \in \mathbb{L}^\varepsilon} \delta(R - r' + r).$$  \hspace{1cm} (129)

By using the previous equations we can verify the formal completeness of the basis set $\chi_{j,n}^\varepsilon(r) = f_j^\varepsilon u_{n,j}^\varepsilon$

$$\sum_{n,j} \overline{\chi}_{j,n}^\varepsilon(r) \chi_{j,n}^\varepsilon(r') = \sum_j f_j^\varepsilon(r) f_j^\varepsilon(r') \sum_{R \in \mathbb{L}^\varepsilon} \delta(R - r' + r).$$  \hspace{1cm} (130)
The completeness follows from Eq. (119). The verification of the orthogonality proceed straightforwardly

\[ \int_{\mathbb{R}^d} \overline{\chi(r)} \chi'(r) \, dr = \frac{|C'|}{(2\pi)^{2d}} \sum_{G,G' \in \mathcal{L}^*} \int_{\mathbb{R}^d} e^{-iR_{ij} \cdot (k' - k)} \mathbb{I}_{B^e}(k') \mathbb{I}_{B^e}(k) \frac{\overline{u}_{n,j}(G') \hat{u}_{n',j'}(G)}{u_{n,j}(G) \hat{u}_{n',j'}(G)} e^{iR_{ij} \cdot (G + k' - k - G')} \, dr \, dk' \, dk \]

\[ = \frac{|C'|}{(2\pi)^d} \sum_{G,G' \in \mathcal{L}^*} \int_{\mathbb{R}^d} \mathbb{I}_{B^e}(k') \mathbb{I}_{B^e}(G - G' + k') \frac{\overline{u}_{n,j}(G') \hat{u}_{n',j'}(G)}{u_{n,j}(G) \hat{u}_{n',j'}(G)} \, dk' \]

\[ = \frac{|C'|}{(2\pi)^d} \int_{\mathbb{R}^d} \mathbb{I}_{B^e}(k') \sum_{G,G' \in \mathcal{L}^*} \delta^K_{G,G'} \frac{\overline{u}_{n,j}(G') \hat{u}_{n',j'}(G)}{u_{n,j}(G) \hat{u}_{n',j'}(G)} \, dk' \]

\[ = \delta^K_{j,j'} \frac{\sum_{G \in \mathcal{L}^*} \overline{u}_{n,j}(G) \hat{u}_{n',j'}(G)}{u_{n,j}(G) \hat{u}_{n',j'}(G)} = \delta^K_{n,n'} \delta^K_{j,j'}, \quad (131) \]

where we used \( \mathbb{I}_{B^e}(G + k') = \mathbb{I}_{B^e}(k') \delta^K_{G,0} \) and Eq. (128).

We address here to the decomposition of the wave function \( \psi \) on the Luttinger-Kohn-Foreman basis in a more rigorous way and we prove the Theorem 2 and 3.

**Proof of Theorem 2:** For any \( \psi \in \mathcal{S} \), where \( \mathcal{S} \) denotes the Schwartz’s space, we have

\[ \psi = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \tilde{\psi}(k)e^{-i\mathbf{k} \cdot \mathbf{r}} \, dk = \frac{1}{(2\pi)^{d/2}} \sum_{G \in \mathcal{L}^*} e^{i\mathbf{r} \cdot \mathbf{G}} \int_{B^e} \tilde{\psi}(k + \mathbf{G}) e^{-i\mathbf{k} \cdot \mathbf{r}} \, dk. \]

The function

\[ g(\mathbf{r}, \mathbf{s}) = \sum_{G \in \mathcal{L}^*} e^{i\mathbf{r} \cdot \mathbf{G}} f_G(\mathbf{s}) \]

with

\[ f_G(\mathbf{s}) = \frac{1}{(2\pi)^{d/2}} \int_{B^e} \tilde{\psi}(k + \mathbf{G}) e^{i\mathbf{s} \cdot \mathbf{k}} \, dk \]

is in \( L^2(C^e, \mathbb{R}^d) \). In particular, \( g(\mathbf{r}, \mathbf{r}) = \psi(\mathbf{r}) \). We have

\[ \int_{C^e} |g(\mathbf{r}, \mathbf{s})|^2 \, d\mathbf{r} = \sum_{G \in \mathcal{L}^*} |f_G(\mathbf{s})|^2 = \frac{1}{(2\pi)^d} \sum_{G \in \mathcal{L}^*} \left| \int_{C^e} \tilde{\psi}(k + \mathbf{G}) e^{i\mathbf{s} \cdot \mathbf{k}} \, dk \right|^2 \]

\[ = \frac{1}{(2\pi)^d} e^{-i\mathbf{s} \cdot \mathbf{G}} \int_{\mathbb{R}^d} \tilde{\psi}(k) e^{i\mathbf{s} \cdot \mathbf{k}} \, dk = |\psi(\mathbf{s})|^2 \]

and \( \|g\|_{L^2(C^e, \mathbb{R}^d)} = \|\psi\|_{L^2(\mathbb{R}^d)} \). We consider

\[ g(\mathbf{r}, \mathbf{s}) = \frac{1}{(2\pi)^{d/2}} \sum_{G \in \mathcal{L}^*} e^{i\mathbf{r} \cdot \mathbf{G}} \int_{B^e} \tilde{\psi}(k + \mathbf{G}) e^{i\mathbf{s} \cdot \mathbf{k}} \, dk \]

\[ = \sum_{\mathbf{R}_i \in \mathcal{L}^*} \frac{1}{|B^e|} \frac{1}{(2\pi)^{d/2}} \int_{B^e} e^{i(s - \mathbf{R}_i) \cdot \mathbf{k}} \, dk' \int_{B^e} e^{i\mathbf{R}_i \cdot \mathbf{k}} \sum_{G \in \mathcal{L}^*} e^{i\mathbf{r} \cdot \mathbf{G}} \tilde{\psi}(k + \mathbf{G}) \, dk 
\]

\[ = \sum_{\mathbf{R}_i \in \mathcal{L}^*} (2\pi)^{d/2} \frac{1}{|B^e|} \delta^e(s - \mathbf{R}_i) \int_{B^e} e^{i\mathbf{R}_i \cdot \mathbf{r}} \sum_{G \in \mathcal{L}^*} e^{i\mathbf{r} \cdot \mathbf{G}} \tilde{\psi}(k + \mathbf{G}) \, dk, \]

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where we used that for all \( g \in L^2(\mathbb{R}^d) \)
\[
\int_{B^e} e^{i s \cdot k} \tilde{g}(k) \, dk = \frac{1}{|B^e|} \int_{B^e} \int_{B^e} \sum_{R_i \in L^e} e^{i s \cdot k} e^{i R_i \cdot (k-k')} \tilde{g}(k) \, dk \, dk'.
\]

Since the function \( \zeta(k) = \sum_{G \in L^e} e^{i R \cdot G} \tilde{\psi}(k + G) \) is \( L^e \)-periodic and the set \( \{ u_{n,j} | n \in \mathbb{N} \} \) is an orthonormal basis of \( L^2(\mathbb{C}^e) \) for all \( j \in \mathbb{Z}^d \), we take the expansion \( \zeta(k) = \sum_{n} u_{j,n}(r) \langle \zeta_k, u_{j,n} \rangle_{L^2(\mathbb{C}^e)} \) where the parenthesis denotes the internal product. We obtain
\[
g(r, s) = \sum_n \sum_{R_i \in L^e} \frac{(2\pi)^d/2}{|B^e|} u_{i,n}(r) \delta^e(s - R_i) \int_{B^e} e^{i R_i \cdot k} \int_{\mathbb{C}^e} \sum_{G \in L^e} \tilde{u}_{i,n}(r') e^{i R_i \cdot G} \tilde{\psi}(k + G) \, dk \, dr'.
\]

We note that for every function \( \zeta \in L^2(\mathbb{R}^d) \) the identity operator can be written as
\[
\zeta(k + G) = (\mathcal{F} \mathcal{F}^{-1} \zeta) (k + G) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} e^{-i r \cdot (k+G) - k'} \zeta(k') \, dr \, dk'.
\]

We obtain
\[
g(r, s) = \frac{1}{|B^e|} \sum_n \sum_{R_i \in L^e} u_{i,n}(r) \delta^e(s - R_i)
\]
\[
\times \int_{\mathbb{R}^d} \int_{B^e} e^{i R_i \cdot k} \, dk \int_{\mathbb{C}^e} \sum_{G \in L^e} u_{i,n}(r') e^{i r' \cdot G} \, dr' \sum_{G' \in L^e} e^{-i r \cdot (G + G')} \tilde{\psi}(k' + G') \, dk' \, dr''
\]
\[
= \sum_n \sum_{R_i \in L^e} \frac{(2\pi)^d/|C^e|}{|B^e|} u_{i,n}(r) \delta^e(s - R_i) \int_{\mathbb{R}^d} \delta^e(r' - R_i) u_{i,n}(r') \psi(r') \, dr'
\]
\[
= \sum_{n,i} |C^e| u_{i,n}(r) \delta^e(s - R_i) \langle \chi^e_{i,n}, \psi \rangle_{L^2(\mathbb{R}^d)}
\]

and for \( s = r \) we have Eq. (53). In conclusion,
\[
\psi(r) = \sum_{n,i} \chi^e_{i,n}(r) \langle \chi^e_{i,n}, \psi \rangle_{L^2(\mathbb{R}^d)}
\]

and the envelope functions are \( \varphi_{n,j} = |C^e|^{-1/2} \langle \chi^e_{i,n}, \psi \rangle_{L^2(\mathbb{R}^d)} \). Moreover,
\[
\| \psi \|^2_{L^2(\mathbb{R}^d)} = \sum_{n,i} \| \chi^e_{i,n} \|^2_{L^2(\mathbb{R}^d)} \left| \langle \chi^e_{i,n}, \psi \rangle_{L^2(\mathbb{R}^d)} \right|^2
\]
\[
\| \varphi \|^2_{L^2(\mathbb{R}^d)} = \sum_{n,i} \| \varphi_{n,j} \|^2 = \| \psi \|^2_{L^2(\mathbb{R}^d)}.
\]

We proved Eq. (53) for Schwartz functions. By using standard arguments based on the density of \( \mathcal{S} \) in \( L^2(\mathbb{R}^d) \), we have that Eq. (133) is true also for \( L^2(\mathbb{R}^d) \) functions.
Finally, we study the convergence of the envelope functions toward the density of particles around an atomic site.

**Proof of the Theorem 3:** From the definition of the envelope functions we have

$$\frac{1}{|C^e|} \sum_n |\varphi_{n,j}|^2 = \sum_n \int_{\mathbb{R}^d} \overline{u_{n,j}^\varepsilon(r)} u_{n,j}^\varepsilon(r) \delta^\varepsilon(r - R_j) \delta^\varepsilon(r' - R_j) \psi(r) \psi(r') \, dr \, dr'. $$

From the definition of the pseudo-Dirac function we obtain

$$\frac{1}{|C^e|} \sum_n |\varphi_{n,j}|^2 = \frac{1}{(2\pi)^d} \sum_n \int_{\mathbb{R}^d} \overline{\psi(r)} u_{n,j}^\varepsilon(r) \delta^\varepsilon(r - R_j) \, dr \times \int_{B^e} \sum_{R \in \mathcal{L}^e} \int_{C^e} \overline{u_{n,j}^\varepsilon(r')} e^{i(R - R_j \cdot k)} \psi(r' + R) \, dk \, dr' \times \int_{B^e} e^{i(R - R_j \cdot k)} \sum_n u_{n,j}^\varepsilon(r) \langle u_{n,j}^\varepsilon, \psi(r' + R) \rangle_{L^2(C^e)} \, dk \, dr', $$

by using that the $u_{n,j}$ are a basis set of $L^2(C^e)$ we have

$$\frac{1}{|C^e|} \sum_n |\varphi_{n,j}|^2 = \sum_{R \in \mathcal{L}^e} \int_{\mathbb{R}^d} \overline{g_j(r)} g_j(r + R) \, dr = \sum_{R \in \mathcal{L}^e} \int_{\mathbb{R}^d} \overline{g_j(r)} \psi(r) \, dr = |g_j|^2 = \left( \int_{B^e} |\psi(r)|^2 \right)^2.$$

where we defined $g_j(r) = \delta^\varepsilon(r - R_j) \psi(r)$ and we have $\|g_j\|_{L^2(\mathbb{R}^d)} \leq |B^e|^{1/2} \|\psi\|_{L^2(\mathbb{R}^d)}$. Furthermore, we defined

$$\mathcal{J} = \sum_{R \in \mathcal{L}^e} \int_{B^e} |\overline{g}(k)|^2 e^{ikR} \mathbb{1}_{B^e}(k) \, dk = |B^e| \int_{B^e} |\overline{g}(0)|^2 = \frac{1}{|C^e|} \left( \int_{B^e} |\delta^\varepsilon(r - R_j) \psi(r) \, dr \right)^2,$$

and

$$\mathcal{R} = \sum_{R \in \mathcal{L}^e} \int_{B^e} |\overline{g}(k)|^2 e^{ikR} (1 - \mathbb{1}_{B^e}) \, dk.$$
Consequently, the $\varphi_{j,n}$ converges toward a continuous function and we have
\[
\lim_{\varepsilon \to 0} \sup_{R_j \in \mathbb{C}, |R_j - R| < |\mathbb{C}|} \left( |\varphi_{n,j}|^2 - |\varphi_n(R)|^2 \right) = 0.
\]
\[\square\]

References


