Asymptotic expansion of wave scattering in a periodic 2d-plane

Vincent Lescarret

Asymptotic expansion of wave scattering in a periodic 2d-plane*

Vincent Lescarret†

Université Paris Saclay,
Fédération de mathématiques de Centralesupelec, CNRS FR3487

March 29, 2024

Abstract

We give a counter part of Sommerfeld outging radiation condition for waves propagating in a 2d periodic medium under generical assumptions and provide a uniqueness theorem for outgoing solutions.

1 Introduction

Asymptotics of the outgoing Green function for the Helmholtz equation with periodic coefficients has been given in [19] for frequencies lying in the first spectral band in any dimensions. We propose to extend the formula in the 2d case to any frequency except for a set of isolated frequencies. Part of this work reproduces the work [24] which the author just became aware by the time of submission of this present work. Despite redundance of some ideas this work adresses many other points and partly lies on [8].

We wish to solve the Helmholtz equation

$$\operatorname{div}(\alpha\nabla u) + k^2\beta u = f \quad \text{in } \mathbb{R}^2 \tag{1}$$

where $f \in L^2(\mathbb{R}^2)$ is compactly supported, k real positive and $\alpha, \beta > 0$. The coefficients α and β are bounded functions, periodic with common period. Let $W = [0, 2\pi]^2$ be a periodicity cell (Wigner-Seitz cell) and $B = [0, 1]^2$ the fundamental periodicity cell of the reciprocical lattice (Brillouin zone).

*The following article has been submitted to AIP Journal of mathematical physics. After publication if any, it would be found at `https://publishing.aip.org/resources/librarians/products/journals/`

†vincent.lescarret@centralesupelec.fr

We look for a formula for u by the mean of the absorption principle as in [19, 21]. A general formula has been given in [21], Theorem 3.31 expressing $u = u_1 + u_2 + r$ where $r \in L^2(\mathbb{R}^2)$, $u_j \in L^2_{loc}$ for $j \in \{1, 2\}$. Then u_1 is a residu while u_2 is a principal Cauchy value. In Remark 3.33 of [21] the author says that u_1 is the leading term and that u_2 is a corrector in some L^p space but Lemma 2.4 of [19] shows that this is wrong. Loosely speaking the term u_2 removes the terms in u_1 which correspond to "incoming" waves and thus $u_1 + u_2$ only keeps "outgoing" waves (see [7] for the idea in the case of a periodic waveguide).

Our calculations closely follow those of [19] (which are based on the method used in the homogeneous (non periodic) case as for instance in Melrose [16] paragraph 1.7) but with two differences. First instead of proving an analogue of Lemma 2.4 of [19] we just use Cauchy residu formula and thus deal with contour complex deformation as in [9, 8]. Then contrary to [19] we consider any k^2 above the bottom of the essential spectrum of $P = -\frac{1}{\beta}\mathrm{div}(\alpha\nabla)$. In [19], k^2 lies on the first band and is close enough to the bottom of the essential spectrum of P so that the level set on the first band is a single smooth cycle (loop). Here generally several bands meet the level k^2 and one requires a refined analysis of the geometry of the level set. Of course ideas are known for a long time in crystallography and in elasticity where level sets are called slowness surfaces (in 3d). See for instance [28, 3].

Before stating the main result let us start with a formal calculation and introduce the main notations.

Let $\varepsilon > 0$ and replace k^2 in (1) by $k_\varepsilon^2 := k^2 + i\varepsilon$. Then applying the Bloch transform:

$$\hat{u}(x, \ell) = \sum_{j \in \mathbb{Z}^2} u(x + 2\pi j) e^{-i\ell\cdot(x+2\pi j)}$$

to equation (1) and using the commutational property of the Bloch transform (see [2]) we get

$$(\mathrm{div} + i\ell\cdot)\,(\alpha(\nabla + i\ell)\hat{u}) + k_\varepsilon^2 \beta \hat{u} = \hat{f} \quad \text{in } W,$$

together with periodic boundary conditions on W. When α is piecewise continuous the underlying operator $P(\ell) := -\beta^{-1}(\mathrm{div} + i\ell)\alpha(\nabla + i\ell)$ is defined as the m-sectorial operator (see [12]) associated to the sectorial sesquilinear form

$$\int_W \alpha(\nabla + i\ell)u(\nabla - i\ell)\bar{v}dx \quad \text{on}$$
$$H^1_{per}(W) = \{v \in H^1(W, \beta dx), \text{ with periodic boundary conditions on } \partial W\}$$

We readily see that $P(\ell)$ is symmetric: $P(\ell)^* = P(\bar{\ell})$ and it is well-known [22] that it has a discrete spectrum which we denote by $\{\lambda_n(\ell)\}_{n>0}$ (counting multiplicity) with $\lambda_n(\ell)$ real for real ℓ and we denote by $e_n(\ell)$ the corresponding eigenvectors. Since $P(\ell)$ is defined through a sesquilinear form the family $P(\ell)$ is analytic of type B (see [12], § 4.2, p.393) thus the functions $\ell \to \lambda_n(\ell)$ are piecewise analytic and continuous on $\mathbb{C}^2$. Besides, the Bloch variety

$$\mathcal{B} = \{(\ell, \lambda) \in \mathbb{C}^3 \text{ such that } \exists n,\ \lambda_n(\ell) = \lambda\}$$

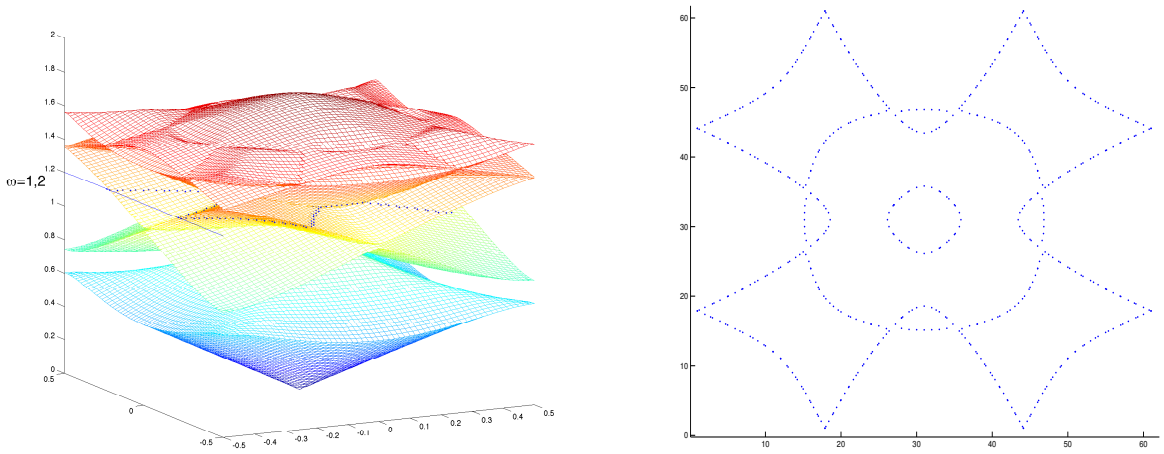

Figure 1: Bloch variety (left) and Fermi level $F^0_{k^2}$ (right) with $k = 1.2$ for $\alpha = 1 + 0.8\cos(x)\cos(y)$ and $\beta = 1$.

is an analytic set because it is the null set of a regularized determinant which is an entire function, see Appendix B where we recall and adapt [13] in this more general setting. See Figure 1 illustrating the Bloch variety.

Expanding the solution in the Hilbert basis $\{e_n\}_{n>0}$ one has

$$u_\varepsilon(x) = \int_B e^{i\ell\cdot x} \sum_{n\in\mathbb{N}^*} \frac{(\hat{f}, e_n(\ell))_{L^2(W)}}{k_\varepsilon^2 - \lambda_n(\ell)} e_n(x,\ell) d\ell. \tag{2}$$

Only a finite number of terms in the sum have singular limit when ε goes to zero. We thus set

$$J_k = \{n,\ \exists \ell \in B,\ \lambda_n(\ell) = k^2\}. \tag{3}$$

Let us introduce the main following geometrical objects:

- For complex λ let us set

$$\mathcal{F}_\lambda = \{\ell \in \mathbb{C}^2, \exists n, \lambda_n(\ell) = \lambda\} = \bigcup_{n>0} \lambda_n^{-1}(\lambda).$$

  which we refer to as the (complex) λ-Fermi level.

- For $\lambda > 0$ we denote by F_λ the set $\mathcal{F}_\lambda \cap \mathbb{R}^2$ which is periodic with B a periodicity cell.

- For $\lambda > 0$ we put $F^0_\lambda = F_\lambda \cap B$.

We give an example of $F^0_{k^2}$ in Figure 1. With these notations we see that the terms in formula (2) whose index belong to J_k are singular on $F^0_{k^2}$ for $\varepsilon = 0$. As in [16, 9] our aim to handle those singular terms is to move B to $\mathbb{C}^2$ (actually a subset of B which is a tubular neighborhood of $F^0_{k^2}$) and use the residu formula. So we need to find a complex deformation of B avoiding the complex Fermi level

$\mathcal{F}_{k^2_\varepsilon}$. To do so we describe a tubular neighborhood of $F^0_{k^2}$ as a union of level sets. These level sets are first indexed by λ in a small open intervall I containing k^2. Then we deform I to a complex curve avoiding k^2_ε.

This procedure can be done for all k^2 except for the critical values of the band functions λ_n and a subset of points of multiple eigenvalues (band crossing) which we call the set of *singular crossing points* (see section 3.1, definition 3.4). The latter set is defined as the complementary set of *regular crossing points* characterized by the fact that up to index relabelling, the (two or more) functions λ_j can be continued analytically through the crossing. In the 1d real case band crossings are regular thanks to Rellich eigenvalue relabelling theorem [23]. In the several dimensional real case this is true [14] except for singular crossing points. We thus exclude the following sets

- the set σ_0 of real critical values of the family $\{\lambda_n\}$,
- the set $\sigma_1 = \{\lambda \in \mathbb{R},\ \exists \ell \in B \mid (\ell, \lambda) \text{ is a singular crossing point}\}$.

That those sets are made of isolated points is a consequence of the stratified structure of the Bloch manifold and the dimension 2 (see Section 3.1).

The set σ_0 is called the set of "Landau resonences" in [8] where it is shown to be made of isolated points. In [8] an other set denoted by σ_∞ is also avoided but it matters only when one considers the global holomorphic extention of the resolvent operator $(P - zI)^{-1}$ from $\mathrm{Im} z > 0$ to a complex neighborhood of $\mathbb{R}$ as an operator from L^2_{comp} to L^2_{loc}. In this paper we are not concerned with σ_∞ since we consider the resolvent in a small neighborhood of $\mathbb{R}$ only. It is shown in [8] that any point of σ_0 is a branch point for the resolvent associated to the equation (1). See section 7.2 where we recall the related expression of the resolvent in the neighborhood of σ_0 in this 2d case. Let us remark that [8] does not address the issue of the assymptotic expansion of the resolvent but only its regularity (holomorphy).

A direct consequence of [14], Theorem 6.7 is that σ_1 is a set of isolated points of the real Bloch variety and the tangent set of such a point is a (non-isotropic) cone which is not a cusp. This is typically the case of Dirac cone [26]. Let us already say that the subsequent analysis takes advantage of the fact that this set is made of isolated points and thus one needs to implement a missing step to deal with higher dimensions where points of σ_1 are generically non isolated.

2 Main results

Our first result is a generic formula for the leading part of the limit of u_ε as ε goes to zero. Generically $F^0_{k^2}$ is 1-dimensional or void. We address the former case (the latter is already well-known and scattering does not take place). The formula we get is an integral on $F^0_{k^2}$ corresponding to the limit of the residu of the expression (2). The expression involves the spectral projector of $P(\ell)$ which is in general position one dimensional and given by $(\hat{f}, e_n(\ell))_{L^2(W)} e_n(x, \ell)$ for $\ell \in \lambda_n^{-1}(k^2)$. This expression is false when $\lambda_n(\ell)$ is multiple.

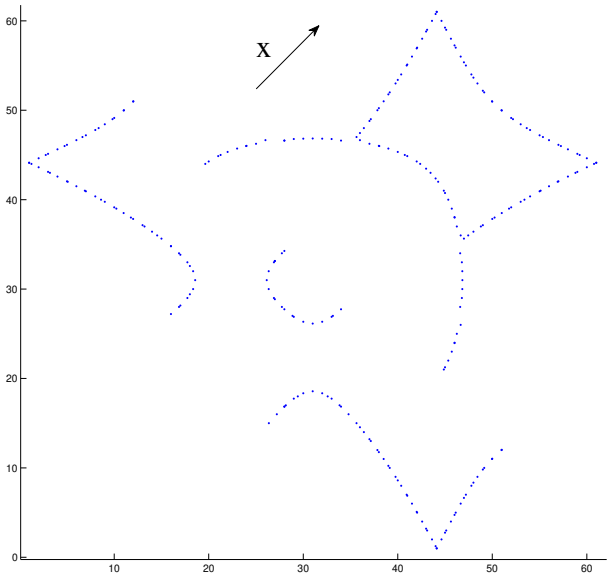

Figure 2: The set $F^+_{k^2}(x)$ with $x = (1, 1)$ and α, k as in Figure 1.

In general position the set $\mathcal{C}_{k^2}$ of points in $F^0_{k^2}$ at which two or more bands cross is generically finite. Thus for $\ell \in F^0_{k^2} \backslash \mathcal{C}_{k^2}$ there is a unique integer $n \in J_k$ such that $\ell \in \lambda_n^{-1}(k^2)$ hence one can define the following two functions a.e. in $F^0_{k^2}$

$$\tilde{\lambda}(\ell) := \lambda_n(\ell) \quad \text{and} \quad \tilde{e}(\ell) := e_n(\ell). \tag{4}$$

Our first result is

Theorem 2.1. *Let k be such that $k^2 \notin \sigma_0 \cup \sigma_1$ in general position. Let*

$$F^+_{k^2}(x) = \{\ell \in F^0_{k^2} \backslash \mathcal{C}_{k^2},\ \nabla \tilde{\lambda}(\ell) \cdot x > 0\}.$$

Then u_ε converges to u in H^1_{loc} expanding

$$u(x) = 2i\pi \int_{F^+_{k^2}(x)} e^{i\ell \cdot x} \frac{(\hat{f}(\ell), \tilde{e}(\ell))_{L^2(W)}}{\|\nabla \tilde{\lambda}(\ell)\|} \tilde{e}(x, \ell) \sigma(d\ell) + R(x) \tag{5}$$

where σ is the length measure on $F^+_{k^2}(x)$ and $R \in H^1(\mathbb{R}^2)$.

See Figure 2 for an example of $F^+_{k^2}(x)$.

Since the integrand is quasiperiodic one can provide a full expansion of the integral as a series of fractional powers of $1/|x|$ by the mean of the stationary phase method. However a difficulty arises because $F^0_{k^2}$ is generically not convex. Using the periodicity of the integrand with respect to the Floquet variable ℓ one can arrange $F^0_{k^2}$ as the union of close smooth curves or periodic smooth curves (see Figure 4). Some curves are convex others have inflexion points $\underline{\ell}_j$.

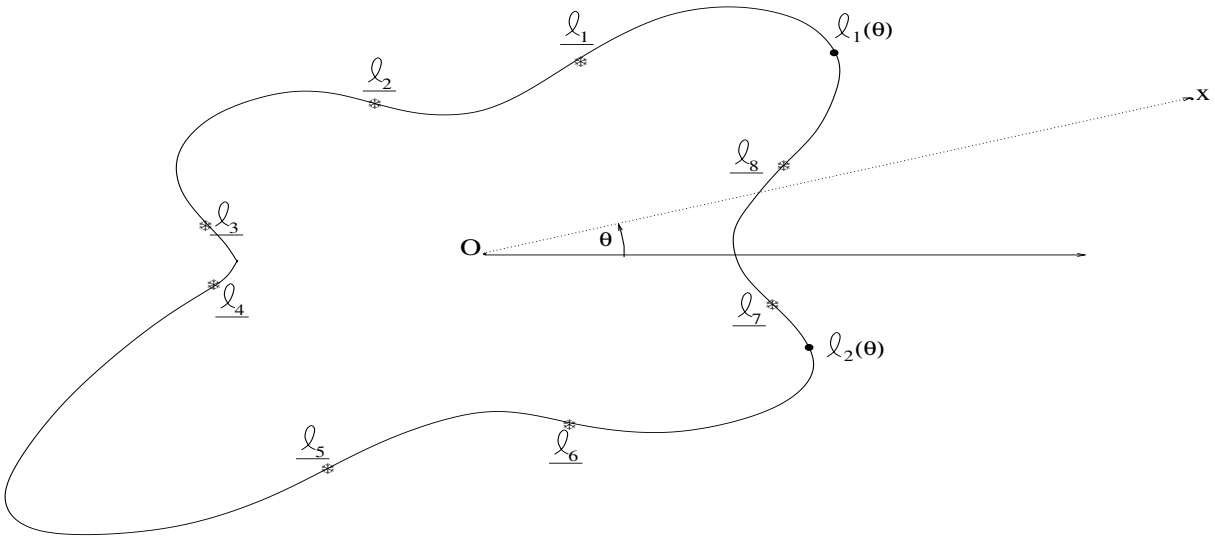

Figure 3: A closed component of $F^0_{k^2}$ with the points $\underline{\ell}_j$ and $\ell_n(\theta) \in F^+_{k^2}(x)$

The stationary phase method shows that critical points of the phase $i\ell \cdot x$ are such that $\nabla\tilde{\lambda}$ is parallell to x at such points. Let us denote them by ℓ_n. Then ℓ_n is a function of $\theta = arg(x)$ and is well defined as long as it does not meet any inflexion point. See Figure 3.2. Again for sake of simplicity we adress the problem in general position assuming that inflexion points are *non degenerated* and two inflexion points correspond to *distinct* angles θ_j. Let us thus denote by $I_n \subset [0, 2\pi]$ the domain of ℓ_n and denote by θ_j the angle for which for some n, $\ell_n(\theta_j) = \underline{\ell}_j$. Finally let $\mathcal{N}_j$ be a small neighborhood of θ_j which does not contain any other inflexion point.

Then the leading term in the expression of u expands asymptotically according to

Theorem 2.2. *Let k as in Theorem 2.1.*

1) For $\theta \in [0, 2\pi]\backslash(\cup_j \mathcal{N}_j)$ there holds for $r = \|x\|$ big

$$u(x) = \frac{i\sqrt{2\pi}}{\sqrt{r}} e^{-i\pi/4} \sum_{n=1} 1_{I_n}(\theta) e^{i\ell_n(\theta)\cdot x} \frac{(\hat{f}(\ell_n), \tilde{e}(\ell_n))_{L^2(W)}}{\|\nabla\tilde{\lambda}(\ell_n)\|\kappa_n^{1/2}} \tilde{e}(x, \ell_n) + \tilde{R}, \tag{6}$$

where κ_n is the curvature of $F^+_{k^2}(x)$ at ℓ_n and $\tilde{R} \in H^1(\mathbb{R}^2)$.

2) For $\theta \in \mathcal{N}_j$ with $\theta_j = \bar{I}_{n_1} \cap \bar{I}_{n_2}$

$$\begin{aligned} u(x) = \frac{e^{i\underline{\ell}_j\cdot x}}{r^{1/3}} \Big(\alpha_j Ai(r^{2/3}\gamma_j(\theta-\theta_j))\tilde{e}(\underline{\ell}_j, x) + \frac{\beta_j}{r^{1/3}} Ai'(r^{2/3}\gamma_j(\theta-\theta_j))w_j(x) \Big) \\ + \frac{i\sqrt{2\pi}}{\sqrt{r}} e^{-i\pi/4} \sum_{n\notin\{n_1,n_2\}} e^{i\ell_n\cdot x} \frac{(\hat{f}(\ell_n), \tilde{e}(\ell_n))_{L^2(W)}}{\|\nabla\tilde{\lambda}(\ell_n)\|\kappa_n^{1/2}} \tilde{e}(x, \ell_n) + \tilde{R} \end{aligned} \tag{7}$$

where Ai is Airy's function, a_j, b_j are non zero real, $\gamma_j(0) = 0$, w_j is periodic and belongs to $H^1(W)$ and $\tilde{R} \in H^1(\mathbb{R}^2)$.

Remark 2.3. *In (7) the decay rate of the first term is $O(r^{-1/2})$ because the oscillatory part of Airy function $Ai(s)$ decays like $O(s^{-1/4})$.*

We expect that the remainder decreases more rapidely in the far. Actually $\tilde{R} = R_1 + R_2$ *where* R_1 *corresponds to terms in* $F^-_{k^2} = F^0_{k^2} - F^+_{k^2}$ *and* R_2 *is related to the stationary phase theorem. We prove that* R_1 *decreases faster than any polynomial and* $R_2 = O(r^{-3/2})$*. However we don't know how to prove any better decrease result for* R *because it is a Bloch inverse transform whose integration set meets* σ_1 *if it is not empty. This prevents the use of the instationary phase theorem.*

Definition 2.4. *A solution to equation* (1) *is called an outgoing solution if there are finitely many open intervals* $(I_n)_n$ *of* $[0, 2\pi]$ *and a neighborhood* $\mathcal{N}$ *of the boundaries* θ_j *of these intervals such that for* $\theta \in [0, 2\pi]\backslash\mathcal{N}$

$$u(x) = \frac{1}{\sqrt{r}} \sum_n 1_{I_n}(\theta) c_n(\theta) e^{i\ell_n \cdot x} \tilde{e}(x, \ell_n) + R \tag{8}$$

where $\ell_n \in F^+_{k^2}$ *and* $\nabla\tilde{\lambda}(\ell_n)$ *is parallell to* x *and* $R \in H^1(\mathbb{R}^2)$ *while for* $\theta \in \mathcal{N}_j$ *a small neighborhood of one extremity* $\theta_j = I_{n_1} \cap I_{n_2}$

(9)

$$u = \frac{e^{ix\cdot\underline{\ell}_j}}{r^{1/3}} \Big(\tilde{c}_j Ai(r^{2/3}\gamma_j(\theta-\theta_j))\tilde{e}(\underline{\ell}_j, x) + \frac{1}{r^{1/3}} Ai'(r^{2/3}\gamma_j(\theta-\theta_j))w_j(x) \Big) + \frac{1}{\sqrt{r}} \sum_{n\notin\{n_1,n_2\}} c_n(\theta) e^{i\ell_n\cdot x}\tilde{e}(x,\ell_n) + R$$

where $\underline{\ell}_j = \ell_{n_1}(\theta_j) = \ell_{n_2}(\theta_j)$*,* w_j *is a periodic fonction belonging to* $H^1(W)$ *and* $R \in H^1(\mathbb{R}^2)$*.*

Uniqueness of outgoing solutions requires that P has no eigenvalue which is the case since the spectrum of P is the union of $\lambda_n(B)$. However P may have singular spectrum corresponding to the fact that one of the λ_n is flat on a non empty ball.

Assumption 2.5. *For all* n*,* λ_n *is a non constant function on any open set.*

Under this assumption the spectrum of P is purely essential [5]. Finally we need a technical assumption to prove uniqueness in Rellich's way: we need that the remainder is smooth enough to consider the trace of ∇R along a circle. This is true if we assume

Assumption 2.6. *The coefficient* α *is either lipschitz or discontinuous along smooth curves as in [15] and in this case we also need* $f \in L^\infty$*.*

Theorem 2.7. *Under Assumptions 2.5 and 2.6 equation* (1) *has a unique outgoing solution.*

3 Limiting absorption principle for the outgoing resolvent

To prove Theorem 2.1 we introduce a smooth cutoff function ψ which vanishes everywhere except in a small neighborhood of k^2 on which the set J_k remains constant.

Then let us split

$$u_\varepsilon = u_{1,\varepsilon} + u_{2,\varepsilon}\ , \qquad u_{1,\varepsilon} = \int_B \sum_{n\in J_k} \psi(\lambda_n(\ell)) \frac{(\hat{f}, e_n(\ell))_{L^2(W)}}{k^2_\varepsilon - \lambda_n(\ell)} e_n(x,\ell) d\ell. \tag{10}$$

Let us first analyze $u_{2,\varepsilon} = u - u_{1,\varepsilon}$. By definition of ψ there is a constant $c > 0$ such that

$$\frac{1-\psi(\lambda_n(\ell))}{|k_\varepsilon^2 - \lambda_n(\ell)|} < c/\lambda_n(\ell) \quad \forall n$$

so the Bloch transform

$$\hat{u}_{2,\varepsilon}(x,\ell) = \sum_{n\in\mathbb{N}^*} (1-\psi(\lambda_n(\ell))) \frac{(\hat{f}, e_n(\ell))_{L^2(W)}}{k_\varepsilon^2 - \lambda_n(\ell)} e_n(x,\ell)$$

belongs to $L^2(B; H^1(W))$. Thus $u_{2,\varepsilon} \in H^1(\mathbb{R}^2)$ (see Appendix A where we collected some classical results about Floquet-Bloch transform on Sobolev spaces).

To analyze and compute the limit of $u_{1,\varepsilon}$ when ε goes to zero we need to modify the integration set B to avoid $\mathcal{F}_{k_\varepsilon^2}$ for all positive ε close to zero. This was done by C. Gerard [8] in a theoretical way using a *complex displacement* according to Pham [20]. Since the Fermi levels are parameterized by λ, a complex displacement amounts to choosing a homotopy for λ from an interval around k^2 to a half loop in the lower complex plane. This allowed to extend the validity of the resolvant associated to (1) in a neighborhood of the real axis but no formula was given to compute the integral defining $u_{1,\varepsilon}$ (except in the difficult case $k^2 \in \sigma_0$).

Here on the contrary in order to compute the limit when ε goes to zero we push λ to the upper complex plane over k_ε^2 and use Cauchy residu formula.

Before going to the details we need more information about the topology of the level sets $F_{k^2}^0$ and explain how to continuously deform it to $\mathcal{F}_\lambda$ when λ goes to the complex domain. This is the aim of the next subsections.

3.1 Geometry of a Fermi level

Let us recall some general facts (see [29]). Since the Bloch variety is an analytic set it possesses a Whitney stratification. This stratification is by regularity and dimension:

$$\mathcal{B} = \mathcal{B}^r \cup \mathcal{B}^\times,$$

where $\mathcal{B}^r$ is the regular part of $\mathcal{B}$ which is open and locally a 2d-manifold and $\mathcal{B}^\times$ the complementary set. The latter is a subset of the points where λ_n are multiple. Indeed, by analytic perturbation theory, any point $(\ell, \lambda_n(\ell))$ where λ_n is simple defines locally a manifold and thus is a regular point of $\mathcal{B}$. Again $\mathcal{B}^\times = (\mathcal{B}^\times)^r \cup \mathcal{B}^{\times\times}$ where $(\mathcal{B}^\times)^r$ is locally a 1d-manifold and any connected component of $\mathcal{B}^r, (\mathcal{B}^\times)^r, \mathcal{B}^{\times\times}$ is called a *stratum*. It is a basic result from [27] that the number of strata is locally finite.

Lemma 3.1. *The set σ_0 is locally finite.*

Proof. Any stratum of $\mathcal{B}^r$ is the graph of a unique analytic function λ_n whose critical values are isolated by [25]. Any stratum S of lower dimension is the graph of finitely many (generically two)

crossing bands $\lambda_{j_1} = \ldots = \lambda_{j_n}$. Since S is a manifold the restriction of $\lambda_k,\ k \in \{j_1, \ldots, j_n\}$ to the set S is holomorphic and thus has at most a finite number of critical points. Finally 0 dimensional strata are isolated. Thus σ_0 is locally finite. □

We call *singular stratum* a stratum of $\mathcal{B}^\times$. Singular strata are in general position the sets of intersection of two bands $\lambda_{n_j},\ j = 1, 2$ which are simple outside the intersection set.

This is a finite dimensional problem for which we can use analyticity results about roots of hermitian matrices.

Let us proceed in details. First we consider the finite dimensional (matrix) reduction of $P(\ell)$ as follows. Since the spectrum of $P(\ell)$ is discrete and locally finite one can introduce the spectral projector on the finite dimensional vector space associated to a finite set of eigenvalues (cf. Kato [12] p.369 and 386). For $(\ell, \lambda_0) \in \mathcal{B}$ with λ_0 a multiple eigenvalue, let us denote by $\pi(\ell, \lambda_0)$ the eigenprojection on the total eigenspace of $P(\ell)$ associated to the eigenvalue branches $\lambda_{n_j},\ j = 1$ or 2 in a neighborhood of λ_0. It reads

$$\pi(\ell, \lambda_0) = \frac{1}{2i\pi} \int_{C(\lambda_0)} (P(\ell) - zI)^{-1} dz,$$

where $C(\lambda_0)$ is a closed curve in the complex plane which encircles only λ_0 for $\ell = \ell_0$. Since $P(\ell)$ is an analytic familly of operators this projector is complex analytic on a small neighborhood of ℓ_0. Let us then set $T(\ell) = P(\ell)\pi(\ell, \lambda_0)$ which is a finite dimensional operator. Since π is analytic T is analytic too. Thus $T(\ell)$ reads as a 2×2 hermitian matrix with complex analytic coefficients. We cannot use 1d Rellich's result [23] about the analytical continuation of eigenvalues of hermitian matrices. In this 2d case one needs to discuss the dimension of the crossing set

$$\mathcal{M} := \{\lambda_{n_1} = \lambda_{n_2}\} \cap V_0$$

in a neighborhood V_0 of ℓ_0 (see [18] paragraph 2.3 for a general discussion). Restricting ourself to real ℓ the authors in [14] give a complete result extending [23] for the analytic continuation of roots of hermitian matrices. In our situation it can be reformulated according to the following

Theorem 3.2 ([14])**.** *Assume $\lambda_0 \notin \sigma_0$. Either $\dim \mathcal{M} = 1$ then λ_{n_j} for $j \in \{1, 2\}$ can be relabelled in such a way that they become (real) analytic functions on V_0 past the crossing. The same relabelling applies to the associated eigenvectors. Either $\dim \mathcal{M} = 0$ and then ℓ_0 is an isolated nodal point which is not a cusp and whose tangent cone lies outside a cone of slope $max\alpha/min\beta$.*

Proof. When $\mathcal{M}$ is a subset of $(\mathcal{B}^\times)^r$ this is [14], Theorem 6.6. When $\mathcal{M} \subset \mathcal{B}^{\times\times}$, upon reducing V_0, $\mathcal{M}$ is the isolated point ℓ_0 and the tangent space of λ_{n_j} at ℓ_0 is a cone which is a basic property of analytic spaces. More precisely let us give the matrix representation of $T(\ell)$:

$$(11)\quad T(\ell) - \lambda_0 I = \begin{pmatrix} a(\ell) & b(\ell) \\ b(\ell) & c(\ell) \end{pmatrix} = \frac{a(\ell) - c(\ell)}{2} + \begin{pmatrix} d(\ell) & b(\ell) \\ b(\ell) & -d(\ell) \end{pmatrix}, \quad d(\ell) = \frac{a(\ell) + c(\ell)}{2}$$

where a, b, c are analytic functions satisfying $a(\ell_0) = b(\ell_0) = c(\ell_0) = 0$. The eigenvalues of the last matrix are $\pm\sqrt{d^2 + b^2}$ whose tangent set at ℓ_0 is a (non isotropic) cone and ℓ_0 is not a cusp because

the minimal homogeneity degree of the roots is 1. Finally by Appendix Lemma C.1 the function λ_n has a gradient bounded by $\max\alpha/\min\beta$.

□

Remark 3.3. *The tangent cone about a nodal point can't be vertical and flat because otherwise* $\lambda_0 \in \sigma_0$.

Definition 3.4. *The first case in the previous theorem will be referred to as* regular crossing. *We denote by* σ_1 *the set of points* ℓ *corresponding to the second case of the theorem. If* $k^2 \notin \sigma_0 \cup \sigma_1$ *we call* $F^0_{k^2}$ *a* regular Fermi level. *For such* k *let us denote by* (μ_n, v_n) *the analytically reordered eigenfunctions and eigenvectors.*

Since λ_n is defined in $\mathbb{R}^2$ the function μ_n is piecewise defined on a subset $\mathcal{D}$ of $\mathbb{R}^2$ avoiding the set of preimages of critical points σ_0 and nodal points σ_1.

By analytic extension theorem μ_n extends analytically in a complex neighborhood of $\mathcal{D}$. Since λ_n are piecewise holomorphic in $\mathbb{C}^2$, μ_n is thus still piecewise defined in term of λ_n in a complex neighborhood of its domain of analyticity. Contrary to (λ_n, e_n) the functions (μ_n, v_n) are not periodic.

3.2 Unfolding a regular real Fermi level

For real k the fiber $\mathrm{F}^0_{k^2}$ is a real stratified set and upon taking $\mathrm{supp}(\psi)$ small enough, the stratification remains invariant. Generically the fiber is a one dimensional set, with finitely many 1d and 0d strata: 1d strata are connected analytic curves c_n and 0d strata are isolated points corresponding to the crossing of generically two band functions and thus the meeting point of two curves $c_n \cap c_j$.

Let us now recall the well-known but non written fact that a Fermi level is actually the folding of closed or periodic analytic curves. To see this we make use of the extended Fermi level F_{k^2} which is periodic with B as a unit cell in $\mathbb{R}^2$. Thus every $c_n \subset F^0_{k^2}$ is repeated by translation of periods of B in F_{k^2}.

Definition 3.5. *Let* c *be a connected curve in* F_{k^2}. *We say that* c *is* p*eriodic modulo* B *if* c *has no boundary or if the vector joining the extremities of* c *is a linear integer combination of the periods of* B.

Lemma 3.6. *There is a familly* $(\tau_n)_n$ *of translations by periods of* B *such that the union over* n *of the translated arcs* $c_n \circ \tau_n$ *can be concatenated into closed or periodic (modulo* B*) analytic curves* $\mathscr{C}_j(k^2)$ *of* F_{k^2}.

Proof. See Figure 4. Let us construct such a set $\mathscr{C}(k^2)$ and prove its analyticity.

Let c be a connected analytical component of $F^0_{k^2}$. It is related to some μ_n. Either it is a closed curve in B and then $c = \mathscr{C}(k^2)$ or both end points (E_1, E_2) belong to ∂B. Since μ_n is piecewise defined in terms of the $(\lambda_n)_n$ we generically have $E_1 \in \lambda_{n_1}^{-1}(k^2)$ and $E_2 \in \lambda_{n_2}^{-1}(k^2)$ for some n_1, n_2 (which can be equal). Let $E_2' \in \partial B$ such that E_2E_2' is a period of B.

Assume that c is the only curve arriving at E_2. This means that λ_{n_2} is analytic around E_2 and by periodicity there is an other curve c' arriving at E_2' such that translating it by $E_2'E_2$ it is an analytic continuation of c.

Assume that two curves c, s meet at E_2. This means that s is associated to λ_{n_3} around E_2 and λ_{n_2} and λ_{n_3} meet at E_2. Then by periodicity of λ_{n_2} and λ_{n_3} there are two curves c', s' arriving at E_2'. The choice of the good continuation is by analyticity. Indeed μ_n continues analytically through E_2 thus one of the translated c', s' is associated to μ_n and thus an analytical continuation of c.

Repeating this procedure one gets a sequence of boundary points $E_1, E_2, \ldots, E_j, \ldots$. We claim that the first redundance modulo B must be E_1 modulo B. Indeed each new connected component which is added to $\mathscr{C}(k^2)$ under construction is a translated component of $F^0_{k^2}$. Moreover there is a finite number of such components. If the first redundance is E_j with $j > 1$ then this would mean that there is some B-periodic subset $\mathscr{C}'(k^2)$ of $\mathscr{C}(k^2)$ which does not go through E_1 but this is wrong since we can reverse the procedure and see that E_j comes from E_1.

□

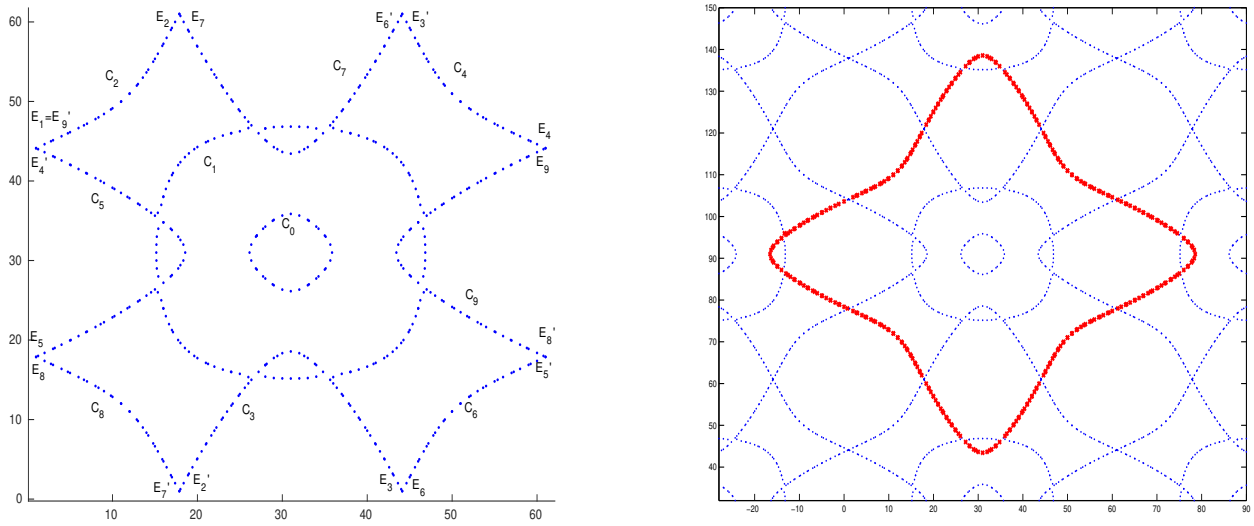

Figure 4: Unfolding the Fermi level for $k = 1.2$ (left) leads (right) to $\mathscr{C}_0(k^2) = c_0$, $\mathscr{C}_1(k^2) = c_1$ and $\mathscr{C}_2(k^2) = \cup_{2 \leqslant j \leqslant 9} c_j$ using B-translations (red curve)

Remark 3.7.

- *From the proof we see that each $\mathscr{C}(k^2)$ is associated to one μ_j and we denote it by $\mathscr{C}_j(k^2)$.*
- *On Figure 4 we only have closed curves in an extended Brillouin zone.*
- *$\partial\mathscr{C}_j(k^2) \neq \varnothing$ if there is a unit vector $\hat{\imath}$ such that the line $t\hat{\imath}$, $t \in \mathbb{R}$ does not meet $F^0_{k^2}$. In other words k^2 lies in a partial gap of P in the direction $\hat{\imath}$. In particular this may happen when bands overlap artificially.*

- *The curves may cross or may be tangent (see Figure 3.2) but this does not make any difference in the subsequent analysis since $k^2 \notin \sigma_1$ and thus the crossing of different μ_j is regular.*

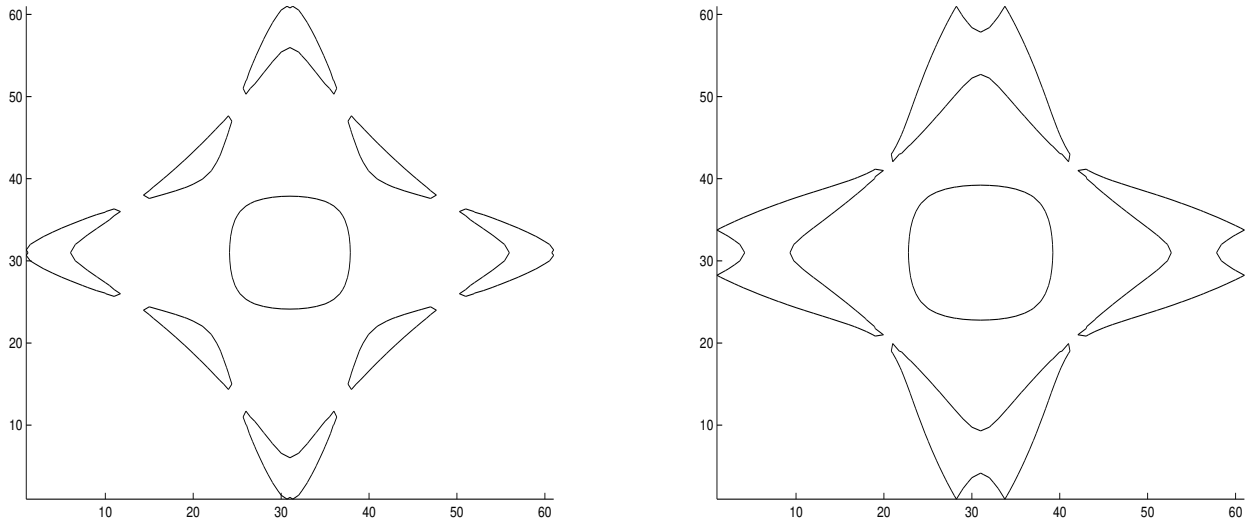

Figure 5: Real Fermi level $F^0_{k^2}$ for $k = 1.06$ (left) and $k = 1.081$ (right, folded)

3.3 Complex extension of a regular real Fermi level

In view of letting k complex we want to extend the definition of $\mathscr{C}_j(k^2)$ to a complex neighborhood of k^2.

Lemma 3.8. *Let $k \in \mathbb{R}$ and let $\ell_{j,0}(t)$, $t \in [0,1]$ be a global (real) parameterization of a curve $\mathscr{C}_j(k^2)$ in $\mathbb{R}^2$. Then for complex λ close to k^2 one defines $\mathscr{C}_j(\lambda)$ through a family of parameterizations $\ell_j(t,\lambda)$, $t \in [0,1]$ such that $\partial \ell_j/\partial\lambda = \nabla\mu_j/(\nabla\mu_j \cdot \nabla\mu_j)$ and $\ell_j(t,k^2) = \ell_{j,0}(t)$ for all $t \in [0,1]$.*

Proof. First ℓ_j is well-defined because away from $\sigma_0 \cup \sigma_1$ the function μ_j is analytic and $\nabla\mu_j(k^2) \neq 0$ so one can apply Cauchy-Lipshitz's Theorem with parameter t and show that there exists a complex ball $\mathscr{B}_{k^2}$ independent of t such that $\ell_j(t,\lambda)$ exists for $\lambda \in \mathscr{B}_{k^2}$.

Let us show that $\mu_j(\ell_j(t,\lambda)) = \lambda$ for all λ in $\mathscr{B}_{k^2}$. For this we just need to show that the initial parameterization is carried along the flow. We compute and find for all $t \in [0,1]$

$$\frac{\partial}{\partial\lambda}\mu_j(\ell_j(t,\lambda)) = 1 \quad \text{with} \quad \mu_j(\ell_j(t,k^2)) = k^2.$$

Thus $\mu_j(\ell_j(t,\lambda)) = \lambda$ for any λ in a small neighborhood of k^2 and $t \in [0,1]$. □

3.4 Complex displacement about a regular k^2-Fermi level

3.4.1 Representation formula

Let us resume the guideline presented just before section 3.1. Let us pick a peculiar $k^2 \notin \sigma_0 \cup \sigma_1$ and denote by K the support of ψ which we take so small that the topology of F^0_λ does not change for $\lambda \in K$. The domain of integration of $u_{1,\varepsilon}$ is $\Psi := \bigcup_{n\in J_k}\{\ell \in B,\ \psi(\lambda_n(\ell)) \neq 0\}$. This set also reads as a union of disjoint Fermi levels: $\Psi \cap \bigcup_{\lambda\in K} F^0_\lambda$. From the previous section we have:

$$\bigcup_{\lambda\in K} F^0_\lambda = \bigcup_j \bigcup_{\lambda\in K} \mathscr{C}_j(\lambda) \quad \text{modulo B}$$

For future use let us denote by

$$\mathcal{A}_j := \bigcup_{\lambda\in K} \mathscr{C}_j(\lambda), \quad \text{and} \quad \mathscr{F} = \bigcup_{\lambda\in K} F^0_\lambda = \bigcup_j \mathcal{A}_j$$

Since λ_n, $e^{i\ell\cdot x}e_n(x,\cdot)$ and $(\hat{f}(\cdot), e_n(\cdot))_{L^2(W)}$ are B-periodic and recalling (4) we get

$$\begin{aligned} u_{1,\varepsilon} &= \sum_{n\in J_k} \int_B e^{i\ell\cdot x}\psi(\lambda_n(\ell))\frac{(\hat{f}, e_n(\ell))_{L^2(W)}}{k^2_\varepsilon - \lambda_n(\ell)} e_n(x,\ell)d\ell \\ &= \int_{\mathscr{F}} e^{i\ell\cdot x}\psi(\tilde{\lambda}(\ell))\frac{(\hat{f}, \tilde{e}(\ell))_{L^2(W)}}{k^2_\varepsilon - \tilde{\lambda}(\ell)} \tilde{e}(x,\ell)d\ell, \\ &= \sum_j w_j \quad \text{with} \quad w_j = \int_{\mathcal{A}_j} e^{i\ell\cdot x}\psi(\tilde{\lambda}(\ell))\frac{(\hat{f}, \tilde{e}(\ell))_{L^2(W)}}{k^2_\varepsilon - \tilde{\lambda}(\ell)} \tilde{e}(x,\ell)d\ell. \end{aligned} \tag{12}$$

Since $\mathscr{C}_j(\lambda)$ is associated to one function μ_j one has $\tilde{e} = v_j$ (recall definition 3.4). Then let us use the explicit parameterization ℓ_j of $\mathscr{C}_j(\lambda)$ according to Lemma 3.8 and compute its Jacobian determinant (here λ is real). First from $\mu_j(\ell_j(t,\lambda)) = \lambda$ we have $\nabla\mu_j \cdot \partial_t\ell_j = 0$ and $\nabla\mu_j \cdot \partial_\lambda\ell_j = 1$ hence

$$|det(\partial_t\ell_j\ \partial_\lambda\ell_j)| = \frac{|\partial_t\ell_j|}{|\nabla\mu_j|}\nabla\mu_j \cdot \partial_\lambda\ell_j = \frac{|\partial_t\ell_j|}{|\nabla\mu_j|}.$$

Finally

$$w_j = \int_K \frac{\psi(\lambda)}{k^2_\varepsilon - \lambda}\int_{\mathscr{C}_j(\lambda)} \frac{e^{i\ell\cdot x}}{|\nabla\mu_j|}(\hat{f}(\ell), v_j(\ell))_{L^2(W)} v_j(\ell,x)d\ell d\lambda.$$

In what follows we consider any w_j so we drop the index j.

3.4.2 Light area and shadow

Before pushing λ to the complex plane note that $e^{i\ell(t,\lambda)\cdot x}$ is a quasi-periodic function with respect to x. When λ is complex then ℓ is complex and the sign of

$$\varphi(t,\lambda) := \ell(t,\lambda)\cdot x$$

can change along $\mathscr{C}(\lambda)$ and thus the asymptotic behaviour of w changes drastically. We thus need to caracterize the zeros of this function for λ in a small neighborhood of k^2.

For complex $\lambda = \tau + iy$ with y close to zero we use Cauchy-Riemann relations to deduce the sign of $\Im\varphi$. Since the parameterization $\ell(t,\cdot)$ is holomorphic and real for $y = 0$ the sign of $\Im\varphi$ for y going to zero is given by the sign of $\partial_y \Im\ell \cdot x$ which is also the sign of $\partial_\tau \ell \cdot x$ for $y = 0$. Now by definition of the parameterization ℓ one has $\partial_\tau \ell \cdot x = (\nabla\mu \cdot x)/|\nabla\mu|^2$ for $y = 0$ thus the sign of $\Im\varphi$ when y is close to zero is given by that of $\nabla\mu \cdot x$.

With the homogeneous case in mind we want to reproduce the proof of the asymptotic expansion as in [16]. Thus we split $\mathscr{C}(k^2)$ in three parts :

- a part $\mathscr{C}_0$ around the shadow transition (i.e. $\nabla\mu(\ell(t,k^2)) \cdot x \approx 0$)
- and two other parts $\mathscr{C}^\pm$ such that $\pm\Im\phi > 0$ for $\varepsilon > 0$ or equivalently such that $\pm\nabla\mu(\ell(t,k^2))\cdot x > 0$.

Because the set $\psi = 1$ is small we perform this splitting uniformly with respect to $\lambda \in K$.

Let us introduce a partition of unity on $\mathscr{C}(k^2)$:

$$1 = \psi_0(t) + \psi_+(t) + \psi_-(t) \quad \text{with } \pm\nabla\mu \cdot x > 0 \quad \text{on} \quad \operatorname{supp}(\psi_\pm).$$

So $w = w_0 + w_+(x) + w_-(x)$ with for $\beta \in \{0, \pm\}$

$$w_\beta = \int_K \frac{\psi(\lambda)}{k_\varepsilon^2 - \lambda} g_\beta(\lambda) d\lambda, \quad g_\beta(\lambda) = \int_0^1 e^{i\ell\cdot x}\psi_\beta(t)\,(\hat{f}(\ell), v(\ell))_{L^2(W)} v(\ell,x) \frac{|\partial_t \ell|}{|\nabla\mu|} dt. \tag{13}$$

3.4.3 Complex displacement

We now consider each term w_β and isolate the leading part.

• For w_+ we can choose the integration path in the first integral going above the residue. For this let $I \subset K$ be such that $\psi = 1$ on I. Then let us consider γ^+ a curve homotopic to I, encircling k_ε^2 for ε small enough. See Figure 3.4.3.

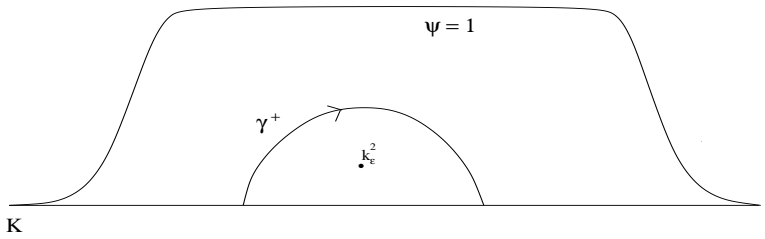

Figure 6: The contour γ^+

Then the integrand g_+ is holomorphic in the region surrounded by γ^+ and I. Indeed, $\psi = 1$ and Lemma 3.8 provides a holomorphic extension of the jacobian determinant in a neighborhood of K

which reads $\pm\det(\partial_t\ell, \partial_\lambda\ell)$ (with fixed sign on K). By the Cauchy-residu formula we get

$$w_+ = 2i\pi g_+(k_\varepsilon^2) + \int_{K\setminus I} \psi(\lambda)\frac{g_+(\lambda)}{k_\varepsilon^2-\lambda}d\lambda + \int_{\gamma^+}\frac{g_+(\lambda)}{k_\varepsilon^2-\lambda}d\lambda \tag{14}$$

where

$$g_+(k_\varepsilon^2) = \int_{\mathscr{C}\cap F^+_{k^2}(x)} \psi_+ e^{i\ell\cdot x}(\hat{f}(\ell), v(\ell))_{L^2(W)} v(\ell,x)\frac{1}{|\nabla\mu|}\sigma(d\ell).$$

• Similarly, for w_- we choose a path γ^- going below the real axis so that there is no residu:

$$w_-(x) = \int_{K\setminus I}\psi(\lambda)\frac{g_-(\lambda)}{k_\varepsilon^2-\lambda}d\lambda + \int_{\gamma^-}\frac{g_-(\lambda)}{k_\varepsilon^2-\lambda}d\lambda.$$

The previous expressions show that $w_\pm$ have limit when ε goes to zero and $g_+(k^2)$ contributes to formula (5).

- As for w_0 one can take the limit when ε goes to zero. This limit involves a principal value:

$$\lim_{\varepsilon\to 0}\frac{1}{k_\varepsilon^2-\lambda} = vp\left(\frac{1}{k_0^2-\lambda}\right) - i\pi\delta_{k_0^2}.$$

The limit thus reads

$$\lim_{\varepsilon\to 0} w_0 = -i\pi g_0(k_0^2) + vp\int_K \frac{\psi(\lambda)}{k_0^2-\lambda}g_0(\lambda)d\lambda,$$

where the principal value is bounded.

4 Boundedness of the residual

Theorem 4.1. *The functions w_0, $w_+ - 2i\pi g_+(k_\varepsilon^2)$ and w_- belong to $H^1(\mathbb{R}^2)$ uniformly with respect to ε (small).*

Proof. Let us first consider w_0 and set

$$pf(\ell,x) = (\hat{f}(\ell), v(\ell))_{L^2(W)}v(\ell,x) \quad \text{and} \quad D_\ell := \pm\det(\partial_t\ell, \partial_\lambda\ell). \tag{15}$$

The choice of $\pm$ is such that $D_\ell > 0$ for real λ. Formula (13) reads

$$w_0 = \int_K\int_0^1 e^{ix\cdot\ell}\psi_0(t)\frac{\psi(\lambda)}{k_\varepsilon^2-\lambda}pf(\ell,x)D_\ell\, dtd\lambda.$$

In view of letting $|x|$ go to infinity Let us redefine the phase as $\varphi = \ell(t,\lambda)\cdot x/|x|$. It is real and instationnary. Indeed, differentiating the relation $\mu(\ell(t,r)) = r$ with respect to t we get $\nabla\mu\cdot\partial_t\ell = 0$. Recalling that ℓ is defined by $\partial_\lambda\ell = \nabla\mu/|\nabla\mu|^2$ we thus get

$$\partial_t\ell\cdot\partial_\lambda\ell = 0. \tag{16}$$

Thus the gradient of the phase φ does not vanish anywhere. Actually on the support of ψ_0 we have $\partial_t\varphi \neq 0$ since $\nabla\mu(\ell)$ and x are approximately orthogonal thus $\partial_t\ell$ and x are approximately collinear. We can thus integrate by parts with respect to t.

Let us note that the amplitude is also oscillatory since it is quasi periodic with respect to ℓ. Integrating by parts requires to differentiate $\hat{f}$ with respect to ℓ and since $\partial_\ell \hat{f} = -i\widehat{xf}$ we need to take f in weighted L^2 space or even in the Schwarz space if one wants to get a full series expansion of w_0 in inverse powers of $|x|$.

In order to prove that $w_0 \in L^2(\mathbb{R}^2)$ we need to integrate twice by parts because $|x|^{-1} \notin L^2(\mathbb{R}^2 \backslash B(0,1))$. Because ψ_0 has compact support we get

$$w_0 = \int_{\mathbb{R}^+} \frac{\psi(r)}{k_\varepsilon^2 - r} \int_0^1 \frac{-1}{|x|^2} e^{i|x|\varphi} \left(\partial_t \frac{1}{\partial_t \varphi} \right)^2 \left(\underbrace{\psi_0(t) pf(\ell, x) D_\ell}_{h} \right) dt dr.$$

The second derivative $(\partial_t \frac{1}{\partial_t \varphi})^2 h$ expresses as a sum of terms of the form

$$\frac{G(t)(\partial_t^a \varphi)^b \partial_t^c pf \partial_t^d D_\ell}{(\partial_t \varphi)^e}, \quad (a,b,c,d,e) \in \mathbb{N}^5 \quad b+c+d \leqslant 2, \quad a \leqslant 3,\ e \leqslant 4,$$

where G is bounded. Since ℓ is analytic with respect to t, $\partial_t^a \varphi$ and $\partial_t^d D_\ell$ are bounded and $\partial_t \varphi$ is lower bounded as we explained above. The only term left is $\partial_t^c pf$ for which one needs to estimate $\partial_\ell^c pf$. More precisely, there is a constant κ such that

$$|x|^2 |w_0| \leqslant \kappa \| pf(\cdot, x) \|_{W^{2,1}(\mathcal{D})}, \quad \text{where} \quad \mathcal{D} = \bigcup_{\lambda \in K} \mathscr{C}(\lambda).$$

Lemma 4.2. *There is a periodic function $q > 0$, $q_{|_W} \in L^2(W)$ such that for any $k \in \mathbb{N}$*

$$\| \partial_\ell^k pf(x, \cdot) \|_{L^1(\mathcal{D})} \leqslant q(x) \| \langle x \rangle^k f \|_{L^2(\mathbb{R}^2)}, \qquad \langle x \rangle = \sqrt{1 + |x|^2}.$$

See the proof of the lemma 4.3 below dealing with a complex extension of this result.

From the previous estimate we finally get the existence of a positive constant c such that

$$\| w_0 \|_{L^2(\mathbb{R}^2)} \leqslant c \| \langle x \rangle^2 f \|_{L^2(\mathbb{R}^2)}.$$

Next, estimating $\|\nabla w_0\|_2$ is equivalent to estimating $\|\sqrt{\alpha} \nabla w_0\|_2$ but

$$\|\sqrt{\alpha} \nabla w_0\|_2^2 = (P w_0, w_0)_2 \leqslant \max_{\ell \in B} \mu(\ell) \|w_0\|_2^2$$

since P commutes with the integrals and $Pv = \mu v$.

Let us now turn to $\tilde{w}_+ = w_+ - 2i\pi g_+$ and w_-. So we consider

$$\tilde{w}_+ = \int_{\gamma^+ \cup K \backslash I} \int_0^1 e^{ix \cdot \ell} \psi_+(t) \frac{\psi(\Re \lambda)}{k_\varepsilon^2 - \lambda} pf(\ell(t,\lambda), x) D_\ell dt d\lambda.$$

The main change is due to complex values and the fact that on the support of ψ_+ the phase $\varphi = \ell \cdot x/|x|$ is not instationnary with respect to t but it is instationnary with respect to λ. Indeed the real part of the phase for $\lambda \in \gamma^+$ is a small perturbation of its values for $\lambda \in I$ and for such real λ the vector $\partial_\lambda \ell$ is collinear to $\nabla \mu$ which is not orthogonal to x.

Let us remark that when the phase takes negative real values these are of order of the imaginary part of γ^+ which is small since we need to remain in the domain of analyticity of μ. So we do not use the exponential decrease but the nonstationarity of the phase. To integrate by parts we just need to provide enough regularity by choosing the contour $\gamma^+ \cup (K\backslash I)$ smooth enough. Integrating twice by parts with respect to λ we get

$$\tilde{w}_+ = -\int_{\gamma^+\cup(K\backslash I)} \int_0^1 \frac{1}{|x|^2} e^{-i|x|\varphi}\psi_+(t)\left(\partial_\lambda \frac{1}{\partial_\lambda\varphi}\right)^2 \frac{\psi(\lambda)}{k_\varepsilon^2-\lambda} pf(\ell(t,\lambda),x) D_\ell dt d\lambda$$

Let $\lambda(s),\ s\in I$ be a parameterization of the curve $\gamma^+ \cup (K\backslash I)$ and let $\phi(t,s)=\ell(t,\lambda(s))$. Also let $\mathscr{C}^+(\lambda)=\mathscr{C}(\lambda)\cap\{\psi^+\neq 0\}$. Then ϕ is a diffeomorphism from $\Delta := [0,1]\times K$ to $\bigcup_{\lambda\in\gamma^+}\mathscr{C}^+(\lambda)$ because $\Im\lambda$ is small and for $\lambda = Id$ it is so by (16). Then we can estimate $\tilde{w}_+$ by

$$|x|^2|\tilde{w}_+(x)| \leqslant \frac{c}{\alpha^3}\|pf(\phi,\cdot)\|_{W^{2,1}(\Delta)},\quad \alpha = \operatorname{dist}(\gamma^+, k_\varepsilon^2).$$

Lemma 4.3. *There is a periodic function $q>0,\ q\in L^2(W)$ and a constant $c>0$ such that*

$$\|\partial_\ell^k pf(x,\phi)\|_{L^1(\Delta)} \leqslant q(x)\| <\cdot>^{k+1} e^{\max|\Im\phi||\cdot|} f\|_{L^2(\mathbb{R}^2)}.$$

Proof. Let us show the lemma for $k=0$ (for bigger k the proof is similar because $\partial_\ell\hat{h} = -i\widehat{xh}$). e being holomorphic and periodic on Δ it is bounded in a small complex neighborhood of the Brillouin zone. Hence v is bounded too and pf can be estimated by

$$\|pf(x,\phi)\|_{L^1(\Delta)} \leqslant \|v(x,\phi)\|_{L^2(\Delta)}\|v(\cdot,\phi)\|_{L^\infty(\Delta;L^2(W))}\|\hat{f}(\phi)\|_{L^2(W\times\Delta)}.$$

Since v is holomorphic with respect to ℓ it is bounded in Δ so that the first term is a $L^2(W)$ periodic function of x. For the second term notice that $\|e(\ell)\|_{L^2(W)}$ (hence $\|v(\ell)\|_{L^2(W)}$) is identically equal to 1 on the real line and continuous by Lebesgue continuity theorem.

Finally we give a crude estimate of $\|\hat{f}(\phi)\|_{L^2(W\times\Delta)}$ as follows. First

$$|\hat{f}(\phi)| \leqslant \sum_{n\in\mathbb{Z}^2} |f(x+2\pi n)| e^{\max|\Im\phi||x+2\pi n|} = \widehat{|f|h}(0) \quad \text{where} \quad h(x) = e^{\max|\Im\phi||x|}.$$

Then setting $g=|f|h$ one has

$$\|\hat{g}(0)\|^2_{L^2(W)} = \sum_{n,m}\int_W g(x+2\pi n)g(x+2\pi m) \leqslant \left(\sum_n \|g\|_{L^2(W+2\pi n)}\right)^2$$

and

$$\sum_n \|g\|_{L^2(W+2\pi n)} \leqslant c\sum_n \frac{\|\langle\cdot\rangle g\|_{L^2(W+2\pi n)}}{<n>}.$$

Now applying Cauchy-Schwarz inequality the last term is bounded by $c\pi^2/6\|\langle\cdot\rangle g\|^2_{L^2(\mathbb{R}^2)}$. Finally $\|\hat{f}(\phi)\|_{L^2(W\times\Delta)} \leqslant \mu(I)c\pi^2/6\|\langle\cdot\rangle g\|^2_{L^2(\mathbb{R}^2)}$ where $\mu(I)$ is the measure of Δ.

□

From the previous estimate and since ϕ is a diffeomorphism one has $\max_D|\Im\phi| \leqslant c\alpha$ hence

$$\|\tilde{w}_+\|_{L^2(\mathbb{R}^2)} \leqslant \frac{c}{\alpha^3}\|\langle x\rangle^3 e^{c\alpha|\cdot|} f\|_{L^2(\mathbb{R}^2)}.$$

This estimate shows that one must take f exponentially decaying for $\tilde{w}_+$ to belong to $L^2(\mathbb{R}^2)$. The same estimate holds for w_-. □

5 Asymptotic behavior

Let us now turn to the far field asymptotics of the residus $g_+(k^2)$. The latter is an oscillatory integral whose phase is stationary on $\mathscr{C}^+(k^2) = \mathscr{C}(k^2) \cap \{\psi_+ \neq 0\}$ when $\partial_t\varphi = \partial_t\ell \cdot x/|x| = 0$. Since φ is analytic as a function of $t \in [0,1]$ it has finitely many extrema. Let t_* and $\ell_* = \ell(t_*)$ be a critical point (resp. value). Since φ depends on $\theta = arg(x)$, t_* is a function of θ. For comparison purpose recall that in the homogeneous case (i.e. α and β constant) there is just one curve $\mathscr{C}$ which is a circle. There is one outgoing stationary point $t = \theta$ defined on $[0, 2\pi[$. When $\mathscr{C}$ is not convex or not closed then t_* is only defined on a subintervall I_* of $[0, 2\pi[$. A point ℓ_* on a convex part of $\mathscr{C}$ moves anti-clockwise as θ increases while points on concave parts move clockwise. The extremities of I_* correspond to inflexion points of $\mathscr{C}$ and there $dt_*/d\theta$ is infinite and two critical values merge or emerge.

The derivative $\partial_t^2\varphi$ is related to the curvature of $\mathscr{C}$. Indeed, since x and $\partial_t\ell$ are orthogonal we have

$$\partial_t^2\varphi = \partial_t^2\ell \times \frac{\partial_t\ell}{|\partial_t\ell|} = \kappa|\partial_t\ell|^2 \tag{17}$$

where κ is the curvature. When the curvature vanishes the phase degenerates. This is a well known situation in optics: if the phase is first order degenerated then it is cubic and the integral around this inflexion point is a Airy function [1]. Let θ_* be such an inflexion point and χ a test function supported about t_* such that $\chi(t_*) = 1$. Let us split $g_+ = g_{+*} + \tilde{g}_+$ where g_{+*} is defined like g_+ but replacing $pf = (\hat{f}, v)v$ by χpf. From [10] Theorem 7.7.18 there are functions α, γ and w_* and $\tilde{w}_*$ such that $r\alpha(\theta_*) = x \cdot \ell_*$, $\gamma(\theta_*) = 0$ and for θ in a neighborhood of θ_* (orthogonal direction to $\partial_t\ell(t_*)$ the following asymptotics holds

$$g_{+*}(x) = \frac{e^{ir\alpha(\theta)}}{r^{1/3}}\left(Ai(\gamma(\theta)r^{2/3})w_*(x) + \frac{1}{r^{1/3}}Ai'(\gamma(\theta)r^{1/3})\tilde{w}_*(x)\right) + O\left(\frac{1}{r^{3/2}}\right) \tag{18}$$

where $O(r^s)$ is with respect to L^∞ norm. Actually [10] is true for pf not depending on x. However the formula still holds true because x can be considered as a parameter and pf is a bounded (periodic) function of x. From Appendix (24) and (25) we find that $\alpha(\theta) = \ell_* x/|x|$ and $w_* = d_* v$ where d_* is a non zero coefficient. Moreover there is a full Taylor expansion in powers $1/r^{1/3+n}$ and $1/r^{2/3+n}$ and the exponent in the $O()$ term is one order bigger than the fisrt term. As for the first term its order is $O(r^{-1/2})$ because the oscillatory part of Ai and Ai' decays like $r^{-1/4}$. Note that non degenerate critical points also give $O(r^{-1/2})$ amplitude. Only the "far field" pattern is different since Ai is exponentially decaying for positive arguments.

To get formula (6) of theorem 2.2 we resume the index j (of the curve $\mathscr{C}_j$) which we dropped in section 3.4. Take k as in Theorem 2.1 and denote by $\underline{\ell}_{jp}$ the finitely many inflexion points of the curve $\mathscr{C}_j$. Denote by t_{jn} the (finitely many) critical points of φ_j and $\ell_{jn} = \ell_j(t_{jn}) \in \mathscr{C}_j^+(k^2)$ the related Floquet numbers. These are analytic functions of $\theta \in I_{jn}$ where I_{jn} is an open intervall whose extremities are the angles θ_{jp} associated to the $\underline{\ell}_{jp}$. Then for θ away from the θ_{jp} the following

asymptotics holds

$$g_{j+}(x,k^2) = i\sqrt{2\pi}e^{-i\pi/4}\sum_n 1_{I_{jn}}(\theta)e^{i\ell_{jn}\cdot x}\frac{(\hat{f}(\ell_{jn}),v_j(\ell_{jn}))_{L^2(W)}}{(\partial_t^2\varphi_j(t_{jn},k^2)|x|)^{1/2}}v_j(\ell_{jn},x)\frac{|\partial_t\ell_j(t_{jn})|}{|\nabla\mu_j(\ell_{jn})|}+R_2 \tag{19}$$

As for θ about θ_{jp} let n_1 and n_2 be the index of the intervals I_{jn} whose mutual end is θ_{jp}. Then splitting $g_{j+}=g_{j+*}+\tilde{g}_{j+}$ as above we find

$$\begin{aligned} g_{j+}(x,k^2) = {} & i\sqrt{2\pi}e^{-i\pi/4}\sum_{n\notin\{n_1,n_2\}} 1_{I_{jn}}(\theta)e^{i\ell_{jn}\cdot x}\frac{(\hat{f}(\ell_{jn}),v_j(\ell_{jn}))_{L^2(W)}}{(\partial_t^2\varphi_j(t_{jn},k^2)|x|)^{1/2}}v_j(\ell_{jn},x)\frac{|\partial_t\ell_j(t_{jn})|}{|\nabla\mu_j(\ell_{jn})|} \\ & +\sum_p \frac{e^{ix\cdot\underline{\ell}_{jp}}}{r^{1/3}}\left(\tilde{c}_j Ai(\gamma_{jp}(\theta-\theta_{jp})r^{2/3})v_j(x,\underline{\ell}_{jp})+\frac{1}{r^{1/3}}Ai'(\gamma_{jp}(\theta-\theta_{jp})r^{2/3})\tilde{w}_{jp}(x)\right)+R_2 \end{aligned} \tag{20}$$

In both cases $R_2=O(r^{-3/2})$. In particular it belongs to $H^1(\mathbb{R}^2)$. Using (17) and recalling (14),(12),(10) and keeping one index on a bigger range we arrive at (6),(7).

6 Uniqueness

Let u be an outgoing solution of (1) according to Definition 3.4 with $f=0$ (no source term). Assumption 2.6 about the regularity of the coefficients entails that ∇u is continuous except across (the smooth) discontinuity of α. Then the same holds for R since the leading terms (of u) are continuous. This allows to integrate ∇R on a curve. Then uniqueness will follow from

Lemma 6.1. *As t goes to infinity*

$$\Im(Pu,u)_{L^2(C_t)} = \sum_k \int_{S_k}\frac{|c_k(\theta)|^2}{(\beta\tilde{e}(\ell_k(\theta)),\tilde{e}(\ell_k(\theta)))_2}\nabla\tilde{\lambda}(\ell_k(\theta))\cdot\vec{n}\,d\sigma+\sum_{k'}\alpha_{k'}|\tilde{c}_{k'}|^2+o(1) \tag{21}$$

where C_t is the circle of radius t and S_k the part of the unit circle related to I_k and $\tilde{e},\tilde{\lambda}$ are defined in (4) and $\alpha_{k'}>0$.

Proof. Integrating by part in the disk D_t of radius t and taking the imaginary part yields

$$0=\Im(Pu,u)_{L^2(D_t)}=\Im(\alpha\partial_n u,u)_{L^2(C_t)}.$$

Let us examine this last expression expanding u according to 3.4((8),(9)). First to avoid explicit bounds in evaluating integrals let us introduce a partition of unity of $[0,2\pi[$:

$$\sum_k\chi_k+\sum_{k'}\tilde{\chi}_{k'}=1$$

where the union of the supports of the χ_k is $[0,2\pi[\backslash\mathcal{N}$ and the support of $\tilde{\chi}_{k'}$ is $\mathcal{N}'_k$ with $\mathcal{N}'_k$ slightly bigger than $\mathcal{N}_k$ centered at θ_k and mutually disjoint. Put

- $u_k(x)=\dfrac{1}{\sqrt{r}}\chi_k(\theta)c_k(\theta)e^{i\ell_k(\theta)\cdot x}v_k(x,\ell_k(\theta))$

- For $\theta \in \mathcal{N}_k'$ set $\tilde{u}_k(x) = \tilde{c}_k \tilde{\chi}_k \frac{e^{ix\cdot \underline{\ell}_k}}{r^{1/3}} \Big(Ai(r^{2/3}\gamma_k(\theta-\theta_k)) v_k(x,\underline{\ell}_k) + \frac{1}{r^{1/3}} Ai'(r^{2/3}\gamma_k(\theta-\theta_k)) \tilde{w}_k(x,\underline{\ell}_k) \Big)$

With these notations (8) and (9) read

$$u(x) = \sum_k u_k + \sum_{k'} \tilde{u}_{k'} + R.$$

Let us break $(\alpha \partial_n u, u)_{L^2(C_t)}$ accordingly :

1. $T_0(t) = (\alpha \partial_n R, R)_{L^2(C_t)}$
2. $T_k(t) = (\alpha \partial_n R, u_k)_{L^2(C_t)}$ or $(\alpha \partial_n u_k, R)_{L^2(C_t)}$
3. $T_{ij} = (\alpha \partial_n u_i, u_j)_{L^2(C_t)}$ where $I_i \cap I_j \neq \varnothing$
4. $\tilde{T}_k = (\alpha \partial_n R, \tilde{u}_k)_{L^2(C_t)}$ or $(\alpha \partial_n \tilde{u}_k, R)_{L^2(C_t)}$
5. $\tilde{T}_{ij} = (\alpha \partial_n u_i, \tilde{u}_j)_{L^2(C_t)}$ or $(\alpha \partial_n \tilde{u}_i, u_j)_{L^2(C_t)}$
6. $T_i^\sharp = (\alpha \partial_n \tilde{u}_i, \tilde{u}_i)_{L^2(C_t)}$

1. Let us first consider the term $T_0(t)$. Since $R \in H^1$ and is piecewise continuous the function T_0 is integrable and continuous on $\mathbb{R}^+$ so $\lim_{t\to\infty} f(t) = 0$.

2. Then we have $T_k(t) = o(1)$ because $u_k \in L^2(C_t)$ uniformly with respect to t and $\|\nabla R\|_{L^2(C_t)}$ is continuous and belongs to $L^2(\mathbb{R}^+)$. Similarly $(\alpha \partial_n u_k, R)_{L^2(C_t)} = o(1)$.

3. First compute the gradient of u_k with respect to x. Since u_k is given by a profile depending on r, θ, x let us set $u_k(x) = U_k(r,\theta,x)$ and let us use the chain rule

$$\nabla u_k(x) = \partial_r U_k(r,\theta,x)\vec{e}_r + \frac{1}{r}\partial_\theta U_k \vec{e}_\theta + \nabla_x U_k$$

$$\nabla u_k(x) = \frac{e^{i\ell_k\cdot x}}{\sqrt{r}} \left(-\frac{c_k(\theta)}{r}\chi_k v_k \vec{e}_r + c_k(\theta)\chi_k(\nabla_x + i\ell_k)v_k + \partial_\theta(c_k\chi_k v_k)\frac{1}{r}\vec{e}_\theta \right).$$

Observe that thanks to the condition of stationary phase $\partial_\theta e^{i\ell_k(\theta)\cdot x} = 0$. Hence

$$T_{ij} = \int_{C_t} \chi_i(\theta)\chi_j(\theta)\frac{\alpha c_i \bar{c}_j}{t} e^{ix\cdot(\ell_i-\ell_j)}((\nabla_x + i\ell_i(\theta))v_i \cdot \vec{n})\bar{v}_j d\sigma + O(t^{-1}), \quad \text{where } \theta = arg(\sigma)$$

For $j \neq i$ we use the stationary phase theorem as we did in the proof of theorem 3.1 to show that the integral is of lower order. Indeed using polar coordinates the phase $\phi(\theta) = t\vec{e}_r(\theta)\cdot(\ell_i - \ell_j)$ has derivative

$$t^{-1}\phi'(\theta) = \vec{e}_\theta(\ell_i - \ell_j) + \vec{e}_r(\ell_i' - \ell_j').$$

where by definition $\ell_k'(\theta)\cdot x = 0$ for all k. Then assuming as in Theorem 2.2 that the phase is a Morse function it has at most a finite number of stationary points. Hence the integral is $O(t^{-1/2})$.

For $i = j$ let us set $p_j(x,\theta) = \alpha(x)\vec{n}(\theta)\cdot(\nabla_x + i\ell_j(\theta))v_j(x,\ell_j(\theta))\bar{v}_j(x,\ell_j(\theta))$ which we consider for any θ and x (not only for $\theta = x/|x|$). This is a periodic function with respect to x which belongs to $L^\infty(W \times I_j)$ thanks to the assumption on α. Rescaling by t we get

$$T_{jj} = \int_{S_j} \chi_j(\theta)|c_j(\theta)|^2 p_j(tx,\theta) d\sigma(x) + O(t^{-1}).$$

From [4] p.94 when t goes to infinity the latter converges to

$$\int_{I_j} \chi_j(\theta)|c_j(\theta)|^2 p_{j0}(\theta) d\theta.$$

Indeed one can uniformly approximate p_j by smooth trigonometric polynomial for which the limit holds using stationary phase theorem. Using identity (23) in Appendix and definition 4 gives the formula of the lemma.

4. First $\tilde{u}_k$ is a sum of two terms

$$\tilde{u}_k = \tilde{u}_{k1} + \tilde{u}_{k2}$$

where the second term is decaying quiker than the first for large r. So it is enough to deal with the first. To show that $\tilde{T}_k = o(1)$ we proceed as for T_k showing that $\tilde{u}_{k1}$ belongs to $L^2(C_t)$ uniformly with respect to t:

$$\|\tilde{u}_k\|^2_{L^2(C_t)} \leqslant |\tilde{c}_k|^2 \|v_k(\underline{\ell}_k)\|_\infty t^{1/3} \int_0^{2\pi} \tilde{\chi}_k^2(\theta) Ai^2(\gamma_k(\theta) t^{2/3}) d\theta.$$

Since $Ai(-\rho) \underset{+\infty}{\sim} |\rho|^{-1/4}$ the last integral is of order $t^{-1/3}$. Hence $\tilde{T}_k = o(1)$.

5. Hiding $\tilde{u}_{k2}$ in a $O(t^{-1/3})$ term we get

$$\tilde{T}_{ik} = \tilde{c}_k \int_{C_t} \frac{\alpha(x) c_i}{t^{5/6}} \chi_i(\theta)\chi_k(\theta) e^{ix\cdot(\ell_i - \underline{\ell}_k)} ((\nabla_x + i\ell_i(\theta)) v_i(x, \ell_i(\theta))\cdot \vec{n}) Ai(\gamma_k(\theta - \theta_k) t^{2/3}) \bar{v}_k(x, \underline{\ell}_k) d\sigma + O(t^{-1/3})$$

When the phase is stationnary at θ_k then the leading term has amplitude $t^{1-5/6-1/2} Ai(\gamma_k(0) t^{2/3}) = O(t^{-1/2})$. Otherwise it is $O(t^{-1})$.

6. As in step 3 we first compute

$$\nabla_x \tilde{u}_{k1} = \tilde{c}_k \tilde{\chi}_k(\theta) \frac{e^{ix\cdot\ell_k}}{r^{1/3}} Ai(\gamma_k(\theta - \theta_k) r^{2/3}) (\nabla + i\underline{\ell}_k) v_k(x, \underline{\ell}_k) + O(r^{-3/2}).$$

shifting by θ_k and setting $p_k = \alpha(x) \vec{e}_r \cdot (\nabla_x + i\ell_k) w_k \bar{w}_k$ yields

$$(\alpha \partial_n \tilde{u}_{k1}, \tilde{u}_{k1})_{L^2(C_t)} = |c_k|^2 t^{1/3} \int_0^{2\pi} \tilde{\chi}_k^2(\theta) Ai^2(t^{2/3}\gamma_k(\theta)) p_k(x, \theta) d\theta + O(t^{-1}).$$

Using again the periodicity of p_k with respect to x as in **3.** we can adapt the stationary phase method to each frequency of p_k giving an integral of size $O(t^{-1/3})$ if the phase is non stationary and $O(t^{-1/4})$ if it is stationary. So only the mean value of p_k contributes at infinity:

$$(\alpha \partial_n \tilde{u}_{k1}, \tilde{u}_{k1})_{L^2(C_t)} = |\tilde{c}_k|^2 (\beta \tilde{e}(\underline{\ell}_k), \tilde{e}(\underline{\ell}_k)) \int_0^{2\pi} \tilde{\chi}_k^2(\theta) t^{1/3} Ai^2(t^{2/3}\gamma_k(\theta)) \nabla \tilde{\lambda}(\underline{\ell}_k) \cdot \vec{e}_r(\theta) d\theta + o(1)$$

When t goes to infinite the last integral converges to $d_k \nabla \tilde{\lambda}(\underline{\ell}_k) \cdot \vec{w}$ which is positive because $d_k > 0$ and $\vec{w}$ is close to $\vec{e}_r(\theta_k)$ which is collinear and directed like $\nabla \tilde{\lambda}(\underline{\ell}_k)$. □

Proof of theorem 2.7. Take two outgoing solutions of (1) and denote by w their difference. It is an outgoing solution of $Pw = 0$. Let us still denote by c_k and $\tilde{c}_{k'}$ its asymptotic coefficients (according to (8) and (9)). Since $\nabla \tilde{\lambda}(\ell_k)\cdot n > 0$ in S_k the previous lemma implies that $c_k(\theta) = 0$ almost everywhere and $\tilde{c}_{k'} = 0$. Thus $w \in H^1(\mathbb{R}^2)$ but since the spectrum of P is purely essential from Assumption 2.5 it follows that $w = 0$. □

7 Singular Fermi levels

7.1 Nodal point

Let us denote by $\lambda_0 = k_0^2$ a point of σ_1. We claim that the resolvent $R(z) := (P-z)^{-1} : L^2_{comp} \to L^2_{loc}$ about such a point is continuous but not holomorphic, a fact that was not mentioned by [8]. Indeed let us consider (11) again which is the case of two bands meeting non critically at a single point ℓ_0 which I assume to be 0.

Then the band functions are of the form

$$\lambda_\pm(\ell) = g(\ell) \pm \sqrt{a^2(\ell) + b^2(\ell)}$$

where g, a, b are analytic, a or b do not vanish identically and the three functions vanish at ℓ_0. Note that if we consider the touching bands together this gives an arc analytic function [14], Theorem 7.2.

Next since $\lambda_\pm$ are non critical at ℓ_0 it implies that the minimal degree of Taylor's expansion of $a^2 + b^2$ has to be less or equal to two thus a or b has to be linear at first order. We thus consider the following functions

$$\lambda_\pm(\ell) = \lambda_0 \pm \sqrt{\ell_1^2 + \ell_2^{2m}}, \quad m \in \mathbb{N}^*.$$

With $z \in \mathbb{C}$ close to λ_0 the leading term of the resolvent $u_1(x,z)$ (it corresponds to $u_{1,\varepsilon}$ when $z = \lambda_0 + i\varepsilon$) reads

$$u_1(x,z) = \int_B e^{i\ell\cdot x} \left(\psi(\lambda_-(\ell)) \frac{pf_-(\ell,x)}{z - \lambda_0 + \sqrt{\ell_1^2 + \ell_2^{2m}}} + \psi(\lambda_+(\ell)) \frac{pf_+(\ell,x)}{z - \lambda_0 - \sqrt{\ell_1^2 + \ell_2^{2m}}} \right) d\ell.$$

For simplicity let us choose $\psi = 1_{[\lambda_0-\alpha,\lambda_0+\alpha]}$. Let us first consider the case $m = 1$ and use polar coordinates

$$u_1(x,z) = \int_{S^1} \int_0^\alpha e^{i\rho u\cdot x} \left(\frac{pf_-(\rho u,x)}{z - \lambda_0 + \rho} + \frac{pf_+(\rho u,x)}{z - \lambda_0 - \rho} \right) \rho d\rho du.$$

Expanding $\rho/(z - \lambda_0 \pm \rho) = \pm 1 \mp \frac{z-\lambda_0}{z-\lambda_0\pm\rho}$ gives

$$u_1(x,z) = \int_{S^1} \int_0^\alpha e^{i\rho u\cdot x} (pf_-(\rho u,x) - pf_+(\rho u,x))\, d\rho du + z \int_{S^1} \int_0^\alpha e^{i\rho u\cdot x} \left(-\frac{pf_-(\rho u,x)}{z - \lambda_0 + \rho} + \frac{pf_+(\rho u,x)}{z - \lambda_0 - \rho} \right) d\rho du$$

The stationary phase method shows that the first term belongs to $H^1(\mathbb{R}^2)$ (exactly as for w_0).

Turning to the second term from [14], Theorem 7.2 $pf_\pm$ are arc analytic functions so there is a function $qf(\rho,u,x)$ analytic with respect to ρ in a neighborhood of 0 such that

$$pf_\pm(\pm\rho u, x) = qf(\pm\rho, u, x).$$

Taking the opposite of u in the integral involving pf_- and then expressing $pf_\pm$ in terms of qf one finds that the second term in the previous expression of $u_1(x,z)$ reads

$$u_1(x,z) = z \int_{S^1} \left(\int_0^{-\alpha} g(\rho,u) d\rho + \int_0^\alpha g(\rho,u) d\rho \right) du, \qquad g(\rho,u) = e^{i\rho u\cdot x} \frac{qf(\rho,u,x)}{z - \lambda_0 - \rho}$$

This expression defines a function of $z\log(z)$ because the integrals in ρ do not combine into one integral running through 0 (similarly as in the homogeneous case). So the resolvent is indeed continuous but not holomorphic about λ_0.

Remark 7.1. *This expansion differs from the homogeneous case ($P=-\Delta$) for which the resolvent about 0 expands $R(z)=P_0\log(z)+P_1+O(z\log(z))$ where P_j are finite rank operators in $L^2(\mathbb{R}^2)$ (see [11]). One could wonder why there is such a difference thinking of 0 as a nodal point of the characteristic manifold of $-\Delta$. This is of course because the characteristic manifold is the set of (ω,ξ) (where ξ is the Fourier variable) such that $\omega=\pm|\xi|$, hence $\lambda=|\xi|^2$. So 0 belongs to σ_0 (see next paragraph).*

Now for k close to k_0 the Fermi curve contains a curve $\mathscr{C}$ which is a small circle whose curvature is proportional to $1/|k-k_0|$. In view of formula (6) taking the limit $k\to k_0$ shows that the leading term whose index is related to $\mathscr{C}$ vanishes. Thus if the Fermi level does not intersect any other band then the resolvent about λ_0 belongs to $O((z-\lambda_0)\log(z-\lambda_0))$.

For $m>1$ odd letting $\ell_2^m=y_2$ we set back to the case $m=1$ up to the jaccobian $|y_2|^{1/m-1}/m$ which is integrable about 0 even and arc-analytic. So the previous resolvent expansion holds. However the previous consideration about the curvature does not hold since it vanishes in the direction $(1,0)$ so (6) does not hold and one needs to adapt item 2 of theorem 2.2 with a higher order Airy-like function. It is very likely that the $O(1)$ term in the resolvent expansion does not vanish.

7.2 Generical critical point

Critical points do not contribute to outgoing waves since the speed vanishes at this point but such points are responsible for some singularity of the resolvent which is logarithmic in the generic 2D case. This situation has been addressed to any dimension by C. Gerard in [8] Theorem 3.6. However the generality of the quoted paper makes it difficult to understand the way the solution is computed. We thus wish to give a very short calculation to give an insight of the result of [8] when $\lambda_0\in\sigma_0$ is a non degenerated Morse critical point of λ_n at $\ell=0$. In such a case let us write λ_n as a quadratic form $\lambda_n(\ell)=\lambda_0+(A(\ell)\ell,\ell)$ where the brackets denote the scalar product in $\mathbb{R}^2$ and A is a smooth 2 by 2 matrix which does not vanish at $\ell=0$. Let us approximate ψ by the characteristic function of a small neighborhood V_0 of 0. Then choosing $\lambda_\varepsilon=\lambda_0+i\varepsilon$ we get

$$u_{1,\varepsilon}=\int_B e^{i\ell\cdot x}\frac{\psi(\ell)}{\lambda_\varepsilon-\lambda_n(\ell)}pf(\ell,x)d\ell=\int_{V_0/\sqrt{\varepsilon}}e^{i\sqrt{\varepsilon}s\cdot x}\frac{1}{i-(A(s\sqrt{\varepsilon})s,s)}pf(s\sqrt{\varepsilon},x)ds.$$

For ε small and $0<\alpha<1/2$ the main contribution reads

$$pf(0,x)\int_{V_0/\varepsilon^\alpha}\frac{1}{i-(A(0)s,s)}ds.$$

Whatever the signature of $A(0)$ the integral diverges like $\mathrm{O}(\ln(\varepsilon))$ as ε goes to zero. If one replaces λ_ε by λ in a complex neighborhood of λ_0 and considers v_0 as a function of λ one readily sees that v_0

is a 2-sheaves analytic function diverging logarithmically at λ_0. This corresponds to the expression of the outgoing resolvent given in [8] Corollary 4.2 where one branch of the resolvent expands as follows

$$(P-\lambda)^{-1} = E_0(\lambda) + C\ln(\lambda-\lambda_0)(M(\lambda_0) + (\lambda-\lambda_0)E_1(\lambda))$$

where C is a constant, M is a finite dimensional operator and E_j are holomorphic operators about λ_0.

8 Greater dimensions

When the dimension d is greater than 2 the set of points of crossing in a Fermi level is generically of dimension $d-2$. One can still use (4) since the latter set is negligible in the Fermi Level. So if for a Fermi level there is only normal crossing then one can straightforwardly extend Theorem 2.1, 2.2 and 2.3.

From [14] the set of points of singular crossing is a $d-2$ dimensional set so we expect σ_1 to be of non zero Lebesgue mesure and needs to be considered for every k. Theorem 7.2 of [14] says that in this case there are blowing ups with smooth centers such that crossing eigenvalues become analytic. So theoretically one can compute u as in paragraph 7.1.

Appendix

A Floquet-Bloch transform and Sobolev spaces

Let $f \in \mathcal{S}(\mathbb{R}^2)$ (Schwarz space). Then its Floquet-Bloch transform defined by

$$\hat{f}(x,\ell) = \sum_{n\in\mathbb{Z}^2} f(x+2\pi n)e^{-i\ell\cdot(x+2\pi n)}$$

is periodic with respect to x and quasi-periodic with respect to ℓ:

$$\hat{f}(x,\ell+a_j) = e^{ix\cdot a_j}\hat{f}(x,\ell),$$

where $a_j,\ j\in\{1,2\}$ are the unit vectors. Then the inverse Floquet-Bloch transform reads

$$f(x) = \int_B e^{i\ell\cdot x}\hat{f}(x,\ell)d\ell.$$

The Floquet-Bloch transform extends by density to $f\in L^2(\mathbb{R}^2)$ and Parceval identity holds so that $\hat{f}\in L^2(W\times B)$ and

$$\|f\|_{L^2(\mathbb{R}^2)} = \|\hat{f}\|_{L^2(B\times W)}.$$

Then the identity $\widehat{(\partial_{x_j}f)}(x,\ell) = (\partial_{x_j}+i\ell_j)\hat{f}(x,\ell)$ for $j\in\{1,2\}$ entails that there is a constant $c>1$ such that

$$\frac{1}{c}\|f\|_{H^n(\mathbb{R}^2)} \leqslant \|\hat{f}\|_{L^2(B,H^n(W))} \leqslant c\|f\|_{H^n(\mathbb{R}^2)}.$$

Here we used the notation

$$L^2(B, H^n(W)) := \{h \in L^2(W \times B),\ \partial_\ell^j h \in L^2(W \times B),\ j \in \{1, \dots, n\}\}.$$

Finally the identity $\widehat{(x_j f)}(x, \ell) = \partial_{\ell_j} \hat{f}(x, \ell)$ for $j \in \{1, 2\}$ implies

$$\| |x|^n f \|_{L^2(\mathbb{R}^2)} \leqslant c \| \hat{f} \|_{L^2(W; H^n(B))},$$

where $L^2(W; H^n(B))$ is defined in a similar way as $L^2(B; H^n(W))$.

B Analyticity of the Bloch variety

Let us recall briefly Kuchment's results [13] about the analyticity of $\mathcal{B}$. For elliptic operators of the form $T := \sum_{|\alpha| \leqslant 2m} b_\alpha(x) \partial^\alpha$ with smooth coefficients b_α, Theorem 3.1.7 ([13]) shows the analyticity of $\mathcal{B}$. Thanks to the smoothness of the coefficients one can use a parametrix which allows to show that the operator $T(\ell)$ resulting from the application of the Floquet-Bloch transform to T and acting on $H^2(B)$ is Fredholm with null index.

Here our operator $P(\ell)$ is of divergence form and with non smooth coefficients. We cannot make use of a parametrix as used in [13] but Theorem 3.1.7 mainly requires a holomorphic family of Fredholm operators with null index (see p. 118). The opertor $P(\ell)$ is Fredholm because it is of compact resolvent type (standard use of Lax-Milgram Lemma and analytic Fredholm theorem) from $H(W)$ to $L^2(W)$ with

$$H(W) = \{u \in H^1_{per}(W), \alpha(\nabla u + i\ell) \in H_{div}(W)\}$$

where $H_{div}(W)$ is the subspace of $L^2(W)$ of W-periodic functions whose divergence belongs to $L^2(W)$.

Then since $P(\ell)$ is symmetric for real ℓ its deficiency index is zero.

The proof of Theorem 3.1.7 needs to be changed because $P(\ell)$ does not map Sobolev spaces to themselves. Moreover the domain of $P(\ell)$ (as operator) depends on ℓ since it requires that $\alpha(\nabla + i\ell)$ belongs to $H_{div}(W)$. We thus consider $p(\ell)$ the associated sesquilinear form on $H^1(W)$ which we expand:

$$p(\ell)(u, v) = (\alpha \nabla u, \nabla v)_2 + i\ell \{(\alpha u, \nabla v)_2 - (\alpha \nabla u, v)_2\} + \ell^2 (\alpha u, v)_2, \qquad u, v \in H^1(W).$$

We decompose it as a sum of three forms $p(\ell) = p_0 + i\ell p_1 + (\ell^2 - 1) p_2$ with

$$p_0(u, v) = (\alpha \nabla u, \nabla v)_2 + (\alpha u, v)_2, \quad p_1(u, v) = (\alpha u, \nabla v)_2 - (\alpha \nabla u, v)_2, \quad p_2(u, v) = (\alpha u, v)_2.$$

Since p_1 is not sectorial on $L^2(W)$ we consider those forms as bounded forms on $H^1_{per}(W, \alpha)$. By Riesz-lemma there are associated operators P_0, P_1 and P_2 defined on $H^1_{per}(W, \alpha)$ endowed with the scalar product p_0. Those operators thus satisfy $p_0(P_j u, v) = p_j(u, v)$. In particular $P_0 = Id$. Then denoting by $\tilde{P}(\ell)$ the operator associated to $p(\ell)$ we have

$$\tilde{P}(\ell) = I + i\ell P_1 + (\ell^2 - 1) P_2 \quad \text{and observe that } ker(P(\ell)) \subset ker(\tilde{P}(\ell)).$$

Thus it is enough to prove Theorem 3.1.7 replacing $P(\ell)$ by $\tilde{P}(\ell)$. One thus only needs to prove that P_j are Schatten class operators on $H^1_{per}(W,\alpha)$. This is greatly eased by making use of the operator $S^2 := (P(0)+\alpha)^{-1}$ for which there holds

$$p_0(S^2u,v) = p_0(Su,Sv) = (u,v)_2, \quad \text{and} \quad P_2 = S^2\alpha.$$

Lemma B.1. *S is a Schatten class operator in $H^1_{per}(W,\alpha)$.*

Proof. First S is compact because if we take a bounded sequence $u_n \in H^1_{per}(W,\alpha)$ then by Rellich theorem there is a subsequence (still denoted by u_n) such that u_n converges to some u in $L^2(W)$. Then let us show that Su_n converges in $H^1_{per}(W,\alpha)$. We have

$$\|S(u_n-u)\|^2_{H^1_{per}(W,\alpha)} = p_0(S(u_n-u),S(u_n-u)) = \|u_n-u\|_2^2$$

which converges to zero.

Then showing that S is a Schatten class operator can be achieved by comparing S to $\tilde{S} := (1-\Delta)^{-1/2}$ which is so in $H^1_{per}(W,1)$. This a simple use of minmax principle. □

As a consequence P_2 is a Schatten class operator.

Lemma B.2. *P_1 is a Schatten class operator of order $p > 2$.*

Proof. Let us split $P_1 = P_{11} - P_{12}$ with

$$p_{11}(u,v) = (\alpha u, \nabla v)_2, \quad \text{and} \quad p_{12}(u,v) = (\alpha\nabla u, v)_2$$

one cannot easily represent P_{11} and show that it is compact. However we remark that $P_{11} = P_{12}^*$. Indeed

$$p_0(P_{11}u,v) = p_{11}(u,v) = (\alpha u,\nabla v)_2 = \bar{p}_{12}(v,u) = p_0(u,P_{12}v).$$

Then remarking that $P_{12} = S^2\alpha\nabla$ one sees that it is a Schatten class operator since $S\alpha\nabla$ is bounded on $H^1_{per}(W,\alpha)$. Then so is P_{11} by duality.

□

C Estimates in Bloch space

The following lemma gives an upper bound for the slope of the real Bloch variety. The calculation is reminiscent of geometric optics [6] and links the gradient of the band function with the metric. It proves in particular that nodal points of the Bloch variety are not cusps.

Lemma C.1. *For all $n > 1$*

$$\|\nabla\sqrt{\lambda_n}\|_{L^\infty(B)} \leqslant \max\alpha/\min\beta. \tag{22}$$

Proof. Let us expand $P(\ell)$:

$$\beta P(\ell) = (\mathrm{div} + i\ell)\alpha(\nabla + i\ell) = \mathrm{div}\alpha\nabla + i\ell(\nabla\alpha + \alpha\nabla) - |\ell|^2.$$

Setting $P_1 = \nabla\alpha + \alpha\nabla$ and then differentiating the relation $P(\ell)e_n(\ell) = -\beta\lambda_n(\ell)e_n(\ell)$ with respect to ℓ we get

$$(P(\ell) - \lambda_n(\ell))\nabla_\ell e_n(\ell) + ((iP_1 + 2\ell\alpha) + \beta\nabla\lambda_n(\ell))e_n(\ell) = 0.$$

Scalarly multiplying by $e_n(\ell)$ which is orthogonal to the first term and a unit vector of $L^2(W)$ gives:

$$\nabla\lambda_n(\ell)(\beta e_n, e_n) = -((iP_1 + 2\ell\alpha)e_n, e_n) = 2\Im(\alpha(\nabla + i\ell)e_n, e_n) \tag{23}$$

Half of the last factor is bounded by $\|\alpha(\nabla + i\ell)e_n\|_2$ which is bounded by α times $\|\sqrt{\alpha}(\nabla + i\ell)e_n\|_2 = \sqrt{(P(\ell)e_n, e_n)} = \sqrt{\lambda_n}$. □

D Scatering expansion under glancing/grazing Bloch vector

Pseudo-differential calculus has been carried out by Melrose and Taylor (see [17]). Here, in this basic scattering approach we only need [10] for adapatation of the stationary phase theorem.

Let us resume notations from begining paragraph 5. Denote by $\ell_{t*} = \partial_t\ell(t_*)$ and let $\delta\theta$ be the angle between x and the orthogonal of ℓ_{t*}. Also let $\vec{u} = x/|x|$ and denote by $\vec{u}_* = \vec{u}(\delta\theta = 0)$. Finally put $\delta t = t - t_*$. Taylor expansion of ℓ with integral remainder about t_* leads

$$\varphi(\delta t, \delta\theta) = \ell_* \cdot \vec{u} + \vec{u} \cdot \vec{\ell}_{t*}(\delta t + a(\delta t)^2) + (\delta t)^3\vec{u} \cdot \vec{g}(\delta t), \quad \vec{u}_* \cdot \vec{g}(0) \neq 0.$$

The coefficient a is a scale factor between $\partial_t\ell(t_*)$ and $\partial_t^2\ell(t_*)$ since they are collinear. When $\delta\theta = 0$ there holds $\vec{u}_* \cdot \vec{\ell}_{t*} = 0$ so using the variable T_* given by the substitution $T_* = \delta t\sqrt[3]{3\vec{u}_* \cdot \vec{g}(\delta t)}$ the phase reads

$$\varphi(\delta t, \delta\theta = 0) = \ell_* \cdot \vec{u} + \frac{T_*^3}{3}.$$

From [10] there is a change of variable $T = T(T_*, \delta\theta)$ with $T = T_*$ for $\delta\theta = 0$ such that the phase reads

$$\varphi(\delta t, \delta\theta) = a(\theta) + b(\theta)T + \frac{T^3}{3} \quad \text{with} \quad a(\theta_*) = \ell_* \cdot \vec{u}_*, \quad \text{and} \quad b(\theta_*) = 0$$

To find T, a, b just write

$$\varphi(\delta t, \theta) = \ell_* \cdot \vec{u} + (\vec{u} \cdot \vec{\ell}_{t*})T_*h(T_*) + m(\theta, T_*)\frac{T_*^3}{3}, \quad m(\theta, T_*) = \frac{\vec{u} \cdot \vec{\tilde{g}}(T_*)}{\vec{u}_* \cdot \vec{\tilde{g}}(T_*)}$$

where $\sqrt[3]{3\vec{u}_* \cdot \vec{g}(0)}h(0) = 1$. Taking $a = \ell_* \cdot \vec{u}$ and $b = \vec{u} \cdot \vec{\ell}_{t*}h(0)$ we see that T is solution of a third degree polynomial equation which has a unique solution for $T \approx T_*$ small since

$$T\left(b(\theta) + \frac{T^2}{3}\right) = T_*\left((b(\theta)\frac{h(T_*)}{h(0)} + m(\theta, T_*)\frac{T_*^2}{3}\right).$$

Hence $dT/dT_*(T_*=0)=1$.

Using this substitution in the integral g_+, and following Hormander's proof of Theorem 7.7.18 one finds

$$(24)\quad g_+ = 2\pi\frac{e^{ix\cdot\ell_*}}{r^{1/3}}\left(Ai\left(\frac{x\cdot\ell_{t*}}{r^{1/3}\sqrt[3]{3\vec{u}_*\cdot\vec{g}(0)}}\right)w_*(x)+\frac{1}{r^{1/3}}Ai'\left(\frac{x\cdot\ell_{t*}}{r^{1/3}\sqrt[3]{3\vec{u}_*\cdot\vec{g}(0)}}\right)\tilde{w}_*(x)\right)+O\left(\frac{1}{r^{3/2}}\right)$$

where w_* (resp. $\tilde{w}_*$) is the zeroth (resp. first) order Taylor expansion in the variable T of the integrand in g_+ (after $t\to T$ substitution). One thus finds

$$(25)\qquad \begin{aligned} w_*(x) &= \sqrt[3]{3\vec{u}_*\cdot\vec{g}(0)}(\hat{f}(\ell_*),v(\ell_*))_{L^2(W)}\frac{|\partial_t\ell(t_*)|}{|\nabla\mu(\ell_*)|}v(\ell_*,x)\\ \tilde{w}_*(x) &= \frac{1}{i}\frac{d}{dt}\left((\hat{f}(\ell),v(\ell))_{L^2(W)}\frac{|\partial_t\ell|}{|\nabla\mu(\ell)|}\frac{d\delta t}{dT}v(\ell,x)\right)(t=t_*)\end{aligned}$$

References

[1] G. B. Airy. On the intensity of light in the neighborhood of a caustic. *Transactions of the Cambridge philisophical society*, 4(3):378–392, 1836.

[2] G. Allaire, C. Conca, and M. Vanninathan. The bloch transform and applications. *ESAIM: Proc.*, 3, 1998.

[3] A. Bamberger, J.C. Guillot, and P. Joly. Numerical diffraction by an uniform grid. *SIAM Journal on Numerical Analysis*, 25(4):753–784, 1988.

[4] A. Bensoussan, J.L. Lions, and G. Papanicolaou. *Asymptotic analysis for periodic structures.* North-Holland, 1978.

[5] M. Sh. Birman and T. A. Suslina. Periodic magnetic hamiltonian with variable metric. the problem of absolute continuity. *Algebra i Analiz*, 11(2):1–40, 1999.

[6] P. Donnat and J. Rauch. Dispersive nonlinear geometric optics. *Journal of Mathematical Physics*, 38(3):1484–1523, 1997.

[7] S. Fliss and P. Joly. Solutions of the time-harmonic wave equation in periodic waveguides: Asymptotic behaviour and radiation condition. *Archive for Rational Mechanics and Analysis*, 219:349–386, 2016.

[8] C. Gérard. Resonance theory for periodic Schrödinger operators. *Bulletin de la Société Mathématique de France*, 118(1):27–54, 1990.

[9] V. Hoang. The limiting absorption principle for a periodic semi-infinite waveguide. *SIAM Journal on Applied Mathematics*, 71(3):791–810, 2011.

[10] L. Hörmander. *The Analysis of Linear Partial Differential Operators*. Number vol. 1 in Grundlehren der mathematischen Wissenschaften. Springer-Verlag, 1990.

[11] A. Jensen and G. Nenciu. A unified approach to resolvent expansions at thresholds. *Reviews in Mathematical Physics*, 13:717–754, 2001.

[12] T. Kato. *Perturbation theory for linear operators; 2nd ed.* Springer, Berlin, 1976.

[13] P. Kuchment. *Floquet Theory for partial differential operators*, volume 37. 1982.

[14] K. Kurdyka and L. Paunescu. Hyperbolic polynomials and multiparameter real-analytic perturbation theory. *Duke Mathematical Journal*, 141(1):123 – 149, 2008.

[15] Y. Li and L. Nirenberg. Estimates for elliptic systems from composite material. *Communications on Pure and Applied Mathematics*, 56:892 – 925, 07 2003.

[16] R. B. Melrose. *Geometric scattering theory*. Standford Lectures. Cambridge University Press, 1995.

[17] R.B. Melrose and M. Taylor. *Boundary Problems for the Wave Equation with Grazing and Gliding Rays*. preprint, 1987.

[18] G. Metivier and K. Zumbrun. Hyperbolic Boundary Value Problems for Symmetric Systems with Variable Multiplicities. *Journal of Differential Equations*, 211:61–134, 2005.

[19] M. Murata and T. Tsuchida. Asymptotics of Green functions and the limiting absorption principle for elliptic operators with periodic coefficients. *Journal of Mathematics of Kyoto University*, 46(4):713 – 754, 2006.

[20] F. Pham. *X. L'analyticité des intégrales dépendant de paramètres*. EDP Sciences, 2021.

[21] M. Radosz. New limiting absorption and limit amplitude principles for periodic operators. *Zeitschrift für angewandte Mathematik und Physik*, 66:253–275, 02 2015.

[22] M. Reed and B. Simon. *Analysis of Operators, Vol. 4*. Methods of Modern Mathematical Physics. Academic Press, 1978.

[23] F. Rellich. *Perturbation Theory of Eigenvalue Problems*. Courant Institute of Mathematical Sciences, New York University. 1954.

[24] Andrey V. Shanin, Raphaël C. Assier, Andrey I. Korolkov, and Oleg I. Makarov. A note on double floquet-bloch transforms and the far-field asymptotics of green's functions tailored to periodic structures. *Arxiv*, 2024.

[25] J. Souček and V. Souček. Morse-sard theorem for real-analytic functions. *Commentationes Mathematicae Universitatis Carolinae*, 13(1):45–51, 1972.

[26] J. Wang, S. Deng, Z. Liu, and Z. Liu. The rare two-dimensional materials with dirac cones. *National Science Review*, 2(1):22–39, 2015.

[27] H. Whitney. Tangents to an analytic variety. *Annals of Mathematics*, 81(3):496–549, 1965.

[28] C. H. Wilcox. Steady-state wave propagation in homogeneous anisotropic media. *Archive for Rational Mechanics and Analysis*, 25:201–242, 1967.

[29] C. H. Wilcox. Theory of bloch waves. *Journal d'Analyse Mathématique*, 33:146–167, 1978.