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ELEMENTARY LINEAR ALGEBRA FOR ADVANCED SPECTRAL PROBLEMS

by Johannes SJÖSTRAND & Maciej ZWORSKI

ABSTRACT. — We describe a simple linear algebra idea which has been used in different branches of mathematics such as bifurcation theory, partial differential equations and numerical analysis. Under the name of the Schur complement method it is one of the standard tools of applied linear algebra. In PDE and spectral analysis it is sometimes called the Grushin problem method, and here we concentrate on its uses in the study of infinite dimensional problems, coming from partial differential operators of mathematical physics.

RÉSUMÉ. — Nous décrivons une idée simple d'algèbre linéaire, qui a été utilisée dans différentes branches des mathématiques, telles que la théorie des bifurcations, les équations aux dérivées partielles et l'analyse numérique. Sous le nom de la méthode des compléments de Schur c'est un des outils standard de l'algèbre linéaire appliquée. En e.d.p. et en analyse spectrale elle est parfois appelée la méthode des problèmes de Grushin, et ici nous nous concentrons sur son utilisation dans l'étude des problèmes en dimension infinie, venant des équations aux dérivées partielles de la physique mathématique.

1. Introduction

The purpose of this article is to discuss a simple linear algebraic tool which has proved itself very useful in the mathematical study of spectral problems arising in electromagnetism and quantum mechanics. Roughly speaking it amounts to replacing an operator of interest by a suitably chosen invertible system of operators.

That approach has a very long tradition and appears constantly under different names and guises in many works of pure and applied mathematics. Our purpose here is not to provide a historical survey but to present an

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account of a specific approach from a personal perspective of the authors. On one hand we hope to provide a source of systematic references for the practitioners of our type of spectral theory and, hopefully, to convince others of the usefulness of this method. We do not know, but find very interesting, if the method which has proved itself so successful in theoretical studies has a chance of being useful numerically.

The key elementary observation goes back — at least — to Schur and his *complement* formula: if for matrices

$$\begin{pmatrix} P & R_- \\ R_+ & 0 \end{pmatrix}^{-1} = \begin{pmatrix} E & E_+ \\ E_- & E_{-+} \end{pmatrix},$$

then P is invertible if and only if E_{-+} is invertible and

$$(1.1) \quad P^{-1} = E - E_+ E_{-+}^{-1} E_-, \quad E_{-+}^{-1} = -R_+ P^{-1} R_-.$$

In fact the equivalence of invertibilities of P and E_{-+} holds for systems with a nonzero lower right hand corner (see Lemma 3.1) but since here we always start with P and choose R_{\pm} we can normally consider these simpler systems. Sometimes, in the context of index theory one considers operators P which are never invertible. In that case the index of P is equal the index of E_{-+} which is trivial to compute if E_{-+} is a matrix — see §2.4.

In the study of linear partial differential equations the use of enlarged systems appeared in Grushin's work [8] on hypoelliptic operators. In a different context they were used in the thesis of the first author [19] and the \pm notation comes from there — see §2.2 for an explanation in the context of linear algebra. As is seen there it is essential that the system is allowed to be non-self-adjoint ^(†). For that historical, if somewhat personal reason, we refer to the problem

$$(1.2) \quad \begin{cases} Pu + R_- u_- = v \\ R_+ u = v_+ \end{cases}$$

$$P : H_1 \rightarrow H_2, \quad R_- : H_- \rightarrow H_2, \quad R_+ : H_1 \rightarrow H_+,$$

as a *Grushin problem*. If it is invertible, we call it *well posed* and we write its inverse as follows

$$(1.3) \quad \begin{pmatrix} u \\ u_- \end{pmatrix} = \begin{pmatrix} E & E_+ \\ E_- & E_{-+} \end{pmatrix} \begin{pmatrix} v \\ v_+ \end{pmatrix}.$$

(†) That distinguishes it from the KKT (for Karush-Kuhn-Tucker) systems popular in numerical studies — see for instance [6] — which seem to be related to §2.1 below.

In this case we will refer to E_{-+} as the *effective Hamiltonian* of P . That effective Hamiltonian normally has its own physical interpretation as will be seen in examples in §§2.5, 5.3 and 5.4.

To illustrate this by a straightforward example consider an operator $P : L^2(\mathbb{R}^n) \rightarrow L^2(\mathbb{R}^n)$ defined as a convolution, $Pu = K \star u$, with $\widehat{K} \in L^\infty(\mathbb{R}^n)$. We can take $H_\pm = L^2(\mathbb{R}^n)$ and put $R_-u_-(x) = -(2\pi)^{-n}\widehat{u}_-(-x)$, the negative of the inverse Fourier transform, and $R_+u(\xi) = \widehat{u}(\xi)$. One easily checks that the resulting Grushin problem is well posed and that E_{-+} is given by multiplication by \widehat{K} . This of course is the effective Hamiltonian for the convolution operator which is invertible on L^2 if and only if $\widehat{K}^{-1} \in L^\infty$.

The main difficulty in constructing useful Grushin problems is the choice of suitable operators R_\pm and of the spaces on which they act. As will be illustrated below that depends on the situation even though one can notice some underlying principles.

The paper is organized as follows. In §2 we present in detail several simple examples showing different ways of constructing Grushin problems. In §3 we review basic linear algebra techniques which are useful when studying Grushin problems arising in spectral theory. In §3.5 we also show a typical parameter dependent estimate. Trace formulæ which are central in the study of classical/quantum correspondence are the subject of §4: we give the basic idea in the context of Grushin problems and use it to prove the Poisson summation formula, in a way which lends itself to many generalizations. Finally, in §5 we describe — without proofs — four advanced examples: a remark on Lidskii-Lusternik-Vishik perturbation theory for matrices [16], [18], the Peierls substitution of solid state physics (from the work of Helffer and the first author [11]), the quantum monodromy approach to the Gutzwiller trace formula, and the asymptotics of scattering poles in electromagnetic scattering by convex bodies (from earlier work of the authors [23], [22]). It would be very hard to survey all the examples in which the Grushin problem appears explicitly — not to mention, those in which it appears implicitly — and we again made some personal choices.

Acknowledgments. — We would like to thank Steve Zelditch for suggesting a talk on Grushin problems during the semi-classical semester at MSRI: this paper is a direct result of that. We are grateful to Michael Overton for the references to Lidskii’s perturbation theory which are the basis of §5.1, and to Michael Hutchings and John Lott for a helpful discussion leading to a simple proof of Proposition 4.2. We are also particularly indebted to Mark Embree whose comments and valuable criticisms eliminated many mistakes in the paper and increased its breadth and readability.

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2. Simple examples

We give five examples. The first two are purely linear algebraic and the third and fifth are intended to show how well known objects in mathematical physics fit in the Grushin problem set up. The fourth example relates Grushin problems to analytic Fredholm theory which is one of the basic tools of spectral theory.

2.1. The Moore-Penrose pseudoinverse

If $P : \mathbb{C}^n \rightarrow \mathbb{C}^m$ is a linear transformation, its Moore-Penrose pseudoinverse is the *unique* transformation $P^+ : \mathbb{C}^m \rightarrow \mathbb{C}^n$ satisfying

$$(2.1) \quad \begin{aligned} PP^+P &= P, & P^+PP^+ &= P^+, \\ (PP^+)^* &= PP^+, & (P^+P)^* &= P^+P. \end{aligned}$$

If P has full rank then

$$P^+ = \begin{cases} (P^*P)^{-1}P^*, & n \leq m \\ P^*(PP^*)^{-1}, & n \geq m \end{cases}.$$

In general P^+ can be expressed by using the standard singular value decomposition $P = U\Sigma V^*$, and inverting the *nonzero* entries in Σ . It is closely related to *least square problems* — see [1, Lecture 11].

Another way to describe the pseudoinverse is as

$$P^+ = (P|_{\ker(P)^\perp})^{-1} \pi_{\operatorname{im}(P)},$$

where π_V is the orthogonal projection on the subspace V , since $P|_{\ker(P)^\perp} : \ker(P)^\perp \rightarrow \operatorname{im}(P)$ is bijective.

The pseudoinverse is a special case of E in (1.3), with $H_1 = \mathbb{C}^n$, $H_2 = \mathbb{C}^m$, and for a natural choice of R_\pm , related to the least squares method. Before describing it, let us give a general statement relating the Grushin problem to (2.1):

PROPOSITION 2.1. — *In the notation of (1.2) and (1.3) we always have*

$$EPE = E,$$

and

$$(R_-E_-)^2 = R_-E_-, \quad (E_+R_+)^2 = E_+R_+,$$

that R_-E_- and E_+R_+ are always projections. In addition the following equivalences hold:

$$\begin{aligned} PEP = P &\iff E_-P = 0 \\ (PE)^* = PE &\iff (R_-E_-)^* = R_-E_- \\ (EP)^* = EP &\iff (E_+R_+)^* = E_+R_+. \end{aligned}$$

In particular, when the conditions on the left hold, $E = P^+$, in the sense that the equations in (2.1) are satisfied.

We can now choose R_{\pm} so that the conditions in Proposition 2.1 are satisfied. For that we simply put

$$\begin{aligned} H_- &= P(H_1)^\perp, \quad H_+ = \ker(P) \\ R_- : H_- &= P(H_1)^\perp \hookrightarrow H_2, \quad R_+ : H_1 \xrightarrow{\perp} \ker(P) = H_+. \end{aligned}$$

This is generalized in §3.6 in order to take into account small eigenvalues of $(P^*P)^{\frac{1}{2}}$ and $(PP^*)^{\frac{1}{2}}$.

Following a suggestion of Mark Embree, we rephrase this linear algebraic example in terms of matrices. Thus let $r = \text{rank}(P)$, and set

$$H_- = \mathbb{C}^{m-r} \simeq \ker(P^*), \quad H_+ = \mathbb{C}^{n-r} \simeq \ker(P).$$

Define $R_- \in M_{m,m-r}(\mathbb{C})$ to have columns that form an orthonormal basis for $\ker(P^*)$, and define $R_+ \in M_{n-r,n}(\mathbb{C})$ such that the columns of R_+^* form an orthonormal basis of $\ker(P)$. This choice of R_- and R_+ makes the Grushin problem (1.2) invertible, and leads to

$$E = P^+, \quad E_+ = R_+^*, \quad E_- = R_-^*, \quad E_{-+} = 0.$$

We note that E_+R_+ and R_-E_- are orthogonal projections for $\ker(P)$ and $\ker(P^*)$ respectively.

2.2. Non-self-adjoint eigenvalue problems

Let J be the $n \times n$ upper triangular Jordan matrix:

$$J = (J_{ij})_{1 \leq i, j \leq n}, \quad J_{ij} = \begin{cases} 1 & \text{for } j = i + 1 \\ 0 & \text{otherwise.} \end{cases}$$

Let

$$e_+ = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad e_- = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}.$$

Then $Je_+ = 0$, $J^*e_- = 0$, $\|e_\pm\| = 1$, and we can set up the following well posed Grushin problem for $\lambda - J$:

$$\mathcal{J}(\lambda) = \begin{pmatrix} \lambda - J & R_- \\ R_+ & 0 \end{pmatrix} : \mathbb{C}^n \oplus \mathbb{C} \longrightarrow \mathbb{C}^n \oplus \mathbb{C},$$

$$R_-u_- = u_-e_-, \quad R_+u = \langle u, e_+ \rangle,$$

where $\langle \bullet, \bullet \rangle$ denotes the standard Hermitian inner product on \mathbb{C}^n . One easily checks that $E_{-+}(\lambda) = \lambda^n$, and that

$$(2.2) \quad E_+v_+ = v_+e_+(\lambda), \quad E_-v = \langle v, e_-(\bar{\lambda}) \rangle,$$

$$e_+(\lambda) = \begin{pmatrix} 1 \\ \lambda \\ \vdots \\ \lambda^{n-1} \end{pmatrix}, \quad e_-(\lambda) = \begin{pmatrix} \lambda^{n-1} \\ \vdots \\ \lambda \\ 1 \end{pmatrix}.$$

If we add a small matrix perturbation, ϵQ to J the same problem remains well posed and, using a Neumann series argument for matrices (see Proposition 3.6 for a proof),

$$E_{-+}^\epsilon(\lambda) = E_{-+}(\lambda) + \sum_{k=1}^\infty (-1)^k \epsilon^k E_-(\lambda) Q (E(\lambda) Q)^{k-1} E_+(\lambda),$$

with uniform convergence for $|\lambda| \leq \theta < 1$ and $\epsilon \leq \epsilon_0$, for some $\epsilon_0 > 0$. Using (2.2) we consequently see that

$$(2.3) \quad E_{-+}^\epsilon(\lambda) = \lambda^n - \epsilon \langle Qe_+(\lambda), e_-(\bar{\lambda}) \rangle + \mathcal{O}(\epsilon^2).$$

Hence when n is large and $|\lambda| < 1$ there will be no spectrum near λ for a generic perturbation Q . This is illustrated in Figure 2.1. The most dramatic perturbation is obtained by taking Q with a large inner product $\langle Qe_+, e_- \rangle$.

This example is a linear algebraic model of the first author’s thesis [19] where the $-+$ notation was introduced. It was motivated by the sign in Hörmander’s commutator condition — see [20] and also [27] for a light-hearted introduction. It is reflected here by the fact that

$$(2.4) \quad [J, J^*]e_\pm = \pm e_\pm, \quad [J, J^*] = JJ^* - J^*J.$$

This example will be revisited in a more general context in §3.5.

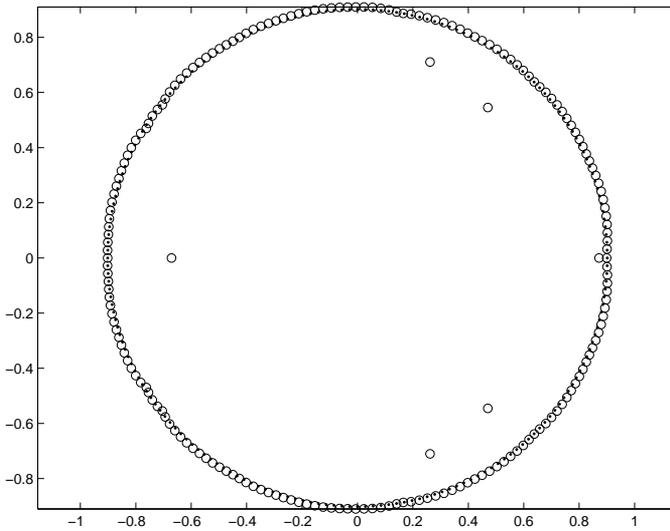


Figure 2.1. Eigenvalues of a small random perturbation of a 200×200 Jordan block matrix (\circ) and of the perturbation $Q = \epsilon e_- \otimes e_+$, $\epsilon = 10^{-9}$ (\cdot). Since the latter lie on the circle of radius $10^{-9/200}$ they are “masked” by the eigenvalues of the random perturbation. An estimate on the number of eigenvalues of a random perturbation not escaping to the boundary, that is the \circ inside the disc, has been recently given by Davies and Hager [3].

2.3. Feshbach method

The Feshbach method which has been useful in the study of quantum resonances fits in the framework of Grushin problems discussed in this paper. To review it we follow [4] and we refer to that paper for pointers to the vast literature on the subject.

Suppose that a Hilbert space \mathcal{H} can be written as a direct sum $\mathcal{H} = \mathcal{H}^v \oplus \mathcal{H}^{\bar{v}}$, and that the operator whose spectrum we want to study decomposes under this splitting as

$$H = \begin{pmatrix} H^{vv} & H^{v\bar{v}} \\ H^{\bar{v}v} & H^{\bar{v}\bar{v}} \end{pmatrix}.$$

Assume now that for $z \in \Omega$, an open set in \mathbb{C} , the operator $(z\mathbb{1}^{\bar{v}\bar{v}} - H^{\bar{v}\bar{v}})$ is invertible. Following [4] we define the resonance function

$$G_v(z) = z\mathbb{1}^{vv} - H^{vv} - H^{v\bar{v}}(z\mathbb{1}^{\bar{v}\bar{v}} - H^{\bar{v}\bar{v}})^{-1}H^{\bar{v}v},$$

which, in classical terminology reviewed in §1 is just the Schur complement of $z\mathbb{1}^{\bar{v}\bar{v}} - H^{\bar{v}\bar{v}}$ in $z - H$.

It then follows, by block Gaussian elimination, that for $z \notin \sigma(H^{\bar{v}\bar{v}})$

$$z \in \sigma(H) \iff 0 \in \sigma(G_v(z)),$$

and moreover it can be verified directly that

$$(2.5) \quad \text{tr} \int_{\gamma_z} (\zeta - H)^{-1} d\zeta = \text{tr} \int_{\gamma_z} \partial_\zeta G_v(\zeta) G_v(\zeta)^{-1} d\zeta,$$

$$\gamma_z(t) = z + \epsilon e^{it}, 0 \leq t \leq 2\pi,$$

that is, the multiplicities agree.

To see how the Schur complement, and hence also the Feshbach method, fit in the Grushin scheme we consider the following larger operator

$$\mathcal{P}(z) = \begin{pmatrix} z - H & R_- \\ R_+ & 0 \end{pmatrix} : \mathcal{D} \oplus \mathcal{H}^v \longrightarrow \mathcal{H} \oplus \mathcal{H}^v,$$

$$R_+ = (\mathbb{1}^{vv} \quad \mathbf{0}^{v\bar{v}}), \quad R_- = \begin{pmatrix} \mathbb{1}^{v\bar{v}} \\ \mathbf{0}^{\bar{v}v} \end{pmatrix}.$$

If $z\mathbb{1}^{\bar{v}\bar{v}} - H^{\bar{v}\bar{v}}$ is invertible then this problem is well posed and Gaussian elimination shows that

$$E_{-+}(z) = -(z\mathbb{1}^{vv} - H^{vv}) + H^{v\bar{v}}(z\mathbb{1}^{\bar{v}\bar{v}} - H^{\bar{v}\bar{v}})^{-1}H^{\bar{v}v} = -G_v(z).$$

The multiplicity formula follows from general principles described in §3.1 but of course it is easy enough to verify directly.

We should stress that converting a linear eigenvalue problem for a matrix H to a nonlinear eigenvalue problem for the *smaller* matrix $G(\lambda)$ is a basis of much numerical linear algebra, developed independently of the work in mathematical physics.

2.4. Analytic Fredholm theory

Here we recall the discussion of the appendix in [10]. For the basic facts from functional analysis we refer to [7] for an in-depth treatment and to [14, Sect.19.1] for a comprehensive introduction.

A bounded operator $P : H_1 \rightarrow H_2$ between two Banach spaces, is called a Fredholm operator if the kernel of P ,

$$\ker P \stackrel{\text{def}}{=} \{u \in H_1 : Pu = 0\},$$

and the cokernel of P ,

$$\text{coker } P \stackrel{\text{def}}{=} H_2 / \{Pu \in H_2 : u \in H_1\},$$

are finite dimensional. It then automatically follows (see for instance [14, Lemma 19.1.1] or the comment after the proof of Proposition 2.2) that PH_1 is closed. For Fredholm operators the index is defined as

$$\text{ind } P = \dim \ker P - \dim \text{coker } P.$$

We have the following

PROPOSITION 2.2. — *Suppose that for some choice of R_{\pm} the Grushin problem (1.2) is well posed. Then $P : H_1 \rightarrow H_2$ is a Fredholm operator if and only if $E_{-+} : H_+ \rightarrow H_-$ is a Fredholm operator, and*

$$\text{ind } P = \text{ind } E_{-+}.$$

Proof. — As for all well posed Grushin problems we have that R_+ , E_- are surjective, and E_+ , R_- are injective.

The equations $Pu = v$, $u_- = 0$ are equivalent to

$$(2.6) \quad u = Ev + E_+v_+, \quad 0 = E_-v + E_{-+}v_+, \quad v_+ = R_+u.$$

This means that

$$E_- : \text{im } P \longrightarrow \text{im } E_{-+},$$

and we can define the induced map

$$E_-^\sharp : H_2/\text{im } P \longrightarrow H_-/\text{im } E_{-+}.$$

Since E_- is surjective, so is E_-^\sharp . Also, $\ker E_-^\sharp = \{0\}$, since if $E_-v \in \text{im } E_{-+}$ then we use (2.6) to see that $v \in \text{im } P$. Hence E_-^\sharp is a bijection of cokernels.

On the other hand,

$$E_+ : \ker E_{-+} \longrightarrow \ker P$$

is a bijection. In fact, if $u \in \ker P$ then $u = E_+v_+$ and $E_{-+}v_+ = 0$ and the map is onto, which is all we need to check as E_+ is always injective.

We conclude that

$$(2.7) \quad \dim \text{coker } P = \dim \text{coker } E_{-+}, \quad \dim \ker P = \dim \ker E_{-+}.$$

In particular the indices are equal. □

For Fredholm operators we can always take H_{\pm} to be finite dimensional: let $n_+ = \dim \ker P$ and $n_- = \dim \text{coker } P$ and choose

$$R_- : \mathbb{C}^{n_-} \longrightarrow H_2, \quad R_+ : H_1 \longrightarrow \mathbb{C}^{n_+},$$

of maximal rank and such that

$$R_-(\mathbb{C}^{n_-}) \cap \text{im } P = \{0\}, \quad \ker(R_+ \upharpoonright_{\ker P}) = \{0\}.$$

In that case $E_{-+} : \mathbb{C}^{n_-} \rightarrow \mathbb{C}^{n_+}$ and its index is, of course, $n_+ - n_-$. This argument also shows that the index does not change under continuous Fredholm deformations of P , and that PH_1 is closed: by Banach's open mapping theorem the operators E_\bullet in (1.3) (constructed using linear algebra only) are continuous.

The following standard result is proved particularly nicely using the Grushin problem framework:

PROPOSITION 2.3. — *Suppose that for $z \in \Omega \subset \mathbb{C}$, a connected open set, $A(z)$ is a family of Fredholm operators depending holomorphically on z . If $A(z_0)^{-1}$ exists at a point $z_0 \in \Omega$, then $\Omega \ni z \mapsto A(z)^{-1}$ is a meromorphic family of operators.*

Proof. — Let $z_0 \in \Omega$ and let $V(z_0)$ be a small neighbourhood of z_0 . We can then form a Grushin problem for $P = A(z_0)$ as described before the statement of the proposition. The same $R_\pm^{z_0}$ give a well posed Grushin problem for $P = A(z)$ for $z \in V(z_0)$, if $V(z_0)$ is sufficiently small. Since the index $A(z)$ is equal to zero we see that $n_+ = n_- = n$ and $E_{-+}^{z_0}(z)$ is an $n \times n$ matrix with holomorphic coefficients. The invertibility of $E_{-+}^{z_0}(z)$ is equivalent to the invertibility of $A(z)$.

This shows that there exists a locally finite covering of Ω , $\{\Omega_j\}$, such that for $z \in \Omega_j$, $A(z)$ is invertible precisely when $f_j(z) \neq 0$, where f_j is holomorphic in Ω_j . Since Ω is connected and since $A(z_1)$ is invertible for at least one $z_1 \in \Omega$ shows that all f_j 's are not identically zero.

That means that $\det E_{-+}(z)$ is a non-vanishing holomorphic function in $V(z_0)$ and consequently $E_{-+}(z)^{-1}$ is a meromorphic family of matrices. Applying (1.1) we conclude that

$$A(z)^{-1} = E(z) - E_+(z)E_{-+}(z)^{-1}E_-(z)$$

is a meromorphic family of operators in $V(z_0)$, and since z_0 was arbitrary, in Ω . □

2.5. Boundary value problems

Let P be an elliptic second order operator on a compact manifold, X , with an orientable smooth boundary, ∂X . For the simplest example we could take $P = -\partial_x^2 + V(x)$ on $[a, b]$, in which case all the objects below are easily described.

We want to pose a Grushin problem for the Dirichlet realization of P :

$$P_D u = f \in L^2(X), \quad u|_{\partial X} = 0.$$

We then put

$$\mathcal{H} = H^2(X) \cap H_0^1(X), \quad \mathcal{H}_- = H^{\frac{3}{2}}(\partial X), \quad \mathcal{H}_+ = H^{\frac{1}{2}}(\partial X).$$

Let $T : H^{\frac{3}{2}}(\partial X) \rightarrow H^2(X)$ be an extension operator, with the following properties:

$$Tv|_{\partial X} = v, \quad \partial_\nu Tv|_{\partial X} = 0,$$

where ∂_ν is the outward normal differentiation at ∂X . The operator T can, for instance, be obtained by introducing normal geodesic coordinates (x, y) in a collar neighbourhood of ∂X , $y \in \partial X$, and putting

$$Tv(x, y) = \chi(x) \exp(x^2 \Delta_{\partial X})v(y), \quad -\Delta_{\partial X} \geq 0,$$

where $\chi \in C_c^\infty([0, \delta])$, $\chi \equiv 1$, near 0.

We then define

$$(2.8) \quad \begin{aligned} R_- : \mathcal{H}_- &\longrightarrow \mathcal{H}, & R_+ : \mathcal{H} &\longrightarrow \mathcal{H}_+ \\ R_- u_- &\stackrel{\text{def}}{=} -PTu_-, & R_+ u &\stackrel{\text{def}}{=} \partial_\nu u|_{\partial X}. \end{aligned}$$

If we denote by P_N the Neumann realization of P ,

$$P_N u = f \in L^2(X), \quad \partial_\nu u|_{\partial X} = 0,$$

we have

PROPOSITION 2.4. — *With R_\pm defined by (2.8) the Grushin problem for P_D is well posed when P_N^{-1} exists. The effective Hamiltonian is given by the Neumann-to-Dirichlet map:*

$$E_{-+} = N, \quad N : \partial_\nu u|_{\partial X} \longmapsto u|_{\partial X}, \quad Pu = 0,$$

where the existence of N is guaranteed by the invertibility of P_N .

Proof. — We can write (1.3) explicitly using the Green operator, $G_N \stackrel{\text{def}}{=} P_N^{-1}$, and the Poisson operator:

$$Q_N f = u, \quad Pu = 0, \quad \partial_\nu u|_{\partial X} = f.$$

It can be easily constructed from P_N^{-1} .

Using this notation we have

$$\begin{aligned} Ev &= G_N v + T((G_N v)|_{\partial X}) \\ E_- v &= (G_N v)|_{\partial X} \\ E_+ v_+ &= Q_N v_+ + TNv_+ \\ E_{-+} v_+ &= (Q_N v_+)|_{\partial X} \end{aligned}$$

A direct verification proves the surjectivity. To prove injectivity we see that injectivity of P_N gives

$$P(u - Tu_-) = 0, \quad \partial_\nu(u - Tu_-) = 0 \implies u - Tu_- = 0.$$

Since $u \upharpoonright_{\partial X} = 0$ this shows that $u_- = Tu_- \upharpoonright_{\partial X} = 0$, and hence $u = 0$, as well. □

A more systematic approach and one related to another use of two-by-two systems [2], [14, Sect.20.4] can be described as follows. Suppose that $P : C^\infty(X) \rightarrow C^\infty(X)$ is an elliptic operator of order m , and that we have two sets of boundary differential operators, with transversal orders $< m$,

$$\begin{aligned} B_j &: C^\infty(X) \rightarrow C^\infty(\partial X), & j &= 1, \dots, J, \\ C_k &: C^\infty(X) \rightarrow C^\infty(\partial X), & k &= 1, \dots, K. \end{aligned}$$

For instance we can consider $P = \Delta$, $B_1u = \partial_\nu u \upharpoonright_{\partial X}$, $C_1u = u \upharpoonright_{\partial X}$, $J = K = 1$.

We want to study the boundary problem

$$(2.9) \quad Pu = f \quad \text{in } X, \quad C_k u = h_k \quad \text{in } \partial X, \quad k = 1, \dots, K,$$

assuming that the boundary problem

$$(2.10) \quad Pu = f \quad \text{in } X, \quad B_j u = g_k \quad \text{in } \partial X, \quad j = 1, \dots, J,$$

is well posed. To avoid technical issues involving Sobolev spaces (see [14, Chapter 20]) we will remain in the C^∞ category. We then put:

$$\begin{aligned} \mathcal{H}_1 &= C^\infty(X), & \mathcal{H}_2 &= C^\infty(X) \otimes C^\infty(\partial X)^K, \\ \mathcal{H}_- &= C^\infty(\partial X)^K, & \mathcal{H}_+ &= C^\infty(\partial X)^J, \end{aligned}$$

writing

$$u_- = \begin{pmatrix} u_-^1 \\ \vdots \\ u_-^K \end{pmatrix} \in \mathcal{H}_-, \quad v = \begin{pmatrix} v_X \\ v_{\partial X}^1 \\ \vdots \\ v_{\partial X}^K \end{pmatrix} \in \mathcal{H}_2,$$

and define

$$(2.11) \quad Qu \stackrel{\text{def}}{=} \begin{pmatrix} Pu \\ C_1u \\ \vdots \\ C_Ku \end{pmatrix}, \quad R_-u_- \stackrel{\text{def}}{=} \begin{pmatrix} 0 \\ u_-^1 \\ \vdots \\ u_-^K \end{pmatrix}, \quad R_+u \stackrel{\text{def}}{=} \begin{pmatrix} B_1u \\ \vdots \\ B_Ju \end{pmatrix}.$$

We have the following *formal*

PROPOSITION 2.5. — *Suppose that the boundary value problem (2.10) is well posed. Then the Grushin problem*

$$Qu + R_-u_- = v, \quad R_+u = v_+,$$

obtained using the operators (2.11) is well posed and the effective Hamiltonian,

$$E_{-+} : C^\infty(\partial X)^J \rightarrow C^\infty(\partial X)^K$$

is a generalization of the Neumann-to-Dirichlet map:

$$(2.12) \quad E_{-+} : \begin{pmatrix} v_+^1 \\ \vdots \\ v_+^J \end{pmatrix} \mapsto \begin{pmatrix} C_1 u \\ \vdots \\ C_K u \end{pmatrix}, \quad Pu = 0, \quad B_j u = v_+^j, \quad j = 1, \dots, J.$$

For boundary value problems one of the basic issues is showing that, on suitably chosen spaces, the operator $u \mapsto (Pu, C_1 u, \dots, C_k u)$ has the Fredholm property. By Proposition 2.2 that is equivalent to showing the Fredholm property of the operator (2.12). The reduction to the boundary described in Proposition 2.5 will furnish us with another example in §3.3.

3. Basic techniques

Here we present some general results about systems arising from considering *Grushin problems* and examples showing how they can be used. We recall that a Grushin problem for an operator $P : H_1 \rightarrow H_2$ is a system

$$(3.1) \quad \begin{cases} Pu + R_- u_- = v \\ R_+ u = v_+ \end{cases}$$

where $R_- : H_- \rightarrow H$, $R_+ : H \rightarrow H_+$. In matrix form we can write

$$\mathcal{P} \stackrel{\text{def}}{=} \begin{pmatrix} P & R_- \\ R_+ & 0 \end{pmatrix} : H_1 \oplus H_- \longrightarrow H_2 \oplus H_+.$$

We say that the Grushin problem is *well posed* if we have the inverse

$$\mathcal{E} = \begin{pmatrix} E & E_+ \\ E_- & E_{-+} \end{pmatrix} : H_2 \oplus H_+ \longrightarrow H_1 \oplus H_-,$$

that is

$$(3.2) \quad \begin{pmatrix} u \\ u_- \end{pmatrix} = \begin{pmatrix} E & E_+ \\ E_- & E_{-+} \end{pmatrix} \begin{pmatrix} v \\ v_+ \end{pmatrix}.$$

In this case we will refer to E_{-+} as the *effective Hamiltonian* of P .

3.1. Two by two systems

Here we consider an invertible system

$$(3.3) \quad \begin{aligned} \mathcal{A} &\stackrel{\text{def}}{=} \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} : H_1 \oplus H_2 \longrightarrow \tilde{H}_1 \oplus \tilde{H}_2, \\ \mathcal{B} &\stackrel{\text{def}}{=} \mathcal{A}^{-1} = \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix} : \tilde{H}_1 \oplus \tilde{H}_2 \longrightarrow H_1 \oplus H_2. \end{aligned}$$

We first recall the formula involving an expression known as the *Schur complement* in linear algebra and as the *Feshbach operator* in mathematical physics:

LEMMA 3.1. — *Suppose that A_{22} is invertible. Then B_{11} is invertible, and*

$$(3.4) \quad B_{11}^{-1} = A_{11} - A_{12}A_{22}^{-1}A_{21}.$$

Proof. — Using $B_{11}A_{11} + B_{12}A_{21} = I$ and $B_{11}A_{12} = -B_{12}A_{22}$ we see that

$$B_{11}A_{11} - B_{11}A_{12}A_{22}^{-1}A_{21} = I - (B_{12} + B_{11}A_{12}A_{22}^{-1})A_{21} = I,$$

and the left inverse property is derived similarly. □

We now allow the entries of \mathcal{A} to depend on a parameter, and denote differentiation with respect to that parameter by $A \mapsto \dot{A}$. The next lemma explicitly shows that the traces of $\dot{B}_{11}B_{11}^{-1}$ and $\dot{A}_{22}A_{22}^{-1}$ differ by terms not involving any inverses. In the case of holomorphic dependence on the parameter that means that these traces differ by holomorphic terms which disappear in contour integration. Before stating this precisely let us recall some basic facts about trace class operators — see [7] or [14, Sect.19.1].

If H_j are infinite dimensional Hilbert spaces, the operator $A : H_1 \rightarrow H_2$ is said to be of *trace class* if the self-adjoint operator $(AA^*)^{\frac{1}{2}} : H_2 \rightarrow H_2$ has a discrete spectrum, $\{\mu_j\}_{j=1}^\infty$, and $\sum_{j=1}^\infty \mu_j < \infty$. If A is of trace class, and $B_1 : H_1 \rightarrow H_1$, $B_2 : H_2 \rightarrow H_2$ are bounded operators then AB_1 and B_2A are of trace class.

If $H = H_1 = H_2$ and A is of trace class we can define the *trace* of A as follows. Let $\{e_j\}_{j=1}^\infty$ be an orthonormal basis of H , then

$$\text{tr } A = \text{tr}_H A \stackrel{\text{def}}{=} \sum_{j=1}^\infty \langle Ae_j, e_j \rangle_H,$$

and this definition is independent of the choice of a basis.

Finally, if $A : H_1 \rightarrow H_2$ is of trace class and $B : H_2 \rightarrow H_1$ is bounded then AB and BA are both of trace class and

$$(3.5) \quad \text{tr}_{H_1} BA = \text{tr}_{H_2} AB.$$

In particular, if $H=H_1=H_2$ then under the same assumptions $\text{tr}[A, B]=0$.

LEMMA 3.2. — *Let \mathcal{A} and \mathcal{B} be as in (3.3). Suppose that the operators \dot{A}_{ij} are of trace class. Then, when A_{22} is invertible, we have*

$$(3.6) \quad \text{tr } B_{11}^{-1} \dot{B}_{11} = \text{tr } A_{22}^{-1} \dot{A}_{22} - \text{tr } \dot{\mathcal{A}}\mathcal{B}.$$

Here the traces are taken in \tilde{H}_1 , H_1 , and $\tilde{H}_1 \oplus \tilde{H}_2$, respectively.

Proof. — This is a straightforward computation based on the formulæ, $\mathcal{A}\mathcal{B} = I$, $\dot{\mathcal{B}} = -\mathcal{B}\dot{\mathcal{A}}\mathcal{B}$, cyclicity of the trace, and Lemma 3.1 (we note that all \dot{B}_{ij} , and in particular \dot{B}_{11} , are of trace class). We obtain

$$\begin{aligned} \text{tr } B_{11}^{-1} \dot{B}_{11} &= \text{tr } A_{22}^{-1} \dot{A}_{22} + \text{tr } E_1 + \text{tr } E_2, \\ E_1 &= -\dot{A}_{11}B_{11} - \dot{A}_{12}B_{21} : \tilde{H}_1 \longrightarrow \tilde{H}_1, \\ E_2 &= -\dot{A}_{21}B_{12} - \dot{A}_{22}B_{22} : \tilde{H}_2 \longrightarrow \tilde{H}_2, \end{aligned}$$

and

$$\text{tr } E_1 + \text{tr } E_2 = -\text{tr } \dot{\mathcal{A}}\mathcal{B} = \text{tr } \dot{\mathcal{A}}\dot{\mathcal{B}}.$$

□

The relevance of this discussion for Grushin problems (which in principle have $B_{22} = 0$) will become apparent in the next subsection.

3.2. From one Grushin problem to another

Suppose that we have a well posed Grushin problem (1.2) with the inverse given by (1.3).

We want to check if another Grushin problem is well posed:

$$(3.7) \quad \begin{cases} Pu + \tilde{R}_- \tilde{u}_- = \tilde{v} \\ \tilde{R}_+ \tilde{u} = \tilde{v}_+ \end{cases}$$

The corresponding operator will be denoted by $\tilde{\mathcal{P}} : H_1 \oplus \tilde{H}_- \rightarrow H_2 \oplus \tilde{H}_+$. If the inverse exists we will denote it by $\tilde{\mathcal{E}}$, with the corresponding notation for the entries.

The simple answer is given in

PROPOSITION 3.3. — *The Grushin problem (3.7) is well posed if and only if the following system of operators obtained from the solution (1.3) of the well posed problem (1.2),*

$$(3.8) \quad \mathcal{G} = \begin{pmatrix} -\tilde{R}_+ E \tilde{R}_- & \tilde{R}_+ E_+ \\ -E_- \tilde{R}_- & E_{-+} \end{pmatrix},$$

is invertible, that is if and only if the matrix of operators has a two sided inverse. In that case

$$(3.9) \quad \mathcal{G}^{-1} = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix} \tilde{\mathcal{G}} \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix},$$

where

$$\tilde{\mathcal{G}} = \begin{pmatrix} -R_+ \tilde{E} R_- & R_+ \tilde{E}_+ \\ -\tilde{E}_- R_- & \tilde{E}_{-+} \end{pmatrix}.$$

Proof. — In place of (3.7) we can consider a larger system

$$\begin{cases} Pu + R_- u_- + \tilde{R}_- \tilde{u}_- = \tilde{v} \\ R_+ u = v_+, \\ \tilde{R}_+ u = \tilde{v}_+ \end{cases}$$

in which \tilde{v} , \tilde{v}_+ , and u_- are given, and u , \tilde{u}_- , and v_+ are unknown. We can solve (3.7) by putting $u_- = 0$. Using (1.3) we can write

$$(3.10) \quad \begin{aligned} u &= E(\tilde{v} - \tilde{R}_- \tilde{u}_-) + E_+ v_+ \\ u_- &= E_-(\tilde{v} - \tilde{R}_- \tilde{u}_-) + E_{-+} v_+, \end{aligned}$$

or, since $\tilde{R}_+ u = \tilde{v}_+$,

$$\begin{aligned} \tilde{R}_+ E_+ v_+ - \tilde{R}_+ E \tilde{R}_- \tilde{u}_- &= \tilde{v}_+ - \tilde{R}_+ E \tilde{v} \\ E_{-+} v_+ - E_- \tilde{R}_- \tilde{u}_- &= u_- - E_- \tilde{v}. \end{aligned}$$

which in turn can be rewritten as

$$\mathcal{G} \begin{pmatrix} \tilde{u}_- \\ v_+ \end{pmatrix} = \begin{pmatrix} \tilde{v}_+ - \tilde{R}_+ E \tilde{v} \\ u_- - E_- \tilde{v} \end{pmatrix}.$$

Hence the invertibility of \mathcal{G} implies that (3.7) is well posed. In fact, we first obtain \tilde{u}_- by inverting \mathcal{G} and then u by using the first equation in (3.10). When $\tilde{v} = 0$ we see that

$$\mathcal{G} \begin{pmatrix} \tilde{u}_- \\ v_+ \end{pmatrix} = \begin{pmatrix} \tilde{v}_+ \\ u_- \end{pmatrix},$$

from which the equivalence and (3.9) follow. □

We illustrate Proposition 3.3 with an example which is also the basis for §4.2 below. Let us consider

$$(3.11) \quad P = P(z) \stackrel{\text{def}}{=} hD_x - z, \quad x \in \mathbb{S}^1 \stackrel{\text{def}}{=} \mathbb{R}/(2\pi\mathbb{Z}).$$

We formulate a Grushin problem as in [23, Sect.2] where it was motivated by [12]. For that we want to find $R_{\pm}(z)$ so that

$$(3.12) \quad \mathcal{P}(z) \stackrel{\text{def}}{=} \begin{pmatrix} P - z & R_-(z) \\ R_+(z) & 0 \end{pmatrix} : H^1(\mathbb{S}^1) \times \mathbb{C} \longrightarrow L^2(\mathbb{S}^1) \times \mathbb{C},$$

is invertible. Rather than give the answer in a “deus ex machina” manner we follow our original reasoning. First, a boundary condition

$$R_+u \stackrel{\text{def}}{=} u(0),$$

is a natural choice. Then we can locally solve

$$\begin{cases} (P - z)u = 0 \\ R_+u = v \end{cases},$$

by putting

$$u = I_+(z)v = \exp(izx/h)v, \quad -\epsilon < x < 2\pi - 2\epsilon.$$

This is the forward solution, and we can also define the backward one by

$$u = I_-(z)v = \exp(izx/h)v, \quad -2\pi + 2\epsilon < x < \epsilon.$$

The monodromy operator $M(z, h) : \mathbb{C} \rightarrow \mathbb{C}$, can be defined by

$$(3.13) \quad I_+(z)v(\pi) = I_-(z)M(z, h)v(\pi),$$

and we immediately see that

$$M(z, h) = \exp(2\pi iz/h).$$

We use $I_{\pm}(z)$ and the point π to work with objects defined on \mathbb{S}^1 rather than on its cover: a more intuitive definition of $M(z, h)$ can be given by looking at a value of the solution after going around the circle.

Let $\chi \in C^\infty(\mathbb{S}^1, [0, 1])$ have the properties

$$\chi(x) \equiv 1, \quad -\epsilon < x < \pi + \epsilon, \quad \chi(x) \equiv 0, \quad -\pi + 2\epsilon < x < -2\epsilon,$$

and put

$$E_+(z) = \chi I_+(z) + (1 - \chi)I_-(z).$$

We see that

$$(P - z)E_+ = [P, \chi]I_+(z) - [P, \chi]I_-(z) = [P, \chi]_-I_+(z) - [P, \chi]_-I_-(z),$$

where $[P, \chi]_-$ denotes the part of the commutator supported near π . This can be simplified using (3.13):

$$(i/h)(P - z)E_+ + (i/h)[P, \chi]_- I_-(z)(I - M(z, h)) = 0,$$

which suggests putting

$$R_-(z) = (i/h)[P, \chi]_- I_-(z),$$

so that the problem

$$\begin{cases} (P - z)u + R_-(z)u_- = 0 \\ R_+(z)u = v \end{cases}$$

has a solution:

$$\begin{cases} u = E_+(z)v \\ u_- = E_{-+}(z)v \end{cases},$$

with $E_{-+}(z) = I - M(z, h)$. In fact, it is much more natural, and easier for full-blown microlocal generalizations, to consider a different $R_+(z)$ so that, with symmetry reminiscent of §2.2,

$$(3.14) \quad \begin{aligned} R_-(z)u_- &= u_- e_-(z), & R_+(z)u &= \langle u, e_+(z) \rangle, \\ e_{\pm}(z, x) &= (i/h)[P, \chi]_{\pm}(\exp(i \bullet z/h))(x). \end{aligned}$$

One can show that with this choice of $R_{\pm}(z)$, (3.12) is invertible and then

$$\mathcal{P}(z)^{-1} = \mathcal{E}(z) = \begin{pmatrix} E(z) & E_+(z) \\ E_-(z) & E_{-+}(z) \end{pmatrix},$$

where all the entries are holomorphic in z , and $E_+(z)$, $E_{-+}(z)$, are as above. The operator $E_{-+}(z)$ is the effective Hamiltonian in the sense that its invertibility controls the existence of the resolvent:

$$(3.15) \quad (P - z)^{-1} = E(z) - E_+(z)E_{-+}(z)^{-1}E_-(z).$$

The invertibility is independent of χ with the properties described above. Hence we can move to a singular limit in the choice of χ and deform π to 0. That means that we consider the following Grushin problem (with suitably modified spaces):

$$\begin{cases} (i/h)(hD_x - z)u(x) - \delta_0(x)u_- = v(x) \\ u(0+) = v_+ \end{cases}.$$

In fact, we can write

$$u = E(z)v + E_+(z)v_+, \quad u_- = E_-(z)v + E_{-+}(z)v_+,$$

where

$$\begin{aligned}
 E(z)v(x) &= \mathbb{1}_{[0,2\pi[} \int_0^x \exp(i(x-y)z/h)v(y)dy, \\
 E_+(z)v_+ &= v_+ \exp(ixz/h) \mathbb{1}_{[0,2\pi[, \\
 E_-(z)v &= -\exp(2\pi iz/h) \int_0^{2\pi} \exp(-iyz/h)v(y)dy, \\
 E_{-+}(z) &= 1 - \exp(2\pi iz/h).
 \end{aligned}
 \tag{3.16}$$

We finally come to an application of Proposition 3.3. In (3.14) it would be nice to be able to take $e_-(z) = e_+(z)$, that is to have a self-adjoint Grushin problem. That would also simplify matters in more complicated situations. Hence suppose that

$$e_{\pm}(z, x) = f(x) \exp(ixz/h).$$

We then have to consider the invertibility of the matrix \mathcal{G} in Proposition 3.3 — * which here is an honest 2×2 matrix. A brief calculation shows that for $z \in \mathbb{R}$, \mathcal{G} is equal to

$$\begin{pmatrix} -A & \overline{B} \\ e^{2\pi iz/h} B & 1 - e^{2\pi iz/h} \end{pmatrix}, \quad A = \int_0^{2\pi} \int_0^x \overline{f(x)} f(y) dy dx, \quad B = \int_0^{2\pi} f(x) dx,$$

and we observe that $|B|^2 = A + \overline{A}$.

Hence the condition for invertibility becomes

$$\operatorname{Re}(Ae^{-\pi iz/h}) \neq 0,$$

and that will always be violated for some $z \in \mathbb{R}$. Hence we cannot have a well posed Grushin problem for all $z \in \mathbb{R}$ with $e_- = e_+$ in (3.14).

3.3. Iterated problems

The Grushin problems can be iterated and this is particularly important when the intermediate Grushin problems are *formal* and only after one or more iterations we obtain a well posed problem. An example of a useful formal problem will be given in §5.2.

Before giving an example of that we start with the following simple

PROPOSITION 3.4. — *Suppose that (1.2) is well posed with the inverse given by (1.3). If*

$$\begin{pmatrix} E_{-+} & N_- \\ N_+ & 0 \end{pmatrix} : H_+ \oplus V_- \longrightarrow H_- \oplus V_+$$

is invertible, with the inverse

$$\mathcal{F} = \begin{pmatrix} F & F_+ \\ F_- & F_{-+} \end{pmatrix},$$

then the new Grushin problem

$$\begin{pmatrix} P & R_- N_- \\ N_+ R_+ & 0 \end{pmatrix} : H \oplus V_- \longrightarrow H \oplus V_+,$$

is well posed with the inverse given by

$$\begin{pmatrix} E - E_+ F E_- & E_+ F_+ \\ F_- E_- & -F_{-+} \end{pmatrix}.$$

Proof. — We need to solve

$$\begin{aligned} Pu + R_- N_- u_- &= v, \\ N_+ R_+ u &= v_+ \end{aligned}$$

Putting $N_- u_- = \tilde{u}_-$, and $R_+ u = \tilde{v}_+$, we obtain

$$\begin{aligned} Pu + R_- \tilde{u}_- &= v, \\ R_+ u &= \tilde{v}_+ \end{aligned}$$

which is solved by taking

$$\begin{aligned} u &= Ev + E_+ \tilde{v}_+, \\ \tilde{u}_- &= E_- v + E_- \tilde{v}_+ \end{aligned}$$

Recalling the definitions of \tilde{u}_- and \tilde{v}_+ this becomes

$$\begin{pmatrix} E_{-+} & N_- \\ N_+ & 0 \end{pmatrix} \begin{pmatrix} \tilde{v}_+ \\ -u_- \end{pmatrix} = \begin{pmatrix} -E_- v \\ v_+ \end{pmatrix}.$$

Solving this using \mathcal{F} gives the lemma. □

We will mention one concrete example for which iterated Grushin problems are useful. In the notation of Proposition 2.5 consider for X an open set in \mathbb{R}^{n+1} , with a smooth boundary Ω , and put $Pu = \Delta u$, $B_1 u = u|_\Omega$, and $C_1 u = Vu|_\Omega$, $K = J = 1$, where V is a vectorfield. If V is not everywhere transversal to Ω we obtain the *oblique derivative problem* and the operator (2.12) is not elliptic and not self-adjoint. As in [19] one can then construct a new Grushin problem for that operator using the structure of the set where V is not transversal to Ω . A “baby” version of that type of problem was presented on the level of matrices in §2.2.

3.4. A Grushin approximation scheme

Let H be a Hilbert space, and H_0 a finite dimensional subspace with an orthonormal basis $\{e_j\}_{j=1}^N$. Let us introduce

$$R_+ : H \rightarrow \mathbb{C}^N, \quad R_- = R_+^* : \mathbb{C}^N \rightarrow H,$$

given by

$$(R_+u)_j = \langle u, e_j \rangle, \quad R_-u_- = \sum_{j=1}^N u_{-,j}e_j.$$

We want to consider the Grushin problem for the operator

$$P = I - T, \quad T : H \rightarrow H.$$

In many interesting situations we can reduce the study of a differential operator to the study of $I - T$ by factoring out an invertible term.

The following lemma is related to the example presented in §2.1:

LEMMA 3.5. — *Let π be the orthogonal projection on the span of e_j 's. With the operators R_{\pm} given above, and $P = (1 - \pi T)$ the problem (1.2) is well posed, and the matrix (1.3) is given by*

$$(3.17) \quad \begin{pmatrix} E^0 & E_+^0 \\ E_-^0 & E_{-+}^0 \end{pmatrix} = \begin{pmatrix} 1 - \pi & R_- \\ R_+(I + T(1 - \pi)) & R_+TR_- - 1 \end{pmatrix}.$$

Proof. — We observe that

$$(3.18) \quad R_-R_+ = \pi, \quad R_+R_- = \text{Id}_{\mathbb{C}^N}, \quad \pi R_- = R_-, \quad R_+\pi = R_+,$$

which leads to an immediate verification of (3.17). □

We can now consider the problem for $1 - T$ and we have

PROPOSITION 3.6. — *If $\|(1 - \pi)T\| < \delta < 1$ then the Grushin problem (1.2) with $P = 1 - T$ and R_{\pm} as in Lemma 3.5, is well posed, and the effective Hamiltonian has the following expansion:*

$$E_{-+} = E_{-+}^0 + \sum_{k=1}^{\infty} R_+T((1 - \pi)T)^k R_-.$$

Proof. — This is a typical Neumann series argument. Using Lemma 3.5, and writing $I - T = I - \pi T - (I - \pi)T$ we see that

$$\begin{pmatrix} I - T & R_- \\ R_+ & 0 \end{pmatrix} = \begin{pmatrix} I - \pi T & R_- \\ R_+ & 0 \end{pmatrix} \left(\text{Id}_{H \oplus \mathbb{C}^N} - \begin{pmatrix} (I - \pi)T & 0 \\ R_+T(I - \pi)T & 0 \end{pmatrix} \right),$$

where we used (3.18) to multiply

$$\begin{pmatrix} 1 - \pi & R_- \\ R_+(I + T(1 - \pi)) & R_+TR_- - 1 \end{pmatrix} \begin{pmatrix} (I - \pi)T & 0 \\ 0 & 0 \end{pmatrix}.$$

Hence

$$\begin{pmatrix} E & E_+ \\ E_- & E_{-+} \end{pmatrix} = \sum_{k=0}^{\infty} \begin{pmatrix} (I-\pi)T & 0 \\ R_+T(I-\pi)T & 0 \end{pmatrix}^k \begin{pmatrix} 1-\pi & R_- \\ R_+(I+T(1-\pi)) & R_+TR_- - 1 \end{pmatrix}.$$

Since

$$\begin{pmatrix} A & 0 \\ B & 0 \end{pmatrix}^k = \begin{pmatrix} A^k & 0 \\ BA^{k-1} & 0 \end{pmatrix},$$

we immediately obtain the formula for E_{-+} . □

The difficulty with the approximation scheme described here is the need for an orthonormal basis. In practice that is rarely given in theoretical and, especially, numerical problems. To some extent that can be remedied as follows.

We replace the condition on the smallness of $(I-\pi)T$ by a different condition. We assume that there exists a finite set, $\{e_j\}_{j=1}^M$, with the following property:

$$(3.19) \quad \forall u \in H, \exists t_j \in \mathbb{C}, r \in H,$$

$$Tu = \sum_1^M t_j e_j + r, \quad \|r\| \leq \delta \|u\|, \quad \frac{1}{C} \|Tu\| \leq \|\vec{t}\|_{\ell^2} \leq C \|Tu\|.$$

As before we would like to construct a well posed (in the sense that its stability constant is controlled, not just that it is invertible) Grushin problem for $I - T$.

First, we need to modify the spanning set, $\{e_j\}_{j=1}^M$. For that we introduce the Grammian matrix,

$$G \stackrel{\text{def}}{=} (\langle e_i, e_j \rangle)_{1 \leq i, j \leq M}.$$

It is positive semi-definite and hence can be diagonalized. We then can, after a unitary (in \mathbb{C}^M) “reorganization”, assume that $\{e_j\}$ satisfy

$$\langle e_i, e_j \rangle = \delta_{ij} \lambda_j, \quad \lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_M \geq 0.$$

Suppose that $\lambda_j > (\epsilon/C)^2$ for $j \leq L$. The condition number, $\|G\| \|G^{-1}\|$, of the Grammian, G , for $\{e_j\}_{j=1}^L$ is now bounded by $C^2 \max |\lambda_j|/\epsilon^2$ so we can use G , and its inverse, to form a well posed Grushin problem. For that we change e_j to $e_j/\sqrt{\lambda_j}$, and denote by π the *orthogonal projection* onto the span of e_j 's. We easily see the following

LEMMA 3.7. — *Condition (3.19) implies*

$$\|(1-\pi)T\| \leq \delta + \epsilon \|T\|.$$

Proof. — In the notation of (3.19) we write

$$\tilde{r} = \sum_{j=L+1}^M t_j e_j + r,$$

and

$$\|Tu - \sum_{j=1}^L t_j e_j\| = \|\tilde{r}\| \leq \delta \|u\| + \left(\sum_{L+1}^M \lambda_j |t_j|^2 \right)^{\frac{1}{2}}.$$

Since $\lambda_j \leq \epsilon^2/C^2$, and $\|\tilde{t}\|_{\ell^2} \leq C\|Tu\|$ the estimate follows. □

We can now proceed as in Proposition 3.6.

3.5. A typical estimate

Specific application of the Grushin problem scheme — see for instance §5 — involve estimates, often depending on a parameter. We would like to illustrate this in a situation loosely related to the approximation scheme described in §3.4, and more concretely to the example in §2.2.

Let us assume that $P = P(h) : \mathcal{H} \rightarrow \mathcal{H}$ is a bounded operator. Suppose that there exist two orthogonal projections $\pi_{\pm} = \pi_{\pm}(h) : \mathcal{H} \rightarrow \mathcal{H}$ satisfying

$$\begin{aligned} (3.20) \quad & \|P^* \pi_{-}\|, \|P \pi_{+}\| = \mathcal{O}(h), \\ & \|\pi_{-} P(I - \pi_{+})\| = o(h), \quad \|\pi_{+} P^*(I - \pi_{-})\| = o(h), \\ & \|P(I - \pi_{+})u\| \geq h\|(I - \pi_{+})u\|, \quad \|P^*(I - \pi_{-})u\| \geq h\|(I - \pi_{-})u\|. \end{aligned}$$

Here by $a(h) = o(h)$ we mean that $\lim_{h \rightarrow 0} a(h)/h = 0$.

We then have

PROPOSITION 3.8. — *With P and π_{\pm} with the properties described above we define*

$$\begin{aligned} \mathcal{H}_{\pm} &\stackrel{\text{def}}{=} \text{im } \pi_{\pm}, \quad R_{-} : \mathcal{H}_{-} \hookrightarrow \mathcal{H}, \quad R_{+} : \mathcal{H} \xrightarrow{\perp} \mathcal{H}_{+}, \\ R_{-}^* R_{-} &= \text{Id}_{\mathcal{H}_{-}}, \quad R_{-} R_{-}^* = \pi_{-}, \quad R_{+} R_{+}^* = \text{Id}_{\mathcal{H}_{+}}, \quad R_{+}^* R_{+} = \pi_{+}. \end{aligned}$$

Then for h small enough the Grushin problem

$$\begin{cases} Pu + R_{-}u_{-} = v \\ R_{+}u = v_{+} \end{cases}$$

is well posed and

$$(3.21) \quad h\|u\| + \|u_{-}\| \leq C(\|v\| + h\|v_{+}\|),$$

where C is independent of h .

Proof. — We start by rewriting our Grushin problem as

$$(3.22) \quad \begin{cases} P\tilde{u} + R_-u_- = \tilde{v} \\ R_+\tilde{u} = 0 \end{cases}$$

$$\tilde{u} \stackrel{\text{def}}{=} u - R_+^*v_+, \quad \tilde{v} \stackrel{\text{def}}{=} v - PR_+^*v_+.$$

We observe that $\pi_-R_- = R_-$, $R_+\pi_+ = R_+$, and $(I - \pi_+)\tilde{u} = \tilde{u}$. From (3.20) we see that

$$\|P\tilde{u}\| = \|P(I - \pi_+)\tilde{u}\| \geq h\|(I - \pi_+)\tilde{u}\| = h\|\tilde{u}\|.$$

Taking the inner product of the first equation in (3.22) with $P\tilde{u}$ gives

$$\|P\tilde{u}\|^2 + \text{Re}\langle P^*\pi_-R_-u_-, \tilde{u} \rangle \leq \|P\tilde{u}\|\|\tilde{v}\|,$$

and we estimate the second term on the left hand side using (3.20):

$$|\langle P^*\pi_-R_-u_-, \tilde{u} \rangle| \leq \|(I - \pi_+)P^*\pi_- \|u_-\|_{\mathcal{H}_-} \|\tilde{u}\| = o(h)\|u_-\|_{\mathcal{H}_-} \|\tilde{u}\|.$$

Putting these inequalities together gives

$$\begin{aligned} \frac{1}{2} (h^2\|\tilde{u}\|^2 + \|P\tilde{u}\|^2) &\leq \|P\tilde{u}\|^2 \leq \|P\tilde{u}\|\|\tilde{v}\| - \text{Re}\langle P^*\pi_-R_-u_-, \tilde{u} \rangle \\ &\leq \frac{1}{4} \|P\tilde{u}\|^2 + \|\tilde{v}\|^2 + o(h)\|u_-\|_{\mathcal{H}_-} \|\tilde{u}\| \\ &\leq \frac{1}{4} \|P\tilde{u}\|^2 + \|\tilde{v}\|^2 + o(h^2)\|\tilde{u}\|^2 + o(1)\|u_-\|_{\mathcal{H}_-}^2. \end{aligned}$$

We conclude that

$$h\|\tilde{u}\| \leq C\|\tilde{v}\| + o(1)\|u_-\|_{\mathcal{H}_-}^2,$$

and also that,

$$\|u_-\|_{\mathcal{H}_-} = \|R_-u_-\| \leq \|P\tilde{u}\| + \|\tilde{v}\| \leq C\|\tilde{v}\| + o(1)\|u_-\|_{\mathcal{H}_-}.$$

Consequently

$$\|u_-\|_{\mathcal{H}_-} + h\|\tilde{u}\| \leq C\|\tilde{v}\|.$$

To obtain (3.21) we estimate $\|\tilde{v}\|$ using (3.20):

$$\|PR_+^*v_+\| = \|P\pi_+R_+^*v_+\| = \mathcal{O}(h)\|v_+\|_{\mathcal{H}_+},$$

so that

$$\|\tilde{v}\| \leq \|v\| + \mathcal{O}(h)\|v_+\|_{\mathcal{H}_+}.$$

Since by definition $\|u\| \leq \|\tilde{u}\| + \|v_+\|_{\mathcal{H}_+}$, the estimate follows.

This shows the injectivity and to see the surjectivity we apply the same proof to the adjoint Grushin problem, observing that the assumptions are symmetric. □

The estimate (3.21) is natural and appears under different assumptions (see for instance [22, Lemma 5.2] for another elementary abstract estimate). In the proof we could have considered $h = 1$ since we can scale h out of the hypotheses:

$$\begin{pmatrix} h^{-1} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} P(h) & R_- \\ R_+ & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & h \end{pmatrix} = \begin{pmatrix} h^{-1}P(h) & R_- \\ R_+ & 0 \end{pmatrix}.$$

3.6. Application to pseudospectral estimates

To see the estimates of §3.5 in use we relate them to the example in §2.2. The general phenomenon observed there is the growth of the resolvent of a non-normal operator away from the spectrum, and the consequent instability of eigenvalues — see [20], [24], [27].

Thus consider a general $n \times n$ matrix A . Let us then put $P = P(\lambda) = A - \lambda$, and

$$\pi_- = \pi_-(\lambda) \stackrel{\text{def}}{=} \mathbb{1}_{P(\lambda)P(\lambda)^* \leq h^2}, \quad \pi_+ = \pi_+(\lambda) \stackrel{\text{def}}{=} \mathbb{1}_{P(\lambda)^*P(\lambda) \leq h^2},$$

where for a selfadjoint matrix B , $\mathbb{1}_{B \leq r}$ denotes the orthogonal projection on the span of eigenvectors of B with eigenvalues less than or equal to r .

A more concrete description of π_{\pm} is given using the singular value decomposition:

$$(3.23) \quad A - \lambda = (U_1 \ U_2) \begin{pmatrix} \Sigma_1 & 0 \\ 0 & \Sigma_2 \end{pmatrix} \begin{pmatrix} V_1^* \\ V_2^* \end{pmatrix},$$

where the singular values of Σ_1 are all greater than h , and those of Σ_2 are less than or equal to h . Then

$$\pi_- = \pi_-(\lambda, h) \stackrel{\text{def}}{=} U_2 U_2^*, \quad \pi_+ = \pi_+(\lambda, h) \stackrel{\text{def}}{=} V_2 V_2^*.$$

We see that the hypothesis (3.20) is satisfied:

$$\begin{aligned} \|P\pi_+u\|^2 &= \langle P^*P\pi_+u, \pi_+u \rangle \leq h^2\|\pi_+u\|^2, \\ \|P^*\pi_-u\|^2 &= \langle PP^*\pi_-u, \pi_-u \rangle \leq h^2\|\pi_-u\|^2, \\ \|P(I - \pi_+)u\|^2 &= \langle P^*P(I - \pi_+)u, (I - \pi_+)u \rangle \geq h^2\|(I - \pi_+)u\|^2, \\ \|P^*(I - \pi_-)u\|^2 &= \langle PP^*(I - \pi_-)u, (I - \pi_-)u \rangle \geq h^2\|(I - \pi_-)u\|^2, \\ \pi_-P(I - \pi_+) &= 0, \quad \pi_+P^*(I - \pi_-) = 0. \end{aligned}$$

To see the last identities we can use (3.23) or note that

$$P : \ker(P^*P - r) \longrightarrow \ker(PP^* - r), \quad P^* : \ker(PP^* - r) \longrightarrow \ker(P^*P - r),$$

implies

$$\mathbb{1}_{P P^* \leq h^2} P \mathbb{1}_{P^* P > h^2} = 0, \quad \mathbb{1}_{P^* P \leq h^2} P^* \mathbb{1}_{P P^* > h^2} = 0.$$

This shows that we can apply Proposition 3.8. In the notation of (3.23) that means putting

$$R_- \stackrel{\text{def}}{=} U_2, \quad R_+ = V_2^*.$$

The corresponding Grushin problem constructed there has the inverse:

$$\begin{pmatrix} E(\lambda, h) & E_+(\lambda, h) \\ E_-(\lambda, h) & E_{-+}(\lambda, h) \end{pmatrix} = \begin{pmatrix} \mathcal{O}(1/h) & \mathcal{O}(1) \\ \mathcal{O}(1) & \mathcal{O}(h) \end{pmatrix} : \mathbb{C}^n \oplus \mathbb{C}^{n(\lambda, h)} \longrightarrow \mathbb{C}^n \oplus \mathbb{C}^{n(\lambda, h)},$$

where $n(\lambda, h) = \text{tr } \mathbb{1}_{(A-\lambda)^*(A-\lambda) \leq h^2}$. Using (1.1) we see in particular that

$$(3.24) \quad \|(A - \lambda)^{-1}\| \simeq \|E_{-+}(\lambda, h)^{-1}\| + \mathcal{O}(1/h),$$

since $\|E_+ v_+\| \simeq \|v_+\|$, and $\|E_-^* u_-\| \simeq \|u_-\|$. Here $a \simeq b$ means that $b/C \leq a \leq Cb$ for a constant independent of h .

In the example presented in §2.2 where A was equal to a Jordan block matrix, we can take any $|\lambda|^n \ll h < |\lambda|$ to obtain a Grushin problem with $n(\lambda, h) = 1$ and

$$E_{-+}(\lambda, h) = -\|(A - \lambda)^{-1}\|^{-1}.$$

The discrepancy with §2.2 was explained to us by Mark Embree as follows. In §2.2 R_- and R_+ were chosen as good “pseudoeigenvectors”, not as *optimal* pseudoeigenvectors. In the present setting, R_- and R_+ are obtained from optimal pseudoeigenvectors (in the sense that they correspond to the minimal singular value of $A - \lambda$). Using the singular value decomposition (3.23) we see that

$$E_{-+}^{-1} = -R_- P^{-1} R_+ = -V_2^* (A - \lambda)^{-1} U_2 = -\Sigma_2^{-1}.$$

Recently this approach to pseudospectral estimates was used in [9] to study random perturbations of nonselfadjoint semiclassical pseudodifferential operators.

4. Trace formulæ

4.1. Basic idea

Suppose that $P = P(z)$. Writing $\partial_z A(z) = \dot{A}(z)$ we have

$$\dot{\mathcal{E}}(z) = -\mathcal{E}(z) \dot{P}(z) \mathcal{E}(z),$$

which gives

$$(4.1) \quad E_-(z)\dot{P}(z)E_+(z) = -\dot{E}_{-+}(z) - E_-(z)\dot{R}_-(z)E_{-+}(z) - E_{-+}(z)\dot{R}_+(z)E_+(z).$$

We recall that, formally,

$$P(z)^{-1} = E(z) - E_+(z)E_{-+}(z)^{-1}E_-(z).$$

Hence, assuming that we have no difficulty in taking traces, we obtain

$$(4.2) \quad \text{tr } \dot{P}(z)P(z)^{-1} = \text{tr } \dot{E}_{-+}(z)E_{-+}(z)^{-1} + \text{tr } E_-(z)\dot{R}_-(z) + \text{tr } \dot{R}_+(z)E_+(z) + \text{tr } \dot{P}(z)E(z),$$

which is a special case of Lemma 3.2. This gives

PROPOSITION 4.1. — *Suppose that $P = P(z)$ is a family of Fredholm operators depending holomorphically on $z \in \Omega$ where $\Omega \subset \mathbb{C}$ is a connected open set. Suppose also that the operators $R_{\pm} = R_{\pm}(z)$ are of finite rank, depend holomorphically on $z \in \Omega$, the corresponding Grushin problem is well posed for $z \in \Omega$, and that $E_{-+}(z_0)^{-1}$ is invertible at some $z_0 \in \Omega$. Let g be holomorphic in Ω . Then for any curve γ homologous to 0 in Ω , and on which $P(z)^{-1}$ exists $\int_{\gamma} \dot{P}(z)P(z)^{-1}g(z)dz$ is of trace class and we have*

$$(4.3) \quad \text{tr} \int_{\gamma} \dot{P}(z)P(z)^{-1}g(z)dz = \text{tr} \int_{\gamma} \dot{E}_{-+}(z)E_{-+}(z)^{-1}g(z)dz.$$

Proof. — Since E_{-+}^{-1} is a finite matrix for $z \in \gamma$ we have that

$$\int_{\gamma} \dot{P}(z)P(z)^{-1}g(z)dz = - \int_{\gamma} \dot{P}(z)E_+(z)E_{-+}(z)^{-1}E_-(z)g(z)dz$$

is an operator of trace class, and, arguing as we did before the statement of the proposition we obtain (4.3). □

The condition that $E_{-+}(z)$ is a finite matrix is often too restrictive. To illustrate this in a simple example we use the results of §2.5. Let Δ_D and Δ_N be the Dirichlet and Neumann Laplacians on a bounded domain X , with a smooth boundary ∂X . We now put $P_{\bullet}(z) = -\Delta_{\bullet} - z$, $\bullet = D, N$. As described in §2.5 we have a well posed problem for $P_D(z)$ if $P_N^{-1}(z)$ exists, and in that case $E_{-+}(z) = N(z)$, the Neumann to Dirichlet operator. Similarly we have a well posed problem for $P_N(z)$ if $P_D^{-1}(z)$ exists, and in that case $E_{-+}(z) = N(z)^{-1}$, the Dirichlet to Neumann operator. Hence if γ_D is a contour homologous to 0 in the region where $P_N(z)^{-1}$ exists we get $-\text{tr} \int_{\gamma_D} P_D(z)^{-1}dz = \text{tr} \int_{\gamma_D} \dot{N}(z)N(z)^{-1}dz$. Strictly speaking we cannot apply Proposition 4.1 directly but as $N(z)$ is a Fredholm operator we can

locally use an iterated problem with R_{\pm} of finite rank. Our contour can be made a sum of contours involving only these local problems.

Similarly we have $\int_{\gamma_D} P_N(z)^{-1} dz = 0$. We can consider an analogous contour γ_N and write any contour γ as $\gamma_D + \gamma_N$. This leads to the following formula:

$$(4.4) \quad \text{tr} \int_{\gamma} ((-\Delta_N - z)^{-1} - (-\Delta_D - z)^{-1}) dz = \text{tr} \int_{\gamma} N(z)^{-1} \frac{d}{dz} N(z) dz,$$

where $N(z)$ is the Neumann to Dirichlet map for $-\Delta - z$. For a non-trivial application of a similar idea in the context of resonances for the elastic Neumann problem see the work of Vodev and the first author [21].

4.2. Classical Poisson formula

To present an application of Proposition 4.1 we use it to derive the classical Poisson summation formula:

$$(4.5) \quad \sum_{n \in \mathbb{Z}} f(n) = \sum_{m \in \mathbb{Z}} \hat{f}(2\pi m), \quad \hat{f} \in C_c^\infty(\mathbb{R}), \quad \hat{f}(\xi) \stackrel{\text{def}}{=} \int f(x) e^{-ix\xi} dx.$$

Our proof here might well be the most complicated derivation of (4.5) but as will be indicated in §5.2 it lends itself to far reaching generalizations.

We start by rewriting (4.5) using the operator $P = hD_x$ on $\mathbb{R}/(2\pi\mathbb{Z})$:

$$(4.6) \quad \text{tr} f(P/h) = \frac{1}{2\pi i} \sum_{|k| \leq N} \int_{\mathbb{R}} f(z/h) \left(e^{2\pi iz/h} \right)^k \frac{d}{dz} \left(e^{2\pi iz/h} \right) dz.$$

The left hand side there can be written using the usual functional calculus based on Cauchy’s formula:

$$(4.7) \quad \text{tr} f \left(\frac{P}{h} \right) = \frac{1}{2\pi i} \text{tr} \int_{\Gamma} f \left(\frac{z}{h} \right) (P - z)^{-1} dz, \\ \Gamma = \Gamma_+ - \Gamma_-, \quad \Gamma_{\pm} = \mathbb{R} \pm iR,$$

where we take the positive orientation of \mathbb{R} and $R > 0$ is an arbitrary constant. We make an assumption on the support of the Fourier transform on f :

$$(4.8) \quad \text{supp } \hat{f} \subset (-2\pi N, 2\pi N).$$

We can now use the Grushin problem (3.12) and its inverse given by (3.16). Applying Proposition 4.1 with $P(z) = (i/h)(P - z)$ and $g(z) = f(z/h)$ we obtain

$$\text{tr} f \left(\frac{P}{h} \right) = -\frac{1}{2\pi i} \int_{\Gamma} f \left(\frac{z}{h} \right) \text{tr} \partial_z E_{-+}(z) E_{-+}(z)^{-1} dz.$$

We now use the expression for E_{-+} from §3.2 to write

$$\begin{aligned} \operatorname{tr} f\left(\frac{P}{h}\right) &= \frac{1}{2\pi i} \int_{\Gamma_+} f\left(\frac{z}{h}\right) \operatorname{tr} \partial_z M(z, h) (I - M(z, h))^{-1} dz \\ &\quad + \frac{1}{2\pi i} \int_{\Gamma_-} f\left(\frac{z}{h}\right) \operatorname{tr} \partial_z M(z, h) M(z, h)^{-1} (I - M(z, h)^{-1})^{-1} dz, \end{aligned}$$

$M(z, h) = \exp(2\pi iz/h)$. The assumption (4.8) and the Paley-Wiener theorem give

$$|\hat{f}(z/h)| \leq e^{2\pi N |\operatorname{Im} z|/h} \langle \operatorname{Re} z/h \rangle^{-\infty}.$$

Writing

$$(I - M(z, h))^{-1} = \sum_{k=0}^{N-1} M(z, h)^k + M(z, h)^N (I - M(z, h))^{-1},$$

for Γ_+ , and

$$\begin{aligned} M(z, h)^{-1} (I - M(z, h)^{-1})^{-1} &= \sum_{k=1}^N M(z, h)^{-k} \\ &\quad + M(z, h)^{-N-1} (I - M(z, h))^{-1}, \end{aligned}$$

for Γ_- , we can eliminate the last terms by deforming the contours to imaginary infinities ($R \rightarrow \infty$ in (4.7)), and this gives (4.6).

4.3. An abstract version

In addition to demanding a finite rank of R_{\pm} , Proposition 4.1 is restrictive in the sense that we need to assume that the family of operators depends holomorphically on the parameter z . Following [17, Appendix A] we present a result without that assumption. Let \mathcal{H} be a complex Hilbert space and let us denote by $\mathcal{L}(\mathcal{H}, \mathcal{H})$ bounded operators on \mathcal{H} . We consider $\mathbb{S}^1 \ni t \mapsto A(t) \in \mathcal{L}(\mathcal{H}, \mathcal{H})$, a \mathcal{C}^1 closed curve of operators, in the sense that $A(t)$ is strongly differentiable with a continuous derivative $\mathbb{S}^1 \ni t \mapsto \dot{A}(t) \in \mathcal{L}(\mathcal{H}, \mathcal{H})$. We write $dA = \dot{A}dt$, and for another such $t \mapsto B(t)$,

$$\int_{\mathbb{S}^1} B(t) \dot{A}(t) dt = \int B dA \in \mathcal{L}(\mathcal{H}, \mathcal{H}).$$

If the values of $A(t)$ are taken in an open subset V of $\mathcal{L}(\mathcal{H}, \mathcal{H})$, we will say that $A(t)$ is *contractible* in V , if $\mathbb{S}^1 \ni t \mapsto A(t) \in V$ has a \mathcal{C}^1 extension $\mathbb{D} \ni z \mapsto A(z) \in V$, $\mathbb{D} = \{|z| < 1\}$, $\partial\mathbb{D} = \mathbb{S}^1$.

With this terminology we have

PROPOSITION 4.2. — *Suppose that*

$$(4.9) \quad \mathbb{S}^1 \ni t \mapsto \mathcal{P}(t) = \begin{pmatrix} P(t) & R_-(t) \\ R_+(t) & 0 \end{pmatrix} : \mathcal{H} \oplus \mathbb{C}^N \longrightarrow \mathcal{H} \oplus \mathbb{C}^N,$$

is contractible in the set of invertible operators on $\mathcal{H} \oplus \mathbb{C}^N$, with $\mathbb{D} \ni z \mapsto \hat{\mathcal{P}}(z)$ continuous with values in operators of trace class.

If $P(t)^{-1}$ exists for all $t \in \mathbb{S}^1$ then

$$(4.10) \quad \text{tr} \int P^{-1} dP = \text{tr} \int E_{-+}^{-1} dE_{-+},$$

where we use the standard Grushin problem notation for the inverse of (4.9).

Proof. — We first note that for $t \in \mathbb{S}^1$ we can smoothly deform $\mathcal{P}(t)$ to

$$\begin{pmatrix} P(t) & 0 \\ 0 & E_{-+}(t)^{-1} \end{pmatrix},$$

within the space of invertible operators. In fact, we define

$$\mathcal{P}(t, s) = \begin{pmatrix} P(t) & (\cos s)R_-(t) \\ (\cos s)R_+(t) & (\sin^2 s)E_{-+}(t)^{-1} \end{pmatrix}, \quad 0 \leq s \leq \pi/2,$$

and we easily check its invertibility for all s , and $t \in \mathbb{S}^1$: since $E_{-+}^{-1} = -R_+ P^{-1} R_-$ we have

$$\mathcal{P}(t, s) = \begin{pmatrix} P(t) & 0 \\ (\cos s)R_+(t) & \text{Id}_{\mathbb{C}^N} \end{pmatrix} \begin{pmatrix} \text{Id}_{\mathcal{H}} & (\cos s)P(t)^{-1}R_-(t) \\ 0 & E_{-+}(t)^{-1} \end{pmatrix}.$$

In the sense of operator valued differential forms in variables $(t, s) \in \mathbb{S}^1 \times [0, \pi/2]$,

$$(4.11) \quad d(\mathcal{P}^{-1} d\mathcal{P}) = -\mathcal{P}^{-1} d\mathcal{P} \wedge \mathcal{P}^{-1} d\mathcal{P}.$$

Also for a differential form μ with values in operators of trace class

$$(4.12) \quad \text{tr} \mu \wedge \mu = 0.$$

Using Stokes's theorem on $\Omega = \mathbb{S}^1 \times [0, \pi/2]$, (4.11), and (4.12), we see that

$$\text{tr} \int \mathcal{P}(\bullet, \pi/2)^{-1} d\mathcal{P}(\bullet, \pi/2) = \text{tr} \int \mathcal{P}(\bullet, 0)^{-1} d\mathcal{P}(\bullet, 0) = 0,$$

where the last equality comes from the contractibility assumption and from another application of Stokes's theorem. The left hand side is clearly equal to $\text{tr} \int P^{-1} dP - \text{tr} \int E_{-+}^{-1} dE_{-+}$ which proves (4.10). □

It is quite possible that Proposition 4.2 follows from some general topological facts. It is not clear what are the weakest assumptions on P and dP to guarantee that $\int PdP$ is of trace class. For a discussion of one case of a weaker assumption see [17, Appendix A].

5. Advanced examples

5.1. Around Lidskii’s perturbation theory for matrices

In §2.2 the equation for the eigenvalues of the perturbation of one Jordan block is easily derived from (2.3):

$$\lambda^n - \epsilon Q_{n1} + \epsilon \mathcal{O}(\lambda) + \mathcal{O}(\epsilon^2) = 0, \quad |\lambda| < 1.$$

and the solutions are

$$\lambda_\ell = \epsilon^{1/n} |Q_{n1}|^{1/n} e^{(2\pi i \ell + \arg Q_{n1})/n} + o(\epsilon^{1/n}), \quad 1 \leq \ell \leq n.$$

Here we consider n fixed and are interested in the $\epsilon \rightarrow 0$ asymptotics.

In this section we will show how the Grushin problem approach applies to the study of perturbation of matrices with arbitrary Jordan structure. We restrict ourselves to an example suggested by Michael Overton which according to him contains the essential elements of the general problem studied in [16] and [18].

Let J_ℓ be the $\ell \times \ell$ upper triangular Jordan bloc matrix. We then consider

$$(5.1) \quad A = J_n \oplus J_n \oplus J_k : \mathbb{C}^n \oplus \mathbb{C}^n \oplus \mathbb{C}^k \longrightarrow \mathbb{C}^n \oplus \mathbb{C}^n \oplus \mathbb{C}^k, \quad k < n,$$

that is

$$A = \begin{pmatrix} J_n & 0_{nn} & 0_{nk} \\ 0_{nn} & J_n & 0_{nk} \\ 0_{kn} & 0_{kn} & J_k \end{pmatrix},$$

where $0_{\ell p}$ denotes the $\ell \times p$ zero matrix.

The Grushin problem for A is a straightforward modification of the one for J_n in §2.2:

$$R_- : \mathbb{C}^3 \longrightarrow \mathbb{C}^n \oplus \mathbb{C}^n \oplus \mathbb{C}^k, \quad R_+ : \mathbb{C}^n \oplus \mathbb{C}^n \oplus \mathbb{C}^k \longrightarrow \mathbb{C}^3.$$

We then obtain the effective Hamiltonian, $E_{-+}(\lambda)$ for $A - \lambda$:

$$E_{-+}(\lambda) = \begin{pmatrix} \lambda^n & 0 & 0 \\ 0 & \lambda^n & 0 \\ 0 & 0 & \lambda^k \end{pmatrix},$$

and $E_{\pm}(\lambda)$ are similarly constructed from the three $e_{\pm}(\lambda)$ vectors.

Suppose we now consider a perturbation of A :

$$(5.2) \quad A_\epsilon = A + \epsilon Q, \quad Q = \begin{pmatrix} Q^{11} & Q^{12} & Q^{13} \\ Q^{21} & Q^{22} & Q^{23} \\ Q^{31} & Q^{32} & Q^{33} \end{pmatrix},$$

$$Q^{ij} : \mathbb{C}^{n_i} \longrightarrow \mathbb{C}^{n_j}, \quad n_i = n, \quad i = 1, 2, \quad n_3 = k.$$

As in §2.2 we see that the effective Hamiltonian for the perturbation is

$$E_{-+}^\epsilon(\lambda) = E_{-+}(\lambda) - \epsilon E_-(\lambda) Q E_+(\lambda) + \mathcal{O}(\epsilon^2).$$

The effective first order perturbation is easily checked to be

$$E_-(\lambda) Q E_+(\lambda) = \begin{pmatrix} Q_{n1}^{11} & Q_{n1}^{12} & Q_{n1}^{13} \\ Q_{n1}^{21} & Q_{n1}^{22} & Q_{n1}^{23} \\ Q_{k1}^{31} & Q_{k1}^{32} & Q_{k1}^{33} \end{pmatrix} + \mathcal{O}(\lambda),$$

where Q_{ij}^{pq} denotes the ij 'th entry of the matrix Q^{pq} .

Suppose that the matrix $(Q_{n1}^{ij})_{1 \leq i, j, \leq 2}$ is diagonalizable with eigenvalues q_1 and q_2 . Then the eigenvalues of A_ϵ are given by the values of λ for which the following matrix is not invertible:

$$\begin{pmatrix} \lambda^n - \epsilon q_1 & 0 & \epsilon \tilde{Q}_{13} \\ 0 & \lambda^n - \epsilon q_2 & \epsilon \tilde{Q}_{23} \\ \epsilon \tilde{Q}_{31} & \epsilon \tilde{Q}_{32} & \lambda^k - \epsilon \tilde{Q}_{33} \end{pmatrix} + \epsilon \mathcal{O}(\lambda) + \mathcal{O}(\epsilon^2).$$

Since $k < n$, and both k and n are fixed, perturbation theory gives

PROPOSITION 5.1. — *The largest modulus eigenvalues of A_ϵ for ϵ small are given by*

$$\lambda_\ell^j = \epsilon^{1/n} |q_j|^{1/n} e^{(2\pi i \ell + \arg q_j)/n} + o(\epsilon^{1/n}), \quad 1 \leq \ell \leq n, \quad j = 1, 2,$$

where q_j are the eigenvalues (assumed to be distinct) of the $(Q_{n1}^{ij})_{1 \leq i, j \leq 2}$ part of the perturbation matrix in (5.2).

A finer perturbation theory for matrices of size given by the number of distinct Jordan blocks will (most likely) give the general results of [16] and [18].

5.2. Generalized Gutzwiller trace formula

Trace formulæ provide one of the most elegant descriptions of the classical-quantum correspondence. One side of such a formula is given by a

trace of a quantum object, typically derived from a quantum Hamiltonian, and the other side is described in terms of closed orbits of the corresponding classical Hamiltonian.

Here we follow [23] and outline the structure of a formula which is derived using a *formal* Grushin problem. It is an intermediate trace formula in which the original trace is expressed in terms of traces of quantum monodromy operators directly related to the classical dynamics. The usual trace formulæ follow and in addition this approach allows handling effective Hamiltonians, such as the one described in §5.3 below.

Let P be a semi-classical, self-adjoint, principal type operator, elliptic in the classical sense, with symbol p , and a compact characteristic variety, $p^{-1}(0)$. Let $\gamma \subset p^{-1}(0)$ be a closed primitive orbit of the Hamilton flow of p . The simplest example, and one discussed in §4.2, $P = hD_x$, on the circle, $p^{-1}(0) = \{(x, 0) \mid x \in \mathbb{S}^1\} \subset T^*\mathbb{S}^1$, and the Hamilton vector field is ∂_x . More interesting examples are $P = -h^2\Delta_g - 1$ on a compact Riemannian manifold, or $P = -h^2\Delta + V(x)$ with a suitable V on \mathbb{R}^n .

We can define the *monodromy operator*, $M(z, h)$ for $P - z$ along γ , acting on functions in one dimension lower, that is, on functions on the transversal to γ in the base. We then have

THEOREM 5.2. — *Suppose that there exists a neighbourhood of γ , Ω , satisfying the condition*

$$(5.3) \quad m \in \Omega \text{ and } \exp tH_p(m) = m, \quad p(m) = 0, \quad 0 < |t| \leq TN \implies m \in \gamma,$$

where T is the primitive period of γ . If $\hat{f} \in \mathcal{C}_c^\infty(\mathbb{R})$, $\text{supp } \hat{f} \subset (-NT, NT) \setminus \{0\}$, $\chi \in \mathcal{C}_c^\infty(\mathbb{R})$, and $A \in \Psi_h^{0,0}(X)$ is a microlocal cut-off to a sufficiently small neighbourhood of γ , then

$$(5.4) \quad \text{tr} f(P/h)\chi(P)A \\ = \frac{1}{2\pi i} \sum_{-N-1}^{N-1} \text{tr} \int_{\mathbb{R}} f(z/h)M(z, h)^k \frac{d}{dz} M(z, h)\chi(z)dz + \mathcal{O}(h^\infty),$$

where $M(z, h)$ is the semi-classical monodromy operator associated to γ .

The dynamical assumption on the operator means that in a neighbourhood of γ there are no other closed orbits of period less than TN , on the energy surface $p = 0$. We avoid a neighbourhood of 0 in the support of \hat{f} to avoid the dependence on the microlocal cut-off A .

The monodromy operator quantizes the Poincaré map for γ and its geometric analysis gives the now standard trace formulæ of Selberg, Gutzwiller

and Duistermaat-Guillemin. The term $k = -1$ corresponds to the contributions from “not moving at all” and the other terms to contributions from going $|k + 1|$ times around γ , in the positive direction when $k \geq 0$, and in the negative direction, when $k < -1$. For non-degenerate orbits the analysis of the traces on monodromy operators recovers the usual semi-classical trace formulæ in our general setting — see [23, Theorem 3].

The proof of the formula follows the lines of the proof of the classical Poisson formula presented in §4.2. In the general situation where the circle is replaced by a closed trajectory of a real principal type operator we can proceed similarly but now *microlocally* in a neighbourhood of that closed orbit on an energy surface. The contour integral formula (4.7) is replaced by the Dynkin-Droste-Helffer-Sjöstrand formula (see [5, Chapter 8])

$$(5.5) \quad \text{tr } f\left(\frac{P}{h}\right) \chi(P)A = -\frac{1}{\pi} \int_{\mathbb{C}} f\left(\frac{z}{h}\right) \bar{\partial}_z \tilde{\chi}(z) (P - z)^{-1} \mathcal{A}\mathcal{L}(dz),$$

where $\tilde{\chi}$ is an *almost analytic extension* of χ , that is an extension satisfying $\bar{\partial}_z \tilde{\chi}(z) = \mathcal{O}(|\text{Im } z|^\infty)$ — see [23, Sect.6] and we want to proceed with a similar reduction to the effective Hamiltonian given in terms of a suitably defined *monodromy operator*.

To construct the monodromy operator we fix two different points on γ , m_0, m_1 (corresponding to 0 and π in (3.12)-(3.13)), and their disjoint neighbourhoods, W_+ and W_- respectively. We then consider local kernels of $P - z$ near m_0 and m_1 (that is, sets of distributions satisfying $(P - z)u = 0$ near m_i 's), $\ker_{m_j}(P - z)$, $j = 0, 1$, with elements microlocally defined in W_\pm . and the forward and backward solutions:

$$I_\pm(z) : \ker_{m_0}(P - z) \longrightarrow \ker_{m_1}(P - z).$$

We then define the *quantum monodromy operator*, $\mathcal{M}(z)$ by

$$I_-(z)\mathcal{M}(z) = I_+(z), \quad \mathcal{M}(z) : \ker_{m_0}(P - z) \longrightarrow \ker_{m_0}(P - z).$$

The operator P is assumed to be self-adjoint with respect to some inner product $\langle \bullet, \bullet \rangle$, and we define the *quantum flux* norm on $\ker_{m_0}(P - z)$ as follows^(‡): let χ be a microlocal cut-off function, with basic properties of the function χ in the example. Roughly speaking χ should be supported near γ and be equal to one near the part of γ between W_+ and W_- . We denote by $[P, \chi]_{W_+}$ the part of the commutator supported in W_+ , and put

$$\langle u, v \rangle_{\text{QF}} \stackrel{\text{def}}{=} \langle [(h/i)P, \chi]_{W_+} u, v \rangle, \quad u, v \in \ker_{m_0}(P - z).$$

(‡) See [12] for an earlier mathematical development of this basic quantum mechanical idea.

As can be easily seen this norm is independent of the choice of χ . This independence leads to the unitarity of $\mathcal{M}(z)$:

$$\langle \mathcal{M}(z)u, \mathcal{M}(z)u \rangle_{\mathbb{QF}} = \langle u, u \rangle_{\mathbb{QF}}, \quad u \in \ker_{m_0}(P - z).$$

For practical reasons we identify $\ker_{m_0}(P - z)$ with $\mathcal{D}'(\mathbb{R}^{n-1})$, microlocally near $(0, 0)$, and choose the identification so that the corresponding monodromy map is unitary (microlocally near $(0, 0)$ where $(0, 0)$ corresponds to the closed orbit intersecting a transversal identified with $T^*\mathbb{R}^{n-1}$). This gives

$$M(z, h) : \mathcal{D}'(\mathbb{R}^{n-1}) \longrightarrow \mathcal{D}'(\mathbb{R}^{n-1}),$$

microlocally defined near $(0, 0)$ and unitary there. This is the operator appearing in Theorem 5.2 and it shares many properties with its simple version $\exp(2\pi iz/h)$ appearing in (3.13) for \mathbb{S}^1 .

As in §3.2 we can construct a Grushin problem with the effective Hamiltonian given by $E_{-+}(z, h) = I - M(z, h)$. However, now the problem is *formal*, that is all the inversion formulæ are only valid microlocally^(*) near γ . Since in Theorem 5.2 we are interested in taking traces, and not, for instance, locating eigenvalues or resonances, that is sufficient.

Nevertheless, as one striking application of this point of view we can explain the way in which complex quasi-modes manifest themselves on compact manifolds [15], a phenomenon which was already explicitly or implicitly noted in the works of Paul-Uribe, Guillemin, and Zelditch — see [25] and references given there.

To explain it, let us recall the now classical fact (Lazutkin, Ralston, Colin de Verdière, Popov) that for an elliptic closed geodesic on a compact manifold M one can construct approximate eigenfunctions concentrating on that trajectory, and that the corresponding approximate eigenvalues are close to actual eigenvalues with arbitrary polynomial accuracy as energy increases. When the trajectory is hyperbolic that procedure no longer makes sense as the formal construction of quasi-modes gives complex numbers. That can lead to the construction of resonances in scattering situations (Ikawa, Gérard, Sjöstrand-Gérard) but cannot have a direct spectral interpretation when the manifold is compact. Despite that they make a direct appearance when traces are considered and we have the following consequence of recent work on inverse spectral problems (see [25] and [15]):

(*) For a review of this important notion see [23, Section 3]. Roughly speaking it corresponds to a localization of the behaviour of quantum states to relevant subsets of classical phase space. It does not guarantee global well-posedness in an *honest* Hilbert space sense.

THEOREM 5.3. — *Let M be a compact Riemannian manifold and γ a closed hyperbolic trajectory of primitive length L_γ . Let λ_j^2 denote the sequence of eigenvalues of the Riemann-Beltrami operator, μ_k the sequence of complex quasi-modes associated to the trajectory γ , $0 < \text{Im } \mu_k$ (well defined modulo $\mathcal{O}(|\text{Re } \mu_k|^{-\infty})$). Suppose that for any $m \in \mathbb{Z} \setminus \{0\}$, mL_γ is different from the length of any closed geodesic on M which is not an iterate of γ . Then, for any $m \in \mathbb{Z} \setminus \{0\}$ there exists a neighbourhood U_m of mL_γ such that*

$$\sum_j e^{i\lambda_j t} - \sum_k e^{i\mu_k t} \in \mathcal{C}^\infty(U_m),$$

where both sums are meant in the sense of distributions on \mathbb{R} , and $\sum_k e^{i\mu_k t}$ is defined only modulo $\mathcal{C}^\infty(\mathbb{R} \setminus 0)$.

In our approach, especially in view of Grushin reductions to the effective Hamiltonians, it is important that we can consider operators with non-linear dependence on the spectral parameter. In that case, motivated by Proposition 4.1, the left hand side of (5.4) is replaced by

$$\frac{1}{\pi} \text{tr} \int f(z/h) \bar{\partial}_z [\tilde{\chi}(z) \partial_z P(z) P(z)^{-1}] A\mathcal{L}(dz),$$

which for $P(z) = P - z$ reduces to (5.5). For a generalized version we refer to [23, Theorem 2].

Finally we point out that the semi-classical Grushin problem point of view taken here, when translated to the special case of \mathcal{C}^∞ -singularities/high energy regime, is close to that of Marvizi-Melrose and Popov (see references in [23]). In those works the trace of the wave group was reduced to the study of a trace of an operator quantizing the Poincaré map.

5.3. Peierls substitution

In this section we will follow [11] to show how the Grushin reduction leads to a natural mathematical explanation of the celebrated Peierls substitution from solid state physics. It gives an effective Hamiltonian for a crystal in a magnetic field. For simplicity of the presentation we will consider the case of dimension two only, and of the first spectral band — we refer to [11] and [12] for the general case and for references to the vast literature on the subject.

First we need to consider the case of no magnetic field. Mathematically this corresponds to considering a Schrödinger operator with a periodic potential:

$$P_0 = -\Delta + V, \quad V \in C^\infty(\mathbb{R}^2), \quad V(x + \gamma) = V(x), \quad \gamma \in \Gamma,$$

where Γ is a lattice in \mathbb{R}^2 . In other words,

$$(5.6) \quad T_\alpha P_0 = P_0 T_\alpha, \quad T_\alpha u(x) \stackrel{\text{def}}{=} u(x - \alpha).$$

The operator P_0 is unitarily equivalent to a direct integral of Floquet operators, P_θ , acting as P_0 on \mathcal{H}_θ :

$$\mathcal{H}_\theta \stackrel{\text{def}}{=} \{u \in L^2_{\text{loc}}(\mathbb{R}^2) : \forall \gamma \in \Gamma \ u(x - \gamma) = e^{i\langle \theta, \gamma \rangle} u(x)\}, \quad \theta \in \mathbb{R}^2/\Gamma^*,$$

where Γ^* is the dual lattice of Γ : $\gamma^* \in \Gamma^* \iff \langle \gamma^*, \alpha \rangle \in 2\pi\mathbb{Z}$ for all $\alpha \in \Gamma$. We denote by E and E^* the fundamental domains of Γ and Γ^* respectively. Explicitly,

$$\begin{aligned} \mathcal{B}P_0\mathcal{C} &= \int^{\oplus} P_\theta d\theta, \\ (\mathcal{B}f)(x, \theta) &= \sum_{\gamma \in \Gamma} e^{-i\langle \theta, \gamma \rangle} f(x - \gamma), \quad (\mathcal{C}g)(x) = \frac{1}{\text{vol}(E^*)} \int_{E^*} g(x, \theta) d\theta, \\ \mathcal{B} : L^2(\mathbb{R}^2) &\longrightarrow L^2(\mathbb{R}^2/\Gamma^*, \mathcal{H}_\theta), \quad \mathcal{C} = \mathcal{B}^* = \mathcal{B}^{-1}. \end{aligned}$$

The spectrum of P_0 is absolutely continuous and equal to $\bigcup_{k \in \mathbb{N}} \{\lambda_k(\theta) : \theta \in \mathbb{R}^2/\Gamma^*\}$, where $\{\lambda_k(\theta)\}_{k=1}^\infty$ is the sequence of eigenvalues of P_θ . Each interval in the union is referred to as a band and we assume that the first band is disjoint from all the other bands.

We now want to find a Grushin problem for $P_0 - z$ which will be well posed near the first band. It turns out (see [10, Lemma 1.1]) that one can choose $\phi(x, \theta)$, $P_\theta \phi(x, \theta) = \lambda_1(\theta) \phi(x, \theta)$, to be holomorphic, as a function of θ , in a complex neighbourhood of \mathbb{R}^n/Γ^* . That implies that

$$\phi_0(x) \stackrel{\text{def}}{=} (\mathcal{C}\phi)(x),$$

has very nice properties: $|\partial_x^\alpha \phi_0(x)| \leq C_\alpha e^{-|x|/C}$. We then define the following Grushin problem:

$$(5.7) \quad \begin{aligned} \mathcal{P}_0(z) &= \begin{pmatrix} P_0 - z & R_-^0 \\ R_+^0 & 0 \end{pmatrix} : H^2(\mathbb{R}^2) \oplus \ell^2(\Gamma) \longrightarrow L^2(\mathbb{R}^2) \oplus \ell^2(\Gamma), \\ R_+^0 &\stackrel{\text{def}}{=} (R_-^0)^*, \quad R_-^0 u_-(x) \stackrel{\text{def}}{=} \sum_{\gamma \in \Gamma} u_-(\gamma) \phi_0(x - \gamma). \end{aligned}$$

It is not hard to see that this problem is well posed for z close to the first band and away from all the other bands. The effective Hamiltonian is given by

$$(E_{-+}^0(z)v_+)(\alpha) = \sum_{\beta \in \Gamma} (z\delta_{\alpha,\beta} - \widehat{E}(\alpha - \beta))v_+(\beta),$$

$$\widehat{E}(\gamma) = \frac{1}{\text{vol}(E^*)} \int_{E^*} \lambda_1(\theta) e^{i\langle \theta, \gamma \rangle} d\theta,$$

which is unitarily equivalent to the multiplication by $z - \lambda_1(\theta)$, the obvious effective Hamiltonian near the first band.

The Grushin problem (5.7) does have the advantage of being stable under small perturbations and we will see it when the magnetic field is turned on. That corresponds to adding a magnetic potential to our operator. Here we consider only a constant weak magnetic field $B = hdx_1 \wedge dx_2$:

$$(5.8) \quad P_B = (D_{x_1} - hx_2)^2 + D_{x_2}^2 + V(x), \quad D_{x_j} = \frac{1}{i} \partial_{x_j}, \quad B = hdx_1 \wedge dx_2.$$

Although the operator P_B is no longer periodic in the sense of (5.6) it commutes with magnetic translations:

$$(5.9) \quad T_\alpha^B P_B = P_B T_\alpha^B, \quad T_\alpha^B u(x) \stackrel{\text{def}}{=} e^{\frac{i}{2} \langle B, x \wedge \alpha \rangle} u(x - \alpha),$$

$$T_\alpha^B T_\beta^B = e^{-i \langle B, \alpha \wedge \beta \rangle} T_\beta^B T_\alpha^B.$$

We now use the magnetic translations to modify the Grushin problem (5.7):

$$(5.10) \quad \mathcal{P}_B(z) = \begin{pmatrix} P_B - z & R_+^B \\ R_-^B & 0 \end{pmatrix} : H_B^2(\mathbb{R}^2) \oplus \ell^2(\Gamma) \longrightarrow L^2(\mathbb{R}^2) \oplus \ell^2(\Gamma),$$

$$(R_-^B u_-)(x) \stackrel{\text{def}}{=} \sum_{\gamma \in \Gamma} u_-(\gamma) T_\gamma^B \phi_0(x), \quad (R_+^B u)(\gamma) \stackrel{\text{def}}{=} \langle u, T_\gamma^B \phi_0 \rangle_{L^2(\mathbb{R}^2)},$$

$$H_B^2 \stackrel{\text{def}}{=} \{u \in L^2(\mathbb{R}^2) : P_B u \in L^2(\mathbb{R}^2)\}.$$

The operator $\mathcal{P}_B(z)$ commutes with

$$\begin{pmatrix} T_\gamma^B & 0 \\ 0 & \tau_\gamma^B \end{pmatrix}, \quad \tau_\gamma^B u(\alpha) \stackrel{\text{def}}{=} e^{\frac{i}{2} \langle B, \alpha \wedge \gamma \rangle} u(\alpha - \gamma).$$

It is shown in [11, Proposition 3.1] that when h is small ($B = hdx_1 \wedge dx_2$) then $\mathcal{P}_B(z)$ is invertible for z near the first band for P_0 . Although it requires some technical work, roughly speaking it follows from the invertibility of \mathcal{P}_0 and the smallness of the magnetic field.

The inverse has the same symmetries as $\mathcal{P}_B(z)$ and in particular $\tau_\alpha^B E_{-+}(B, z) = E_{-+}(B, z) \tau_\alpha^B$ for all $\alpha \in \Gamma$. That implies that $E_{-+}(z, B)$

is given by a “twisted convolution”:

$$(5.11) \quad \begin{aligned} (E_{-+}(z, B)v_+) (\alpha) &= \sum_{\beta \in \Gamma} e^{\frac{i}{2}\langle B, \alpha \wedge \beta \rangle} f_{B,z}(\alpha - \beta)v_+(\beta), \\ |f_{B,z}(\gamma)| &\leq C e^{|\gamma|/C}. \end{aligned}$$

Operators with kernels satisfying these properties form an algebra sometimes called the algebra of *magnetic matrices*. In [11, Proposition 5.1] it is shown that the invertibility of a magnetic matrix as an operator on $\ell^2(\Gamma)$ is equivalent to its invertibility in the algebra of magnetic matrices. Let $\mathcal{M}_B(f)$ denote the magnetic matrix associated to an exponentially decaying function on Γ , f :

$$\mathcal{M}_B(f)(\alpha, \beta) = e^{\frac{i}{2}\langle B, \alpha \wedge \beta \rangle} f(\alpha - \beta) = e^{\frac{i}{2}h\sigma(\alpha, \beta)} f(\alpha - \beta),$$

where σ is the standard symplectic form on \mathbb{R}^2 . It is easy to check that

$$(5.12) \quad \mathcal{M}_B(f)\mathcal{M}_B(g) = \mathcal{M}_B(f\#_B g), \quad f\#_B g(\gamma) = \sum_{\alpha+\beta=\gamma} e^{\frac{i}{2}\langle B, \alpha \wedge \beta \rangle} f(\alpha)g(\beta).$$

We are now getting close to the Peierls substitution which provides an elegant microlocal description of $E_{-+}(z, B)$. We can take the Fourier transform of an exponentially decaying function on Γ , f ,

$$\widehat{f}(\theta) \stackrel{\text{def}}{=} \sum_{\gamma \in \Gamma} e^{i\langle \theta, \gamma \rangle} f(\gamma),$$

to obtain a Γ^* -periodic analytic function on \mathbb{R}^2 .

To simplify the presentation we assume now that $\Gamma = \mathbb{Z}^2$. Then one can check [11, §6] the following fact:

$$(5.13) \quad \text{Op}_h^w(\widehat{f\#_B g}) = \text{Op}_h^w(\widehat{f})\text{Op}_h^w(\widehat{g}),$$

where Op_h^w denotes the semi-classical Weyl quantization of a function on \mathbb{R}^2 :

$$a(x, \xi) \mapsto a^w(x, hD) : L^2(\mathbb{R}) \longrightarrow L^2(\mathbb{R}),$$

provided that a and all of its derivatives are bounded (see [5]). In view of (5.12) and (5.13) it is not surprising that the invertibility of $\mathcal{M}_B(f)$ in the algebra of magnetic matrices is equivalent to the invertibility of $\text{Op}_h^w(\widehat{f})$ in the algebra of of pseudodifferential operators. This leads to

THEOREM 5.4. — *Suppose that the first spectral band of a Schrödinger operator with a \mathbb{Z}^2 -periodic smooth potential is separated from other bands, with $\theta \mapsto E(\theta)$, the $(2\pi\mathbb{Z})^2$ -periodic first Floquet eigenvalue. Suppose that P_B is the corresponding magnetic Schrödinger operator with $B = hdx_1 \wedge dx_2$.*

Then there exists $(2\pi\mathbb{Z})^2$ -periodic (in θ) analytic function, $E = E(\theta, z, h)$, such that for z in a neighbourhood of the first band, and h small

$$z \in \sigma(P_B) \iff 0 \in \sigma(\text{Op}_h^w(E(\bullet, z, h))),$$

$$E(\theta, z, h) \sim E(\theta) - z + hE_1(\theta) + h^2E_2(\theta, z) + \dots$$

For the formulation for a general lattice and any dimension (in particular dimension three) we refer to [11] where one can also find the discussion of the coefficients in the expansion of $E(\theta, z, h)$. Considering the spectrum of the leading term, $E(x, hD_x)$, already shows how dramatic is the introduction of the magnetic field from the spectral point of view — see [12] and the references given there.

5.4. High frequency scattering by a convex obstacle

In this section we will outline the construction of a Grushin problem which reduces an exterior resonance problem to a problem on the surface of the obstacle. It was used in [22] to describe the asymptotic distribution of resonances in scattering by a convex obstacle satisfying a natural (at least from the point of view of our Grushin problem) curvature pinching conditions.

The study of resonances, or scattering poles, for convex bodies has a very long tradition going back to Watson's 1918 work on electromagnetic scattering by the earth. He was motivated by the description of the field in the deep shadow. It provided impetus for the work on the distribution of zeros of Hankel functions which are the resonances for the case of the sphere. For general convex obstacles the distribution of resonances was studied, among others, by Buslaev, Fock, Babich-Grigoreva, Bardos-Lebeau-Rauch, and Hargé-Lebeau. We refer to [22] for pointers to the literature on the subject.

The problem can be described as follows. Let $\mathcal{O} \subset \mathbb{R}^n$ be a strictly convex compact set with a \mathcal{C}^∞ boundary. We consider the Dirichlet (or Neumann) Laplacian on $\mathbb{R}^n \setminus \mathcal{O}$, $-\Delta_{\mathbb{R}^n \setminus \mathcal{O}}$, and its resolvent,

$$R_{\mathcal{O}}(\lambda) \stackrel{\text{def}}{=} (-\Delta_{\mathbb{R}^n \setminus \mathcal{O}} - \lambda^2)^{-1} : L^2(\mathbb{R}^n \setminus \mathcal{O})$$

$$\longrightarrow H^2(\mathbb{R}^n \setminus \mathcal{O}) \cap H_0^1(\mathbb{R}^n \setminus \mathcal{O}), \quad \text{Im } \lambda > 0.$$

When we allow $R_{\mathcal{O}}(\lambda)$ to act on a smaller space with values in a larger space, it becomes meromorphic in λ :

$$R_{\mathcal{O}}(\lambda) : L^2_{\text{comp}}(\mathbb{R}^n \setminus \mathcal{O}) \longrightarrow H^2_{\text{loc}}(\mathbb{R}^n \setminus \mathcal{O}) \cap H^1_{0,\text{loc}}(\mathbb{R}^n \setminus \mathcal{O}),$$

$$\lambda \in \begin{cases} \mathbb{C} & \text{when } n \text{ is odd} \\ \Lambda & \text{when } n \text{ is even} \end{cases}$$

where Λ is the logarithmic plane. The poles of this meromorphic family of operators are called *resonances* or *scattering poles*. They constitute a natural replacement of discrete spectral data for problems on non-compact domains — see [26] for an introduction and references.

The first step of the argument is a deformation of $\mathbb{R}^n \setminus \mathcal{O}$ to a totally real submanifold, Γ , with boundary $\partial\Gamma = \partial\mathcal{O}$ in \mathbb{C}^n . The Laplacian $-\Delta_{\mathbb{R}^n \setminus \mathcal{O}}$ on $\mathbb{R}^n \setminus \mathcal{O}$ can be considered as a restriction of the holomorphic Laplacian on \mathbb{C}^n and it in turn restricts to an operator on Γ , $-\Delta_{\Gamma}$. When Γ is equal to $e^{i\theta_0}\mathbb{R}^n$ near infinity then the resonances of $-\Delta_{\mathbb{R}^n \setminus \mathcal{O}}$ coincide with the complex eigenvalues of Δ_{Γ} in a conic neighbourhood of \mathbb{R} . That is the essence of the well known complex scaling method adapted to this setting.

Normal geodesic coordinates are obtained by taking x' as coordinates on $\partial\mathcal{O}$ and x_n as the distance to $\partial\mathcal{O}$. In these coordinates the Laplacian near the boundary is approximated by

$$(5.14) \quad D^2_{x_n} - 2x_n Q(x', D_{x'}) + R(x', D_{x'})$$

where R is the induced Laplacian on the boundary and the principal symbol of Q is the second fundamental form of the boundary. The complex deformation near the boundary can be obtained by rotating x_n in the complex plane: $x_n \mapsto e^{i\theta}x_n$ which changes (5.14) to

$$(5.15) \quad e^{-2i\theta}D^2_{x_n} - 2e^{i\theta}x_n Q(x', D_{x'}) + R(x', D_{x'}).$$

The natural choice of θ comes from the homogeneity of the equation: $\theta = \pi/3$.

It is also natural to work in the semi-classical setting, that is, to consider resonances of $-h^2\Delta_{\mathbb{R}^n \setminus \mathcal{O}}$ near a fixed point, say 1. Letting $h \rightarrow 0$ gives then asymptotic information about resonances of $-\Delta_{\mathbb{R}^n \setminus \mathcal{O}}$.

Hence we are lead to an operator which near the boundary is approximated by

$$(5.16) \quad P_0(h) = e^{-2\pi i/3}((hD_{x_n})^2 + 2x_n Q(x', hD_{x'})) + R(x', hD_{x'}),$$

and we are interested in its eigenvalues close to 1. Let us consider the principal symbol of (5.16) in the tangential variables. That gives

$$p_0(h) = e^{-2\pi i/3}((hD_{x_n})^2 + 2x_n Q(x', \xi')) + R(x', \xi').$$

We are interested in the invertibility of $P_0(h) - \zeta$ for ζ close to 1 and that should be related to invertibility of the operator valued symbol $p_0(h) - \zeta$. We rewrite it as

$$(5.17) \quad \begin{aligned} p_0(h) - \zeta &= h^{\frac{2}{3}} \left(e^{-2\pi i/3} (D_t^2 + t\mu) + \lambda - z \right), \\ t &= h^{-\frac{2}{3}} x_n, \quad \lambda = h^{-\frac{2}{3}} (R(x', \xi') - 1), \\ z &= h^{-\frac{2}{3}} (\zeta - 1), \quad \mu = 2Q(x', \xi'), \end{aligned}$$

that is, we rescale the variables using the natural homogeneity of $p_0(h) - \zeta$. On the symbolic level the operator (5.16) can be analyzed rather easily. We can describe $(p_0(h) - \zeta)^{-1}$ using the Airy function:

$$(D_t^2 + t)Ai(t) = 0, \quad Ai(-\zeta_j) = 0, \quad Ai \in L^2([0, \infty)).$$

Thus we consider

$$(5.18) \quad \begin{aligned} P_\lambda - z &= e^{-2\pi i/3} (D_t^2 + \mu t) + \lambda - z, \\ \lambda &\in \mathbb{R}, \quad 1/C \leq \mu \leq C, \quad |\text{Im } z| < C_1, \end{aligned}$$

where C_1 will remain large but fixed. To simplify the notation we shall now put $\mu = 1$ (all the estimates will clearly be uniform with respect to μ with all derivatives).

Let $0 > -\zeta_1 > -\zeta_2 > \dots > -\zeta_k > \dots$ be the zeros of the Airy function and let $e_j(t) = c_j Ai(t - \zeta_j)$ be the normalized eigenfunctions of

$$\begin{cases} (D_t^2 + t)e_j(t) = \zeta_j e_j(t), & t \geq 0 \\ e_j(0) = 0. \end{cases}$$

We recall that the eigenfunctions e_j decay rapidly since for $t \rightarrow +\infty$ we have

$$Ai(t) \sim (2\sqrt{\pi})^{-1} t^{-\frac{1}{4}} \exp(-2t^{\frac{3}{2}}/3).$$

We now take $N = N(C_1)$ to be the largest number such that

$$|\text{Im } e^{-i2\pi/3} \zeta_N| \leq C_1.$$

To set up the model Grushin problem we define

$$(5.19) \quad \begin{aligned} R_+^0 : L^2([0, \infty)) &\longrightarrow \mathbb{C}^N, \quad R_+^0 u(j) = \langle u, e_j \rangle, \quad 1 \leq j \leq N, \\ R_-^0 : \mathbb{C}^N &\longrightarrow L^2([0, \infty)), \quad R_-^0 = (R_+^0)^*. \end{aligned}$$

Using this we put

$$\begin{aligned}
 (5.20) \quad \mathcal{P}_\lambda^0(z) &= \begin{pmatrix} P_\lambda - z & R_-^0 \\ R_+^0 & 0 \end{pmatrix} : B_\lambda \times \mathbb{C}^N \longrightarrow L^2 \times \mathbb{C}^N, \\
 B_\lambda &= \{u \in L^2 : D_t^2 u, tu \in L^2, u(0) = 0\}, \\
 \|u\|_{B_{z,\lambda}} &= \langle \lambda - \operatorname{Re} z \rangle \|u\|_{L^2} + \|D_t^2 u\|_{L^2} + \|tu\|_{L^2}.
 \end{aligned}$$

Since the eigenvalues of P_λ are given by $\lambda + e^{-2\pi i/3} \zeta_j$ and e_j are the corresponding eigenfunctions, we see that $\mathcal{P}_\lambda^0(z)$ is bijective with a bounded inverse.

As in §5.3 our Grushin problem becomes “stable under perturbations”. However, because of the rescaling, the symbol class of the inverse is very bad in the original coordinates: we lose $h^{-\frac{2}{3}}$ when differentiating in the direction transversal to the hypersurface $R - 1 = 0$. Overcoming that requires some second microlocal techniques. Once that is in place the invertibility of $P_0(h) - (1 + h^{\frac{2}{3}}z)$ for $|\operatorname{Im} z| \leq C$ is controlled by invertibility of an operator on the boundary with the principal symbol given by

$$\begin{aligned}
 (5.21) \quad E_{-+}^0 &\in \operatorname{Hom}(\mathbb{C}^N, \mathbb{C}^N), \quad (E_{-+}^0)_{1 \leq i, j \leq N} = -(\lambda - z + \mu^{\frac{2}{3}} e^{-2\pi i/3} \zeta_j) \delta_{ij}, \\
 \lambda &= h^{-\frac{2}{3}}(R(x', \xi') - 1), \quad \mu = 2Q(x', \xi').
 \end{aligned}$$

Here N depends on C which controls the range of $\operatorname{Im} z$.

The passage to a global operator on the boundary, $E_{-+}(z)$, with poles of $E_{-+}(z)^{-1}$ corresponding to the rescaled resonances is rather delicate. We use [22, Section 6] a symbolic calculus which takes into account lower order terms near the boundary. This results in an effective Hamiltonian, $E_{-+}(z)$, described in Theorem 5.5. In a suitable sense it is close to the model operator E_{-+}^0 described above. It has to be stressed that a restriction on the range of $\operatorname{Re} z$ has to be made: for every large constant L we construct a different $E_{-+}(z)$ which works for $|\operatorname{Re} z| \leq L$. The properties of the leading symbol remain unchanged but the lower order terms and the symbolic estimates depend on L .

The detailed description of the effective Hamiltonian is quite technical and involves the second microlocal classes of pseudodifferential operators introduced in [22, Section 4]. Nevertheless from a computational point of view the construction is quite straightforward relying on the Grushin problem described above and the Taylor expansion of the coefficients of the Laplacian (in normal geodesic coordinates) at the boundary.

THEOREM 5.5. — *Let $W \Subset (0, \infty)$ be a fixed set. For every $w \in W$ and $z \in \mathbb{C}$, $|\operatorname{Re} z| \ll 1/\sqrt{\delta}$, $|\operatorname{Im} z| \leq C_1$ there exists $E_{w,-+}(z)$, a second*

microlocal pseudodifferential operator associated to $\Sigma_w = \{p \in T^*\partial\mathcal{O} : R(p) = w\}$, $N = N(C_1)$ such that for $0 < h < h_0(\delta)$:

(i) If the multiplicity of the pole of the meromorphic continuation of $(\Delta_{\mathbb{R}^n} \setminus \mathcal{O} - \zeta)^{-1}$ is given by $m_{\mathcal{O}}(\zeta)$ then

$$(5.22) \quad m_{\mathcal{O}}(h^{-2}(w + h^{\frac{2}{3}}z)) = \frac{1}{2\pi i} \operatorname{tr} \oint_{|\tilde{z}-z|=\epsilon} E_{w,-+}(\tilde{z})^{-1} \frac{d}{d\tilde{z}} E_{w,-+}(\tilde{z}) d\tilde{z},$$

$0 < \epsilon \ll 1.$

(ii) If $E_{w,-+}^0(z; p) = \sigma_{\Sigma_w, h}(E_{w,-+}(z))(p; h)$, $p \in T^*\partial\mathcal{O}$, $\sigma_{\Sigma_w, h}$, the second microlocal symbol map,

$$E_{w,-+}^0(z; p; h) = \mathcal{O}(\langle \lambda - \operatorname{Re} z \rangle).$$

In addition for $|\lambda| \leq 1/(C\sqrt{\delta})$ we have

$$(5.23) \quad \|E_{w,-+}^0(z; p; h) - \operatorname{diag}(z - \lambda - e^{-2\pi i/3}\zeta_j(p))\|_{\mathcal{L}(\mathbb{C}^N, \mathbb{C}^N)} \leq \epsilon \ll 1,$$

and

$$(5.24) \quad \det E_{w,-+}^0(z; p; h) = 0 \iff z = \lambda + e^{-2\pi i/3}\zeta_j(p) \text{ for some } 1 \leq j \leq N$$

where the zero is simple. Here $\zeta_j(p) = \zeta_j(2Q(p))^{\frac{2}{3}}$.

(iii) For $|\lambda| \geq 1/(C\sqrt{\delta})$, $E_{w,-+}^0$ is invertible and

$$E_{w,-+}^0(z; p; h)^{-1} = \mathcal{O}(\langle \lambda - \operatorname{Re} z \rangle^{-1}).$$

In [22, Section 9] we give a trace formula for $E_{-+}(z)$. For that we start with the obvious observation that the trace of the integral of $E_{-+}(z)^{-1}(d/dz)E_{-+}(z)$ against a holomorphic function f over a closed curve gives the sum of values of f at resonances enclosed by the curve. The proof of the trace formula involves a further Grushin reduction, a local lower modulus theorem and a good choice of contours. The gain is in obtaining an integral in the region where the operator $E_{-+}(z)$ is elliptic (roughly speaking in the pole free region). A good choice of f , yields an asymptotic formula (see [22, Theorem 1.2]) for the number of resonances in bands

$$\begin{aligned} \kappa\zeta_j(\operatorname{Re} \lambda)^{\frac{1}{3}} - C < -\operatorname{Im} \lambda < K\zeta_j(\operatorname{Re} \lambda)^{\frac{1}{3}} + C, \quad j \leq j_0 \\ \kappa = 2^{-\frac{1}{3}} \cos \frac{\pi}{6} \min_{S\partial\mathcal{O}} Q^{\frac{2}{3}}, \quad K = 2^{-\frac{1}{3}} \cos \frac{\pi}{6} \max_{S\partial\mathcal{O}} Q^{\frac{2}{3}}, \end{aligned}$$

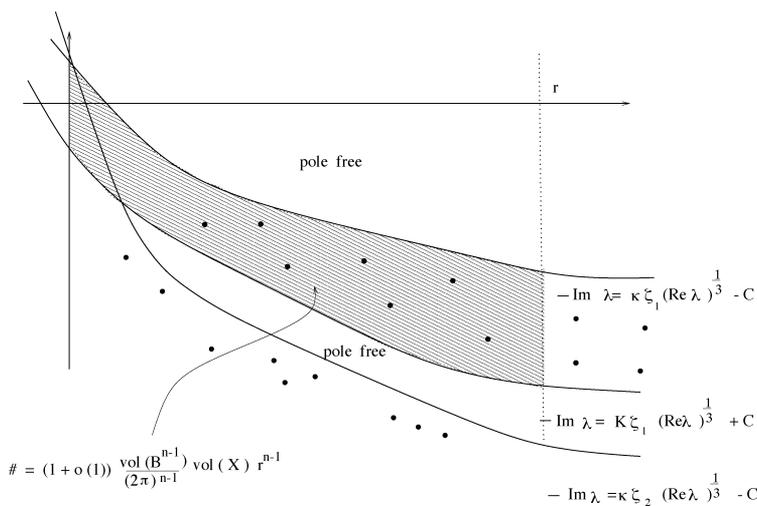


Figure 5.1. The distribution of resonances for a convex obstacle satisfying the pinched curvature assumption (5.25) with $j_0 = 1$.

where, as above, Q is the second fundamental form of $\partial\mathcal{O}$ and $S\partial\mathcal{O}$ the sphere bundle of $\partial\mathcal{O}$, provided that we have the pinched curvature condition:

$$(5.25) \quad \frac{\max_{S\partial\mathcal{O}} Q}{\min_{S\partial\mathcal{O}} Q} < \left(\frac{\zeta_{j_0+1}}{\zeta_{j_0}} \right)^{\frac{3}{2}}.$$

Under this assumption the regions between the bands are resonance free — this is shown in Figure 5.1 which illustrates the result.

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