REGULARITY FOR EIGENFUNCTIONS OF SCHRÖDINGER OPERATORS

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ABSTRACT. We prove a regularity result in weighted Sobolev (or Babuška–Kondratiev) spaces for the eigenfunctions of certain Schrödinger-type operators. Our results apply, in particular, to a non-relativistic Schrödinger operator of an N-electron atom in the fixed nucleus approximation. More precisely, let $\mathcal{K}_a^m(\mathbb{R}^{3N}, r_S)$ be the weighted Sobolev space obtained by blowing up the set of singular points of the potential $V(x) = \sum_{1\le j\le N} \frac{b_j}{|x_j|} + \sum_{1\le i<j\le N} \frac{c_{ij}}{|x_i - x_j|}$, $x \in \mathbb{R}^{3N}$, $b_j, c_{ij} \in \mathbb{R}$. If $u \in L^2(\mathbb{R}^{3N})$ satisfies $(-\Delta + V)u = \lambda u$ in distribution sense, then $u \in \mathcal{K}_a^m$ for all $m \in \mathbb{Z}_+$ and all $a \le 0$. Our result extends to the case when b_j and c_{ij} are suitable bounded functions on the blown-up space. In the single-electron, multi-nuclei case, we obtain the same result for all $a < 3/2$.

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1. Introduction

We prove a global regularity result for the eigenfunctions of a non-relativistic Schrödinger operator $\mathcal{H} := -\Delta + V$ of an N-electron atom. More precisely, let

$$V(x) = \sum_{1\le j\le N} \frac{b_j}{|x_j|} + \sum_{1\le i<j\le N} \frac{c_{ij}}{|x_i - x_j|}, \tag{1}$$

where $x = (x_1, x_2, \ldots, x_N) \in \mathbb{R}^{3N}$, $x_j \in \mathbb{R}^3$, and b_j and c_{ij} are suitable smooth functions. This potential can be used to model the case of a single, heavy nucleus, in which case b_j are negative constants, arising from the attractive force between the nucleus and the j-th electron, whereas the c_{ij} are positive constants, arising from the repelling forces between electrons. Our results, however, will not make use of sign assumptions on the coefficients b_j, c_{ij}. We also study the case of one electron and several fixed nuclei, which is important for the study of Density Functional Theory, Hartree, and Hartee-Fock equations. In that case, our regularity results are optimal. Our method can also be applied to the case of several light nuclei and to the study of wave packets, as in [38].

Let $u \in L^2(\mathbb{R}^{3N})$ be an eigenfunction of $\mathcal{H} := -\Delta + V = -\sum_{i=1}^{3N} \frac{\partial^2}{\partial x_i^2} + V$, the Schrödinger operator associated to this potential, that is, a non-trivial solution of

$$\mathcal{H}u := -\Delta u + Vu = \lambda u \tag{2}$$

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in the sense of distributions, where $\lambda \in \mathbb{R}$. Our main goal is to study the regularity of u. One can replace the Laplacian Δ with any another uniformly strongly elliptic operator on $\mathbb{R}^n$. Typically the negativity of the b_j implies that infinitely many eigenfunctions of $\mathcal{H}$ exist, see for instance the discussion in [48, XIII.3]. In physics, an eigenfunction of $\mathcal{H}$ (associated to a discrete eigenvalue with finite multiplicity) is interpreted as a bound electron, as its evolution under the time-dependent Schrödinger equation is $e^{-i\lambda t}u(x)$ and thus the associated probability distribution $|u(x)|^2$ does not depend on t.

The potential V is singular on the set $S := \bigcup_j \{x_j = 0\} \cup \bigcup_{i<j}\{x_i = x_j\}$. The planes in the union defining S describe the collision of at least two particles, thus we also call them collision planes, as customary. Basic elliptic regularity [17, 50] shows that $u \in H^s_{\mathrm{loc}}(\mathbb{R}^{3N} \smallsetminus S)$ for all $s \in \mathbb{R}$, which is however not strong enough for the purpose of approximating the eigenvalues and eigenvectors of $\mathcal{H}$. Moreover, it is known classically that u is not in $H^s(\mathbb{R}^{3N})$ for all $s \in \mathbb{R}$ [24, 33, 50]. If the coefficient b_j and c_{ij} are real-analytic, then it follows from analytic regularity theory (see e.g. [47, Theorem 6.8.1]) that u is analytic on $\mathbb{R}^{3N} \setminus S$. In this case a strong local regularity result was obtained in [24] in the neighborhood of the simple coalescence points, where it was shown that locally $u(x) = u_1(x) + |l(x)|u_2(x)$ with u_1 and u_2 real analytic and l linear. See also [8, 10, 11, 16, 20, 22, 21, 23, 25, 36, 38, 51, 54, 55, 56] and references therein for more results on the regularity of the eigenfunctions of Schrödinger operators. Related is [19] which was circulated after this article has been submitted.

Our approach is to use the "weighted Sobolev spaces," or "Babuška-Kondratiev spaces,"

$$\mathcal{K}^m_a(\mathbb{R}^n, r_S) := \{u : \mathbb{R}^n \to \mathbb{C} \,|\, r_S^{|\alpha|-a}\partial^\alpha u \in L^2(\mathbb{R}^n),\ |\alpha| \le m\}, \tag{3}$$

where $a \in \mathbb{R}$ and $m \in \mathbb{N} \cup \{0\}$. The weight function $r_S(x)$ is the smoothed distance from x to S, however the distance r_S is not measured with respect to euclidean distance, but with respect to a metric on the ball compactification of $\mathbb{R}^n$. This modified choice does not effect $\mathcal{K}^m_a(\mathbb{R}^n, r_S)$ on closed balls, but globally. The main result of our paper (Theorem 4.3) is that

$$u \in \mathcal{K}^m_a(\mathbb{R}^{3N}, r_S) \tag{4}$$

for $a \le 0$ and for *arbitrary* $m \in \mathbb{N}$. For a single electron, we prove the same result for $a < 3/2$ and conjecture that this holds true in general. Let us notice that we obtain higher regularity results, which were not available before (for instance, the results in [38], yield the boundedness of eigenfunctions and of their gradients, but no results on the higher derivatives).

The proof of our main result uses a suitable compactification $\mathbb{S}$ of $\mathbb{R}^{3N} \smallsetminus S$ to a manifold with corners, which turns out to have a Lie manifold structure. Then we use the regularity result for Lie manifolds proved in [2]. The weighted Sobolev spaces $\mathcal{K}^m_a(\mathbb{R}^{3N}, r_S)$ then identify with some geometrically defined Sobolev spaces (also with weight).

To obtain the space $\mathbb{S}$, we compactify $\mathbb{R}^{3N}$ to a ball. This ball carries a Lie manifold structure, which describes the geometry underlying the scattering calculus, recalled later. The space $\mathbb{S}$ is then blown up along the closure of the singular set S in $\mathbb{R}^{3N}$. For this we decompose S in its strata of different dimensions and then blow up the 0-dimensional stratum first and then successively the strata of higher and higher dimension. The resulting compact space is a manifold with corners $\mathbb{S}$ whose interior is naturally diffeomorphic to $\mathbb{R}^{3N} \setminus S$. Roughly speaking, the blow-up-compactification procedure amounts to define generalized polar coordinates close to the singular set in which the analysis simplifies considerably. Each singular stratum of the singular set S gives rise to a boundary hyperface, corresponding to the collision planes, in the blown-up manifold with corners $\mathbb{S}$, and the distance functions to the strata turn into boundary defining functions. (These kind of hyperfaces are called also 'hyperfaces at infinity'.) The construction of the manifold with corners $\mathbb{S}$ is a standard technique, see e.g. [46] for a similar construction.

We show then that, additionally, the compactification $\mathbb{S}$ carries a Lie structure at infinity $\mathcal{W}$, a geometric structure developed in [3, 4], which extends work by Melrose, Schrohe, Schulze, Vasy and their collaborators, which in turn build on earlier results by Cordes [12], Parenti [42], and others. More precisely, $\mathcal{W}$ is a Lie subalgebra of vector fields on $\mathbb{S}$ with suitable properties (all vector fields are tangent to the boundary, $\mathcal{W}$ is a finitely generated projective $C^\infty(\mathbb{S})$-module, there are no restrictions on $\mathcal{W}$ in the interior of $\mathbb{S}$). There is a natural algebra $\mathrm{Diff}_{\mathcal{W}}(\mathbb{S})$ of differential operators on $\mathbb{S}$, defined as the set of differential operators generated by $\mathcal{W}$ and $C^\infty(\mathbb{S})$. This Lie structure is obtained iteratively as well. On the ball compactification of $\mathbb{R}^{3N}$ this is just the Lie structure underlying the scattering calculus. We will show in Section 3 that each time we blow up a Lie manifold along a suitable submanifold, then the blown-up manifold inherits the structure of a Lie manifold as well. In particular, we obtain a Lie manifold structure on the blown-up manifold without assuming any additional condition at infinity, in contrast to the existing literature where Lie manifold structures on blow-ups have only been developed under quite restrictive conditions. The Lie structure on $\mathbb{S}$ provides a Lie algebroid A on $\mathbb{S}$, a structure which, in particular, is a vector bundle A over $\mathbb{S}$. It comes with an anchor map $\rho : A \to T\mathbb{S}$, a vector bundle homomorphism which is an isomorphism in the interior of $\mathbb{S}$. A metric on A gives rise to a complete metric g on the interior $\mathbb{S}_0$ of $\mathbb{S}$. Metrics on $\mathbb{S}_0 \cong \mathbb{R}^{3N} \setminus S$ obtained this way are said to be compatible with the Lie structure. Our blow-up procedure yields such a compatible metric on $\mathbb{R}^{3N} \setminus S$ with the additional property to be conformal to the euclidean metric.

Our analytical results will be obtained by studying the properties of the differential operators in $\mathrm{Diff}_{\mathcal{W}}(\mathbb{S})$ and then by relating our Hamiltonian to $\mathrm{Diff}_{\mathcal{W}}(\mathbb{S})$. Here $\mathcal{W}$ is the Lie algebra of vector fields defining the Lie manifold structure of $\mathbb{S}$. Some of the relevant results in this setting were obtained in [2]. More precisely, let $\rho := \prod_{1\leq i\leq k} x_{H_i}$, where $\mathcal{B} = \{H_1, \ldots, H_k\}$ is the set of boundary hyperfaces of $\mathbb{S}$ that are obtained by blowing up the singular set (corresponding to the collision planes) and x_{H_i} is a defining function of the hyperface H_i. An important step in our approach is to show that $\rho^2\mathcal{H} \in \mathrm{Diff}_{\mathcal{W}}(\mathbb{S})$, where $\mathcal{H} = -\Delta + V$ is as in Equation (2) (see Theorem 4.2).

Let $H^m(\mathbb{S})$ be the Sobolev spaces associated to a metric g on $\mathbb{R}^{3N} \smallsetminus S$ compatible with the Lie manifold structure on $\mathbb{S}$, namely

$$H^m(\mathbb{S}) := \{u \in L^2(\mathbb{R}^{3N}) \mid Du \in L^2(\mathbb{R}^{3N} \smallsetminus S, d\,\mathrm{vol}_g),\ \forall\ D \in \mathrm{Diff}^m_{\mathcal{W}}(\mathbb{S})\}. \tag{5}$$

For any vector $\vec{\mathbf{a}} = (a_H)_{H\in\mathcal{B}} \in \mathbb{R}^k$, where again $k := \#\mathcal{B}$ is the number of hyperfaces of $\mathbb{S}$ corresponding to the singular set (the collision planes), we define $H^m_{\vec{\mathbf{a}}}(\mathbb{R}^{3N}) := \chi H^m(\mathbb{S})$, with $\chi := \prod_{H\in\mathcal{B}} x_H^{a_H}$. In particular, $H^m_{\vec{\mathbf{0}}}(\mathbb{R}^{3N}) = H^m(\mathbb{S})$. This allows us to use the regularity result of [2] to conclude that $u \in H^m_{\vec{\mathbf{a}}}(\mathbb{R}^N)$ for all m, whenever $u \in H^0_{\vec{\mathbf{a}}}(\mathbb{R}^N)$. Since $H^0_{\vec{\mathbf{a}}}(\mathbb{R}^{3N}) = L^2(\mathbb{R}^{3N})$ for suitable $\vec{\mathbf{a}} = (a_H)$, this already leads to a regularity result on the eigenfunctions u of $\mathcal{H}$, which is however not optimal in the range of a, as we show for the case of a single electron (but multiple nuclei). Future work will therefore be needed to make our results fully applicable to numerical methods. One will probably have to consider also regularity in anisotropically weighted Sobolev spaces as in [7].

We now briefly review the contents of this paper. In Section 2, we describe the differential structure of the blow-up of a manifold with corners by a family of submanifolds that intersect cleanly. In particular, we define the notion of iterated blow-up in this setting. In Section 3, we review the main definitions of manifolds with a Lie structure at infinity and of lifting vector fields to the blown-up manifold. The main goal is to show that the iterated blow-up of a Lie manifold inherits such a structure (see Theorem 3.10). We give explicit descriptions of the relevant Lie algebras of vector fields, study the geometric differential operators on blown-up spaces and describe the associated Sobolev spaces. Finally, in Section 4, we consider the Schrödinger operator with interaction potential (1) and apply the results of the previous sections to obtain our main regularity result, Theorem 4.3, whose main conclusion is Equation (4) stated earlier. The range of the index a in Equation (4) is not optimal. New ideas are needed to improve the range of a. We show how this can be done for the case of a single electron, but multi-nuclei, in which case we do obtain the optimal range $a < 3/2$. When b_j and c_{ij} are constants, our regularity result in the single electron case is also a consequence of [23, 24].

In fact, for the case of a single electron and several nuclei, our result is more general, allowing for the potentials that arise in applications to the Hartree-Fock equations and the Density Functional Theory. As such, they can be directly used in applications to obtain numerical methods with optimal rates of convergence in $\mathbb{R}^3$. For several electrons, even after obtaining an optimal range for the constant a, our results will probably need to be extended before being used for numerical methods. The reason is that the resulting Riemannian spaces have exponential volume growth. This problem can be fixed by considering anisotropically weighted Sobolev spaces, as in [7]. The results for anisotropically weighted Sobolev spaces however are usually a consequence of the results for the usual weighted Sobolev spaces. For several electrons, one faces additional difficulties related to the high dimension of the corresponding space (curse of dimensionality).

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2. Differential structure of blow-ups

2.1. **Overview.** The main goal of this section is to establish a natural procedure to desingularize a manifold with corners M along finitely many submanifolds $X_1, X_2, \ldots, X_k$ of M. This construction is often useful in studying singular spaces such as polyhedral domains and operators with singular potentials [5, 6, 31, 40]. Its origins in the setting of pseudodifferential calculus on singular spaces can be traced to the work of Melrose, Schulze, and their collaborators, building on earlier work by Cordes, Parenti, Taylor, and others, see [44, 43, 30] and references therein. See also the notes [46] for more on the constructions below. In what follows, by a *manifold* we will mean a manifold that may have corners. On the other hand, by a *smooth manifold* we shall understand a manifold that does **not** have a boundary (so no corners either). In addition, a submanifold is always required to be a *closed* subset.

If X is a submanifold of M, then the desingularization procedure yields a new manifold, called the *blow-up* of M along X, denoted by $[M : X]$. Roughly speaking, $[M : X]$ is obtained by removing X from M and gluing back the unit sphere bundle of the normal bundle of X in M. If M is a manifold without boundary, then $[M : X]$ is a manifold whose boundary is the total space of that sphere bundle. More details will be given below. There is also an associated natural *blow-down map* $\beta : [M : X] \to M$ which is the identity on $M \setminus X$.

Then we want to desingularize along a second submanifold X' of M, typically we will have $X \subset X' \subset M$. In this situation, the inclusion $X' \hookrightarrow M$ lifts to an embedding $[X' : X] \hookrightarrow [M : X]$. Then we blow-up $[M : X]$ along $[X' : X]$, obtaining a manifold with corners. An iteration will then yield the desired blown-up manifold. Since we are interested in applying our results to the Schrödinger equation, we have to allow that submanifolds intersect each other. These intersection will be blown up first before the submanifold themselves are blown up. So even if one is interested just in smooth manifolds without boundary, a repeated blow up will lead to manifolds with corners.

2.2. **Blow-up in smooth manifolds.** It is convenient to first understand some simple model cases. If $M = \mathbb{R}^{n+k}$ and $X = \mathbb{R}^n \times \{0\}$, then we define

$$[\mathbb{R}^{n+k} : \mathbb{R}^n \times \{0\}] := \mathbb{R}^n \times S^{k-1} \times [0, \infty), \tag{6}$$

with blow-down map

$$\beta : \mathbb{R}^n \times S^{k-1} \times [0, \infty) \to \mathbb{R}^{n+k}, \quad (y, z, r) \mapsto (y, zr). \tag{7}$$

If $x \in \mathbb{R}^n \times S^{k-1} \times (0, \infty)$, then we identify x with $\beta(x)$, in the sense that $\mathbb{R}^n \times S^{k-1} \times (0, \infty)$ is interpreted as polar coordinates for $\mathbb{R}^{n+k} \setminus \mathbb{R}^n$. In the following we use the symbol $\sqcup$ for the *disjoint* union. We obtain (as sets)

$$[\mathbb{R}^{n+k} : \mathbb{R}^n \times \{0\}] = (\mathbb{R}^{n+k} \setminus \mathbb{R}^n \times \{0\}) \sqcup \mathbb{R}^n \times S^{k-1}.$$

Remark 2.1. An alternative way to define $[\mathbb{R}^{n+k} : \mathbb{R}^n \times \{0\}]$ is as follows. For any $v \in \mathbb{R}^{n+k} \setminus \mathbb{R}^n \times \{0\}$ define the $(n+1)$-dimensional half-space $E_v := \{x + tv \mid x \in \mathbb{R}^n \times \{0\},\ t \geq 0\}$ and $G := \big\{E_v \mid v \in \mathbb{R}^{n+k} \setminus \mathbb{R}^n \times \{0\}\big\} \cong S^{k-1}$. Then

$$[\mathbb{R}^{n+k} : \mathbb{R}^n \times \{0\}] := \{(x, E) \mid E \in G,\ x \in E\}$$

and $\beta(x, E) := x$. The equation $x \in E$ defines a submanifold with boundary of $\mathbb{R}^{n+k} \times G$, and its boundary is $\{(x, E) \mid E \in G,\ x \in \mathbb{R}^n \times \{0\}\} \cong \mathbb{R}^n \times S^{k-1}$.

If V is an open subset of $\mathbb{R}^{n+k}$ and $X = (\mathbb{R}^n \times \{0\}) \cap V$, then the blow-up of V along X is defined as

$$[V : X] := \beta^{-1}(V) = V \setminus X \sqcup \beta^{-1}(X)$$

for the above map $\beta : [\mathbb{R}^{n+k} : \mathbb{R}^n \times \{0\}] \to \mathbb{R}^{n+k}$, and the new blow-down map is just the restriction of β to $[V : X]$.

Lemma 2.2. *Let $\phi : V_1 \to V_2$ be a diffeomorphism between two open subsets of $\mathbb{R}^{n+k}$, mapping $X_1 := V_1 \cap \mathbb{R}^n \times \{0\}$ onto $X_2 := V_2 \cap \mathbb{R}^n \times \{0\}$. Then ϕ uniquely lifts to a diffeomorphism*

$$\phi^\beta : [V_1 : X_1] \to [V_2 : X_2]$$

covering ϕ in the sense that $\beta \circ \phi^\beta = \phi \circ \beta$.

Proof. For $x \in V_1 \setminus X_1 \subset [V_1 : X_1]$ we set $\phi^\beta(x) := \phi(x)$. Elements in $\beta^{-1}(X_1)$ will be written as (x, v) with $x = \beta(x, v) \in X_1 \subset \mathbb{R}^n$ and $v \in S^{k-1} \subset \mathbb{R}^k$. Note that $d_x\phi \in \mathrm{End}(\mathbb{R}^{n+k})$ maps $\mathbb{R}^n \times \{0\}$ to itself, and thus has block-form

$$\begin{pmatrix} A & B \\ 0 & D \end{pmatrix}.$$

We then define $\phi^\beta(x, v) := (\phi(x), \frac{Dv}{\|Dv\|}, 0) \in \mathbb{R}^n \times S^{k-1} \times [0, \infty)$. The smoothness of $\phi^\beta : [V_1 : X_1] \to [V_2 : X_2]$ can be checked in polar coordinates.

Alternatively using the above remark, one can express this map as $\phi^\beta(x, E_x) = (\phi(x), E_{\phi(x)})$ for $x \in V_1 \setminus X_1$ and $\phi^\beta(x, E) := (\phi(x), d_x\phi(E))$ if $x \in X_1$. In this alternative expression the smoothness of ϕ^β is an immediate consequence of the definition of derivative as a limit of difference quotients. □

Now let M be an arbitrary smooth manifold (without boundary) of dimension $n + k$ and X a (closed) submanifold of M of dimension n. We choose an atlas $\mathcal{A} := \{\psi_i\}_{i\in I}$ of M consisting of charts $\psi_i : U_i \to V_i$ such that $X_i := X \cap U_i = \psi_i^{-1}\big(V_i \cap (\mathbb{R}^n \times \{0\})\big)$. Note that we do not exclude the case $X \cap U_i = \emptyset$. Then the previous lemma tells us that the transition functions

$$\phi_{ij} := \psi_i \circ \psi_j^{-1} : V_{ij} := \psi_j(U_i \cap U_j) \to V_{ji} := \psi_i(U_i \cap U_j)$$

can be lifted to maps

$$\phi_{ij}^\beta : [V_{ij} : X_{ij}] \to [V_{ji} : X_{ji}],$$

where $X_{ij} := \psi_j(U_i \cap U_j \cap X)$.

Gluing the manifolds with boundary $[V_i : X_i]$, $i \in I$ with respect to the maps ϕ_{ij}^β, $i, j \in I$ we obtain a manifold with boundary denoted by $[M : X]$ and gluing together the blow-down maps yields a map $\beta : [M : X] \to M$. The boundary of $[M : X]$ is $\beta^{-1}(X)$. The restriction of β to the interior $[M : X] \setminus \beta^{-1}(X)$ is a diffeomorphism onto $M \setminus X$ which will be used to identify these sets.

Recall that the *normal bundle* of X in M is the bundle $N^M X \to X$, whose fiber over $p \in X$ is the quotient $N_p^M X := T_pM/T_pX$. Fixing a Riemannian metric g on M, the normal bundle is isomorphic to $T^\perp X = \{v \in T_pM \,|\, p \in X, \quad v \perp T_pX\}$. We shall need also the normal sphere bundle $S^M X$ of X in M, that is, the sphere bundle over X whose fiber $S_p^M X$ over $p \in X$ consists of all unit length vectors in $N_p^M X$ with respect the metric on $N^M X$. The choice of g will not affect our construction. The restriction of $\beta|_{\beta^{-1}(X)} : \beta^{-1}(X) \to X$ is a fiber bundle over X with fibers S^{k-1}, which is isomorphic to the normal sphere bundle.

Let us summarize what we know about the blow-up $[M : X]$ thus obtained. As sets we have $[M : X] = M \setminus X \sqcup S^M X$. The set $S^M X$ is the boundary of $[M : X]$, and the exact way how this boundary is attached to $M \setminus X$ is expressed by the lifted transition functions ϕ_{ij}^β. More importantly, we have seen that the construction of the blow-up is a local problem, a fact that will turn out to be useful below when we discuss the blow-up of manifolds with corners.

2.3. **Blow-up in manifolds with corners.** Now let M be an m-dimensional manifold with corners. Recall that by a hyperface of M we shall mean a boundary face of codimension 1. The intersection of s hyperfaces $H_1 \cap \ldots \cap H_s$, if non-empty, is then a union of boundary faces of codimension s of M. We shall follow the definitions and conventions from [3]. In particular, we shall always assume that each hyperface is embedded and has a defining function. We also say that points x in the interior of $H_1 \cap \ldots \cap H_s$ are points of boundary depth s, in other word the boundary faces of codimension k contain all points of boundary depth $\geq k$. Points in the interior of M are points of boundary depth 0 in M. In the case $s = 0$ the intersection $H_1 \cap \ldots \cap H_s$ denotes M.

Definition 2.3. A closed subset $X \subset M$ is called a *submanifold with corners* of codimension k if any point $\overline{x} \in X$ of boundary depth $s \in \mathbb{N} \cup \{0\}$ in M has an open neighborhood U in M and smooth functions $y_1, \ldots, y_k : U \to \mathbb{R}$ such that the following hold:

(i) $X \cap U = \{x \in U \mid y_1(x) = y_2(x) = \cdots = y_k(x) = 0\}$
(ii) Let $H_1, \ldots, H_s$ be the boundary faces containing $\overline{x}$ (which is equivalent to saying that $\overline{x}$ is in the interior of $H_1 \cap \ldots \cap H_s$). Let $x_1, \ldots, x_s$ be boundary defining functions of $H_1, \ldots, H_s$. Then $dy_1, \ldots, dy_k, dx_1, \ldots, dx_s$ are linearly independent at $\overline{x}$.

Remark 2.4. Similar notions were also introduced and studied by Melrose in [46], however with a different aim and a slightly different terminology. A submanifold with corners in the above sense, is the same as a p-submanifold with $l = k$ in [46, Sec. 1.7], and this is equivalent to an interior p-submanifold in later sections of [46]. Such blow-ups are iterated in [46] as well, and the iterated constructions coincide with our iterated blow-up described below in the case of chains. However, in contrast to [46], if a clean family of submanifolds (definition see below) contains submanifolds X_1 and X_2 with $X_1 \not\subset X_2$ and $X_2 \not\subset X_1$, we will always blow-up $X_1 \cap X_2$ before blowing up X_1 and X_2 which yields stronger analytic properties.

A simple example of a submanifold with corners X of a manifold with corners M is

$$X := [0, \infty)^{m-k} \times \{0\} \subset M := [0, \infty)^{m-k} \times \mathbb{R}^k.$$

Here the codimension is k, and as y_i we can choose the standard coordinate functions of $\mathbb{R}^k$, and as x_i the coordinate functions of $[0, \infty)^{m-k}$.

On the other hand this simple example already provides models for all kind of local boundary behavior of a submanifold with corners X of a manifold with corners M with codimension k, and $m = \dim M$. More precisely, a subset X of a manifold with corners M is a submanifold with corners in the above sense if, and only if, any $x \in X$ has an open neighborhood U and a diffeomorphism $\phi : U \to V$ to an open subset V of $[0, \infty)^{m-k} \times \mathbb{R}^k$ with $\phi(X \cap U) = ([0, \infty)^{m-k} \times \{0\}) \cap V$.

As before, all submanifolds with corners shall be *closed* subsets of M, contrary to the standard definition of a smooth submanifold of a smooth manifold. The definition of a submanifold with corners gives right away:

(i) *Interior submanifold*: the interior of X is a closed submanifold of codimension k of the interior of M, in the usual sense.
(ii) *Constant codimension*: If F is the interior of a boundary face of M of codimension s, then $F \cap X$ is an $(m - k - s)$-dimensional submanifold of F, that is, $F \cap X$ is also a submanifold (in the usual sense) of codimension k in F.
(iii) *Clean intersections*: If F is as above and $x \in F \cap X$, then $T_x(F \cap X) = T_xF \cap T_xX$

The use of the term "clean" goes back to the work of Bott, and was then used again in [46].

Let $N^M X$ denote the normal bundle of X in M. Now, if F is the interior of a boundary face, then the inclusion $F \hookrightarrow M$ induces a vector bundle isomorphism

$$N^F(X \cap F) \cong N^M X|_{X\cap F}.$$

Similarly, we obtain for the interior F of any boundary face an isomorphism for normal sphere bundles

$$S^F(X \cap F) \cong S^M X|_{X\cap F}.$$

Now we will see how to blow-up a manifold M with corners along a submanifold X with corners. For simplicity of presentation let $k \geq 1$. As before, we have as sets $[M : X] = M \setminus X \sqcup S^M X$, but here $M \setminus X$ will, in general, have boundary components, each boundary face F of M will give rise to one (or several) boundary faces for $[M : X]$. The total space of $S^M X$ yields new boundary hyperfaces.

To construct the manifold structure on $[M : X]$ one can proceed as in the smooth setting. Let $\beta : [\mathbb{R}^{n+k} : \mathbb{R}^n \times \{0\}]$ be the blow-down map. Then the blow-up of

$$\mathbb{R}^{n-s} \times [0,\infty)^s \times \{0\} \subset \mathbb{R}^{n-s} \times [0,\infty)^s \times \mathbb{R}^k$$

is just the restriction of $[\mathbb{R}^{n+k} : \mathbb{R}^n \times \{0\}] \to \mathbb{R}^{n+k}$ to $\beta^{-1}(\mathbb{R}^{n-s} \times [0,\infty)^s \times \mathbb{R}^k)$. Similarly, Lemma 2.2 still holds if V_i are open subsets of $\mathbb{R}^{n-s} \times [0,\infty)^s \times \mathbb{R}^k$, and gluing together charts with the lifted transition functions ϕ_{ij}^β yields a manifold with corners $[M : X]$ in a completely analogous way as in the previous section. In this way, we have defined $[M : X]$ if M is a manifold with corners, and if X is a submanifold with corners of M.

For the convenience of the reader, we now describe an alternative way to define $[M : X]$. Let $\mathcal{B} = \{H_1, \dots, H_k\}$ be the set of (boundary) hyperfaces of M. We first realize M as the set $\{x \in \widetilde{M} \,|\, x_H \geq 0,\ \forall H \in \mathcal{B}\}$, for $\widetilde{M}$ an enlargement of M to a smooth manifold, such that $X = \widetilde{X} \cap M$, for a smooth submanifold $\widetilde{X}$ of $\widetilde{M}$. Here $\{x_H\}$ is a set of boundary defining functions of M, extended smoothly to $\widetilde{M}$. Let $\beta : [\widetilde{M} : \widetilde{X}] \to \widetilde{M}$ be the blow-down map. Then we can define $[M : X] := \beta^{-1}(M) = \{x \in [\widetilde{M} : \widetilde{X}], x_H(\beta(x)) \geq 0\}$, and, slightly abusing notation, we will write again x_H for $x_H \circ \beta$. The definition of a submanifold with corners ensures that $[M : X]$ is still a manifold with corners. Note that smooth functions on M (respectively $[M : X]$) are given by restriction of smooth functions on $\widetilde{M}$ (respectively $[\widetilde{M} : \widetilde{X}]$).

It also is helpful to describe the set of boundary hyperfaces of $[M : X]$. Some of them arise from boundary hypersurfaces of M and some of them are new. Let H be a connected boundary hyperface of M. All connected components of $H \setminus (X \cap H)$ give rise to a connected hyperface of $[M : X]$. The other connected hyperfaces of $[M : X]$ arise from connected components of X. Each connected component of X yields a boundary hyperface for $[M : X]$, which is diffeomorphic to the normal sphere bundle of X restricted to that component. (Such a hyperface arising from X is said to be an hyperface at infinity.) The boundary hyperfaces of X then induce codimension 2 boundary faces for $[M : X]$ each of which is the common boundary of a hyperface arising from M and a hyperface arising from X.

One can describe similarly the codimension 2 boundary faces of $[M : X]$. Some of them arise from boundary hyperfaces of X, as described in the paragraph above, the others arise from boundary faces of M of codimension 2. More precisely, let F be the interior of such a face, then any connected component of $F \setminus X$ is a connected component of a boundary face of codimension 2 of $[M : X]$.

As for boundary defining functions, let $\overline{g}$ be a *true* Riemannian metric on M, that is a smooth metric on M, defined and smooth up to the boundary. We shall denote by $r_X : M \to [0,1]$ a continuous function on M, smooth outside X that close to X is equal to the distance function to X with respect to $\overline{g}$ and $r_X^{-1}(0) = X$. A function with these properties will be called *a smoothed distance function to* X. If X and all $H \setminus (X \cap H)$ are connected, then x_H, $H \in \mathcal{B}$ and r_X (identified with their lifts to the blow-up) are boundary defining functions of $[M : X]$. This statement generalizes in an obvious way to the non-connected case.

2.4. **Blow-up in submanifolds.** For the iterated blow-up construction we have to consider the following situation.

Proposition 2.5. *Let Y be a submanifold with corners of M and $X \subset Y$ be a submanifold with corners of Y. Then there is a unique embedding $[Y : X] \to [M : X]$ as a submanifold with corners such that*

$$\begin{array}{ccc} [Y:X] & \to & [M:X] \\ \downarrow \beta_Y & & \downarrow \beta_M \\ Y & \to & M \end{array}$$

commutes. The range of the embedding $[Y : X] \to [M : X]$ is the closure of $Y \setminus X$ in $[M : X]$.

Proof. The statement of the proposition is essentially a local statement. Let us find good local models first. We assume $n = \dim X$, $n + \ell = \dim Y$ and $n + k = \dim M$. As described above X is locally diffeomorphic to an open subset of $[0,\infty)^n$. The definition of submanifolds with corners implies that X does not meet boundary faces of Y or M of codimension $> n$. Thus any point $x \in X$ has an open neighborhood in M where the iterated submanifold structure $X \subset Y \subset M$ is locally diffeomorphic to

$$[0,\infty)^n \times \{0\} \subset [0,\infty)^n \times \mathbb{R}^\ell \times \{0\} \subset [0,\infty)^n \times \mathbb{R}^k.$$

A more precise version of this is the following obvious lemma. Here $A \supset\!\!\!\supset B$ stands for an open inclusion map (so B is an open subset of A).

Lemma 2.6. *Let Y be a submanifold with corners of M and $X \subset Y$ be a submanifold with corners of Y. Then any $x \in X$ has an open neighborhood U in M such that there is a diffeomorphism $\phi : U \to V$ to an open subset V of $[0,\infty)^n \times \mathbb{R}^k$ for which the diagram*

$$\begin{array}{ccccc} X & \supset\!\!\!\supset & U \cap X & \cong & V \cap [0,\infty)^n \times \{0\} \\ \downarrow & & \downarrow & & \downarrow \\ Y & \supset\!\!\!\supset & U \cap Y & \cong & V \cap [0,\infty)^n \times \mathbb{R}^\ell \times \{0\} \\ \downarrow & & \downarrow & & \downarrow \\ M & \supset\!\!\!\supset & U & \cong & V \cap [0,\infty)^n \times \mathbb{R}^k \end{array}$$

commutes.

It is easy to see that Proposition 2.5 holds for the local model as the embedding $S^{\ell-1} \times \{0\} \hookrightarrow S^{k-1}$ induces an embedding

$$\begin{aligned} [U \cap Y : U \cap X] &\cong V \cap [0,\infty)^n \times S^{\ell-1} \times [0,\infty) \times \{0\} \\ \hookrightarrow [U : U \cap X] &\cong V \cap [0,\infty)^n \times S^{k-1} \times [0,\infty). \end{aligned}$$

The local embeddings thus obtained then can be glued together using Lemma 2.2 to get a global map $[Y : X] \to [M : X]$. The other statements of the proposition are then obvious. □

2.5. **Iterated blow-up.** We now want to blow up a finite family of submanifolds.

Definition 2.7. A finite set of connected submanifolds with corners $\mathcal{X} = \{X_1, \dots, X_k\}$, $X_i \neq \emptyset$, of M is said to be a *clean family of submanifolds* if, for any indices $i_1, \dots, i_t \in \{1, 2, \dots, k\}$, one has the following properties:

- Any connected component of $\bigcap_{j=1}^t X_{i_j}$ is in $\mathcal{X}$, that is, the family $\mathcal{X}$ is closed under intersections.
- For any $x \in \bigcap_{j=1}^t X_{i_j}$ one has $\bigcap_{j=1}^t T_x X_{i_j} = T_x \left(\bigcap_{j=1}^t X_{i_j} \right)$.

Examples:

(i) $M = \mathbb{R}^6 = \mathbb{R}^3 \times \mathbb{R}^3$, $X_1 := \mathbb{R}^3 \times \{0\}$, $X_2 := \{0\} \times \mathbb{R}^3$, X_3 the diagonal of $\mathbb{R}^3 \times \mathbb{R}^3$, $X_4 := \{0\}$. Then $\mathcal{X} := \{X_1, X_2, X_3, X_4\}$ is a clean family.

(ii) Using the same notations as in (i), $\mathcal{X}_0 := \{M, X_1, X_2, X_3, X_4\}$, $\mathcal{X}_1 := \{M, X_1, X_2, X_4\}$ and $\mathcal{X}_2 := \{M, X_1\}$ are also clean families.

(iii) More generally, let M be a vector space and $\mathcal{X} = \{X_i\}$ a finite family of affine subspaces closed under intersections. Then $\mathcal{X}$ is a clean family.

If $\mathcal{X} = \{X_i\}$ is a clean family of submanifolds and the submanifolds X_i are also *disjoint*, then we define $[M : \mathcal{X}]$ by successively blowing up the manifolds X_i. The iteratively blown-up space $[M : \mathcal{X}] := [\dots[[M : X_1] : X_2] : \dots : X_k]$ is independent of the order of the submanifolds X_i, as the blow-up structure given by Lemma 2.2 is local.

Let us consider now a general clean family $\mathcal{X}$, and let us define the new family $\mathcal{Y} := \{Y_\alpha\}$ consisting of the *minimal* submanifolds of $\mathcal{X}$ (i. e. submanifolds that do not contain any other proper submanifolds in $\mathcal{X}$). By the assumption that the family $\mathcal{X}$ is closed under intersections, the family $\mathcal{Y}$ consists of disjoint submanifolds of M. Let $M' := [M : \mathcal{Y}]$ be the manifold with corners obtained by blowing up the submanifolds Y_α. Assuming that $\mathcal{Y} \neq \mathcal{X}$, we set $\mathcal{Y}_j := \{Y \in \mathcal{Y} \,|\, Y \subset X_j\}$, for $X_j \in \mathcal{X} \setminus \mathcal{Y}$, and define $X'_j := [X_j : \mathcal{Y}_j]$. By Proposition 2.5 X'_j is the closure of $X_j \smallsetminus \cup Y_\alpha$ in M'. Let also $d_{\mathcal{X}}$ be the minimum of the dimensions of the minimal submanifolds of $\mathcal{X}$ (i. e. the minimum of the dimensions of the submanifolds in $\mathcal{Y}$). We then have the following theorem.

Theorem 2.8. *Assume $\mathcal{Y} \neq \mathcal{X}$. Then, using the notation of the above paragraph, the family $\mathcal{X}' := \{X'_j\}$ is a clean family of submanifolds of M'. Moreover, the minimum dimension $d_{\mathcal{X}'}$ of the family $\mathcal{X}'$ is greater that the minimum dimension $d_{\mathcal{X}}$ of the family $\mathcal{X}$.*

Proof. By Proposition 2.5, the sets X'_j are submanifolds with corners of M'. Let $j_1 < j_2 < \dots < j_t$ and let $Z' := X'_{j_1} \cap X'_{j_2} \cap \dots \cap X'_{j_t}$. We first want to show that $Z' \in \mathcal{X}'$. Assume that $Z' \cap (M \smallsetminus \bigcup Y_\alpha)$ is not empty. Then $Z := X_{j_1} \cap X_{j_1} \cap \ldots \cap X_{j_1} \in \mathcal{X}$ and hence $Z = X_i$, for some i, by the assumption that $\mathcal{X}$ is a clean family. We only need to show that $Z' = X_i'$.

We have that $X_i \cap (M \smallsetminus \bigcup Y_\alpha) \subset X_{j_s} \cap (M \smallsetminus \bigcup Y_\alpha)$, so $X_i' \subset X_{j_s}'$, and hence $X_i' \subset Z' := \bigcap X_{j_s}'$. We need now to prove the opposite inclusion. Let $x \in Z'$. If $\beta(x) \notin Y_\alpha$ for any α, then $x = \beta(x) \in Z = X_i$ and hence $x \in X_i'$. Let us assume then that $y := \beta(x) \in Y_\alpha$ for some α. By definition, this means that $x \in T_yM/T_yY_\alpha$ (and is a vector of length one, but this makes no difference). Our assumption is that $x \in T_yX_{j_s}/T_yY_\alpha$, for all s. But our cleanness assumption then implies $x \in T_yX_i/T_yY_\alpha$, which means $x \in X_i'$, as desired.

It remains to prove that $TX_i' = \bigcap TX_{j_s}'$, where $X_i' = Z' = X_{j_1}' \cap X_{j_2}' \cap \ldots \cap X_{j_t}'$, as above. The inclusion $TX_i' \subset \bigcap TX_{j_s}'$ is obvious. Let us prove the opposite inclusion. Let then $\xi \in \bigcap T_xX_{j_s}'$, $x \in M' = [M : \mathcal{Y}]$. If $\beta(x) \notin Y_\alpha$, for any α, then $\xi \in TX_i'$, by the assumption that $\mathcal{X}$ is a clean family. Let us assume then that $y := \beta(x) \in Y_\alpha$. Since our statement is local, we may assume that $Y_\alpha = \mathbb{R}^{n-s} \times [0,\infty)^s \times \{0\}$ and that $M = \mathbb{R}^{n-s} \times [0,\infty)^s \times \mathbb{R}^k$. Then the tangent spaces $T_yX_{j_s}$ identify with subspaces of $\mathbb{R}^{n+k}$. Let us identify $[M : Y_\alpha]$ with the set of vectors in M at distance ≥ 1 to Y_α. We then use this map to identify all tangent spaces to subspaces of $\mathbb{R}^{n+k}$. With this identification, T_xX_j' identifies with T_yX_j. Therefore, if $\xi \in \bigcap T_xX_{j_s}'$, then $\xi \in \bigcap T_yX_{j_s} = T_yX_i = T_xX_i'$.

For each manifold X_j', we have $\dim X_j' = \dim X_j > \dim Y_\alpha$, for some α, so $d_{\mathcal{X}'} > d_{\mathcal{X}}$. $\square$

We are ready now to introduce the blow-up of a clean family of submanifolds of a manifold with corners M.

Definition 2.9. Let $\mathcal{X} = \{X_j\}$ be a non-empty clean family of submanifolds with corners of the manifold with corners M. Let $\mathcal{Y} = \{Y_\alpha\} \subset \mathcal{X}$ be the non-empty subfamily of minimal submanifolds of $\mathcal{X}$. Let us define $M' := [M : \mathcal{Y}]$, which makes sense since $\mathcal{Y}$ consists of disjoint manifolds. If $\mathcal{X} = \mathcal{Y}$, then we define $[M : \mathcal{X}] = M'$. If $\mathcal{X} \neq \mathcal{Y}$, let $d_{\mathcal{X}}$ be the minimum dimension of the manifolds in $\mathcal{Y}$ and we define $[M : \mathcal{X}]$ by induction on $\dim(\mathcal{X}) - d_{\mathcal{X}}$ as follows. Let $\mathcal{X}' := \{X_j'\}$, where X_j' is the closure of $X_j \smallsetminus (\cup Y_\alpha)$ in M', provided that the later is not empty (thus $\mathcal{X}'$ is in bijection with $\mathcal{X} \smallsetminus \mathcal{Y}$). Then $\dim(M') - d_{\mathcal{X}'} < \dim(M) - d_{\mathcal{X}}$, and $\mathcal{X}'$ is a clean family of submanifolds with corners of M', so $[M' : \mathcal{X}']$ is defined. Finally, we define

$$[M : \mathcal{X}] := [M' : \mathcal{X}'] = [[M : \mathcal{Y}] : \mathcal{X}'].$$

Another equivalent definition of $[M : \mathcal{X}]$ is the following. Assume $\mathcal{X} = \{X_i \,|\, i = 1, 2, \ldots, k\}$. Then we say that $\mathcal{X}$ is *admissibly ordered* if, for any $\ell \in \{1, 2 \ldots, k\}$, the family $\mathcal{X}_\ell = \{X_i \,|\, i = 1, 2, \ldots, \ell\}$ is a clean family as well, or equivalently, if it is closed under intersections. After possibly replacing the index set and reordering the X_i, any $\mathcal{X}$ is admissibly ordered. Let us denote $\mathcal{Y} := \{X_1, \ldots, X_r\}$ for $r := \#\mathcal{Y}$, with $\mathcal{Y}$ the family of minimal submanifolds in $\mathcal{X}$ as before, and X_{r+1} corresponds to a submanifold X_{r+1}' in the family $\mathcal{Y}'$ of minimal submanifolds in $\mathcal{X}'$. This gives the following iterative description of the blow-up:

$$[M : \mathcal{X}] = [[\ldots[M : X_1] : X_2] : \ldots : X_r] : X_{r+1}'] : \ldots : X_k''']$$

where $'''$ stands for an appropriate number of $'$-signs.

For $\ell \in \{1, 2 \ldots, k\}$, let us then denote

$$M^{(\ell)} := [[\ldots[M : X_1] : X_2] : \ldots : X_r] : X_{r+1}'] : \ldots : X_\ell'''] \qquad Y^{(\ell)} := X_\ell''' \subset M^{(\ell-1)}$$

where again $'''$ stands for an appropriate number of $'$-signs. Then $M = M^{(0)}$, $M^{(\ell)} = [M^{(\ell-1)} : Y^{(\ell)}]$ and $M^{(k)} = [M : \mathcal{X}]$.

Definition 2.10. The sequences $Y^{(1)}, Y^{(2)}, \ldots, Y^{(k)}$ and $M^{(0)}, M^{(1)}, \ldots, M^{(k)}$ are called the *canonical sequences* associated to M and the admissibly ordered family $\mathcal{X}$.

Let $\beta_\ell : M^{(\ell)} = [M^{(\ell-1)} : Y^{(\ell)}] \to M^{(\ell-1)}$ for $\ell \in \{1, 2, \ldots, k\}$ be the corresponding blow-down maps. Then we define the blow-down map $\beta : [M : \mathcal{X}] \to M$ as the composition

$$\beta := \beta_1 \circ \beta_2 \circ \ldots \circ \beta_k : M^{(k)} = [M : \mathcal{X}] \to M = M^{(0)}. \tag{8}$$

3. Lie structure at infinity

Manifolds with a Lie structure at infinity were introduced in [3] (see also [44] for the general ideas related to this definition). In this section, we consider the blow-up of a Lie manifold by a submanifold with corners and show that the blown-up space also has a Lie manifold structure. To this effect, we start with describing lifts of vectors fields to the blow-up. By the results of the previous section, we can then blow up with respect to a clean family of submanifolds with corners. We also investigate the effect of the blow-ups on the metric and Laplace operators (and differential operators in general).

Let M be a manifold with corners and let $\mathcal{B}_M = \{H_1, \ldots, H_k\}$ be its set of boundary hyperfaces. As usual, we define

$$\mathcal{V}_M := \{V \in \Gamma(TM) \,|\, V|_H \text{ is tangent to } H \ , \ \forall H \in \mathcal{B}_M\} \,. \tag{9}$$

That is, $\mathcal{V}_M$ denotes the Lie algebra of vector fields on M that are tangent to all boundary faces of M. It is the Lie algebra of the group of diffeomorphisms of M.

3.1. **Lifts of vector fields.** Let M be a manifold with corners. As in the smooth case, we identify the set $\Gamma(TM)$ of smooth vector fields on M with the set of derivations of $C^\infty(M)$, that is, the set of linear maps $V : C^\infty(M) \to C^\infty(M)$ satisfying $V(fg) = fV(g) + V(f)g$. With this identification, the Lie subalgebra $\mathcal{V}_M \subset \Gamma(TM)$ identifies with the set of derivations V that satisfy $V(x_H C^\infty(M)) \subset x_H C^\infty(M)$, for all boundary defining functions x_H [45].

Let M and P be manifolds with corners and $\beta : P \to M$ a smooth, surjective, map. Regarding vector fields as derivations, it is then clear what one should mean by "lifting vector fields from M to P," namely that the following diagram commutes

$$\begin{array}{ccc} C^\infty(P) & \xrightarrow{W} & C^\infty(P) \\ {\scriptstyle\beta^*}\uparrow & & \uparrow{\scriptstyle\beta^*} \\ C^\infty(M) & \xrightarrow{V} & C^\infty(M) \end{array} \tag{10}$$

where $\beta^* f = f \circ \beta$. Given two vector fields V on M and W on P , we say that V *lifts* to W along β, if $V(f) \circ \beta = W(f \circ \beta)$, for any $f \in C^\infty(M)$. Considering the differential $\beta_* : T_pP \to T_{\beta(p)}M$, we then say that V *lifts to* W along β if, and only if, $\beta_* W_p = V_{\beta(p)}$, for all $p \in P$.

For a vector field W on P, $\beta_* W$ does not define in general a vector field on M. If W is the lift of a vector field V on M, then $\beta_* W_p$ only depends on $\beta(p)$, i.e. $\beta_* W_p = \beta_* W_q$ for all $p, q \in P$ with $\beta(p) = \beta(q)$. We denote by $\Gamma_\beta(TP)$ the set of all vector fields on P that are lifts along β of some vector field on M. For any $W \in \Gamma_\beta(TP)$, the push-forward $\beta_* W$ is well defined as a vector field on M. By definition, we have a map

$$\beta_* : \Gamma_\beta(TP) \to \Gamma(TM), \quad (\beta_* W)_x := \beta_* W_p, \; \beta(p) = x. \tag{11}$$

If β is a diffeomorphism, then $\Gamma_\beta(TP) = \Gamma(TP)$ and any vector field on M can be lifted uniquely to P. Note that $\Gamma_\beta(TP)$ is always a Lie subalgebra of $\Gamma(TP)$, since $\beta_*([W_1, W_2]_p) = [\beta_* W_1, \beta_* W_2]_x$, if $\beta(p) = x$.

If β is a submersion, then any vector field on M lifts to P along β, and the lift is unique mod $\ker \beta_*$, that is, after fixing a Riemannian structure on P, there is an unique horizontal lift W such that $W_p \in (\ker \beta_*)^\perp$, $p \in P$.

3.2. **Lifts and products.** Let P, M and β as above. We assume in this subsection that any vector field $V \in \Gamma(TM)$ has *at most one lift* $W_V \in \Gamma(TP)$. We now take product with a further manifold N with corners. Then $T(M \times N) = TM \times TN$. Accordingly, a vector field $\widetilde{V} \in \Gamma(T(M \times N))$ is then naturally the sum of its M- and N-components: $\widetilde{V}(x, y) = \widetilde{V}_M(x, y) + \widetilde{V}_N(x, y)$, $x \in M$, $y \in N$.

The following lemma answers when such a vector field lifts with respect to $\beta \times \mathrm{id} : P \times N \to M \times N$.

Lemma 3.1. *Under the above assumptions (including uniqueness of the lift), any vector field $\widetilde{V} \in \Gamma(T(M \times N))$ has a lift $\widetilde{W} \in \Gamma(T(P \times N))$ if, and only if, for any $y \in N$, the vector field $\widetilde{V}_M(\,.\,, y) \in \Gamma(TM)$ lifts to a vector field W_y on P. In this case, the lift is $\widetilde{W}(x, y) = W_y(x) + \widetilde{V}_N(x, y)$, in particular, the lift $\widetilde{W}$ is uniquely determined.*

Proof. The only non-trivial statement in the lemma is to prove that the vector field $\widetilde{W}$ defined by $\widetilde{W}(x, y) = W_y(x) + \widetilde{V}_N(x, y)$ is smooth, provided that the right hand side exists.

The uniqueness of the lift implies that the map $\Gamma_\beta(TP) \to \Gamma(TM)$ is an isomorphism of vector spaces, and thus its inverse, being a linear map, is a smooth map $\Gamma(TM) \to \Gamma_\beta(TP)$, where we always assume the C^∞-Frechet topology in these spaces. The composition map $Y \to \Gamma(TM) \to \Gamma_\beta(TP)$, $y \mapsto V_M(\,.\,, y) \mapsto W_y$ is thus smooth as well. We have proven the smoothness of $\widetilde{W}$. $\square$

3.3. **Lifting vector fields to blow-ups.** Let M be a manifold with corners, X a submanifold with corners. We are interested in studying lifts of Lie algebras of vector fields on M, tangent to all faces, along the blow-down map $\beta : [M : X] \to M$.

For simplicity of presentation, *we shall restrict to the case* $\dim X < \dim M$, in what follows (even if most of our results hold for $\dim X = \dim M$). We adopt from now on the convention that *any submanifold (with corners) is of smaller dimension than its ambient manifold (with corners).* The map β is then surjective and it yields a diffeomorphism $[M : X] \smallsetminus \beta^{-1}(X) \to M \smallsetminus X$. The problem of lifting vector fields thus is an extension problem, so the lift is unique if it exists. The uniqueness implies that lifts exist on M if and only if they exist on each open subset of M, i.e. the lifting problem is a local problem. Recall that $\mathcal{V}_M$ was defined in Equation (9).

In this subsection, we will show the following proposition on lifts of vector fields to blow-ups. A proof of this result can be found in Section 5.3 of the unpublished manuscript [46], so we include a proof for completeness. Notice, however, that the extension of this result to

Lie manifolds is a new result, which is surprising, in part, because it requires no additional assumptions on the Lie manifold structure, see Subsection 3.5.

Proposition 3.2. *Let M be a manifold with corners, X a submanifold with corners, and $V \in \mathcal{V}_M$. Then, there exists a vector field $W \in \mathcal{V}_{[M:X]}$ that lifts V if, and only if, V is tangent to X.*

The proposition should be seen as an infinitesimal version of Lemma 2.2. Let us denote by $\mathrm{Diffeo}(M/X)$ the group of diffeomorphisms of M mapping X onto itself. Then let $\mathrm{Diffeo}(M) := \mathrm{Diffeo}(M/\emptyset)$. In the case that M is an open subset of $[0,\infty)^n \times \mathbb{R}^k$, and $X = M \cap [0,\infty)^n \times \{0\}$, Lemma 2.2 states that a Lie group homomorphism $\alpha : \mathrm{Diffeo}(M/X) \to \mathrm{Diffeo}([M : X])$ exists such that $\alpha(\phi)$ coincides with ϕ on $M \setminus X$. It thus implies a Lie algebra homomorphism α_* between the corresponding Lie algebras. The Lie algebra of $\mathrm{Diffeo}(M/X)$ consists of those vector fields in $\mathcal{V}_M$ whose restriction to X is tangent to X. The Lie algebra of $\mathrm{Diffeo}([M : X])$ is $\mathcal{V}_{[M:X]}$. The image of α_* is $\Gamma_\beta(T[M : X])$. As lifting vector fields is a local property, these considerations already provide a proof of Proposition 3.2, assuming facts from the theory of infinite-dimensional Lie groups and algebras.

In order to be self-contained we will also include a direct proof. As before we will study a simple model situation first.

Lemma 3.3. *Let $M = [0,\infty)^n \times \mathbb{R}^k$ and $X = [0,\infty)^n \times \{0\} \subset M$, and thus $[M : X] = [0,\infty)^n \times S^{k-1} \times [0,\infty)$. Let $V \in \mathcal{V}_M$ be a vector field that is tangent to $[0,\infty)^n \times \{0\}$, that is we assume that V is a vector field on M tangent to the boundary of M and to the submanifold X. Then there exists a lift of V in $\mathcal{V}_{[M:X]}$, that is, there is a vector field $W \in \mathcal{V}_{[M:X]}$ with $\beta_* W = V$ that is tangent to all boundary hyperfaces of $[M : X]$.*

Proof. At first, we assume $n = 0$. Denoting $f_\lambda(x) = f(\lambda x)$, a differential operator $D \in \mathrm{Diff}(\mathbb{R}^k \setminus \{0\})$ is homogeneous of degree h if $(Df)_\lambda = \lambda^h D f_\lambda$ for all $\lambda \in (0,\infty)$. Radially constant vector fields on $\mathbb{R}^k \setminus \{0\}$ thus define first order homogeneous differential operators homogeneous of degree -1.

For $y = (y_1, ..., y_k) \in \mathbb{R}^k \setminus 0$ (defining X) and $(r,\omega) \in [0,\infty) \times S^{k-1}$, $x = \beta(r,\omega) = r\omega$, we can write in polar coordinates, for $r \neq 0$,

$$\partial_{y_j} = \frac{\partial y_j}{\partial r}\partial_r + S_j(r) = \omega_j \partial_r + \frac{1}{r} S_j(1) \tag{12}$$

where $S_j(r)$ is a vector field on S^{k-1}, depending smoothly on $r \in (0,\infty)$. Note that since both ∂_{y_j} and ∂_r are homogeneous of degree -1, the component S_j is again of degree -1, and this means $S_j(r) = \frac{1}{r} S_j(1)$ for all $r \in (0,\infty)$. A vector field V on $\mathbb{R}^k$ vanishes at 0 if, and only if, it can be written as $V = \sum a_{ij}(y) y_i \partial_{y_j}$, $x \in \mathbb{R}^k$. Since a_{ij} lifts to $\beta^* a_{ij} = a_{ij} \circ \beta$ and since, writing $y = r\omega$,

$$y_i \partial_{y_j} = r\omega_i\omega_j \partial_r + \omega_i S_j(1) \tag{13}$$

clearly extends to $r = 0$, we have that V lifts to $[\mathbb{R}^k : 0]$ and it is tangent to S^{k-1} at $r = 0$. The statement for $n = 0$ follows. The case for general n then follows from Lemma 3.1. $\square$

Now, as the existence of a lift is a local property, Lemma 3.3 also holds if M is an open subset of $[0,\infty)^n \times \mathbb{R}^k$ with $X = M \cap [0,\infty)^n \times \{0\}$. If M is a manifold with corners and if

X is submanifold with corners of it, then we obtain that a vector field on M can be lifted in any coordinate neighborhood, if it is tangent to X. As the lifts are unique we obtain sufficiency in Proposition 3.2 by gluing together the local lifts. Note that we obtain from Equation (13) that lifts of vector fields tangent to X are in fact tangent to the fibers of $\beta^{-1}(X) = S^M X \to X$.

It also follows from (12) that a vector field $V \in \Gamma(TM)$ for which $V|_X$ is not tangential to X does not lift to a vector field in $\mathcal{V}_{[M:X]}$, so we finish the proof of Proposition 3.2.

We now choose a true Riemannian metric $\overline{g}$ on M (i. e. smooth up to the boundary). In contrast to the $\mathcal{V}$-metric, introduced later, this is a metric in the usual sense, i.e. a smooth section of $T^*M \otimes T^*M$ which is pointwise symmetric and positive definite. Recall that we denoted by $r_X : M \to [0,\infty)$ a smoothed distance function to X, that is, a continuous function on M, smooth outside X that close to X is equal to the distance function to X with respect to $\overline{g}$ and $r_X^{-1}(0) = X$.

Corollary 3.4. *Let M be a manifold with corners, X a submanifold with corners, and $r_X : M \to [0,\infty)$ be a smoothed distance function to X. Let $V \in \mathcal{V}_M$. Then there exists a vector field $W \in \mathcal{V}_{[M:X]}$ such that $W = r_X V$ on $M \smallsetminus X \subset [M : X]$.*

Proof. Again, it is sufficient to check the lifting property locally. We assume that U is open in M and that $y_1, \dots, y_k$ are functions defining X as in Definition 2.3 (i). We can assume that $r_X^2 = \sum_i y_i^2$. We then can write

$$r_X V = \sum_i \frac{y_i}{r_X}\, y_i V. \tag{14}$$

Proposition 3.2 says that the vector fields $y_i V$ lift to $\Gamma(T[M : X])$ as vector fields tangent to the faces. The functions $\frac{y_i}{r_X}$, defined a priori on $U \setminus (U \cap X)$, extend to smooth functions on $\beta^{-1}(U)$. Thus $r_X V$ has a lift locally on U, and by uniqueness of the local lifts, these lifts match together to a global lift. ☐

If X is connected, then $\{r_X\} \cup \{x_H \mid H \in \mathcal{B}\}$ is a set of boundary defining functions for $[M : X]$, where each x_H is the defining function for the hyperface H of M. Furthermore $W \in \mathcal{V}_{[M:X]}$ if, and only if, $W(x_H f) = x_H \widetilde{f}$ and $W(r_X f) = r_X \widetilde{f}$ (where we are actually considering lifts of x_H and r_X to $[M : X]$). For non-connected X, the distance to X has to be replaced by the distance functions to the connected components in the obvious way, and the same result remains true.

The set of vector fields in $\mathcal{V}$ which are tangent to X forms a sub-Lie algebra of $\mathcal{V}$ which is also a $C^\infty(M)$-submodule. This is the Lie-algebra of Diffeo(M/X). Inside this sub-Lie algebra, the vector fields *vanishing* on X form again a sub-Lie algebra, which is again a $C^\infty(M)$-submodule. This is the Lie algebra to the group Diffeo$(M; X)$ the Lie group of diffeomorphisms of M that fix X pointwise.

We can characterize the lifts of such vector fields. Let $V \in \mathcal{V}_M$ with lift $W \in \mathcal{V}_{[M:X]}$. It follows from the definition that $\beta_*(W(p)) = V_{\beta(p)}$. Hence, $V|_X \equiv 0$ is equivalent to

$$\beta_*(W(p)) = 0 \qquad \forall p \in \beta^{-1}(X). \tag{15}$$

We obtain that V vanishes on X if, and only if, $W|_{S^M X}$ is a vector field on $\beta^{-1}X = S^M X \subset \partial[M : X]$ which is tangent to the fibers of $S^M X \to X$. With (14) we see that lifts of vector fields $r_X V$ from $M \setminus X$ to $[M : X]$ are also tangent to these fibers.

3.4. **Lie manifolds.** Let us recall the definition of a Lie manifold and of its Lie algebroid [3, 4]. Let M be a compact manifold with corners. We say that a Lie subalgebra $\mathcal{V} \subset \mathcal{V}_M$ is a *structural Lie algebra of vector fields* if it is a finitely generated, projective $C^\infty(M)$-module. The Serre-Swan theorem then yields that there exists a vector bundle A satisfying $\mathcal{V} \cong \Gamma(A)$. In particular, $\Gamma(A)$ is a Lie algebra. Moreover,

(1) there is a map $\rho : A \to TM$, called the *anchor map*, which induces the inclusion map $\rho : \Gamma(A) \to \Gamma(TM)$;
(2) ρ is a Lie algebra homomorphism and $[V, fW] = f[V,W] + (\rho(V)f)\,W$.

The vector bundle A is then what is called a *Lie algebroid*.

Definition 3.5. A *Lie manifold* M_0 is given by a pair $(M, \mathcal{V})$ where M is a compact manifold with corners with $M_0 = int(M)$, and $\mathcal{V}$ is structural Lie algebra of vector fields such that $\rho_{|M_0} : A|_{M_0} \to TM_0$ is an isomorphism. A $\mathcal{V}$*-metric* is a smooth section of $A^* \otimes A^*$ which is pointwise symmetric and positive definite.

A $\mathcal{V}$-metric defines a Riemannian metric on the interior M_0 of M. If $\mathcal{V}$ is fixed, then any two such metrics are bi-Lipschitz equivalent. The geometric properties of Riemannian Lie manifolds were studied in [3]. It is known that any such M_0 is necessarily complete and has positive injectivity radius by the results of Crainic and Fernandes [15].

To avoid a misunderstanding, we emphasize that the metric $\overline{g}$ introduced in Subsection 3.3, and used to define smoothed distance functions, is not a $\mathcal{V}$-metric. The metric $\overline{g}$ extends to the boundary as a smooth section of $T^*M \otimes T^*M$, whereas a $\mathcal{V}$-metric does not. One can also use the terminology that $\overline{g}$ is a true metric on TM, whereas $\mathcal{V}$-metrics are usually called metrics on A.

To each Lie manifold we can associate an algebra of $\mathcal{V}$-differential operators $\mathrm{Diff}_{\mathcal{V}}(M)$, the enveloping algebra of $\mathcal{V}$, generated by $\mathcal{V}$ and $C^\infty(M)$. If E, F are vector bundles over M, then we define $\mathrm{Diff}_{\mathcal{V}}(M; E, F) := e_F M_N(\mathrm{Diff}_{\mathcal{V}}(M))e_E$, where e_E, e_F are projections onto $E, F \subset M \times \mathbb{C}^N$.

It is shown in [3] that all geometric differential operators associated to a compatible metric on a Lie manifold are $\mathcal{V}$-differential, including the classical Dirac operator and other generalized Dirac operators. In particular, the de Rham differential defines an operator $d : \Gamma(\bigwedge^q A^*) \to \Gamma(\bigwedge^{q+1} A^*)$ and $d \in \mathrm{Diff}^1_{\mathcal{V}}(M; \bigwedge^q A^*, \bigwedge^{q+1} A^*)$, and its formal adjoint d^* is an operator in $\mathrm{Diff}^1_{\mathcal{V}}(M; \bigwedge^{q+1} A^*, \bigwedge^q A^*)$. By composition, we know that the *Hodge-Laplace operator*

$$\Delta := (d + d^*)^2 = dd^* + d^*d \in \mathrm{Diff}^2_{\mathcal{V}}(M; {\textstyle\bigwedge}^q A^*), \tag{16}$$

is thus $\mathcal{V}$-differential as well. It is moreover elliptic in that algebra, in the sense that its principal symbol, a function defined on A^*, is invertible, see [3].

We shall need the following regularity result from [2, Theorem 5.1]. The Sobolev space $H^k(M, \mathcal{V})$ associated to a Lie manifold $(M, \mathcal{V})$ with a $\mathcal{V}$-metric g on its Lie algebroid A is defined in [2] as

$$H^k(M, \mathcal{V}) := \{u : M \to \mathbb{C} \mid V_1 \dots V_j u \in L^2(M, d\,\mathrm{vol}_g)\ \forall V_1, \dots, V_j \in \mathcal{V},\ j \le k\} \tag{17}$$

Note that these Sobolev spaces are not the Sobolev spaces with respect to the euclidean metric, but with respect to the blown-up metric g, and they depend only on the Lie manifold structure defined by $\mathcal{V}$.

Theorem 3.6. *Let $m \in \mathbb{Z}^+$, $s \in \mathbb{Z}$. Let $P \in \mathrm{Diff}^m_{\mathcal{V}}(M, \mathcal{V})$ be elliptic and $u \in H^r(M, \mathcal{V})$ be such that $Pu \in H^s(M, \mathcal{V})$. Then $u \in H^{s+m}(M, \mathcal{V})$. The same result holds for systems.*

3.5. **Blow-up of Lie manifolds.** Let M carry a Lie manifold structure, and X be a submanifold with corners of M. We want to define a Lie structure on $[M : X]$.

We begin by choosing a true metric $\overline{g}$ on TM, that is, $\overline{g}$ is smooth up to the boundary. Let $U_\epsilon(X)$ be an ϵ-neighborhood of X in M with respect to $\overline{g}$. Later on we will need that the distance function to X with respect to $\overline{g}$ is a smooth function on $U_\epsilon(X) \smallsetminus X$ for sufficiently small $\epsilon > 0$. Unfortunately, such an $\epsilon > 0$ does not exists for arbitrary metrics $\overline{g}$ on M. On the other hand, such an $\epsilon > 0$ exists if a certain compatibility condition between M, X and $\overline{g}$ holds, and for given M and X a compatible $\overline{g}$ exists. More precisely, the compatibility condition is that there is an $\epsilon > 0$ such that for any $V \in T_xM$, $x \in X$, $V \perp T_xX$, the curve $\gamma_V : t \mapsto \exp_x(tV)$ is defined for $|t| < \epsilon$ and the boundary depth is constant along such curves. For example metrics $\overline{g}$ whose restriction to a tubular neighborhood of X are product metrics of $\overline{g}|_X$ with a metric on a transversal section, satisfy this compatibility condition. However, we cannot assume without loss of generality that for given M and X there is a metric $\overline{g}$ providing such a product structure. (For example, consider the case that the normal bundle of X in M is non-trivial. Then there is no product metric on a neighborhood of X, whereas a compatible metric exists.)

Now let r_X denote the smoothed distance function to X with respect to a true metric $\overline{g}$ that satisfies the compatibility condition of the previous paragraph. The function r_X thus coincides with the distance function to X on $U_\epsilon(X)$, for some $\epsilon > 0$, and is smooth and positive on $M \setminus X$. We will also assume $r_X \leq 1$.

Any $x \in X$ has an open neighborhood U in M and a submersion $y = (y_1, \ldots, y_k) : U \to \mathbb{R}^k$ with $X \cap U = y^{-1}(0)$ and $r_X = |y| = \sqrt{\sum_i y_i^2}$.

Lemma 3.7. *Let $(M, \mathcal{V})$ be a Lie manifold, $X \subset M$ be a submanifold with corners. Then*

$$\mathcal{V}_0 := \big\{ \sum f_i V_i \,|\, f_i \in C^\infty(M), \quad f_i|_X \equiv 0, \quad V_i \in \mathcal{V} \big\}$$

is a $C^\infty(M)$-submodule and a Lie subalgebra of $\mathcal{V}$. The lift

$$\mathcal{W}_0 := \{ W \in \Gamma_\beta(T[M : X]) \,|\, \beta_*(W) \in \mathcal{V}_0 \}$$

is isomorphic to $\mathcal{V}_0$ as a $C^\infty(M)$-module and as a Lie algebra. Let $\mathcal{W}$ be the $C^\infty([M : X])$-submodule of $\mathcal{V}_{[M:X]}$ generated by $\mathcal{W}_0$, i. e.

$$\mathcal{W} := \big\{ \sum_i f_i W_i \,|\, f_i \in C^\infty([M : X]), \, W_i \in \mathcal{W}_0 \, \big\}.$$

Then, for any vector field $W \in \mathcal{W}$, its restriction $W|_{S^M X}$ is tangent to the fibers of $S^M X$ and $\mathcal{W}$ is closed under the Lie bracket.

Proof. The vector space $\mathcal{V}_0$ is a Lie subalgebra of $\mathcal{V}_{[M:X]}$ as

$$[f_1V_1, f_2V_2] = f_1f_2[V_1, V_2] + f_1V_1(f_2)V_2 - f_2V_2(f_1)V_1.$$

Incidentally, the same equation shows that $\mathcal{W}$ is closed under the Lie bracket.

By Propositon 3.2, any vector field in $\mathcal{V}_0$ can be lifted uniquely and smoothly to the blow-up. The map $\beta_* : \Gamma_\beta(T[M : X]) \to \Gamma(TM)$ is obviously an isomorphism of $C^\infty(M)$-modules and of Lie algebras. Then $\mathcal{W}_0$ is a Lie algebra of vector fields in $\mathcal{V}_{[M:X]}$, and so is $\mathcal{W}$. It follows from the definition of lift that $W|_{S^M X}$ is tangent to the fibers for all $W \in \mathcal{W}$ (see the remarks at the end of Section 3.3). $\square$

Lemma 3.8. *Let $(M, \mathcal{V})$ be a Lie manifold, $X \subset M$ be a submanifold with corners. Let r_X be a smoothed distance function to X. Then*

$$\mathcal{W}_1 := \{W \in \Gamma(T[M : X]) \mid \exists V \in \mathcal{V} \text{ with } W|_{M \setminus X} = r_X V|_{M \setminus X}\}$$

is isomorphic to $\mathcal{V}$ as a $C^\infty(M)$-module. Furthermore the natural multiplication map

$$\mu : C^\infty([M : X]) \otimes_{C^\infty(M)} \mathcal{W}_1 \to \mathcal{W} \subset \mathcal{V}_{[M:X]}$$

is an isomorphism of $C^\infty([M : X])$-modules, and hence $\mathcal{W}$ is a projective $C^\infty([M : X])$-module.

Remark 3.9. The previous two lemmata imply that there are surjective linear maps $C^\infty([M : X]) \otimes_{C^\infty(M)} \mathcal{W}_i \to \mathcal{W}$ for $i = 0, 1$. As stated above, the resulting map for $i = 1$ is an isomorphism. However, one can show that the resulting map is not injective for $i = 0$.

Often $W \in \mathcal{W} \subset \mathcal{V}_{[M:X]}$ will be identified in notation with $W|_{M \setminus X}$ and with $\beta_* W \in \mathcal{V}_M$ if it exists. (Recall that $\mathcal{V}_M$ was defined in Equation (9).)

Proof of Lemma 3.8. Let us denote $P := [M : X]$, to simplify notation. The map $\mathcal{V} \to \mathcal{W}_1$, which associates to a vector field $V \in \mathcal{V}$ a lift of $r_X V$, is obviously an isomorphism of $C^\infty(M)$-modules.

Now, we will show $\mathcal{W}_1 \subset \mathcal{W}$. This means that for $V \in \mathcal{V}$ we will show that $r_X V$ lifts to a vector field in $\mathcal{W}$. With a partition of unity argument we see that without loss of generality we can assume that the support of V is contained in an open set U, such that a function $y : U \to \mathbb{R}^k$ as above exists. We choose $\chi \in C^\infty(M)$ with support in U and such that $\chi \equiv 1$ on the support of V. We then write

$$r_X V = \sum_i \frac{\chi y_i}{r_X} \, \chi y_i V.$$

Since $\chi y_i V \in \mathcal{V}_0$ and $\chi y_i / r_X \in C^\infty(P)$, the assertion follows.

In order to show that $\mathcal{W}_1$ generates $\mathcal{W}$, we take a function $f \in C^\infty(M)$, vanishing on X, and $V \in \mathcal{V}$. We have to show that fV is in the $C^\infty(P)$-module spanned by $\mathcal{W}_1$. Similarly to above, we can assume that the support of f is in an open set U, such that y exists on U. We then can write $f = \sum h_i y_i$ with $h_i \in C^\infty(M)$ and support in U. We write

$$fV = \sum \frac{h_i y_i}{r_X} \, r_X V.$$

The vector field $r_X V$ lifts to a vector field in $\mathcal{W}_1$. Since $\frac{y_i}{r_X} \in C^\infty(P)$, the claim that $\mathcal{W}_1$ generates $\mathcal{W}$ follows.

Finally, to prove that the multiplication map $\mu : C^\infty(P) \otimes_{C^\infty(M)} \mathcal{W}_1 \to \mathcal{W}$ is an isomorphism of $C^\infty(P)$-modules, it is enough to show μ is injective (since we have just proved that it is surjective). Using the isomorphism from above $\mathcal{W}_1 = r_X \mathcal{V} \simeq \mathcal{V}$ as $C^\infty(M)$-modules. Hence by the projectivity of $\mathcal{V}$ as a $C^\infty(M)$–module, we can choose an embedding $\iota : \mathcal{W}_1 \to C^\infty(M)^N$ with retraction $C^\infty(M)^N \to \mathcal{W}_1$, where both ι and r are morphisms of $C^\infty(M)$-modules and $r \circ \iota = id$, the identity. The embedding ι corresponds to an embedding $j : A \to \mathbb{R}^N$ of vector bundles. By definition, $A|_{M \smallsetminus X} = TM|_{M \smallsetminus X}$. We can therefore identify the restrictions of the vector fields in $\mathcal{W}$ to sections of $A|_{M\smallsetminus X}$, which then yields an embedding $\iota_0 : \mathcal{W} \hookrightarrow \Gamma(M \smallsetminus X, \mathbb{R}^N) = C^\infty(M \smallsetminus X)^N$. Let us denote by res the restriction from P to $M \setminus X$. We thus obtain the diagram

$$\begin{array}{ccc} C^\infty(P) \otimes_{C^\infty(M)} \mathcal{W}_1 & \xrightarrow{\mu} & \mathcal{W} \\ {\scriptstyle \mathrm{id}\otimes\iota}\big\downarrow & & \big\downarrow{\scriptstyle \iota_0} \\ C^\infty(P) \otimes_{C^\infty(M)} C^\infty(M)^N & \xrightarrow{res} & C^\infty(M \smallsetminus X)^N \\ {\scriptstyle =}\big\downarrow & & \big\downarrow{\scriptstyle =} \\ C^\infty(P)^N & \xrightarrow{res} & C^\infty(M \smallsetminus X)^N \end{array} \tag{18}$$

This diagram is commutative by the definition of i_0.

We have that $(id \otimes r) \circ (id \otimes \iota) = id$, and hence $id \otimes \iota$ is injective. Moreover, all the other vertical maps and the restriction maps are injective. It follows from the commutativity of the diagram that μ is injective as well. ☐

In the following we write $r_X\mathcal{V}$ for $\mathcal{W}_1$, and for $\mathcal{W}$ which is the $C^\infty(P)$-module generated by it, with $P := [M : X]$, we also write $C^\infty(P)r_X\mathcal{V}$. We obtain

Theorem 3.10. *Let $(M, \mathcal{V})$ be a Lie manifold, $X \subset M$ be a submanifold with corners, and r_X be a smoothed distance function to X. Denote by $P := [M : X]$ the blow-up of M along X. Then the $C^\infty(P)$-module $\mathcal{W} := C^\infty(P)r_X\mathcal{V}$ defines a Lie manifold structure on P, which is independent of the choice of r_X.*

Proof. Clearly $\mathcal{W}$ consists of vector fields. The previous lemma shows that $\mathcal{W}$ is a projective $C^\infty(P)$–module. Proposition 3.2 shows that $\mathcal{W} \subset \mathcal{V}_P$, that is, that $\mathcal{W}$ consists of vector fields tangent to all faces of P (Equation (9)). Lemma 3.7 shows that $\mathcal{W}$ is a Lie algebra (for the Lie bracket). Moreover, if V is any vector field on the interior P and U is an open set whose closure does not intersect the boundary of P, then there exits $V_0 \in \mathcal{V}$ such that $V_0 = r_X^{-1}V$ on U. Then $r_XV_0 \in \mathcal{W}$ restricts to V on U. This shows that there are no restrictions on the vector fields in $\mathcal{W}$ in the interior of P. This completes the proof. ☐

3.6. **Direct construction of the blown-up Lie-algebroid.** We keep the notation of the previous subsection, especially of Theorem 3.10. In particular, let $X \subset M$ be a submanifold with corners. Since $\mathcal{W}$ (introduced in Theorem 3.10) is projective, there is a Lie algebroid B over $[M : X]$ such that $\mathcal{W}$ is isomorphic to $\Gamma(B)$ as $C^\infty([M : X])$-modules and Lie algebras. We now provide a direct construction of B. We will denote by $T^{bX}[M : X]$ the vector bundle whose sections are the vector fields on $[M : X]$ tangent to all the faces obtained by blowing up X in M.

In the following we will always use a smoothing r_X of the distance function to X, and we again assume r_X takes values in $[0, 1]$. Different choices of metrics $\overline{g}$ or different smoothing will provide different functions r_X. However, if r'_X comes from other choices than r_X, then there is a constant $C > 0$ with $C^{-1} \leq r'_X/r_X \leq Cr_X$ and due to compactness all derivatives of r'_X/r_X are bounded. We start with a preparatory lemma.

Lemma 3.11. *Let X be a submanifold of M, and r_X be a smoothed distance function to X. Then the map $T(M \setminus X) \to T(M \setminus X)$, $V \mapsto r_X^{-1} V$ extends to a bundle isomorphism*

$$\kappa : T^{bX}[M : X] \to \beta^* TM.$$

The proof is straightforward. Note that κ is not the map $\beta_* : T^{bX}[M : X] \to \beta^* TM$, but we have $\beta_* = r_X \kappa$.

As a vector bundle we then simply define

$$B := \beta^* A = \{(V, x) \in A \times [M : X] \mid V \in A_{\beta(x)}\}.$$

The anchor map $\rho_A : A \to TM$ pulls back to a map $\beta^* \rho : \beta^* A \to \beta^* TM$, and we define the anchor ρ_B of B to be the composition

$$B = \beta^* A \xrightarrow{\beta^* \rho_A} \beta^* TM \xrightarrow{\kappa^{-1}} T^{bX}[M : X] \longrightarrow T[M : X]$$

In order to turn B into a Lie algebroid, one has to specify a compatible Lie bracket on sections of B. The Lie bracket $[.,.]_A$ on $\Gamma(A)$ will not be compatible with the previous structures. However the Lie bracket $[.,.]_B$ given by

$$[V, W]_B := r_X [V, W]_A + (\partial_V r_X) W - (\partial_W r_X) V,$$

for all $V, W \in \Gamma(A) \overset{\beta^*}{\hookrightarrow} \Gamma(B)$ can be extended in the obvious way to $\Gamma(B)$, and this bracket is compatible in the following sense:

(a) $[f_1 W_1, f_2 W_2]_B = f_1 f_2 [W_1, W_2]_B + f_1 (\partial_{\rho_B(W_1)} f_2) W_2 - f_2 (\partial_{\rho_B(W_2)} f_1) W_1$

(b) The map $\Gamma(B) \to \Gamma(T[M : X])$ induced by ρ_B is a Lie-algebra homomorphism.

One checks that $\Gamma(B) = \mathcal{W}$.

Remark 3.12. The constructions in this section depend on r_X, and thus on the choices of $\overline{g}$ and the smoothing. Let r_X' be a different choice of a function with the properties of r_X. Using r_X' instead of r_X will lead to a different κ' B', and ρ' replacing κ, B, and ρ. However, the new choices only differ by a r_X'/r_X-factor from the old ones. In particular the bundles B and B' thus obtained are isomorphic.

3.7. **Geometric differential operators on blown-up manifolds.** We now study the relation between the Laplace operator on M and the one on $[M : X]$.

Proposition 3.13. *Let $(M, \mathcal{V})$ be a manifold with a Lie structure at infinity, $\mathcal{V} = \Gamma(A)$, for some vector bundle $A \to M$. Assume that M carries both a $\mathcal{V}$-metric g on A, and a true metric $\overline{g}$ on TM which is compatible with a submanifold X of M in the sense of subsection 3.5. Let r_X denote a smoothed distance function to X with respect to the metric $\overline{g}$. Then*

$$\operatorname{grad}_g r_X^2 \in \mathcal{W}$$

or more exactly the vector field $\operatorname{grad}_g r_X^2 \in \Gamma(A)$ has a unique lift in $\mathcal{W}$. Furthermore $\|\operatorname{grad}_g r_X\|^2 \in C^\infty([M : X])$.

Proof. We write $r_X^2 \in C^\infty(M)$ locally as $\sum_i y_i^2$. As g is a metric on A, it is fiberwise non-degenerate so it also defines a metric g^b on A^*. This dual metric g^b is locally given by $\sum_i e_i \otimes e_i$ where e_i is a local g-orthonormal frame, and is a section of $A \otimes A$. Let $\rho : A \to TM$ be the anchor map of A. The dual map of ρ, i. e. fiberwise composition with ρ, yields a smooth map $\rho^* : T^*M \to A^*$, $T^*_pM \ni \alpha \mapsto \alpha \circ \rho \in A^*$. The contraction $T^*M \to A$ of this map with g^b will be denoted as $T^*M \ni \alpha \to \alpha^\# \in A^*_p$. The g-gradient of a smooth function is by definition $\operatorname{grad}_g f := (df)^\# \in \Gamma(A)$. Thus we have

$$\operatorname{grad} r_X^2 = (dr_X^2)^\# = 2\sum_i y_i (dy_i)^\#.$$

Obviously the last equation only holds locally. From the remarks above one sees that $(dy_i)^\# = \operatorname{grad}_g y_i$ is a local section of A, and thus using Lemma 3.7 it we see that $y_i \operatorname{grad}_g y_i$ lifts to $\mathcal{W}$. This implies that $\operatorname{grad}_g r_X^2$ locally lifts to $\mathcal{W}$, and thus globally.

The proof of the second statement is a bit subtle. The first subtle point is that $\|\operatorname{grad}_g r_X\|^2$ is not well-defined as a function on M, but only as a function on $[M : X]$. The second subtle point is that the Gauss lemma does not provide $\|\operatorname{grad}_g r_X\|^2 = 1$ close to X as r_X is a smoothed distance with respect to the metric $\overline{g}$, whereas the gradient is taken with respect to g.

However the Gauss lemma (applied for the metric $\overline{g}$) does provide that dr_X is a well-defined smooth function $[M : X] \to T^*M$ commuting with the maps to M. Thus $\rho^* \circ dr_X \otimes \rho^* \circ dr_X$ is a smooth function $[M : X] \to A^* \otimes A^*$. The contraction with $g^b \circ \beta$ then yields $\|\operatorname{grad}_g r_X\|^2 = \|dr_X\|^2 \in C^\infty([M : X])$. □

Let us now examine the effect of blow-up on Sobolev spaces. Recall that the Sobolev space $W^{k,p}(M, \mathcal{V})$ associated to a Lie manifold $(M, \mathcal{V})$ with a $\mathcal{V}$-metric g on its Lie algebroid A is defined in [2]

$$W^{k,p}(M, \mathcal{V}) := \{u : M \to \mathbb{C} \mid V_1 \dots V_j u \in L^p(M, d\operatorname{vol}_g)\ \forall V_1, \dots, V_j \in \mathcal{V},\ j \le k\} \tag{19}$$

Lemma 3.14. *Using the notation of the Lemmma 3.7, we have*

$$W^{k,p}([M : X], \mathcal{W}) = \{u : M \to \mathbb{C} \mid r_X^j V_1 \dots V_j u \in L^p(M, d\operatorname{vol}_g)\ \forall V_1, \dots, V_j \in \mathcal{V},\ j \le k\}$$

Proof. We have that M and $[M : X]$ coincide outside a set of measure zero, hence we can replace integrable functions on $[M : X]$ by functions on M integrable over $M \setminus X$. The result for $k = 1$ follows from Lemma 3.8; for $k > 1$, use induction on k together with the fact that $V_i r_X - r_X V_i = V_i(r_X) \in C^\infty([M : X])$ is a bounded function, so that $(r_X V_i)(r_X V_j)u = r_X^2 V_i V_j u + V_i(r_X) r_X V_j u \in L^p(M \setminus X)$. □

Let us record also the effect of the blow-up on metrics and differential operators.

Lemma 3.15. *We continue to use the notation of Lemmas 3.7 and 3.8, in particular, r_X is a smoothed distance function to X. Let $A \to M$ be the Lie algebroid associated to $\mathcal{V}$, so that $\mathcal{V} \simeq \Gamma(A)$. Let us choose a metric g on A. Let B be the Lie algebroid associated to $([M : X], \mathcal{W})$. Then the restriction of $r_X^{-2} g$ to $M \smallsetminus X$ extends to a smooth metric h on B. Let Δ_g and Δ_h be the associated Laplace operators. Then the operator*

$$u \mapsto D(u) := r_X^{\frac{n+2}{2}} \Delta_g (r_X^{-\frac{n-2}{2}} u) - \Delta_h u.$$

is given by multiplication with a smooth function on $[M : X]$, that is $D \in \operatorname{Diff}^0_{\mathcal{W}}([M : X])$. Furthermore

$$r_X^2 \Delta_g - \Delta_h \in \operatorname{Diff}^1_{\mathcal{W}}([M : X]).$$

In particular, $r_X^2 \Delta_g$ is elliptic in $\operatorname{Diff}^2_{\mathcal{W}}([M : X])$.

Proof. The operator $r_X^{\frac{n+2}{2}}\Delta_g r_X^{-\frac{n-2}{2}}$ and Δ_h have the same principal symbol, are symmetric with respect to $d\,\mathrm{vol}_h$, and are smoth differential operators on $[M:X]$. Thus D is in $C^\infty([M:X]) = \mathrm{Diff}^0_{\mathcal{W}}([M:X])$.

Applying the formula $\Delta(uv) = v\Delta u + u\Delta v + 2g(\mathrm{grad}_g u, \mathrm{grad}_g v)$ we obtain

$$\begin{aligned} {r_X}^{\frac{n+2}{2}}\Delta_g({r_X}^{-\frac{n-2}{2}}u) &= r_X^2\Delta_g u + {r_X}^{\frac{n+2}{2}}(\Delta_g {r_X}^{-\frac{n-2}{2}})u - 2\frac{n-2}{2}r_x(\mathrm{grad}\, r_X)(u) \\ &= r_X^2\Delta_g u + {r_X}^{\frac{n+2}{2}}(\Delta_g {r_X}^{-\frac{n-2}{2}})u - \frac{n-2}{2}(\mathrm{grad}\, r_X^2)(u) \end{aligned}$$

The formula $\Delta r^\alpha = \alpha r^{\alpha-1}\Delta r + \alpha(\alpha-1)r^{\alpha-2}\|\,\mathrm{grad}\, r\|^2$ applied for $r = r_X$ yields

$${r_X}^{2-\alpha}\Delta_g {r_X}^\alpha = \alpha r_X \Delta_g r_X + \alpha(\alpha-1)\|\,\mathrm{grad}_g r_X\|_g^2.$$

We apply this for $\alpha = -(n-2)/2$ and $\alpha = 2$ and obtain

$${r_X}^{\frac{n+2}{2}}\Delta_g {r_X}^{-\frac{n-2}{2}} = -\frac{n-2}{4}\Delta_g r_X^2 + \frac{n^2-4}{4}\|\,\mathrm{grad}_g r_X\|_g^2.$$

From the Gauss lemma applied to $\overline{g}$ it follows that $r_X^2 \in C^\infty(M)$. In Proposition 3.13 we have shown that $\|\,\mathrm{grad}_g r_X\|_g^2 \in C^\infty([M:X])$, thus

$${r_X}^{\frac{n+2}{2}}\Delta_g {r_X}^{-\frac{n-2}{2}} \in C^\infty([M:X]).$$

Using then $\mathrm{grad}_g r_X^2 \in \mathcal{W}$, also proven in Proposition 3.13, the lemma follows. □

We shall need the following result as well.

Lemma 3.16. *Using the notation of Lemma 3.15, let $X \subset Y \subset M$ be submanifolds with corners. Let d_g (respectively, d_h) be a smoothed distance function to Y in the metric g (respectively, in the metric $h = r_X^{-2}g$). Then the quotient $r_X^{-1}d_g/d_h$, defined on $M \smallsetminus (Y \cup \partial M)$, extends to a smooth function on $[M:X]$.*

Proof. This is a local statement, so it can be proved using local coordinates. See [6] for a similar result. □

3.8. **Iterated Blow-ups of Lie-manifolds.** We now iterate the above constructions to blow up a clean family of submanifolds.

Let us fix for the remainder of this section the following notation: $(M, \mathcal{V})$ is a fixed Lie manifold and $\mathcal{X}$ is a fixed clean family of submanifolds with corners. As discussed at the end of Section 2, we can assume that $\mathcal{X} = (X_i \,|\, i = 1, 2, \ldots, k)$ is admissibly ordered. We denote by $P = [M : \mathcal{X}]$ the blow-up of M with respect to $\mathcal{X}$ and by $\beta : P \to M$ the blow-down map. Again let $Y^{(1)}, Y^{(2)}, \ldots, Y^{(k)}$ and $M^{(0)}, M^{(1)}, \ldots, M^{(k)}$ be the canonical sequences associated to M and the admissibly ordered family $\mathcal{X}$, see Section 2, Definition 2.10. Let $r_\ell : M^{(\ell-1)} \to [0,\infty)$ be a smoothed distance function to $Y^{(\ell)}$, $1 \le \ell \le k$ in a true metric on $M^{(\ell-1)}$ (in particular smooth up to the boundary). Then we denote

$$\rho := r_1 r_2 \ldots r_k, \tag{20}$$

where the product is first defined away from the singularity, and then it is extended to be zero on the singular set. Let us notice that r_j is a defining function for the face corresponding to $Y^{(j)}$ in the blow-up manifold M.

We also denote by $r_{\mathcal{X}}(x)$ the distance from x to $\bigcup \mathcal{X} := \bigcup_{i=1}^{k} X_i$, again in a true metric. Let us note for further use the following simple fact.

Lemma 3.17. *Using the notation just introduced, we have that the quotient $r_{\mathcal{X}}/\rho$, defined first on $M \smallsetminus (\bigcup \mathcal{X})$, extends to a continuous, nowhere zero function on P. In particular, there exists a constant $C > 0$ such that*

$$C^{-1}\rho \leq r_{\mathcal{X}} \leq C\rho.$$

Proof. This follows by induction from Lemma 3.16, as in [6]. □

We now show that we can blow up Lie manifolds with respect to a clean family to obtain again a Lie manifold. Recall that the blow-down map $\beta : P \to M$ was introduced in Equation (8) as the composition $\beta := \beta_1 \circ \beta_2 \circ \ldots \circ \beta_k : P = M^{(k)} = [M : \mathcal{X}] \to M = M^{(0)}$.

Proposition 3.18. *Using the above notation, we have that*

$$\mathcal{W}_0 := \{W \in \Gamma_\beta(TP),\ \beta_*(W|_{M\smallsetminus\bigcup\mathcal{X}}) \in \rho(\mathcal{V}|_{M\smallsetminus\bigcup\mathcal{X}})\}$$

is isomorphic to $\mathcal{V}$ as a $C^\infty(M)$-module. Let

$$\mathcal{W} := \{fW,\ W \in \mathcal{W}_0, f \in C^\infty(P)\}.$$

Then $\mathcal{W}$ is a Lie algebra isomorphic to $C^\infty(P) \otimes_{C^\infty(M)} \mathcal{V}$ as a $C^\infty(P)$-module and hence $\mathcal{W}$ is a finitely generated, projective module over $C^\infty(P)$, and $(P, \mathcal{W})$ is a Lie manifold, which is isomorphic to the Lie manifold obtained by iteratively blowing up the Lie manifold $(M, \mathcal{V})$ along the submanifolds $Y^{(\ell)}$, $1 \leq \ell \leq k$.

Proof. Again, this follows by induction from Lemmas 3.16, 3.17, and Theorem 3.10. □

The Lie manifold $(P, \mathcal{W}) = ([M : \mathcal{X}], \mathcal{W})$ is called the *blow-up of the Lie manifold $(M, \mathcal{V})$ along the clean family $\mathcal{X}$.*

Proposition 3.19. *Using the notation of the Proposition 3.18, let $A \to M$ be the Lie algebroid associated to $\mathcal{V}$, so that $\mathcal{V} \simeq \Gamma(A)$. Let us choose a metric g on A. Let B be the Lie algebroid associated to $(P, \mathcal{W})$. Then the restriction of $\rho^{-2}g$ to $M \smallsetminus (\bigcup \mathcal{X} \cup \partial M)$ extends to a smooth metric h on B. Let Δ_g and Δ_h be the associated Laplace operators. Then*

$$\rho^2 \Delta_g - \Delta_h \in \mathrm{Diff}^1_{\mathcal{W}}(P).$$

In particular, $\rho^2\Delta_g$ is elliptic in $\mathrm{Diff}^2_{\mathcal{W}}(P)$.

Proof. This proposition follows from Lemma 3.15 by induction. □

We complete this section with a description of the Sobolev space of the blow-up.

Proposition 3.20. *Using the notation of Lemma 3.17 and of Proposition 3.18, we have*

$$W^{k,p}(P, \mathcal{W}) := \{u : M \to \mathbb{C}, \rho^j V_1 \ldots V_j u \in L^p(M, d\,\mathrm{vol}_g),\ \forall V_1, \ldots, V_j \in \mathcal{V},\ j \leq k\}.$$

Proof. This follows from Lemmas 3.14 and 3.17. □

4. Regularity of eigenfunctions

We now provide the main application of the theory developed in the previous sections.

4.1. **Regularity of multi-electron eigenfunctions.** Let us consider $\mathbb{R}^{3N}$ with the standard Euclidean metric. We radially compactify $\mathbb{R}^{3N}$ as follows. Using the diffeomorphism $\phi : \mathbb{R}^{3N} \to B_1(0)$, $x \mapsto \frac{2\arctan|x|}{\pi|x|}x$ we view $\mathbb{R}^{3N}$ as the open standard ball $\mathbb{R}^{3N}$. The compactification $M = \overline{\mathbb{R}^{3N}}$ is then a manifold with boundary together with a diffeomorphisms from M to the closed standard ball, extending ϕ. The compactification M carries a Lie structure at infinity $\mathcal{V}_{sc}$ [3, 13, 41, 42, 45] which is defined as follows. Let r_∞ be a defining function of the boundary of $M = \overline{\mathbb{R}^{3N}}$, for example, we can take $r_\infty(x) = (1 + |x|^2)^{-1/2}$. We extend $x_1 := r_\infty$ locally to coordinates $x_1, x_2, \ldots, x_N$, defined on a neighborhood of a boundary point. In particular $x_2, \ldots, x_N$ are coordinates of the boundary. In these coordinates $\mathcal{V}_{sc}$ is generated by $r_\infty^2\partial_{r_\infty}, r_\infty\partial_{x_j}$, $j = 2, \ldots, N$. Thus $\mathcal{V}_{sc} = r_\infty\mathcal{V}_M$, with $\mathcal{V}_M$ defined in Equation (9). We can then choose the metric on $\mathcal{V}_{sc}$ so that the induced metric on M_0, the interior of M, is the usual Euclidean metric on $\mathbb{R}^{3N}$.

Motivated by the specific form of the potential V introduced in Equation (1), let us now introduce the following family of submanifolds of $M = \overline{\mathbb{R}^{3N}}$. Let X_j be the closure in M of the set $\{x = (x_1, \ldots, x_N), x_j = 0 \in \mathbb{R}^3\}$. Let us define similarly X_{ij} to be the closure in M of the set $\{x = (x_1, \ldots, x_N), x_i = x_j \in \mathbb{R}^3\}$. Let $\mathcal{S}$ be the family of consisting of all manifolds X_j, X_{ij} for which the parameter functions b_j and c_{ij} are non-zero, together with their intersections. The family $\mathcal{S}$ will be called the *multi-electron* family of singular manifolds.

Proposition 4.1. *The multi-electron family of singular manifolds $\mathcal{S}$ is a clean family.*

Proof. Let $\mathcal{Y} = \{Y_j\}$ be the family of all finite intersections of the sets X_j. We need to prove that $T_x(\bigcap Y_{j_k}) = \bigcap T_x Y_{j_k}$. At a point $x \in \mathbb{R}^{3N}$ this is obvious, since each Y_j is (the closure of) a linear subspace close to x. For x on the boundary of M, we notice that $\mathcal{Y}$ has a product structure in a tubular neighborhood of the boundary of M. □

Let $(\mathbb{S}, \mathcal{W}) := ([M : \mathcal{S}], \mathcal{W})$ be the blow-up of the Lie manifold $(M = \overline{\mathbb{R}^{3N}}, \mathcal{V}_{sc})$, given by Proposition 3.18, and ρ be the function introduced in (20). Note that the definition of $\mathbb{S}$ and $\mathcal{W}$ depend on which of the b_j and c_{ij} are allowed to be non-zero. Let V be the potential considered in Equation (1):

$$V(x) = \sum_{1\le j\le N} \frac{b_j}{|x_j|} + \sum_{1\le i<j\le N} \frac{c_{ij}}{|x_i - x_j|},$$

where $x = (x_1, x_2, \ldots, x_N) \in \mathbb{R}^{3N}$, $x_j \in \mathbb{R}^3$. We allow $b_j, c_{ij} \in C^\infty(\mathbb{S})$, which is important for some applications to the Hartree–Fock and Density Functional Theory. We endow $\mathbb{S}$ with the volume form defined by a compatible metric and we then define $L^p(\mathbb{S})$ accordingly.

Theorem 4.2. *The blow-up $(\mathbb{S}, \mathcal{W})$ of the scattering manifold $(M = \overline{\mathbb{R}^{3N}}, \mathcal{V}_{sc})$ has the following properties:*

(i) $\rho V \in r_\infty C^\infty(\mathbb{S})$.
(ii) $\rho^2(-\Delta + V) \in \mathrm{Diff}_{\mathcal{W}}(\mathbb{S})$ *and is elliptic in that algebra.*
(iii) Let x_H be a defining function of the face H and $a_H \in \mathbb{R}$, for each hyperface H of $\mathbb{S}$. Denote $\chi = \prod_H x_H^{a_H}$ and assume that $u \in \chi L^p(\mathbb{S})$ satisfies $(-\Delta+V)u = \lambda u$, $1 < p < \infty$, for some $\lambda \in \mathbb{R}$. Then $u \in \chi W^{m,p}(\mathbb{S}, \mathcal{W})$ for all $m \in \mathbb{Z}_+$.

Proof. (i) Let us choose the compatible metric to be the Euclidean metric and choose the boundary defining function r_∞ for the boundary (sphere) at infinity of $\mathbb{R}^{3N}$ to satisfy $r_\infty(x) = 1/|x|$ for $|x|$ large. Let X be any of the manifolds $X_j := \overline{\{x_j = 0\}}$ or $X_{ij} := \overline{\{x_i = x_j\}}$ defining $\mathcal{S}$ (the closures are all in M). We shall denote by r_X the distance to X in a true (bounded) metric on M and by d_X the distance to X in the Euclidean metric. For example, if $X \cap \mathbb{R}^{3N} = X_j \cap \mathbb{R}^{3N} = \{x_j = 0 \in \mathbb{R}^3\}$, then $d_X(x) = |x_j|$. We claim that the function $\phi := r_\infty d_X/r_X$ extends to a smooth and positive function on $[M : X]$. We will assume that the bounded metric is a product metric near the boundary in the standard (polar coordinates) tubular neighborhood $U = S^{3N-1} \times [0, \epsilon)$ of S^{3N-1}. We can also assume $r_\infty(x', t) = t$. In the interior of M, the smoothness and positivity of ϕ follows from the fact that if V is a linear subspace of $\mathbb{R}^{3N}$ and if g_1 and g_2 are two scalar products on $\mathbb{R}^{3N}$ with associated distance functions d_1 and d_2, then $x \mapsto d_1(x, V)/d_2(x; V)$ extends to a smooth and positive function on $[\mathbb{R}^{3N} : V]$. At the boundary of M the argument uses also homogeneity. Both functions $r_X(x', t)$ and $r_\infty(x', t)d_X(x', t)$ are in fact independent of $t \in [0, \epsilon)$. Therefore $\phi(x', t)$ is independent of t for t small. Since the function ϕ was proved to be smooth for $t > 0$, the claim follows.

It follows that ϕ is a smooth function also on $\mathbb{S} = [M : \mathcal{S}]$, because $C^\infty([M : X]) \subset C^\infty([M : \mathcal{S}])$. Moreover, ϕ is nowhere zero, so we also have $\phi^{-1} \in C^\infty(\mathbb{S})$. Since V is a sum of terms of the form d_X^{-1}, it is enough to show that $\rho/d_X \in r_\infty C^\infty(\mathbb{S})$. But $\rho = \psi r_X$ for some smooth function $\psi \in C^\infty(\mathbb{S})$ and hence

$$\rho/d_X = \psi r_X/d_X = \psi\phi^{-1} r_\infty \in r_\infty C^\infty(\mathbb{S}).$$

(ii) follows from Propositions 3.19 and 4.1 using also (i) just proved.

(iii) is a direct consequence of the regularity result in [2], Theorem 3.6, because $\rho^2(-\Delta + V - \lambda)$ is elliptic, by (ii). The proof is now complete. □

Note that it follows from Proposition 3.20 and the definition of $\mathcal{V}_{sc}$ that

$$W^{k,p}(\mathbb{S}, \mathcal{W}) := \{u : \mathbb{R}^{3N} \to \mathbb{C}, \rho^{|\alpha|+3N/2}\partial^\alpha u \in L^p(\mathbb{R}^{3N}),\ \ |\alpha| \le k\}\,. \tag{21}$$

We are now ready to prove our main result, as stated in Equation (4).

Theorem 4.3. *Assume $u \in L^2(\mathbb{R}^{3N})$ is an eigenfunction of $\mathcal{H} := -\Delta + V$, then*

$$u \in \mathcal{K}^m_a(\mathbb{R}^{3N}, r_S) = \rho^{a-3N/2} W^{m,2}(\mathbb{S}, \mathcal{W})$$

for all $m \in \mathbb{Z}_+$ and for all $a \le 0$.

Proof. We have that $L^2(\mathbb{R}^{3N}) = \rho^{-3N/2}L^2(\mathbb{S})$ since the metric on $\mathbb{S}$ is $g_\mathbb{S} = \rho^{-2}g_{\mathbb{R}^{3N}}$. The function ρ is a product of defining functions of faces at infinity, so $\rho^{-3N/2} = \chi$, for some χ as in Theorem 4.2 (iii). The result then follows from Theorem 4.2 (iii). □

4.2. **Regularity in the case of one electron and several heavy nuclei.** Let us now consider $S = \{P_1, P_2, \dots P_m\} \in \mathbb{R}^3$, let M be the scattering calculus Lie manifold obtained by radially compactifying $\mathbb{R}^3$, as in the previous subsection. So $N = 1$ in this section, but we allow several fixed nuclei. Let us blow it up with respect to the set S, obtaining a manifold with boundary $\mathbb{S}$. Let $\mathcal{W}$ be the structural Lie algebra of vector fields on $\mathbb{S}$ obtained blowing up the scattering calculus on M.

Let $V_0, k_j : \mathbb{S} \to \mathbb{R}$ be smooth functions, $j = 1, 2, 3$. Let $r_S : \mathbb{S} \to [0, 1]$ be a smooth function that is equal to 0 on the faces corresponding to the singular points in S and equal to 1 in a neighborhood of the hyperface coming from the ball compactification of $\mathbb{R}^3$, i. e. the face at infinity before the blowup. We assume that $dr_S \neq 0$ on the faces corresponding to the set of singular points S. As S is a compact set, we can assume in this subsection that $r_S(x)$ is the euclidian distance from x to S if $x \in \mathbb{R}^3 \smallsetminus S$ is close to S. We have $r_S = \rho$ in the notation of the previous subsection.

In view of further applications to operators that arise in the study of periodic potentials, in this subsection we shall consider eigenfunctions of the operator

$$\mathcal{H}_m = -\sum_{j=0}^{3} (\partial_j - ik_j)^2 + V_0/r_S, \tag{22}$$

which is the *magnetic* version of the Schrödinger operator (2). For possible applications to the periodic case, the case where k_j are constants is the most important case, but our results are more general. Recall that the spaces $H^m(\mathbb{S})$ were introduced in Equation (5). Also, let us notice that $e^{-\epsilon|x|}$ is a smooth function on $\mathbb{S}$, so multiplication by this function maps the spaces $H^m(\mathbb{S})$ to themselves.

Theorem 4.4. *Let $u \in L^2(\mathbb{R}^3)$ be such that $\mathcal{H}_m u = \lambda u$, in distribution sense. Then*

(i) $r_S^2 e^{\mu|x|} \mathcal{H}_m e^{-\mu|x|} \in \mathrm{Diff}_{\mathcal{W}}(\mathbb{S})$, $\mu \in \mathbb{R}$, is elliptic.

(ii) $u \in r_S^{-3/2} H^m(\mathbb{S}) = \mathcal{K}_0^m(\mathbb{R}^3, r_S)$ for all m.

(iii) If $-\lambda > \epsilon > 0$, then $u \in r_S^{-3/2} e^{-\epsilon|x|} H^m(\mathbb{S})$ for all m.

Proof. The first part, (i), is a direct calculation, completely similar to Theorem 4.2. To prove (*ii*), we notice that $L^2(\mathbb{R}^3) = r_S^{-3/2} H^0(\mathbb{S})$. Then (ii) is an immediate consequence of the regularity theorem of [2]. Finally, we have that $v = e^{\epsilon|x|} u \in L^2(\mathbb{R}^3) = r_S^{-3/2} H^0(\mathbb{S})$ by [1], since $-\lambda > \epsilon > 0$. It is also an eigenfunction of $H_1 := e^{\epsilon|x|} \mathcal{H}_m e^{-\epsilon|x|}$. The result of (iii) then follows from the ellipticity of $r_S^2 H_1$, by (i), and by the regularity theorem of [2], Theorem 3.6. □

See also [9, 14, 27, 35, 52] and the references therein for more on the decay of eigenfunctions. See also [37, 39] for additional general properties of the Hamiltonian operators arising in Quantum Mechnics.

To get an improved regularity in the index a, we shall need the following result of independent interest. Let us replace $\mathbb{R}^3$ by $\mathbb{R}^N$ in the following result, while keeping the rest of the notation unchanged. In particular, $S \subset \mathbb{R}^N$ is a finite subset and $r_S(x) \in [0, 1]$ is the distance from x to S for x close to S and is equal to 1 in a neighborhood of the hyperface at infinity before the blow-up of the singular points.

As usual we define $\mathcal{K}_{-a}^{-m}(\mathbb{R}^N, r_S)$ to be the dual of $\mathcal{K}_a^m(\mathbb{R}^N, r_S)$ with respect to the pairing $(f_1, f_2) := \int_{\mathbb{R}^N} f_1 f_2$, where $\mathcal{K}_a^m(\mathbb{R}^N, r_S)$ was defined in (3).

Theorem 4.5. *Let $|a| < (N-2)/2$, then*

$$\Delta - \mu : \mathcal{K}_{a+1}^{m+1}(\mathbb{R}^N, r_S) \to \mathcal{K}_{a-1}^{m-1}(\mathbb{R}^N, r_S)$$

is an isomorphism for $\mu > 0$ large enough.

Proof. We begin by recalling the classical Hardy's inequality, valid for $u \in H^1(\mathbb{R}^N)$:

$$c_N^2 \int_{\mathbb{R}^N} \frac{|u|^2}{|x|^2} dx \leq \int_{\mathbb{R}^N} |\nabla u|^2 dx, \tag{23}$$

with $c_N = (N-2)/2$ (see for example [53] and the references therein). A partition of unity argument then implies that for any $\delta > 0$ there exists $\mu = \mu_\delta > 0$ such that

$$(1-\delta)c_N^2 \int_{\mathbb{R}^N} |r_S^{-1} u|^2 dx \leq \int_{\mathbb{R}^N} \big(|\nabla u|^2 + \mu |u|^2\big) dx. \tag{24}$$

We can assume that $|\nabla r_S| \leq 1$. Let us assume $u \in C_c^\infty(\mathbb{R}^3 \smallsetminus S)$, which is a dense subset of $\mathcal{K}_a^m(\mathbb{R}^N, r_S)$ for all m and a, by [2]. Let $|a| < (N-2)/2$. We shall denote $(u,v) = \int_{\mathbb{R}^N} uv\, dx$, as usual. Let us regard r^a and r^{-a} as multiplication operators. Let us now multiply Equation (24) with $1-\delta$ and use $\nabla(r_S^a u) = a r_S^{a-1} u \nabla r_S + r_S^a \nabla u$ to obtain

$$\begin{aligned}
\big((\mu - r_S^{-a}\Delta r_S^a)u, u\big) &= \mu(u,u) + (\nabla r_S^a u, \nabla r_S^{-a} u) \\
&= \mu(u,u) + (r_S^a \nabla u, r_S^{-a}\nabla u) + a(r_S^{-1}(\nabla r_S)u, \nabla u) \\
&\quad -a(\nabla u, r_S^{-1}(\nabla r_S)u) - a^2(r_S^{-1}(\nabla r_S)u, r_S^{-1}(\nabla r_S)u) \\
&\geq \mu(u,u) + (\nabla u, \nabla u) - a^2(r_S^{-1}u, r_S^{-1}u) \\
&\geq ((1-\delta)^2 c_N^2 - a^2)(r_S^{-1}u, r_S^{-1}u) + \delta(\nabla u, \nabla u) \\
&\geq \delta \|u\|_{\mathcal{K}_1^1}^2.
\end{aligned}$$

For $\delta > 0$ small enough $((1-\delta)^2 c_N^2 - \delta \geq a^2)$. This means that the continuous map

$$P_{a,\mu} := \mu - r_S^{-a}\Delta r_S^a : \mathcal{K}_1^1(\mathbb{R}^N, r_S) \to \mathcal{K}_{-1}^{-1}(\mathbb{R}^N, r_S)$$

satisfies

$$\|P_{a,\mu}u\|_{\mathcal{K}_{-1}^{-1}} \|u\|_{\mathcal{K}_1^1} \geq (P_{a,\mu}u, u) \geq \delta \|u\|_{\mathcal{K}_1^1}^2,$$

and hence $\|P_{a,\mu}u\|_{\mathcal{K}_{-1}^{-1}(\mathbb{R}^N)} \geq \delta \|u\|_{\mathcal{K}_1^1(\mathbb{R}^N)}$, for $\mu > 0$ large and some $\delta > 0$. It follows that $P_{a,\mu}$ is injective with closed range for all $|a| < (N-2)/2$. Since the adjoint of $P_{a,\mu}$ is $P_{-a,\mu}$, it follows that $P_{a,\mu}$ is also surjective, and hence an isomorphism by the Open Mapping Theorem. The regularity result of [2] (Theorem 3.6) shows that $P_{a,\mu} := \mu - r_S^{-a}\Delta r_S^a : \mathcal{K}_1^{m+1}(\mathbb{R}^N, r_S) \to \mathcal{K}_{-1}^{m-1}(\mathbb{R}^N, r_S)$ is also an isomorphism for all m. The result follows from the fact that $r_S^b : \mathcal{K}_c^m(\mathbb{R}^N, r_S) \to \mathcal{K}_{c+b}^m(\mathbb{R}^N, r_S)$ is an isomorphism for all b, c, and m [5]. □

We are ready to prove the main result of this subsection.

Theorem 4.6. *Let $u \in L^2(\mathbb{R}^3)$ be such that $\mathcal{H}_m u = \lambda u$, in distribution sense. Then $u \in \mathcal{K}_a^m(\mathbb{R}^3, r_S) = r_S^{a-3/2} H^m(\mathbb{S})$ for all $m \in \mathbb{Z}_+$ and all $a < 3/2$.*

Proof. Let us first notice that the operator $Q := \mathcal{H}_m + \Delta$ is a bounded operator $\mathcal{K}_a^m(\mathbb{R}^3, r_S) \to \mathcal{K}_{a-1}^{m-1}(\mathbb{R}^3, r_S)$ for all a and m. Assume that $u \in L^2(\mathbb{R}^3)$ satisfies $-\mathcal{H}_m u = \lambda u$. Then we know that $u \in \mathcal{K}_0^m(\mathbb{R}^3, r_S)$ for all m by Theorem 4.4. Hence

$$f := (\Delta - C)u = Qu + (\lambda - C)u \in \mathcal{K}_{-1}^{m-1}(\mathbb{R}^3, r_S).$$

For large C we can invert $\Delta - C$, and thus we obtain $u = (\Delta - C)^{-1} f \in \mathcal{K}_1^{m+1}(\mathbb{R}^3, r_S) = (\Delta - C)^{-1}\mathcal{K}_{-1}^{m-1}(\mathbb{R}^3, r_S)$, by Theorem 4.5. But then $f = Qu + (\lambda - C)u \in \mathcal{K}_0^m(\mathbb{R}^3, r_S) \subset$

$\mathcal{K}^{m-1}_{-1+a}(\mathbb{R}^3, r_S)$ for any $a < 1/2$. We can then repeat this argument to obtain $u = (\Delta - C)^{-1} f \in \mathcal{K}^{m+1}_{1+a}(\mathbb{R}^3, r_S)$ for any $a < 1/2$ and any m, as claimed. $\square$

See [18, 22, 33] for an approach to the singularities of one electron Hamiltonians using the theory of singular functions for problems with conical singularities. The regularity at the origin in the above theorem is, in fact, a simple consequence of the theory of singular functions. For V_0 real analytic and $k_j = 0$, the regularity at the origin is also an immediate consequence of the analytic regularity result proved in [23].

It would be interesting to extend our results in the case of magnetic fields [26, 33, 34, 32]. In addition to the above extensions, one would have to look into the issues that arise in the numerical approximation of solutions of partial differential equations in spaces of high dimension (the so called "curse of dimensionality"). Let us mention in this regard the papers [29, 28, 49] and the references therein, where the issue of approximation in high dimension is discussed.

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