



Institut für Numerische Simulation

Rheinische Friedrich-Wilhelms-Universität Bonn

Friedrich-Hirzebruch-Allee 7 • 53115 Bonn • Germany
phone +49 228 73-69828 • fax +49 228 73-69847
www.ins.uni-bonn.de

H.J. Flad, G. Flad-Harutyunyan, M. Griebel

**Higher Order Singularities in Configuration
Space. I. Quantum Many-Particle Coulomb
Systems**

INS Preprint No. 2601

May 2026

Higher Order Singularities in Configuration Space.

I. Quantum Many-Particle Coulomb Systems

Heinz-Jürgen Flad[†], Gohar Flad-Harutyunyan^{*} and Michael Griebel[‡]

[†]Institut für Numerische Simulation, Universität Bonn, Friedrich-Hirzebruch-Allee 7 53115 Bonn

^{*}Fachgruppe Mathematik, RWTH Aachen University, Pontdriesch 14-16, 52062 Aachen

[‡]Fraunhofer Institut für Algorithmen und Wissenschaftliches Rechnen SCAI,
Schloss Birlinghoven 1, 53757 Sankt Augustin

Abstract

Configuration spaces of many-particle systems represent a generic class of high-dimensional problems where various types of singularities appear at coalescence points of particles. These singularities can be classified into conic, edge and higher order corner singularities depending on the number of particles involved. Within the present work, we consider the configuration space of quantum many-particle Coulomb systems as a generic example with a wide range of applications in physics, chemistry and material sciences. Singularities at coalescence points have a severe impact on regularity issues and approximation properties of mathematical models for numerical simulations.

Our focus is on the functional analytic setting including stratification, function spaces and a pseudo-differential calculus that enables parametrix constructions for elliptic operators. In particular, we discuss explicit local coordinates systems that are adapted to the canonical stratification of the configuration space and the corresponding degenerate structure of Hamilton operators. Furthermore, we provide an explicit construction of appropriately weighted Sobolev type function spaces which incorporate asymptotic information in the neighbourhood of the singularities of the Hamilton operator. The construction involves a recursive scheme from singular analysis based on so called order reducing operators. Explicit formulas are given which connect different asymptotics and Sobolev scales to a common reference space.

1 Introduction

Let us briefly introduce the concept of a configuration space. Given a set X , for example the domain $\mathbb{R}^3$, whose elements $x \in X$ represent possible positions of a particle. For a system of N particles, we take the product X^N , where each N -tuple $\mathbf{x} := (x_1, \dots, x_N) \in X^N$ represents a possible arrangement of the considered particles. In physics, the configuration space of all N particles is taken to be X^N , whereas in mathematics $X(N) := X^N \setminus \Delta_\ell$, with

$$\Delta_\ell := \{\mathbf{x} \in X^N \mid x_i = x_j \text{ for some } i \neq j, i, j = 1, \dots, N\},$$

is employed.¹ In the following, we refer to Δ_ℓ as the large diagonal of X^N which simply consists of every element of the X^N where two or more of the components coincide. The study of topological and geometrical properties of the configuration space $X(N)$ is a well established mathematical subject, see e.g. [8] and the references cited therein.

Despite its origin in statistical and many-particle physics, the concept of a configuration space can be considered as a paradigm for a much larger class of problems. To this end, we might think of the Cartesian product of domains of a multivariate quantity. Whenever the variables of a multivariate quantity are defined on a collective domain, we might think of the Cartesian product of

¹ X^N and $X(N)$ are also called unconstrained and constrained configuration space, respectively.

the domain as the underlying configuration space. It is quite common that the considered quantity shows a special behaviour if two or more variables coincide. In terms of configuration space, it means that the large diagonal should be considered as a singularity. In general, the large diagonal has a rather complex geometrical structure which must be appropriately resolved for example by a *stratification* of the configuration space. Then, as a next step, tensor product approximations can be employed on top of such a stratification. Their potential ability to circumvent the curse of dimension in numerical simulations makes them particularly attractive for higher dimensional problems. However the presence of singularities on the large diagonal might cause a severe deterioration of the convergence rates of tensor product approximations compared to models where such "singular behaviour" is absent. It is the purpose of the present work to set the ground for a singular asymptotic analysis that can be used to mitigate this problem. From the computational point of view it is important to note that singular behaviour does not necessarily require the presence of a real world singularity, whatever it means, or even of an analytic singularity of the mathematical model. What only matters is the presence of a singular *asymptotic* behaviour on the length scales of the model which are to be resolved in a simulation. This asymptotic behaviour determines the computational complexity with respect to a given approximation scheme. Therefore it is often beneficial to consider a mathematical model with analytic singularities that correctly describes the asymptotic behaviour instead of a regularized variant without analytic singularities. The latter has just the same type of asymptotic behaviour and therefore the same computational complexity on the scale of interest but conceals this information by using regularized quantities.

To get a better understanding of possible bottlenecks for tensor product approximations, it is important to have analytical tools available that provide explicit information concerning the asymptotic behaviour of the quantity of interest in the neighbourhood of a singularity. Especially for higher order singularities such tools are not commonly available and a universally applicable scheme to deal with singular high-dimensional quantities seems presently out of reach. Instead, we want to focus on a particular example which appears sufficiently significant to us and exhibits some characteristic features that might also be of interest in a broader context. Thus, we restrict our discussion to a physical model that has been devised to describe the behaviour of many-particle systems and allows the computation of its characteristic properties. To be specific, we consider Schrödinger's equation for Coulomb systems which represents the fundamental model of electronic structure theory. The treatment of such a specific application has a long and fruitful tradition in numerical analysis where in particular quantum many-particle theory delivered important concepts that had been later generalized to a broader class of problems.

The remainder of the paper is organized as follows: In Section 2, we provide a detailed discussion of our particular stratification for many-particle Coulomb systems and introduce a special kind of hyperspherical coordinates which are adapted to the stratification. We show that the Hamilton operator for a Coulomb systems, expressed in terms of these hyperspherical coordinates, has the proper degeneracies required by our approach for its singular analysis. The main part of the paper, contained in Section 3, deals with appropriately weighted Sobolev spaces. They can be employed to study the asymptotic behaviour of solutions of Schrödinger's equation in the neighbourhood of strata. In particular, we explicitly construct so called order reducing operators which are used to refer these function spaces to a common reference space.² Finally, we close with a brief outlook on future research.

²This concept is standard for ordinary Sobolev spaces $H^s(\mathbb{R}^n)$, $s \in \mathbb{R}$, which can be related by such operators to $L_2(\mathbb{R}^n)$.

2 Configuration space of quantum many-particle Coulomb systems

At the fundamental level, quantum many-particle systems can be described by Schrödinger's equation. In this context, we consider a system of N identical particles governed by the stationary Schrödinger equation within the Born-Oppenheimer approximation

$$H\Psi(x_1, \dots, x_N) = E\Psi(x_1, \dots, x_N) \quad x_i \in \mathbb{R}^3, \quad i = 1, \dots, N \quad (2.1)$$

with Hamilton operator³

$$H = -\frac{1}{2} \sum_{i=1}^N \Delta_i + \sum_{i < j} \frac{1}{|x_i - x_j|} - \sum_{i=1}^N \sum_{k=1}^K \frac{Z_k}{|a_k - x_i|}, \quad (2.2)$$

where the K nuclei of charge Z_k are fixed and located at $a_k \in \mathbb{R}^3$, $k = 1, \dots, K$. Thus, the set $\mathcal{V} := \{a_1, \dots, a_K\} \subset \mathbb{R}^3$ specifies the locations of point-like singularities originating from the Coulomb potentials of the nuclei. These many-particle Coulomb systems represent for example electrons in atoms, molecules, cluster or solids⁴. We consider many-particle Coulomb systems as the generic case because Coulomb potentials fit all the requirements of the pseudo-differential calculus which our approach relies on. In principle any potential with $r^2 v(r) \in C^\infty(\mathbb{R}_+)$ that belongs to the Rollnik class [26], like the Yukawa potential, would be suitable. To simplify our presentation, unless otherwise mentioned, we suppress possible spin degrees of freedom. In the absence of spin-dependent operators, e.g. spin-orbit couplings, one can chose a spin free formalism, where the wavefunction and related quantities belong to an irreducible representation of the symmetric group S_N that reflects the spin state of the system.

Let us consider the configuration space of N particles $\mathcal{M}[N] := \mathbb{R}^{3N} \setminus \mathcal{M}_0$, with $\mathcal{M}_0 := \Delta_\ell \cup S$, where Δ_ℓ is the large diagonal of $\mathbb{R}^{3N}$ and

$$S := \{x \in \mathbb{R}^{3N} \mid x_i \in \mathcal{V}, \text{ for some } i = 1, \dots, N\}$$

contains additional point like singularities due to the singular behaviour of the one-particle potential. In other words $\mathcal{M}_0$ contains all points of $\mathbb{R}^{3N}$ where the potential part of the Hamiltonian H becomes singular. The set of coalescence points has an obvious hierarchical structure in terms of two-, three-, ..., N -particle coalescence points, which can be represented by a stratified space defined by intersecting subspaces.

The Hamilton operator of an interacting many-particle systems corresponds to an elliptic partial differential operator under rather general assumptions concerning its local potential. However, in order to apply the singular pseudo-differential calculus that guarantees existence of a corresponding parametrix and Green operator, further restrictions have to be imposed. Thus, it is necessary to introduce appropriate local coordinate systems in configuration space which reflect the hierarchy of singularities to be discussed below. In these particular local coordinates, the coefficients of the Hamiltonian have to satisfy certain smoothness conditions up to the singularities and in addition it's hierarchy of symbols has to fulfill appropriate ellipticity conditions which reflect the hierarchical structure of the underlying stratified configuration space. Moreover, the choice of coordinates determines the structure of the weighted Sobolev spaces on which the singular operator algebras act.

2.1 Hyperspherical coordinates and the stratified Laplace operator

In the following, we discuss a particular choice of hyperspherical coordinates which seem to be appropriate for our purpose. The general definition for the N -particle case has been given by

³In the present work all equations are given in atomic units.

⁴Solids require periodic boundary conditions and a modified treatment of the Coulomb potentials. This can be achieved, e.g., by replacing the Coulomb by periodic Ewald potentials.

Granzow [18], a special case of these coordinates appeared already in [21]. The case of two particles and a fixed nucleus has been treated in [9, 12, 13]. Let us therefore focus on the three-particle case, which is general enough to be easily carried over to a larger number of particles and is still simple enough to avoid a cumbersome notation. In the following discussion we want to consider the unconstrained configuration space $\mathbb{R}^9$ of three particles as a stratified manifold with embedded edge and corner singularities. The singularities, to be specified below, correspond to coalescence points of particles plus the origin.⁵ Let us define a point in $\mathbb{R}^9$ by $\mathbf{x} := (x_1, x_2, x_3)$, where x_i , $i = 1, 2, 3$, denote the $3d$ Cartesian coordinates of the particles. The coalescence points of particles (including the origin) give rise to the following hierarchy of strata, cf. Fig. 1:

- $s_0(\mathbb{R}^9)$ ($\dim s_0 = 9$):

1. Here the stratum is the constrained configuration space $\mathcal{M}[3]$ which corresponds to $\mathbb{R}^9$ minus all coalescence points of particles and the origin.

- $s_1(\mathbb{R}^9) := s_{1,a}(\mathbb{R}^9) \cup s_{1,b}(\mathbb{R}^9)$ ($\dim s_1 = 6$):

1. Strata in $s_{1,a}(\mathbb{R}^9)$ and $s_{1,b}(\mathbb{R}^9)$ correspond to coalescence points of two particles and of one particle with the origin, respectively.

$$s_{1,a}(\mathbb{R}^9) = \{\tilde{S}_{12}, \tilde{S}_{13}, \tilde{S}_{23}\}, \quad \tilde{S}_{ij} := \{\mathbf{x} \in \mathbb{R}^9 \mid x_i = x_j \neq x_k \neq 0\}, \quad (2.3)$$

$$s_{1,b}(\mathbb{R}^9) = \{S_1, S_2, S_3\}, \quad S_i := \{\mathbf{x} \in \mathbb{R}^9 \mid x_i = 0, x_j \neq x_k \neq 0\}. \quad (2.4)$$

2. Model space of a neighbourhood of a stratum: $Y_1 \times \mathcal{C}^\Delta(S^2)$, with

$$\mathcal{C}^\Delta(S^2) := \overline{\mathbb{R}}_+ \times S^2 / \{0\} \times S^2,$$

and $Y_1 \subset \mathbb{R}^6$ open, where Y_1 has embedded singularities.

- $s_2(\mathbb{R}^9) := s_{2,a}(\mathbb{R}^9) \cup s_{2,b}(\mathbb{R}^9) \cup s_{2,c}(\mathbb{R}^9)$ ($\dim s_2 = 3$):

1. Strata in $s_{2,a}(\mathbb{R}^9)$, $s_{2,b}(\mathbb{R}^9)$ and $s_{2,c}(\mathbb{R}^9)$ correspond to coalescence points of three particles, of two particles with the origin and of two particles when the third particle is at the origin, respectively.

$$s_{2,a}(\mathbb{R}^9) = \{\tilde{S}_{123}\}, \quad \tilde{S}_{123} := \{\mathbf{x} \in \mathbb{R}^9 \mid x_1 = x_2 = x_3 \neq 0\}, \quad (2.5)$$

$$s_{2,b}(\mathbb{R}^9) = \{S_{12}, S_{13}, S_{23}\}, \quad S_{ij} := \{\mathbf{x} \in \mathbb{R}^9 \mid x_i = x_j = 0, \mathbf{x} \neq 0\}, \quad (2.6)$$

$$s_{2,c}(\mathbb{R}^9) = \{\hat{S}_{(12)3}, \hat{S}_{(13)2}, \hat{S}_{(23)1}\}, \quad \hat{S}_{(ij)k} := \{\mathbf{x} \in \mathbb{R}^9 \mid x_i = x_j \neq 0, x_k = 0\}. \quad (2.7)$$

2. Model space of a neighbourhood of a stratum: $Y_2 \times B_1^\Delta$, with

$$B_1^\Delta := \overline{\mathbb{R}}_+ \times (S^2 \times \mathcal{C}^\Delta(S^2)) / \{0\} \times (S^2 \times \mathcal{C}^\Delta(S^2)).$$

with $Y_2 \subset \mathbb{R}^3$ open.⁶

- $s_3(\mathbb{R}^9)$ ($\dim s_3 = 0$):

⁵It is convenient to consider the origin as a stratum of its own, either for formal reasons, or due to the fact that the origin is occupied by another particle which is kept fixed, like an atomic nucleus in the Born-Oppenheimer approximation.

⁶Alternatively, the model space can be expressed as: $Y_2 \times (\overline{\mathbb{R}}_+ \times S^5 / \{0\} \times S^5)$, where Y_2 and S^5 have embedded singularities.

1. The only stratum $S_O \in s_3(\mathbb{R}^9)$ corresponds to the coalescence point of all three particles with the origin.
2. Model space of a neighbourhood of a stratum: $B_2^\Delta := \overline{\mathbb{R}}_+ \times (S^2 \times B_1^\Delta) / \{0\} \times (S^2 \times B_1^\Delta)$.
3. Global singular model space: $\overline{\mathbb{R}}_+ \times S^8 / \{0\} \times S^8$, where S^8 has embedded singularities.

To each stratum, let us assign a distance variable, i.e., r_1 , r_2 and t to the strata in $s_1(\mathbb{R}^9)$, $s_2(\mathbb{R}^9)$ and $s_3(\mathbb{R}^9)$, respectively. These distance variables reflect the degree of degeneracy of a singularity.

The hyperspherical coordinate system of Granzow [18] for $\mathbb{R}^9$ is given by

$$x_1 = t \sin(r_2) \sin(r_1) \Phi(\theta_1, \varphi_1), \quad x_2 = t \sin(r_2) \cos(r_1) \Phi(\theta_2, \varphi_2), \quad x_3 = t \cos(r_2) \Phi(\theta_3, \varphi_3), \quad (2.8)$$

with radial variable $t := \sqrt{|x_1|^2 + |x_2|^2 + |x_3|^2}$ and standard spherical coordinates

$$\Phi(\theta, \varphi) := \begin{pmatrix} \sin(\theta) \cos(\varphi) \\ \sin(\theta) \sin(\varphi) \\ \cos(\theta) \end{pmatrix},$$

where the range of variables is given by $0 < t < \infty$, $0 < r_1, r_2 < \pi/2$ and $0 < \theta_i < \pi$, $0 < \varphi_i < 2\pi$ for $i = 1, 2, 3$.

To apply these coordinates to our stratified space, it becomes necessary to introduce an atlas with specific local charts in the neighbourhoods of the strata. Let us exemplify this for the case of the stratum $S_1 \in s_{1,b}(\mathbb{R}^9)$ where the first particle is located at the origin, i.e., $|x_1| = 0$. The stratum S_1 meets a stratum $S_{12} \in s_{2,b}(\mathbb{R}^9)$ in a corner singularity, if e.g. $|x_2|$ also vanishes and eventually these strata merge at the stratum $S_O \in s_3(\mathbb{R}^9)$ with the stratum $S_3 \in s_{1,b}(\mathbb{R}^9)$ given by $|x_3| = 0$. This particular part of configuration space is appropriately described in a local chart, cf. Fig. 2, denoted *Chart-1* in the following, by the hyperspherical coordinates

$$\text{Chart-1: } (x_1, x_2, x_3) = t \begin{cases} \sin(r_2), & \begin{cases} \sin(r_1) \Phi(\theta_1, \varphi_1), \\ \cos(r_1) \Phi(\theta_2, \varphi_2), \end{cases} \\ \cos(r_2) & \Phi(\theta_3, \varphi_3), \end{cases} \quad (2.9)$$

where r_1 , r_2 and t control the distance to the strata S_1 , S_{12} and S_O , respectively.

Similar considerations apply if particles meet each other. It is only the initial set of Cartesian coordinates which has to be modified. Let us exemplify this for a specific stratum $\tilde{S}_{12} \in s_{1,a}(\mathbb{R}^9)$ which represents the coalescence points of the first and second particle. To handle this case with our hyperspherical coordinates, we have to switch to the Cartesian coordinates

$$z_{12} := \frac{1}{\sqrt{2}}(x_1 - x_2), \quad u_3 := \sqrt{\frac{2}{3}}\left(\frac{1}{2}(x_1 + x_2) - x_3\right), \quad s := \frac{1}{\sqrt{3}}(x_1 + x_2 + x_3), \quad (2.10)$$

which satisfy

$$|z_{12}|^2 + |u_3|^2 + |s|^2 = |x_1|^2 + |x_2|^2 + |x_3|^2,$$

and therefore

$$\Delta_{x_1} + \Delta_{x_2} + \Delta_{x_3} = \Delta_{z_{12}} + \Delta_{u_3} + \Delta_s,$$

where Δ_y , with $y = x_1, x_2, x_3, z_{12}, u_3, s$, denotes the Laplace operator in $\mathbb{R}^3$. Once appropriate Cartesian coordinates have been defined, we can consider the corresponding hyperspherical coordinates

$$z_{12} = t \sin(r_2) \sin(r_1) \Phi(\theta_1, \varphi_1), \quad u_3 = t \sin(r_2) \cos(r_1) \Phi(\theta_2, \varphi_2), \quad s = t \cos(r_2) \Phi(\theta_3, \varphi_3). \quad (2.11)$$

The stratum $\tilde{S}_{12} \in s_{1,a}(\mathbb{R}^9)$ meets the stratum $\tilde{S}_{123} \in s_{2,a}(\mathbb{R}^9)$ in an edge type singularity if x_3 approaches the center of mass of the first and second particle and eventually these two strata approach the stratum $S_O \in s_3(\mathbb{R}^9)$ at the origin. The corresponding part of configuration space can be described in a local chart, denoted as *Chart-2* in the following, by hyperspherical coordinates replacing (x_1, x_2, x_3) by (z_{12}, u_3, s) in (2.9), where r_1, r_2 and t now control the distance to the strata $\tilde{S}_{12}, \tilde{S}_{123}$ and S_O , respectively.

2.1.1 Stratified Laplace operator

We are now prepared to consider the Laplace operator in hyperspherical coordinates [18] from the point of view of singular analysis. The Laplace operator in any of the local charts is given by

$$\begin{aligned} \Delta_{hc} = & \frac{1}{t^2} \left\{ (-t\partial_t)^2 - 7(-t\partial_t) + \frac{\Omega_3}{\cos^2(r_2)} \right. \\ & + \frac{1}{\sin^2(r_2)} \left[(-\sin(r_2)\partial_{r_2})^2 - h_2(r_2)(-\sin(r_2)\partial_{r_2}) + \frac{\Omega_2}{\cos^2(r_1)} \right] \\ & \left. + \frac{1}{\sin^2(r_2)} \frac{1}{\sin^2(r_1)} \left[(-\sin(r_1)\partial_{r_1})^2 - h_1(r_1)(-\sin(r_1)\partial_{r_1}) + \Omega_1 \right] \right\} \end{aligned} \quad (2.12)$$

with

$$h_1(r_1) := \frac{\cos^2(r_1) - 2\sin^2(r_1)}{\cos(r_1)}, \quad h_2(r_2) := \frac{4\cos^2(r_2) - 2\sin^2(r_2)}{\cos(r_2)},$$

where $\Omega_i, i = 1, 2, 3$ denotes the Laplace-Beltrami operator on corresponding copies of S^2 . To simplify our further discussion, (2.12) has been already brought into a form suitable for the singular calculus. Following the recursive approach of [3, 4], it can be easily seen that it has the right degenerate behaviour near the singular strata. Let us start with the highest order corner singularity S_O . The Laplace operator (2.12) locally belongs to $\text{Diff}_{deg}^2(B_2^\Delta)$, which consists of degenerate differential operators of the form

$$A = t^{-2} \sum_{j \leq 2} a_j(t) (-t\partial_t)^j \quad (2.13)$$

with coefficients $a_j(t) \in C^\infty(\overline{\mathbb{R}}_+, \text{Diff}_{deg}^{2-j}(S^2 \times B_1^\Delta))$. The recursive approach for higher order singularities requires coefficients of the form

$$a_j(t) = \sin^{-2}(r_2) \sum_{k+|\alpha| \leq 2-j} b_{jk,\alpha}(t, r_2, \theta_3, \varphi_3) (-\sin(r_2)\partial_{r_2})^k (\sin(r_2)^{|\alpha|} D_{\theta_3, \varphi_3}^\alpha),$$

with $b_{jk,\alpha} \in C^\infty(\overline{\mathbb{R}}_+ \times S^2, \text{Diff}_{deg}^{2-j-|\alpha|}(S^2 \times C^\Delta(S^2)))$ and edge variables θ_3, φ_3 . In the case of (2.12), we can use a slightly simplified representation, namely

$$a_j(t) = \sin^{-2}(r_2) \sum_{k+2p \leq 2-j} b_{jk,(2p)}(t, r_2, \theta_3, \varphi_3) (-\sin(r_2)\partial_{r_2})^k (\sin^2(r_2)\Omega_3)^p.$$

According to it, a_2 and a_1 are constant coefficients, whereas a_0 has the nonvanishing coefficients

$$b_{02,0} = 1, \quad b_{01,0}(r_2) = -h_2(r_2), \quad b_{00,2}(t, r_2) = \frac{t^2}{\cos^2(r_2)}$$

and

$$b_{00,0}(t) = \sin^{-2}(r_1) \left[(-\sin(r_1)\partial_{r_1})^2 - h_1(r_1)(-\sin(r_1)\partial_{r_1}) + t^2\Omega_1 + \frac{t^2 \sin^2(r_1)\Omega_2}{\cos^2(r_1)} \right]. \quad (2.14)$$

Finally, the latter has to be an element of $\text{Diff}_{deg}^2(S^2 \times C^\Delta(S^2))$, with edge variables θ_2, φ_2 , i.e.,

$$b_{00,0}(t) = \sin^{-2}(r_1) \sum_{l+2p \leq 2} c_{l,(2p)}(t, r_1, r_2, \theta_3, \varphi_3) (-\sin(r_1) \partial_{r_1})^l (\sin^2(r_1) \Omega_2)^p,$$

with $c_{l,(2p)} \in C^\infty(S^2, \text{Diff}^{2-j-|\alpha|}(S^2))$. Inspection of (2.14) gives

$$c_{2,0} = 1, \quad c_{1,0}(r_1) = -h_1(r_1), \quad c_{0,0}(t) = t^2 \Omega_1, \quad c_{0,2}(t, r_1) = \frac{t^2}{\cos^2(r_1)},$$

and completes our recursive discussion of the stratified Laplace operator.

2.1.2 Stratified Hamilton operator

To demonstrate the existence of a stratified Hamilton operator in the singular calculus, we have to consider the behaviour of the Coulomb potential in the neighbourhoods of the strata. Let us consider the generic case of three electrons and a nucleus, where the Coulomb potential is given by

$$V(x_1, x_2, x_3) = -\frac{Z}{|x_1|} - \frac{Z}{|x_2|} - \frac{Z}{|x_3|} + \frac{1}{|x_1 - x_2|} + \frac{1}{|x_1 - x_3|} + \frac{1}{|x_2 - x_3|}. \quad (2.15)$$

The Coulomb potential (2.15) has in *Chart-1* the following form

$$\begin{aligned} V_{Chart-1}(t, r_1, r_2, \dots) = & -\underbrace{\frac{Z}{t \sin(r_1) \sin(r_2)}}_{S_1, S_{12}, S_O} - \underbrace{\frac{Z}{t \cos(r_1) \sin(r_2)}}_{S_2, S_{12}, S_O} - \underbrace{\frac{Z}{t \cos(r_2)}}_{S_O} \\ & + \underbrace{\frac{1}{t \sin(r_2) |\sin(r_1) \Phi_1 - \cos(r_1) \Phi_2|}}_{S_{12}, S_O} + \underbrace{\frac{1}{t |\sin(r_1) \sin(r_2) \Phi_1 - \cos(r_2) \Phi_3|}}_{S_O} \\ & + \underbrace{\frac{1}{t |\cos(r_1) \sin(r_2) \Phi_2 - \cos(r_2) \Phi_3|}}_{S_O}, \end{aligned} \quad (2.16)$$

where the strata on which Coulomb potentials becomes singular have been indicated under the parentheses, cf. (2.4) and (2.6). Because of $|\Phi_i| = 1$, $i = 1, 2, 3$, we get for r_1, r_2 sufficiently small, the estimates

$$\begin{aligned} 0 &< |\sin(r_1) - \cos(r_1)| \leq |\sin(r_1) \Phi_1 - \cos(r_1) \Phi_2|, \\ 0 &< |\sin(r_1) \sin(r_2) - \cos(r_2)| \leq |\sin(r_1) \sin(r_2) \Phi_1 - \cos(r_2) \Phi_3|, \\ 0 &< |\cos(r_1) \sin(r_2) - \cos(r_2)| \leq |\cos(r_1) \sin(r_2) \Phi_2 - \cos(r_2) \Phi_3|. \end{aligned}$$

Taking into account these estimates and the respective degeneracies of the strata, we can bring (2.16) into the form

$$\begin{aligned} V_{Chart-1}(t, r_1, r_2, \dots) = & \frac{1}{t^2} \left[-\frac{Zt}{\cos(r_2)} + \frac{t}{|\sin(r_1) \sin(r_2) \Phi_1 - \cos(r_2) \Phi_3|} \right. \\ & + \frac{t}{|\cos(r_1) \sin(r_2) \Phi_2 - \cos(r_2) \Phi_3|} \\ & + \frac{1}{\sin^2(r_2)} \left(-\frac{Zt \sin(r_2)}{\cos(r_1)} + \frac{t \sin(r_2)}{|\sin(r_1) \Phi_1 - \cos(r_1) \Phi_2|} \right) \\ & \left. - \frac{1}{\sin^2(r_1) \sin^2(r_2)} (Zt \sin(r_1) \sin(r_2)) \right], \end{aligned}$$

which demonstrates that the corresponding Hamiltonian with Coulomb interactions in the local chart belongs to the class $\text{Diff}_{deg}^2(B_2^\Delta)$.

Let us also briefly discuss the Coulomb potential in *Chart-2*, where it is sufficient to consider the interaction part, i.e., the last three terms in (2.15). We have, cf. (2.10),

$$|x_1 - x_2| = \sqrt{2}|z_{12}|, \quad |x_1 - x_3| = \frac{1}{\sqrt{2}}|\sqrt{3}u_3 + z_{12}|, \quad |x_2 - x_3| = \frac{1}{\sqrt{2}}|\sqrt{3}u_3 - z_{12}|,$$

which yields the interaction potential

$$\begin{aligned} V_{Chart-2}^{(2)}(t, r_1, r_2, \dots) = & \frac{1}{\sqrt{2}} \left[\underbrace{\frac{1}{t \sin(r_1) \sin(r_2)}}_{\tilde{S}_{12}, \tilde{S}_{123}, S_O} + \underbrace{\frac{2}{t \sin(r_2) |\sqrt{3} \cos(r_1) \Phi_2 + \sin(r_1) \Phi_1|}}_{\tilde{S}_{123}, S_O} \right. \\ & \left. + \underbrace{\frac{2}{t \sin(r_2) |\sqrt{3} \cos(r_1) \Phi_2 - \sin(r_1) \Phi_1|}}_{\tilde{S}_{123}, S_O} \right], \end{aligned}$$

where the strata have been indicated on which Coulomb potentials become singular, cf. (2.3) and (2.5). Taking into account the corresponding degeneracies and the estimate

$$0 < |\sqrt{3} \cos(r_1) - \sin(r_1)| \leq |\sqrt{3} \cos(r_1) \Phi_2 \pm \sin(r_1) \Phi_1|$$

for r_1 sufficiently small, it shows that the Coulomb potential satisfies the requirements of the singular calculus.

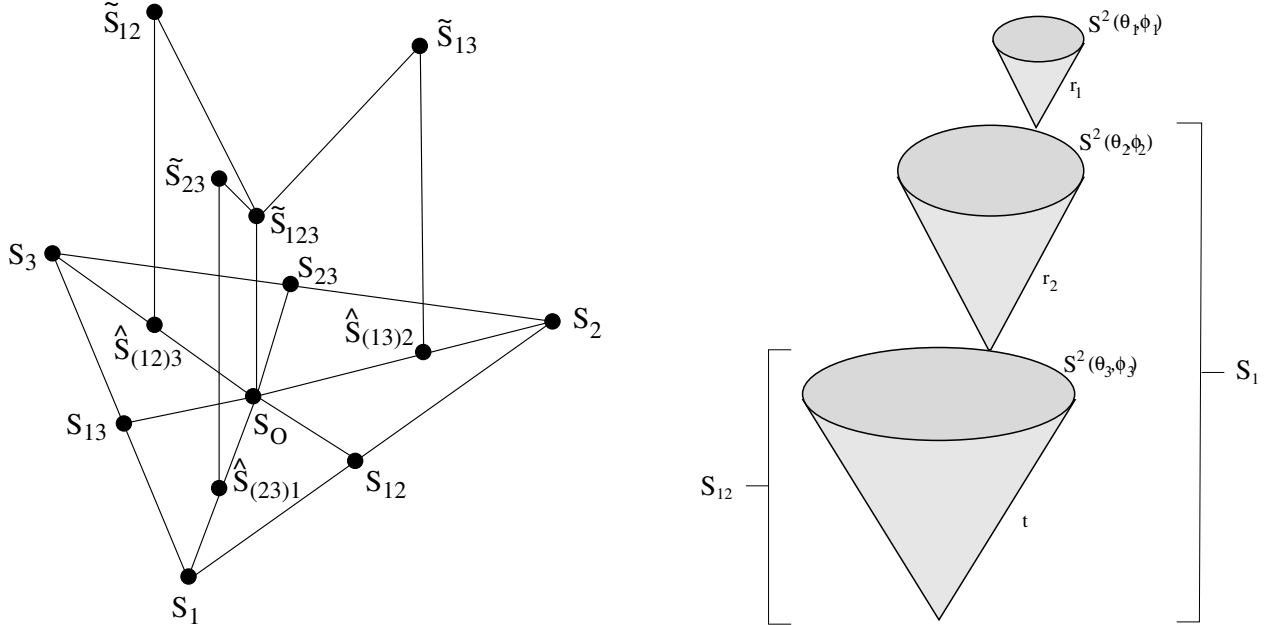


Figure 1: Global and local structure of a stratified three-particle configuration space. a) Net of connectivity for strata of the configuration space, cf. (2.3), (2.4), (2.5), (2.6) and (2.7) for definitions. b) Stratification of configuration space in the local coordinates (2.9). Here S^2 submanifolds are represented by circles for reasons of graphical representability.

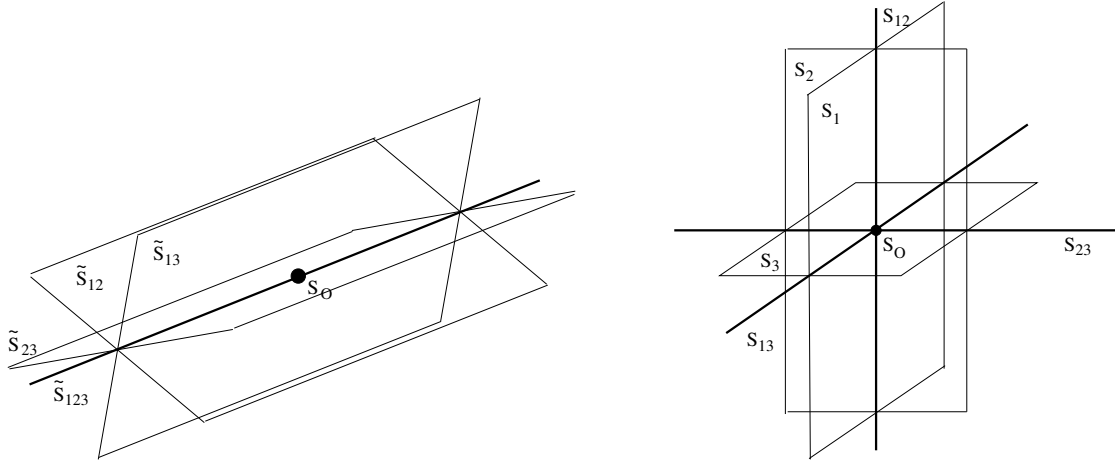


Figure 2: Strata of the configuration space represented as arrangements of intersecting hyperplanes. a) Strata of $s_{1,a}(\mathbb{R}^9)$ and $s_{2,a}(\mathbb{R}^9)$. b) Strata of $s_{1,b}(\mathbb{R}^9)$ and $s_{2,b}(\mathbb{R}^9)$.

3 Function spaces on corner manifolds

To take advantage of the stratification of the configuration space it is necessary to use an appropriate functional analytic set up that enables us to extract the desired asymptotic information of solutions of PDEs related to the stratified Hamilton operator discussed in Subsections 2.1.1 and 2.1.2. The tools we want to employ have been developed over decades by Schulze and collaborators, see for example the monographs [6, 19, 23, 24] and references therein. In the present work, we use the most recent approach to higher singularities outlined in [3, 4]. The characteristic feature of this approach is the recursive construction of new function spaces via non-direct sums of Hilbert spaces and by taking projective limits. For the convenience of the reader, we provide in Appendix A some facts about non-direct sums that will be used in the following.

3.1 Kegel spaces on corner manifolds and wedge spaces along their strata

Within the present work, we want to study triple asymptotics with respect to edge and corner singularities corresponding to coalescence points of two, three and four⁷ particles, respectively. This requires weighted Sobolev spaces with three different asymptotic directions given by the hyperspherical coordinates t, r_1, r_2 . The recursive construction of function spaces for higher order corner singularities has been given in [3, 4] which we follow with minor modifications.

Our focus on the asymptotic behaviour leads us to Kegel spaces with asymptotics. These spaces are subspaces of larger Kegel spaces where only the weights but no explicitly given asymptotic type have been presumed. For the sake of a concise presentation, we consider only Kegel spaces with asymptotics. However, we refer in the following presentation to norms of underlying Kegel spaces without asymptotics. For the convenience of the reader, we summarized the construction of these norms in Appendix C. For further details we refer to [3, 4].

Due to the fact that the highest order corner singularity corresponds to a single point, we have some simplifications in contrast to the general case where the corner represents a higher dimensional stratum in configuration space. According to the stratification discussed in Subsection 2.1, we start

⁷Here the fourth particle is considered to be a nucleus at rest.

on the highest level with the Kegel space

$$\mathcal{K}_{P_1, P_2, P_3}^{s, \gamma_1, \gamma_2, \gamma_3}(B_2^\wedge) = \mathcal{E}_{(P_1, P_2)P_3}^{(\gamma_1, \gamma_2), \gamma_3}(B_2^\wedge) + \mathcal{K}_{P_1, P_2, \Theta_3}^{s, \gamma_1, \gamma_2, \gamma_3}(B_2^\wedge), \quad (3.1)$$

which is of triple asymptotic type⁸ and represents a direct sum of the flattened Kegel space of double asymptotic type $\mathcal{K}_{P_1, P_2, \Theta_3}^{s, \gamma_1, \gamma_2, \gamma_3}(B_2^\wedge)$ with the asymptotic space $\mathcal{E}_{(P_1, P_2)P_3}^{(\gamma_1, \gamma_2), \gamma_3}(B_2^\wedge)$. Both spaces are defined in a recursive manner with respect to function spaces of lower asymptotic type. The Kegel space (3.1) has to be considered as a subspace of the Kegel space $\mathcal{K}^{s, \gamma_1, \gamma_2, \gamma_3}(B_2^\wedge)$ with norm (C.3), c.f. Appendix C for further details.

The *flattened* Kegel space $\mathcal{K}_{P_1, P_2, \Theta_3}^{s, \gamma_1, \gamma_2, \gamma_3}(B_2^\wedge)$ is given by the projective limit

$$\mathcal{K}_{P_1, P_2, \Theta_3}^{s, \gamma_1, \gamma_2, \gamma_3}(B_2^\wedge) := \varprojlim_{\epsilon > 0} \mathcal{K}_{P_1, P_2}^{s, \gamma_1, \gamma_2, \gamma_3 - \vartheta_3 - \epsilon}(B_2^\wedge) = \bigcap_{\epsilon > 0} \mathcal{K}_{P_1, P_2}^{s, \gamma_1, \gamma_2, \gamma_3 - \vartheta_3 - \epsilon}(B_2^\wedge)$$

for the weight intervall $\Theta_3 = (\vartheta_3, 0]$, $-\infty \leq \vartheta_3 < 0$, of Kegel spaces $\mathcal{K}_{P_1, P_2}^{0, \gamma_1, \gamma_2, \tilde{\gamma}}(B_2^\wedge)$ which are of double asymptotic type. The latter can be defined via order reducing operators R^t , $t \in \mathbb{R}$, cf. [3] [Def. 3.8], i.e.,

$$\mathcal{K}_{P_1, P_2}^{s, \gamma_1, \gamma_2, \tilde{\gamma}}(B_2^\wedge) := R_3^{-s}(\mathcal{K}_{\tilde{P}_1, \tilde{P}_2}^{0, \gamma_1 - s, \gamma_2 - s, \tilde{\gamma} - s}(B_2^\wedge)), \quad (3.2)$$

from the composite Kegel space

$$\begin{aligned} \mathcal{K}_{\tilde{P}_1, \tilde{P}_2}^{0, \tilde{\gamma}_1, \tilde{\gamma}_2, \tilde{\gamma}}(B_2^\wedge) &:= \omega_3 \omega_2 \mathcal{H}^{0, \tilde{\gamma}}(\mathbb{R}_+ \times S^2, \mathcal{K}_{\tilde{P}_1, \tilde{P}_2}^{0, \tilde{\gamma}_1, \tilde{\gamma}_2}(B_1^\wedge)) + (1 - \omega_3) \omega_2 \mathcal{H}^{0, 0}(\mathbb{R}_+ \times S^2, \mathcal{K}_{\tilde{P}_1, \tilde{P}_2}^{0, \tilde{\gamma}_1, \tilde{\gamma}_2}(B_1^\wedge)) \\ &\quad + \omega_3 (1 - \omega_2) \mathcal{K}_{\tilde{P}_1}^{0, \tilde{\gamma}_1, \tilde{\gamma}}((2\mathbb{B}_2)^\wedge) + (1 - \omega_3) (1 - \omega_2) \mathcal{K}_{\tilde{P}_1}^{0, \tilde{\gamma}_1, 0}((2\mathbb{B}_2)^\wedge), \end{aligned} \quad (3.3)$$

where $C_0^\infty(\overline{\mathbb{R}}_+)$ cut-off functions $\omega_3 := \omega(t)$, $\omega_2 := \omega(r_2)$ are choosen such that $\omega(r) = 1$ in a neighbourhood of $r = 0$. The Kegel space (3.3) can be actually considered as a non-direct sum of Frechet spaces, cf. [3] for further details. It should be mentioned that this function space does not depend on the specific choice of the cut-off function ω . In Subsection 3.2 below, we give a more detailed discussion of order reducing operators and provide an explicit constructions of such an operator for the Kegel space (3.3). At this point, let us just mention that these operators map specific asymptotic types $\tilde{P}_1, \tilde{P}_2$ into the asymptotic types P_1, P_2 . The first two terms of the composite Kegel space (3.3) consists of $\mathcal{H}^{s, \tilde{\gamma}}(\mathbb{R}_+ \times S^2, \mathcal{K}_{\tilde{P}_1, \tilde{P}_2}^{s, \tilde{\gamma}_1, \tilde{\gamma}_2}(B_1^\wedge))$ spaces which can be considered as the completion of $C_0^\infty(\mathbb{R}_+ \times S^2, \mathcal{K}_{\tilde{P}_1, \tilde{P}_2}^{s, \tilde{\gamma}_1, \tilde{\gamma}_2}(B_1^\wedge))$ with respect to the norm

$$\|u\|_{\mathcal{H}^{s, \tilde{\gamma}}(\mathbb{R}_+ \times S^2, \mathcal{K}_{\tilde{P}_1, \tilde{P}_2}^{s, \tilde{\gamma}_1, \tilde{\gamma}_2})} := \left\{ \int_{S^2} \int_{\Gamma_{3-\tilde{\gamma}}} \langle w, \eta \rangle^{2s} \|\kappa_{\langle w, \eta \rangle}^{-1} M_{r_2 \rightarrow w} F_{y \rightarrow \eta}(u)(w, \eta)\|_{\mathcal{K}^{s, \tilde{\gamma}_1, \tilde{\gamma}_2}(B_1^\wedge)}^2 dw d\eta \right\}^{\frac{1}{2}}, \quad (3.4)$$

where $\langle w, \eta \rangle := (1 + |w|^2 + |\eta|^2)^{\frac{1}{2}}$ and κ_λ , $\lambda \in \mathbb{R}$, represents a group action on $\mathcal{K}_{\tilde{P}_1, \tilde{P}_2}^{s, \tilde{\gamma}_1, \tilde{\gamma}_2}(B_1^\wedge)$ with

$$\kappa_\lambda u(r_2, y) = \lambda^3 u(\lambda r_2, y), \quad u \in \mathcal{K}_{\tilde{P}_1, \tilde{P}_2}^{s, \tilde{\gamma}_1, \tilde{\gamma}_2}(B_1^\wedge). \quad (3.5)$$

In the definition (3.4), the integrand depends on the norm of the Kegel space $\mathcal{K}^{s, \tilde{\gamma}_1, \tilde{\gamma}_2}(B_1^\wedge)$ which is given by (C.2), c.f. Appendix C for further details. Moreover, $M_{r_2 \rightarrow w}$ refers to a Mellin transform of the cone coordinate r_2 taken on the line $\Gamma_{3-\tilde{\gamma}} := \{w \in \mathbb{C} \mid \operatorname{Re} w = 3 - \tilde{\gamma}\}$, and $F_{y \rightarrow \eta}$ refers to a

⁸The subscripts γ_i and P_i , $i = 1, 2, 3$, refer to weights and asymptotic types, respectively. They specify the asymptotic behaviour of functions near strata. A complete definition of these parameters will be given in our discussion of the asymptotic part $\mathcal{E}_{(P_1, P_2)P_3}^{(\gamma_1, \gamma_2), \gamma_3}(B_2^\wedge)$ below.

partial Fourier transform⁹ with respect to the sphere coordinates $y \in S^2$. Finally, the last two terms in (3.3) represent Kegel spaces $\mathcal{K}_{\tilde{P}_1}^{0, \tilde{\gamma}_1, \tilde{\gamma}}((2\mathbb{B}_2)^\wedge)$ of single asymptotic type with respect to the base $2\mathbb{B}_2$ which can be obtained by gluing together two copies of $\mathbb{B}_2 := B_2 \setminus s_2 = S^2 \times B_1^\wedge$ along their common boundaries which gives $2\mathbb{B}_2 \equiv \mathbb{R} \times S^2 \times B_1$.

The asymptotic space

$$\mathcal{E}_{(P_1, P_2)P_3}^{(\gamma_1, \gamma_2), \gamma_3}(B_2^\wedge) := \left\{ \omega_3(t) \sum_j \sum_{k=0}^{m_j} b_{jk} t^{-p_j} \ln^k t, \ b_{jk} \in H_{P_1, P_2}^{\infty, \gamma_1, \gamma_2}(B_2) \right\}$$

is characterized by a sequence $p_j \in \mathbb{C}$ which is taken from a strip of the complex plane, i.e.,

$$p_j \in \left\{ z : \frac{9}{2} - \gamma_3 + \vartheta_3 < \operatorname{Re} z < \frac{9}{2} - \gamma_3 \right\},$$

where the width and location of this strip are determined by its *weight data* (γ_3, Θ_3) . Each substrip of finite width contains only a finite number of p_j . These asymptotic data are summarized in the *asymptotic type* $P_3 := \{(p_j, m_j)\}_{j \in \mathbb{Z}_+}$. The coefficients b_{jk} belong to a weighted corner Frechet space of double asymptotic type

$$H_{P_1, P_2}^{\infty, \gamma_1, \gamma_2}(B_2) = \bigcap_s H_{P_1, P_2}^{s, \gamma_1, \gamma_2}(B_2),$$

with

$$H_{P_1, P_2}^{s, \gamma_1, \gamma_2}(B_2) := \omega_2 \mathcal{W}^s(S^2, \mathcal{K}_{P_1, P_2}^{s, \gamma_1, \gamma_2}(B_1^\wedge)) + (1 - \omega_2) H_{P_1}^{s, \gamma_1}(2\mathbb{B}_2). \quad (3.6)$$

Here, the spaces $H_{P_1, P_2}^{s, \gamma_1, \gamma_2}(B_2)$ are composed of the wedge Sobolev spaces $\mathcal{W}^s(S^2, \mathcal{K}_{P_1, P_2}^{s, \gamma_1, \gamma_2}(B_1^\wedge))$ which represent the completion of $C^\infty(S^2, \mathcal{K}_{P_1, P_2}^{s, \gamma_1, \gamma_2}(B_1^\wedge))$ with respect to the norm¹⁰

$$\|u\|_{\mathcal{W}^s(S^2, \mathcal{K}^{s, \gamma_1, \gamma_2})} := \left\{ \int_{S^2} \langle \eta \rangle^{2s} \| \kappa_{\langle \eta \rangle}^{-1} F_{y \rightarrow \eta}(u)(\eta) \|_{\mathcal{K}^{s, \gamma_1, \gamma_2}(B_1^\wedge)}^2 d\eta \right\}^{\frac{1}{2}},$$

with group action (3.5), $\langle \eta \rangle := (1 + |\eta|^2)^{\frac{1}{2}}$, and weighted corner Sobolev spaces $H_{P_1}^{s, \gamma_1}(2\mathbb{B}_2)$ of single asymptotic type

$$H_{P_1}^{s, \gamma_1}(2\mathbb{B}_2) := \omega_1 \mathcal{W}^s(\mathbb{R} \times S^2, \mathcal{K}_{P_1}^{s, \gamma_1}(C^\wedge)) + (1 - \omega_1) H^s(2(2\mathbb{B}_2)).$$

Moreover, the Sobolev space $H^s(2(2\mathbb{B}_2))$ refers to the smooth manifold $2(2\mathbb{B}_2)$ obtained by gluing together two copies of $2\mathbb{B}_2 \setminus s_1 = S^2 \times \mathbb{R} \times (B_1 \setminus s_1)$ along their common boundaries which gives $2(2\mathbb{B}_2) \equiv \mathbb{R}^2 \times S^2 \times S^2 \times S^2$.

We can now continue our discussion on the next lower level with the Kegel space of double asymptotic type

$$\mathcal{K}_{P_1, P_2}^{s, \gamma_1, \gamma_2}(B_1^\wedge) = \mathcal{E}_{(P_1), P_2}^{(\gamma_1), \gamma_2}(B_1^\wedge) + \mathcal{K}_{P_1, \Theta_2}^{s, \gamma_1, \gamma_2}(B_1^\wedge), \quad (3.7)$$

which shows up in (3.3), (3.6) and represents a direct sum of the flattened Kegel space $\mathcal{K}_{P_1, \Theta_2}^{s, \gamma_1, \gamma_2}(B_1^\wedge)$ of single asymptotic type and the asymptotic space $\mathcal{E}_{(P_1), P_2}^{(\gamma_1), \gamma_2}(B_1^\wedge)$. The Kegel space (3.7) is a subspace of the Kegel space $\mathcal{K}^{s, \gamma_1, \gamma_2}(B_1^\wedge)$ with norm (C.2), cf. Appendix C for further details. Once again, both spaces are defined in a recursive manner with respect to function spaces of lower asymptotic type. The flattened Kegel space with weight intervall $\Theta_2 = (\vartheta_2, 0]$, $-\infty \leq \vartheta_2 < 0$, is given by the projective limit

$$\mathcal{K}_{P_1, \Theta_2}^{s, \gamma_1, \gamma_2}(B_1^\wedge) := \varprojlim_{\epsilon > 0} \mathcal{K}_{P_1}^{s, \gamma_1, \gamma_2 - \vartheta_2 - \epsilon}(B_1^\wedge)$$

⁹For Fourier integrals, we use the common notation $d\eta := \frac{1}{(2\pi)^d} d\eta$.

¹⁰The integrand refers to the norm of the Kegel space $\mathcal{K}^{s, \gamma_1, \gamma_2}(B_1^\wedge)$ which is given by (C.2), c.f. Appendix C for further details.

of Kegel spaces $\mathcal{K}_{P_1}^{s,\gamma_1,\gamma_2-\vartheta_2-\epsilon}(B_1^\wedge)$ which are of single asymptotic type. Again, these Kegel spaces can be defined via an order reducing operator, cf. [3] [Def. 3.8],

$$\mathcal{K}_{P_1}^{s,\gamma_1,\tilde{\gamma}}(B_1^\wedge) := R_2^{-s}(\mathcal{K}_{\tilde{P}_1}^{0,\gamma_1-s,\tilde{\gamma}-s}(B_1^\wedge)), \quad (3.8)$$

from the composite Kegel space

$$\begin{aligned} \mathcal{K}_{\tilde{P}_1}^{0,\tilde{\gamma}_1,\tilde{\gamma}}(B_1^\wedge) &:= \omega_2 \omega_1 \mathcal{H}^{0,\tilde{\gamma}}(\mathbb{R}_+ \times S^2, \mathcal{K}_{\tilde{P}_1}^{0,\tilde{\gamma}_1}(C^\wedge)) + (1 - \omega_2) \omega_1 \mathcal{H}^{0,0}(\mathbb{R}_+ \times S^2, \mathcal{K}_{\tilde{P}_1}^{0,\tilde{\gamma}_1}(C^\wedge)) \\ &\quad + \omega_2(1 - \omega_1) \mathcal{K}^{0,\tilde{\gamma}}((2\mathbb{B}_1)^\wedge) + (1 - \omega_2)(1 - \omega_1) \mathcal{K}^{0,0}((2\mathbb{B}_1)^\wedge). \end{aligned} \quad (3.9)$$

Like the Kegel space (3.3), the Kegel space (3.9) can be also considered as a non-direct sum of Frechet spaces. The composition consists of $\mathcal{H}^{s,\tilde{\gamma}}(\mathbb{R}_+ \times S^2, \mathcal{K}_{\tilde{P}_1}^{s,\tilde{\gamma}_1}(C^\wedge))$ spaces which can be considered as the completion of $C_0^\infty(\mathbb{R}_+ \times S^2, \mathcal{K}_{\tilde{P}_1}^{s,\tilde{\gamma}_1}(C^\wedge))$ with respect to the norm

$$\|u\|_{\mathcal{H}^{s,\tilde{\gamma}}(\mathbb{R}_+ \times S^2, \mathcal{K}_{\tilde{P}_1}^{s,\tilde{\gamma}_1})} := \left\{ \int_{S^2} \int_{\Gamma_{3/2-\tilde{\gamma}}} \langle w, \eta \rangle^{2s} \|\kappa_{\langle w, \eta \rangle}^{-1} M_{r_1 \rightarrow w} F_{y \rightarrow \eta}(u)(w, \eta)\|_{\mathcal{K}^{s,\tilde{\gamma}_1}(C^\wedge)}^2 dw d\eta \right\}^{\frac{1}{2}}, \quad (3.10)$$

where the norm of the Kegel space $\mathcal{K}^{s,\gamma_1}(C^\wedge)$ given by (C.1), with group action

$$\kappa_\lambda u(r_1, y) = \lambda^{\frac{3}{2}} u(\lambda r_1, y), \quad u \in \mathcal{K}^{s,\tilde{\gamma}_1}(C^\wedge), \quad (3.11)$$

and integrated along the line $\Gamma_{\frac{3}{2}-\tilde{\gamma}} := \{w \in \mathbb{C} \mid \operatorname{Re} w = \frac{3}{2} - \tilde{\gamma}\}$. The Kegel spaces $\mathcal{K}^{0,\tilde{\gamma}}((2\mathbb{B}_1)^\wedge)$ have a smooth base $2\mathbb{B}_1$ that can be obtained by gluing together two copies of $\mathbb{B}_1 := B_1 \setminus s_1 = S^2 \times C^\wedge$ along their common boundaries which gives $2\mathbb{B}_1 = \mathbb{R} \times S^2 \times S^2$. The asymptotic space

$$\mathcal{E}_{(P_1),P_2}^{(\gamma_1),\gamma_2}(B_1^\wedge) := \left\{ \omega_2(r_2) \sum_j \sum_{k=0}^{m_j} c_{jk} r_2^{-p_j} \ln^k r_2, \quad c_{jk} \in H_{P_1}^{\infty,\gamma_1}(B_1) \right\}$$

is characterized by a sequence $p_j \in \mathbb{C}$ taken from the strip

$$p_j \in \{z : 3 - \gamma_2 + \vartheta_2 < \operatorname{Re} z < 3 - \gamma_2\}.$$

Therefore, $\mathcal{E}_{(P_1),P_2}^{(\gamma_1),\gamma_2}(B_1^\wedge)$ is characterized by the asymptotic type $P_2 := \{(p_j, m_j)\}_{j \in \mathbb{Z}_+}$ and weight data (γ_2, Θ_2) . The coefficients c_{jk} in the asymptotic space belong to a weighted corner Sobolev space of single asymptotic type

$$H_{P_1}^{\infty,\gamma_1}(B_1) = \bigcap_s H_{P_1}^{s,\gamma_1}(B_1),$$

with

$$H_{P_1}^{s,\gamma_1}(B_1) := \omega_1 \mathcal{W}^s(S^2, \mathcal{K}_{P_1}^{s,\gamma_1}(C^\wedge)) + (1 - \omega_1) H^s(2\mathbb{B}_1).$$

The space $H_{P_1}^{s,\gamma_1}(B_1)$ represents a non-direct sum of the wedge Sobolev space $\mathcal{W}^s(S^2, \mathcal{K}_{P_1}^{s,\gamma_1}(C^\wedge))$, which represents the completion of $C^\infty(S^2, \mathcal{K}_{P_1}^{s,\gamma_1}(C^\wedge))$ with respect to the norm

$$\|u\|_{\mathcal{W}^s(S^2, \mathcal{K}_{P_1}^{s,\gamma_1})} := \left\{ \int_{S^2} \langle \eta \rangle^{2s} \|\kappa_{\langle \eta \rangle}^{-1} F_{y \rightarrow \eta}(u)(\eta)\|_{\mathcal{K}^{s,\gamma_1}(C^\wedge)}^2 d\eta \right\}^{\frac{1}{2}},$$

and the standard Sobolev space $H^s(2\mathbb{B}_1)$ which refers to the smooth manifold $2\mathbb{B}_1$. On the lowest level, we finally get

$$\mathcal{K}_{P_1}^{s,\gamma_1}(C^\wedge) = \mathcal{E}_{P_1}^{\gamma_1}(C^\wedge) + \mathcal{K}_{\Theta_1}^{s,\gamma_1}(B_1^\wedge), \quad (3.12)$$

which is of single asymptotic type and represents a direct sum of the flattened Kegel space

$$\mathcal{K}_{\Theta_1}^{s, \gamma_1}(C^\wedge) := \varprojlim_{\epsilon > 0} \mathcal{K}^{s, \gamma_1 - \vartheta_1 - \epsilon}(C^\wedge)$$

with weight intervall $\Theta_1 = (\vartheta_1, 0]$, $-\infty \leq \vartheta_1 < 0$, and the asymptotic space

$$\mathcal{E}_{P_1}^{\gamma_1}(C^\wedge) := \left\{ \omega_1(r_1) \sum_j \sum_{k=0}^{m_j} d_{jk} r_1^{-p_j} \ln^k r_1 \right\}.$$

is characterized by a sequence $p_j \in \mathbb{C}$ taken from the strip

$$p_j \in \left\{ z : \frac{3}{2} - \gamma_1 + \vartheta_1 < \operatorname{Re} z < \frac{3}{2} - \gamma_1 \right\}.$$

The asymptotic space is characterized by the asymptotic type $P_1 := \{(p_j, m_j)\}_{j \in \mathbb{Z}_+}$ and weight data (γ_1, Θ_1) . Its coefficients d_{jk} belong to a finite dimensional subspaces of $C^\infty(S^2)$. For further details concerning Kegel spaces $\mathcal{K}^{s, \gamma}$ we refer to Appendix B.

3.2 Explicit construction of order reducing operators

The definition of Kegel spaces for higher order singularities in [3, 4] is based on order reducing operators which induce isomorphisms between Kegel spaces of different Sobolev regularities, cf. (3.2) and (3.8).

The basic idea can be simply illustrated for ordinary Sobolev spaces $H^s(\mathbb{R}^n)$, where the pseudo-differential operator

$$\mathcal{P}_s u(x) = \iint e^{i(x-\tilde{x})\xi} (1 + |\xi|^2)^{\frac{s}{2}} u(\tilde{x}) d\tilde{x} d\xi.$$

induces an isomorphism $\mathcal{P}_s : H^t(\mathbb{R}^n) \rightarrow H^{t-s}(\mathbb{R}^n)$ for $s, t \in \mathbb{R}$. We denote such isomorphism inducing operators as order reducing operators. It is obvious that this concept is compatible with the Hilbert space structure of Sobolev spaces $H^s(\mathbb{R}^n)$ which are induced by the L_2 scalar product via

$$\langle u_1, u_2 \rangle_{H^s} = \langle v_1, v_2 \rangle_{L_2},$$

for $u_i = \mathcal{P}_s v_i$, $i = 1, 2$.

The construction of order reducing operators for the Kegel spaces of Subsection 3.1 can be done in a recursive manner. Let us first consider the Kegel spaces $\mathcal{K}^{s, \gamma}(X^\wedge)$ with a smooth base manifold $X = S^n$. According to the recipe of Schulze, cf. [3, 24], one has to consider an elliptic operator in the space

$$L_{cl}^s(S^n, \mathbb{R}_\mu^p \times \Gamma_{\frac{n+1}{2} - \gamma} \times \mathbb{R}_{\tilde{\eta}}^q), \text{ with } \Gamma_{\frac{n+1}{2} - \gamma} := \{w \in \mathbb{C} \mid \operatorname{Re} w = \frac{n+1}{2} - \gamma\},$$

of classical parameter-dependent pseudo-differential operators on S^n . We deliberately choose an elliptic pseudo-differential operator with symbol

$$\tilde{a}_s(w, \mu, \tilde{\eta}) = (-w^2 + 2(\frac{n+1}{2} - \gamma)w - \Omega_{S^n} + |\mu|^2 + |\tilde{\eta}|^2)^{\frac{s}{2}}, \quad (3.13)$$

where Ω_{S^n} denotes the Laplace-Beltrami operator on S^n and $\mu \in \mathbb{R}^p$, $\tilde{\eta} \in \mathbb{R}^d$ represent auxiliary parameters and additional covariables, respectively. Taking $w = \frac{n+1}{2} - \gamma + i\rho \in \Gamma_{\frac{n+1}{2} - \gamma}$, the symbol becomes¹¹

$$\tilde{a}_s(\rho, \mu, \tilde{\eta}) = \left(\rho^2 + \left(\frac{n+1}{2} - \gamma \right)^2 - \Omega_{S^n} + |\mu|^2 + |\tilde{\eta}|^2 \right)^{\frac{s}{2}}.$$

¹¹By a slight abuse of notation we write $\tilde{a}_s(\rho, \mu, \tilde{\eta})$, instead of $\tilde{a}_s(\frac{n+1}{2} - \gamma + i\rho, \mu, \tilde{\eta})$

The ellipticity condition for parameter dependent symbols, cf. [24] [Section 1.2.3], is obviously satisfied, i.e., there exists a constant $c > 0$ such that

$$|\tilde{\sigma}_s(\rho, \xi, \mu, \tilde{\eta})| = \left(\rho^2 + \left(\frac{n+1}{2} - \gamma \right)^2 + \sigma_{S^n}(\xi) + |\mu|^2 + |\tilde{\eta}|^2 \right)^{\frac{s}{2}} \geq c(1 + |\rho, \xi, \tilde{\eta}|)^s,$$

for $|\rho, \xi, \tilde{\eta}| := \sqrt{\rho^2 + |\xi|^2 + |\tilde{\eta}|^2} \geq \tilde{c}$ with $\tilde{c}$ sufficiently large. In the next step one has to perform a kernel cut-off [24] [Section 2.2.2] in order to obtain a parameter dependent symbol in the class of holomorphic symbols, cf. [3] [Defs. 2.2, 2.6], i.e.,

$$M_{\mathcal{O}}^s(S^n; \mathbb{R}_\mu^p \times \mathbb{R}_{r\eta}^p) := \{h(w, \mu, r\eta) : h(w, \mu, \tilde{\eta}) \in \mathcal{A}(\mathbb{C}_w, L_{cl}^\mu(S^n; \mathbb{R}_s^p \times \mathbb{R}_{\tilde{\eta}}^d))\}.$$

For the degenerate symbol $a_s(r, w, \mu, \eta) := \tilde{a}_s(w, \mu, r\eta)$, we define the kernel function

$$k_s(r, \varrho, \mu, \eta) := \int_{\Gamma_{\frac{n+1}{2}-\gamma}} \varrho^{-w} a_s(r, w, \mu, \eta) \tilde{d}w, \quad (3.14)$$

which, for $s < -1$, represents an absolutely convergent integral and, for $s \geq -1$, has to be considered in the distributional sense as an oscillatory integral. Choosing a cut-off function $\phi \in C_0^\infty(\mathbb{R}_+)$, which takes the value 1 in a neighbourhood of 1, one defines the kernel cut-off operator

$$H(\phi) : L_{cl}^s(S^n, \mathbb{R}_\mu^p \times \Gamma_{\frac{n+1}{2}-\gamma} \times \mathbb{R}_{\tilde{\eta}}^q) \rightarrow M_{\mathcal{O}}^\mu(S^n; \mathbb{R}_s^p \times \mathbb{R}_{r\eta}^d)$$

via the weighted Mellin transformation

$$h_s(r, w, \mu, \eta) := \mathcal{M}_{\gamma-\frac{n}{2}, \varrho \rightarrow w}(\phi(\varrho)k_s(r, \varrho, \mu, \eta)).$$

The symbol $h_s(r, w, \mu, \eta) \in M_{\mathcal{O}}^\mu(S^n; \mathbb{R}_\mu^p \times \mathbb{R}_{r\eta}^p)$ defines an order reducing Mellin pseudo-differential operator

$$R^s(\mu, \eta)u(r) := r^{-s} \text{op}_M^{\gamma-\frac{n}{2}}(h_s(r, \mu, \eta))u,$$

with

$$\text{op}_M^{\gamma-\frac{n}{2}}(h_s(r, \mu, \eta))u := \int_{\mathbb{R}} \int_{\mathbb{R}_+} \left(\frac{r}{\tilde{r}} \right)^{-(\frac{n+1}{2}-\gamma+i\rho)} h_s(r, \frac{n+1}{2} - \gamma + i\rho, \mu, \eta) u(\tilde{r}) \frac{d\tilde{r}}{\tilde{r}} d\rho \quad (3.15)$$

for $|\mu|, |\eta|$ sufficiently large. The order reducing operators can be as well expressed by the kernel function (3.14) via

$$R^s(\mu, \eta)u(r) := r^{-s} \int_0^\infty \phi\left(\frac{r}{\tilde{r}}\right) k_s(r, \frac{r}{\tilde{r}}, \mu, \eta) u(\tilde{r}) \frac{d\tilde{r}}{\tilde{r}}. \quad (3.16)$$

It is instructive to see how the operator (3.16) acts on a function of specific asymptotic type

$$u_{p,m}(r) = \omega(r) r^{-p} \ln^m(r),$$

where $\omega \in C_0^\infty(\overline{\mathbb{R}_+})$ is equal to 1 in a neighbourhood of 0. Then an order reducing operator yields

$$\begin{aligned} R^s(\mu, \eta)u_{p,m}(r) &= r^{-s} \int_0^\infty \phi\left(\frac{r}{\tilde{r}}\right) k_s(r, \frac{r}{\tilde{r}}, \mu, \eta) u_{p,m}(\tilde{r}) \frac{d\tilde{r}}{\tilde{r}} \\ &= r^{-s} \int_0^\infty \phi(t) k_s(r, t, \mu, \eta) u_{p,m}\left(\frac{r}{t}\right) \frac{dt}{t} \\ &= r^{-(s+p)} \int_0^\infty \phi(t) k_s(r, t, \mu, \eta) \omega\left(\frac{r}{t}\right) t^p (\ln(r) - \ln(t))^m \frac{dt}{t} \\ &= r^{-(s+p)} \sum_{j=0}^m (-1)^{m-j} \binom{m}{j} \ln^j(r) \int_0^\infty \phi(t) k_s(r, t, \mu, \eta) \omega\left(\frac{r}{t}\right) t^p \ln^{m-j}(t) \frac{dt}{t}. \end{aligned}$$

For r sufficiently small, we can assume $\phi(t)\omega(\frac{r}{t}) = \phi(t)$, $t \in \mathbb{R}_+$, and therefore the asymptotic behaviour does not depend on the explicit choice of the cut-off function ω , i.e.,

$$R^s(\mu, \eta)u_{p,m}(r) \sim r^{-(s+p)} \sum_{j=0}^m (-1)^{m-j} \binom{n}{j} \ln^j(r) \int_0^\infty \phi(t)k_s(0, t, \mu, \eta)t^p \ln^{m-j}(t) \frac{dt}{t} + \mathcal{O}(r^{-(s+p)+1}).$$

In the following we want to focus on explicit calculations of the kernel functions (3.14) for $s < s_0 < 0$ where s_0 has been chosen small enough to handle the oscillatory integrals without further regularization. This range is sufficient for our envisaged applications. If an order reducing operator for $s \geq s_0$ is indeed required it can be easily constructed by composition

$$R^s = R^{2m} R^{s-2m}, \quad (3.17)$$

with $m \in \mathbb{N}$ large enough such that $s - 2m < s_0$. The order reducing operators R^{2m} , with $m \in \mathbb{N}$, correspond to ordinary elliptic partial differential operators with holomorphic symbol, cf. (3.13), and a kernel cut-off is therefore not necessary.

For $s < 0$, we can perform explicit calculations for the kernel function (3.14). It is convenient to use a spectral resolution with respect to the Laplace-Beltrami operator Ω_{S^n} , which has a pure point spectrum with eigenvalues $\lambda_\ell = -\ell(\ell + n - 1)$, $\ell = 0, 1, 2, \dots$ and multiplicities

$$2\ell + 1 \text{ for } n = 2, \quad \text{and} \quad \frac{(\ell + (n-1)/2) \prod_{j=1}^{n-2} (\ell + j)}{((n-1)/2) \cdot (n-2)!} \text{ for } n \geq 3,$$

cf. [22] for further details. The spectral resolution becomes

$$\Omega_{S^n} = - \sum_{\ell=0}^{\infty} \ell(\ell + n - 1) P_\ell \quad (3.18)$$

where P_ℓ , $\ell = 0, 1, 2, \dots$, denotes projection operators from $L^2(S^n)$ onto the corresponding eigenspaces of the eigenvalues λ_ℓ . From it we get the spectral resolution of the symbol

$$a_s(r, w, \mu, \eta) = \sum_{l=0}^{\infty} a_{\ell,s}(r, w, \mu, \eta) P_l,$$

with

$$a_{\ell,s}(r, w, \mu, \eta) = \left(\rho^2 + \left(\frac{n+1}{2} - \gamma \right)^2 + \ell(\ell + n - 1) + |\mu|^2 + |r\eta|^2 \right)^{\frac{s}{2}}.$$

Finally, the spectral resolution of the kernel function becomes

$$k_{\ell,s}(r, \varrho, \mu, \eta) = \sum_{l=0}^{\infty} k_{\ell,s}(r, \varrho, \mu, \eta) P_l, \quad (3.19)$$

with

$$k_{\ell,s}(r, \varrho, \mu, \eta) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \varrho^{\gamma - \frac{n+1}{2} - i\rho} \left(\rho^2 + \left(\frac{n+1}{2} - \gamma \right)^2 + \ell(\ell + n - 1) + |\mu|^2 + |r\eta|^2 \right)^{\frac{s}{2}} d\rho.$$

Taking

$$f_\ell(r, \mu, \eta) := \sqrt{\left(\frac{n+1}{2} - \gamma \right)^2 + \ell(\ell + n - 1) + |\mu|^2 + |r\eta|^2}$$

with $|\mu| > 0$, the integral becomes

$$\begin{aligned}
k_{\ell,s}(r, \varrho, \mu, \eta) &= \frac{1}{2\pi} \varrho^{\gamma - \frac{n+1}{2}} f_{\ell}(r, \mu, \eta)^{s+1} \int_{-\infty}^{\infty} \varrho^{-i f_{\ell}(r, \mu, \eta) \tilde{\rho}} (\tilde{\rho}^2 + 1)^{\frac{s}{2}} d\tilde{\rho} \\
&= \frac{1}{\pi} \varrho^{\gamma - \frac{n+1}{2}} f_{\ell}(r, \mu, \eta)^{s+1} \int_0^{\infty} \cos(\ln(\varrho) f_{\ell}(r, \mu, \eta) \tilde{\rho}) (\tilde{\rho}^2 + 1)^{\frac{s}{2}} d\tilde{\rho} \\
&= \frac{\varrho^{\gamma - \frac{n+1}{2}}}{\sqrt{\pi} \Gamma(-\frac{s}{2})} \left(\frac{2 f_{\ell}(r, \mu, \eta)}{|\ln(\varrho)|} \right)^{\frac{s+1}{2}} K_{\frac{s+1}{2}}(|\ln(\varrho)| f_{\ell}(r, \mu, \eta)), \tag{3.20}
\end{aligned}$$

where we have used [1] [9.6.25] and $K_{\nu}(\cdot) = K_{-\nu}(\cdot)$, $\nu \in \mathbb{R}$, in the last line. For $\varrho = r/\tilde{r}$, we can further decompose (3.20) using the series for modified Bessel functions, cf. [28] [p.365] and [7] [p.44f],

$$\frac{K_{\nu}(u)}{u^{\nu}} = 2^{\nu} \Gamma(\nu) \sum_{m=0}^{\infty} (\nu + m) \frac{K_{\nu+m}(w)}{w^{\nu}} \frac{I_{\nu+m}(v)}{v^{\nu}} C_m^{\nu}(\cos(\varphi)), \quad \nu \neq 0, -1, -2, \dots, \quad w > v > 0, \tag{3.21}$$

with $u := \sqrt{v^2 + w^2 - 2vw \cos(\varphi)}$ and Gegenbauer polynomials, cf. [28] [p.363],

$$C_m^{\nu}(\cos(\varphi)) = \sum_{k=0}^{\lfloor m/2 \rfloor} \frac{(-1)^k 2^{m-2k} \Gamma(\nu + m - k) \cos^{m-2k}(\varphi)}{(m-2k)! k! \Gamma(\nu)}.$$

Furthermore, let us note the special case

$$K_0(u) = K_0(w) I_0(v) + 2 \sum_{m=1}^{\infty} K_m(w) I_m(v) \cos(m\varphi), \quad w > v > 0. \tag{3.22}$$

For an application of (3.21) and (3.22) to (3.20) let us take

$$|\ln(\varrho)| f_{\ell}(r, \mu, \eta) = \sqrt{v^2 + w^2 - 2vw \cos(\varphi)}, \quad \cos(\varphi) = \pm 1,$$

with $v := f_{\ell}(r, \mu, \eta) |\ln(\tilde{r})|$, $w := f_{\ell}(r, \mu, \eta) |\ln(r)|$. For $r < \tilde{r}$, we get

$$\begin{aligned}
k_{\ell,s}(r, r/\tilde{r}, \mu, \eta) &= \left(\frac{r}{\tilde{r}} \right)^{\gamma - \frac{n+1}{2}} \frac{2^{s+1} \Gamma(\frac{s+1}{2})}{\sqrt{\pi} \Gamma(-\frac{s}{2})} \sum_{m=0}^{\infty} \left(\frac{s+1}{2} + m \right) C_m^{\frac{s+1}{2}}(\cos(\varphi)) \\
&\quad \times \frac{K_{\frac{s+1}{2}+m}(f_{\ell}(r, \mu, \eta) |\ln(r)|)}{|\ln(r)|^{\frac{s+1}{2}}} \frac{I_{\frac{s+1}{2}+m}(f_{\ell}(r, \mu, \eta) |\ln(\tilde{r})|)}{|\ln(\tilde{r})|^{\frac{s+1}{2}}}, \quad s \neq 0, -1, -3, -5, \dots, \tag{3.23}
\end{aligned}$$

and

$$\begin{aligned}
k_{\ell,-1}(r, r/\tilde{r}, \mu, \eta) &= \left(\frac{r}{\tilde{r}} \right)^{\gamma - \frac{n+1}{2}} \frac{1}{\sqrt{\pi} \Gamma(\frac{1}{2})} \left[K_0(f_{\ell}(r, \mu, \eta) |\ln(r)|) I_0(f_{\ell}(r, \mu, \eta) |\ln(\tilde{r})|) \right. \\
&\quad \left. + 2 \sum_{m=1}^{\infty} K_m(f_{\ell}(r, \mu, \eta) |\ln(r)|) I_m(f_{\ell}(r, \mu, \eta) |\ln(\tilde{r})|) \cos(m\varphi) \right]. \tag{3.24}
\end{aligned}$$

The formulas (3.23) and (3.24) greatly simplify explicit asymptotic calculations involving order reducing operators. Using (3.16) and (3.19) together with an appropriate cut-off function ϕ , we obtain an explicit expression of the order reducing operators for $s < 0$ in the form

$$R^s(\mu)u(r) := r^{-s} \sum_{l=0}^{\infty} \int_0^{\infty} \phi(r/\tilde{r}) k_{\ell,s}(r, r/\tilde{r}, \mu) P_{\ell} u(\tilde{r}) \frac{d\tilde{r}}{\tilde{r}}, \tag{3.25}$$

which is suitable for our envisaged calculations.

Let us now turn to the general case of order reducing operators for Kegel spaces on corner manifolds. We explicitly consider the three-particle case, where we start with the elliptic symbol

$$a_s(w_1, w_2, w_3, r_1, r_2, \mu) := \left(- (r_1 r_2 w_3)^2 + 2r_1 r_2 \left(\frac{9}{2} - \gamma_3 \right) (r_1 r_2 w_3) - r_1^2 r_2^2 \Omega_3 - (r_1 w_2)^2 \right. \\ \left. + 2r_1 (3 - \gamma_2) (r_1 w_2) - r_1^2 \Omega_2 - w_1^2 + \left(\frac{3}{2} - \gamma_1 \right) w_1 - \Omega_1 + |\mu|^2 \right)^{\frac{s}{2}} \quad (3.26)$$

with $\mu \in \mathbb{R}$ being an auxiliary parameter. This symbol has been derived from the Laplace operator (2.12) represented in hyperspherical coordinates and takes into account the characteristic degeneracies with respect to the distances to various strata. The corresponding composed Mellin pseudo-differential operator is given by

$$\mathcal{A}^s u = (r_1 r_2 t)^{-s} \text{op}_M^{\gamma_3 - \frac{9}{2}} \left[\text{op}_M^{\gamma_2 - 3} \left[\text{op}_M^{\gamma_1 - \frac{3}{2}} (a_s) u \right] \right], \quad (3.27)$$

with individual Mellin pseudo-differential operators given by (3.15). Taking $w_3 = \frac{9}{2} - \gamma_3 + i\rho_3 \in \Gamma_{\frac{9}{2} - \gamma_3}$, $w_2 = 3 - \gamma_2 + i\rho_2 \in \Gamma_{3 - \gamma_2}$ and $w_1 = \frac{3}{2} - \gamma_1 + i\rho_1 \in \Gamma_{\frac{3}{2} - \gamma_1}$ in (3.26), the pseudo-differential operator (3.27) becomes

$$\mathcal{A}^s u = (r_1 r_2 t)^{-s} \int_{\mathbb{R}} \int_0^\infty \left(\frac{t}{\tilde{t}} \right)^{-(\frac{9}{2} - \gamma_3 + i\rho_3)} \left[\int_{\mathbb{R}} \int_0^\infty \left(\frac{r_2}{\tilde{r}_2} \right)^{-(3 - \gamma_2 + i\rho_2)} \left(\int_{\mathbb{R}} \int_0^\infty \left(\frac{r_1}{\tilde{r}_1} \right)^{-(\frac{3}{2} - \gamma_1 + i\rho_1)} \right. \right. \\ \left. \left. \times a_s(r_1, r_2, \rho_1, \rho_2, \rho_3, \mu) u(\tilde{r}_1, \tilde{r}_2, \tilde{t}) \frac{d\tilde{r}_1}{\tilde{r}_1} d\tilde{\rho}_1 \right) \frac{d\tilde{r}_2}{\tilde{r}_2} d\tilde{\rho}_2 \right] \frac{d\tilde{t}}{\tilde{t}} d\rho_3,$$

with symbol

$$a_s(r_1, r_2, \rho_1, \rho_2, \rho_3, \mu) = \left((r_1 r_2 \rho_3)^2 + (r_1 r_2)^2 \left(\frac{9}{2} - \gamma_3 \right)^2 - r_1^2 r_2^2 \Omega_3 + (r_1 \rho_2)^2 \right. \\ \left. + r_1^2 (3 - \gamma_2)^2 - r_1^2 \Omega_2 + \rho_1^2 + \left(\frac{3}{2} - \gamma_1 \right)^2 - \Omega_1 + |\mu|^2 \right)^{\frac{s}{2}}. \quad (3.28)$$

The corresponding kernel function is given by the oscillatory integral¹²

$$k_s(r_1, r_2, \varrho_1, \varrho_2, \varrho_3, \mu) = \frac{1}{(2\pi)^3} \varrho_1^{\gamma_1 - \frac{3}{2}} \varrho_2^{\gamma_2 - 3} \varrho_3^{\gamma_3 - \frac{9}{2}} \int_{\mathbb{R}} \int_{\mathbb{R}} \int_{\mathbb{R}} \varrho_3^{-i\rho_3} \varrho_2^{-i\rho_2} \varrho_1^{-i\rho_1} \\ \times a_s(r_1, r_2, \varrho_1, \varrho_2, \varrho_3, \mu) d\rho_1 d\rho_2 d\rho_3, \quad (3.29)$$

with $\varrho_1 := \frac{r_1}{\tilde{r}_1}$, $\varrho_2 := \frac{r_2}{\tilde{r}_2}$ and $\varrho_3 := \frac{t}{\tilde{t}}$. Performing appropriate kernel cut-offs by a sequence of weighted Mellin transformations

$$h_s(r_1, r_2, w_1, w_2, w_3, \mu) := \mathcal{M}_{\gamma - \frac{9}{2}, \varrho_3 \rightarrow w_3} \left\{ \phi_3(\varrho_3) \mathcal{M}_{\gamma_2 - 3, \varrho_2 \rightarrow w_2} \left[\phi_2(\varrho_2) \right. \right. \\ \left. \left. \times \mathcal{M}_{\gamma_1 - \frac{3}{2}, \varrho_1 \rightarrow w_1} \left(\phi_1(\varrho_1) k_s(r_1, r_2, \varrho_1, \varrho_2, \varrho_3, \mu) \right) \right] \right\},$$

we obtain a holomorphic symbol h_s in the class

$$M_{\mathcal{O}}^s(S^2 \times S^2 \times S^2; \mathbb{R}_\mu) := \left\{ h(w_1, w_2, w_3, \mu) : h(w_1, w_2, w_3, \mu) \in \mathcal{A}(\mathbb{C}_{w_1, w_2, w_3}^3, L_{cl}^s(S^2 \times S^2 \times S^2; \mathbb{R}_\mu)) \right\}.$$

¹²The integral is absolutely convergent only for $s < -3$.

For sufficiently large values of $|\mu|$, the symbol $h_s \in M_{\mathcal{O}}^s(S^2 \times S^2 \times S^2; \mathbb{R}_\mu)$ defines an order reducing operator

$$R^s u = (r_1 r_2 t)^{-s} \text{op}_M^{\gamma_3 - \frac{9}{2}} \left[\text{op}_M^{\gamma_2 - 3} \left[\text{op}_M^{\gamma_1 - \frac{3}{2}} (h_s) u \right] \right], \quad (3.30)$$

which provides the isomorphism (3.2).

To evaluate the integral (3.29) and to obtain the kernel function in a form suitable for further considerations, we perform spectral resolutions of the Laplace-Beltrami operators on the spheres (3.18) and a Laplace transform of the whole symbol in order to separate the variables. First, spectral resolutions give us the decomposition

$$k_s(r_1, r_2, \varrho_1, \varrho_2, \varrho_3, \mu, \eta) = \sum_{\ell_1=0}^{\infty} \sum_{\ell_2=0}^{\infty} \sum_{\ell_3=0}^{\infty} k_{\ell_1, \ell_2, \ell_3, s}(r_1, r_2, \varrho_1, \varrho_2, \varrho_3, \mu, \eta) P_{\ell_1} P_{\ell_2} P_{\ell_3},$$

and, second, a Laplace transform, cf. [17] [p.1110, Eq. (26)],

$$\int_0^\infty \lambda^{\beta-1} e^{-a\lambda} d\lambda = \Gamma(\beta) a^{-\beta}, \quad \beta > 0, \text{ Re } a > 0, \quad (3.31)$$

enables a separation of variables for symbols with $s < 0$, i.e., we get

$$\begin{aligned} k_{\ell_1, \ell_2, \ell_3, s}(r_1, r_2, \varrho_1, \varrho_2, \varrho_3, \mu, \eta) &= \frac{1}{(2\pi)^3 \Gamma(-\frac{s}{2})} \varrho_1^{\gamma_1 - \frac{3}{2}} \varrho_2^{\gamma_2 - 3} \varrho_3^{\gamma_3 - \frac{9}{2}} \int_{\mathbb{R}} \int_{\mathbb{R}} \int_{\mathbb{R}} \varrho_3^{-i\rho_3} \varrho_2^{-i\rho_2} \varrho_1^{-i\rho_1} \\ &\times \int_0^\infty \lambda^{-\frac{s+2}{2}} \exp[-b_{\ell_1, \ell_2, \ell_3}(r_1, r_2, \rho_1, \rho_2, \rho_3, \mu)\lambda] d\lambda d\rho_1 d\rho_2 d\rho_3, \end{aligned} \quad (3.32)$$

with

$$\begin{aligned} b_{\ell_1, \ell_2, \ell_3}(r_1, r_2, \rho_1, \rho_2, \rho_3, \mu) &= (r_1 r_2 \rho_3)^2 + (r_1 r_2)^2 \left(\frac{9}{2} - \gamma_3\right)^2 + r_1^2 r_2^2 \ell_3(\ell_3 + 1) + (r_1 \rho_2)^2 \\ &+ r_1^2 (3 - \gamma_2)^2 + r_1^2 \ell_2(\ell_2 + 1) + \rho_1^2 + \left(\frac{3}{2} - \gamma_1\right)^2 + \ell_1(\ell_1 + 1) + |\mu|^2. \end{aligned}$$

To proceed with our calculations, let us tentatively assume $s < -3$. According to Fubini's theorem, we can interchange the order of integrations and calculate the separate integrals

$$\begin{aligned} \int_{\mathbb{R}} e^{-i\rho_1 \ln(\varrho_1)} e^{-\rho_1^2 \lambda} d\rho_1 &= \sqrt{\frac{\pi}{\lambda}} e^{-\frac{|\ln(\varrho_1)|^2}{4\lambda}}, \\ \int_{\mathbb{R}} e^{-i\rho_2 \ln(\varrho_2)} e^{-r_1^2 \rho_1^2 \lambda} d\rho_2 &= \sqrt{\frac{\pi}{\lambda}} r_1^{-1} e^{-\frac{|\ln(\varrho_2)|^2}{4r_1^2 \lambda}}, \\ \int_{\mathbb{R}} e^{-i\rho_3 \ln(\varrho_3)} e^{-(r_1 r_2)^2 \rho_3^2 \lambda} d\rho_3 &= \sqrt{\frac{\pi}{\lambda}} (r_1 r_2)^{-1} e^{-\frac{|\ln(\varrho_3)|^2}{4(r_1 r_2)^2 \lambda}}. \end{aligned}$$

Putting things together, we finally obtain

$$\begin{aligned} k_{\ell_1, \ell_2, \ell_3, s}(r_1, r_2, \varrho_1, \varrho_2, \varrho_3, \mu) &= \frac{1}{\Gamma(-\frac{s}{2})} \frac{\varrho_1^{\gamma_1 - \frac{3}{2}}}{2\sqrt{\pi}} \frac{\varrho_2^{\gamma_2 - 3}}{2\sqrt{\pi}} \frac{\varrho_3^{\gamma_3 - \frac{9}{2}}}{2\sqrt{\pi}} r_1^{-2} r_2^{-1} \\ &\times \int_0^\infty \lambda^{-\frac{s+5}{2}} e^{-z_{\ell_1, \ell_2, \ell_3}^2(r_1, r_2)\lambda} e^{-\frac{u^2(r_1, r_2, \varrho_1, \varrho_2, \varrho_3)}{4\lambda}} d\lambda, \end{aligned} \quad (3.33)$$

with

$$\begin{aligned} z_{\ell_1, \ell_2, \ell_3}^2(r_1, r_2) &:= f_{\ell_1}^2 + g_{\ell_2}^2(r_1) + h_{\ell_3}^2(r_1, r_2), \\ u^2(r_1, r_2, \varrho_1, \varrho_2, \varrho_3) &:= |\ln(\varrho_1)|^2 + r_1^{-2} |\ln(\varrho_2)|^2 + r_1^{-2} r_2^{-2} |\ln(\varrho_3)|^2, \end{aligned}$$

and

$$\begin{aligned} f_{\ell_1}^2 &:= \left(\frac{3}{2} - \gamma_1\right)^2 + \ell_1(\ell_1 + 1) + |\mu_1|^2, \\ g_{\ell_2}^2(r_1) &:= r_1^2(3 - \gamma_2)^2 + r_1^2 \ell_2(\ell_2 + 1) + |\mu_2|^2, \\ h_{\ell_3}^2(r_1, r_2) &:= (r_1 r_2)^2 \left(\frac{9}{2} - \gamma_3\right)^2 + r_1^2 r_2^2 \ell_3(\ell_3 + 1) + |\mu_3|^2. \end{aligned}$$

The integral in (3.33) corresponds to a modified Bessel function. This can be easily seen from the following formula [5] [(10.32.10)]

$$K_\nu(x) = \frac{1}{2} \left(\frac{x}{2}\right)^\nu \int_0^\infty \lambda^{-(\nu+1)} e^{-\lambda} e^{-\frac{x^2}{4\lambda}} d\lambda,$$

which yields

$$\begin{aligned} &\int_0^\infty \lambda^{-\frac{s+5}{2}} e^{-z_{\ell_1, \ell_2, \ell_3}^2(r_1, r_2)\lambda} e^{-\frac{u^2(r_1, r_2, \varrho_1, \varrho_2, \varrho_3)}{4\lambda}} d\lambda \\ &= 2^{\frac{s+5}{2}} \left(\frac{z_{\ell_1, \ell_2, \ell_3}(r_1, r_2)}{u(r_1, r_2, \varrho_1, \varrho_2, \varrho_3)} \right)^{\frac{s+3}{2}} K_{\frac{s+3}{2}}(z_{\ell_1, \ell_2, \ell_3}(r_1, r_2) u(r_1, r_2, \varrho_1, \varrho_2, \varrho_3)), \end{aligned}$$

so that the final expression for the kernel function becomes

$$\begin{aligned} k_{\ell_1, \ell_2, \ell_3, s}(r_1, r_2, \varrho_1, \varrho_2, \varrho_3, \mu) &= \frac{1}{\Gamma(-\frac{s}{2})} \frac{\varrho_1^{\gamma_1 - \frac{3}{2}}}{2\sqrt{\pi}} \frac{\varrho_2^{\gamma_2 - 3}}{2\sqrt{\pi}} \frac{\varrho_3^{\gamma_3 - \frac{9}{2}}}{2\sqrt{\pi}} r_1^{-2} r_2^{-1} 2^{\frac{s+5}{2}} z_{\ell_1, \ell_2, \ell_3}^{s+3}(r_1, r_2) \\ &\quad \times \frac{K_{\frac{s+3}{2}}(z_{\ell_1, \ell_2, \ell_3}(r_1, r_2) u(r_1, r_2, \varrho_1, \varrho_2, \varrho_3))}{(z_{\ell_1, \ell_2, \ell_3}(r_1, r_2) u(r_1, r_2, \varrho_1, \varrho_2, \varrho_3))^{\frac{s+3}{2}}}. \end{aligned} \quad (3.34)$$

It remains to verify (3.34) in the case $-3 \leq s < 0$. Here we must treat (3.32) as an oscillatory integral, i.e.,

$$\begin{aligned} &\int_0^\infty \int_0^\infty \int_0^\infty k_{\ell_1, \ell_2, \ell_3, s}(r_1, r_2, r_1/\tilde{r}_1, r_2/\tilde{r}_2, t/\tilde{t}, \mu) u_{\ell_1, \ell_2, \ell_3}(\tilde{r}_1, \tilde{r}_2, \tilde{t}) \frac{d\tilde{r}_1}{\tilde{r}_1} \frac{d\tilde{r}_2}{\tilde{r}_2} \frac{d\tilde{t}}{\tilde{t}} \\ &:= \lim_{\epsilon_1, \epsilon_2, \epsilon_3 \rightarrow 0} \int_0^\infty \int_0^\infty \int_0^\infty k_{\ell_1, \ell_2, \ell_3, s}^{\epsilon_1, \epsilon_2, \epsilon_3}(r_1, r_2, r_1/\tilde{r}_1, r_2/\tilde{r}_2, t/\tilde{t}, \mu) u_{\ell_1, \ell_2, \ell_3}(\tilde{r}_1, \tilde{r}_2, \tilde{t}) \frac{d\tilde{r}_1}{\tilde{r}_1} \frac{d\tilde{r}_2}{\tilde{r}_2} \frac{d\tilde{t}}{\tilde{t}}, \end{aligned}$$

with $u_{\ell_1, \ell_2, \ell_3} \in C_0^\infty(\mathbb{R}_+ \times S^2 \times \mathbb{R}_+ \times S^2 \times \mathbb{R}_+ \times S^2)$ given by

$$u_{\ell_1, \ell_2, \ell_3}(\tilde{r}_1, \tilde{r}_2, \tilde{t}) := P_{\ell_1} P_{\ell_2} P_{\ell_3} u(\tilde{r}_1, \tilde{r}_2, \tilde{t})$$

and regularized kernel function

$$\begin{aligned} k_{\ell_1, \ell_2, \ell_3, s}^{\epsilon_1, \epsilon_2, \epsilon_3}(r_1, r_2, \varrho_1, \varrho_2, \varrho_3, \mu) &:= \frac{1}{(2\pi)^3 \Gamma(-\frac{s}{2})} \varrho_1^{\gamma_1 - \frac{3}{2}} \varrho_2^{\gamma_2 - 3} \varrho_3^{\gamma_3 - \frac{9}{2}} \int_{\mathbb{R}} \int_{\mathbb{R}} \int_{\mathbb{R}} \varrho_3^{-i\rho_3} \varrho_2^{-i\rho_2} \varrho_1^{-i\rho_1} \\ &\quad \times \chi_{\epsilon_1}(\rho_1) \chi_{\epsilon_2}(\rho_2) \chi_{\epsilon_3}(\rho_3) \int_0^\infty \lambda^{-\frac{s+2}{2}} \exp[-b_{\ell_1, \ell_2, \ell_3}(r_1, r_2, \rho_1, \rho_2, \rho_3, \mu)\lambda] d\lambda d\rho_1 d\rho_2 d\rho_3, \end{aligned} \quad (3.35)$$

where $\chi \in C_0^\infty(\mathbb{R})$, $0 \leq \chi \leq 1$, is equal to 1 in $(-1, 1)$ and $\chi_{\epsilon_i}(\rho_i) := \chi(\epsilon_i \rho_i)$, $i = 1, 2, 3$.

Lemma 1. *For $s < 0$, the kernel function of the operator $\mathcal{A}^s$, cf. (3.27), is given by (3.34).*

Proof. The case $s < -3$ of absolutely convergent integrals has been already discussed. Let us therefore consider the limits $\epsilon_i \rightarrow 0$, $i = 1, 2, 3$, in the case $-3 \leq s < 0$. Because of the regularized integral (3.35), we can apply (3.31) and freely interchange in (3.35) the order of integration. Like before, the integrand splits up into separated ρ -integrals. Here to avoid cumbersome notations, we consider, instead of (3.32), a simplified oscillatory integral of the form

$$\begin{aligned}
k_s^\epsilon(\varrho) &= \frac{1}{2\pi\Gamma(-\frac{s}{2})} \varrho^{\gamma-\frac{n}{2}} \int_{-\infty}^{\infty} \varrho^{-i\rho} \chi_\epsilon(\rho) \left(\int_0^{\infty} \lambda^{-\frac{s+2}{2}} e^{-(\rho^2+1)\lambda} d\lambda \right) d\rho \\
&= \frac{1}{2\pi\Gamma(-\frac{s}{2})} \varrho^{\gamma-\frac{n}{2}} \int_0^{\infty} \lambda^{-\frac{s+2}{2}} e^{-\lambda} \left(\int_{-\infty}^{\infty} \varrho^{-i\rho} \chi_\epsilon(\rho) e^{-\rho^2\lambda} d\rho \right) d\lambda \\
&= \frac{1}{2\pi\Gamma(-\frac{s}{2})} \varrho^{\gamma-\frac{n}{2}} \int_0^{\infty} \lambda^{-\frac{s+2}{2}} e^{-\lambda} \left(\int_{-\infty}^{\infty} \varrho^{-i\rho} e^{-\rho^2\lambda} d\rho \right) d\lambda \\
&\quad + \frac{1}{2\pi\Gamma(-\frac{s}{2})} \varrho^{\gamma-\frac{n}{2}} \int_0^{\infty} \lambda^{-\frac{s+2}{2}} e^{-\lambda} \left(\int_{-\infty}^{\infty} \varrho^{-i\rho} (1 - \chi_\epsilon(\rho)) e^{-\rho^2\lambda} d\rho \right) d\lambda \\
&= \underbrace{\frac{2^{\frac{s+1}{2}}}{\sqrt{\pi}\Gamma(-\frac{s}{2})} \varrho^{\gamma-\frac{n}{2}} \frac{\ln K_{\frac{s+1}{2}}(|\ln(\varrho)|)}{|\ln(\varrho)|^{\frac{s+1}{2}}}}_{=:k_s(\varrho)} \\
&\quad + \underbrace{\frac{1}{2\pi\Gamma(-\frac{s}{2})} \varrho^{\gamma-\frac{n}{2}} \int_0^{\infty} \lambda^{-\frac{s+2}{2}} e^{-\lambda} \left(\int_{-\infty}^{\infty} \varrho^{-i\rho} (1 - \chi_\epsilon(\rho)) e^{-\rho^2\lambda} d\rho \right) d\lambda}_{=:kc_s^\epsilon(\varrho)}.
\end{aligned}$$

We are left to consider the oscillatory integral acting in the distributional sense on a test function $u \in C_0^\infty(\mathbb{R}_+)$. For this let us first consider the oscillatory integral

$$\begin{aligned}
&\int_{-\infty}^{\infty} (1 - \chi_\epsilon(\rho)) e^{-\rho^2\lambda} \left[\int_0^{\infty} \left(\frac{r}{\tilde{r}} \right)^{\gamma-\frac{n}{2}-i\rho} u(\tilde{r}) \frac{d\tilde{r}}{\tilde{r}} \right] d\rho \\
&= \int_{-\infty}^{\infty} r^{\gamma-\frac{n}{2}-i\rho} (1 - \chi_\epsilon(\rho)) e^{-\rho^2\lambda} \mathcal{M}u\left(\frac{n}{2} - \gamma + i\rho\right) d\rho, \quad (3.36)
\end{aligned}$$

where $\mathcal{M}u$ denotes the Mellin transform of u . According to [20] [Theorem 3], we have for $u \in C_0^\infty(\mathbb{R}_+)$, with $\text{supp } u \in [a^{-1}, a]$ ($a > 0$), the estimate

$$|\mathcal{M}u| \lesssim (1 + |z|)^{-m} a^{|\text{Re } z|}, \quad z \in \mathbb{C}, \text{ for all } m \in \mathbb{N}.$$

With this, we can estimate (3.36) by using Hölder's inequality with $\frac{1}{p} + \frac{1}{q} = 1$, and obtain

$$\begin{aligned}
& \left| \int_{-\infty}^{\infty} (1 - \chi_{\epsilon}(\rho)) e^{-\rho^2 \lambda} \left[\int_0^{\infty} \left(\frac{r}{\tilde{r}} \right)^{\gamma - \frac{n}{2} - i\rho} u(\tilde{r}) \frac{d\tilde{r}}{\tilde{r}} \right] d\rho \right| \\
& \leq \int_{-\infty}^{\infty} |r^{\gamma - \frac{n}{2}} (1 - \chi_{\epsilon}(\rho)) e^{-\rho^2 \lambda} \mathcal{M}u(\tfrac{n}{2} - \gamma + i\rho)| d\rho \\
& \leq \|u\|_{L_p} \left(\int_{-\infty}^{\infty} |r^{\gamma - \frac{n}{2}} (1 - \chi_{\epsilon}(\rho)) e^{-\rho^2 \lambda}|^q d\rho \right)^{\frac{1}{q}} \\
& \stackrel{\tilde{\rho} = \sqrt{q\lambda}\rho}{=} \|u\|_{L_p} r^{\gamma - \frac{n}{2}} (q\lambda)^{-\frac{1}{2q}} \left(\int_{-\infty}^{\infty} |1 - \chi_{\epsilon}(\tilde{\rho}/\sqrt{q\lambda})|^q e^{-\tilde{\rho}^2} d\tilde{\rho} \right)^{\frac{1}{q}} \\
& \leq \|u\|_{L_p} r^{\gamma - \frac{n}{2}} \left(\frac{2}{\sqrt{q\lambda}} \right)^{\frac{1}{q}} \left(\int_{\frac{\sqrt{q\lambda}}{\epsilon}}^{\infty} e^{-\tilde{\rho}^2} d\tilde{\rho} \right)^{\frac{1}{q}} \\
& \leq \|u\|_{L_p} r^{\gamma - \frac{n}{2}} \left(\frac{2}{\sqrt{q\lambda}} \right)^{\frac{1}{q}} e^{-\frac{\lambda}{\epsilon^2}} \left(\frac{\sqrt{q\lambda}}{\epsilon} + \sqrt{\frac{q\lambda}{\epsilon^2} + \frac{4}{\pi}} \right)^{-\frac{1}{q}} \\
& \leq \|u\|_{L_p} r^{\gamma - \frac{n}{2}} \left(\frac{\pi}{q\lambda} \right)^{\frac{1}{2q}} e^{-\frac{\lambda}{\epsilon^2}},
\end{aligned}$$

where in the second to last line, we used the estimate, cf. [1] [7.1.13],

$$\int_a^{\infty} e^{-t^2} dt \leq \frac{e^{-a^2}}{a + \sqrt{a^2 + \frac{4}{\pi}}},$$

for the complementary error function. It remains to consider the limit $\epsilon \rightarrow 0$, where we perform the decomposition

$$\int_0^{\infty} k_s^{\epsilon}(r/\tilde{r}) u(\tilde{r}) \frac{d\tilde{r}}{\tilde{r}} = \int_0^{\infty} k_s(r/\tilde{r}) u(\tilde{r}) \frac{d\tilde{r}}{\tilde{r}} + \int_0^{\infty} k_c^{\epsilon}(r/\tilde{r}) u(\tilde{r}) \frac{d\tilde{r}}{\tilde{r}}$$

and use the estimate

$$\begin{aligned}
\left| \int_0^{\infty} k_c^{\epsilon}(r/\tilde{r}) u(\tilde{r}) \frac{d\tilde{r}}{\tilde{r}} \right| & \leq \|u\|_{L_p} \frac{1}{2\pi\Gamma(-\frac{s}{2})} r^{\gamma - \frac{n}{2}} \left(\frac{\pi}{q\lambda} \right)^{\frac{1}{2q}} \int_0^{\infty} \lambda^{-\frac{s+2}{2}} e^{-\lambda} e^{-\frac{\lambda}{\epsilon^2}} d\lambda \\
& \leq \|u\|_{L_p} \frac{1}{2\pi\Gamma(-\frac{s}{2})} r^{\gamma - \frac{n}{2}} \left(\frac{\pi}{q} \right)^{\frac{1}{2q}} \epsilon^{-s - \frac{1}{q}} \int_0^{\infty} \tilde{\lambda}^{-\frac{s+2}{2} - \frac{1}{2q}} e^{-\tilde{\lambda}} d\tilde{\lambda} \\
& \sim \mathcal{O}(\epsilon^{-s - \frac{1}{q}}) \quad \text{for } s < -\frac{1}{q}.
\end{aligned}$$

For any $s < 0$, we can choose q sufficiently small to fulfill this requirement and thus obtain the desired result

$$\lim_{\epsilon \rightarrow 0} \int_0^{\infty} k_s^{\epsilon}(r/\tilde{r}) u(\tilde{r}) \frac{d\tilde{r}}{\tilde{r}} = \int_0^{\infty} k_s(r/\tilde{r}) u(\tilde{r}) \frac{d\tilde{r}}{\tilde{r}}.$$

□

With appropriately chosen cut-off functions ϕ_i , $i = 1, 2, 3$, we can now define the order reducing operator (3.30) for $s < 0$ by

$$\begin{aligned}
R^s u &= \sum_{\ell_1=0}^{\infty} \sum_{\ell_2=0}^{\infty} \sum_{\ell_3=0}^{\infty} \int_0^{\infty} \int_0^{\infty} \int_0^{\infty} \phi_1(r_1/\tilde{r}_1) \phi_2(r_2/\tilde{r}_2) \phi_3(t/\tilde{t}) \\
& \quad \times k_{\ell_1, \ell_2, \ell_3, s}(r_1, r_2, r_1/\tilde{r}_1, r_2/\tilde{r}_2, t/\tilde{t}, \mu) P_{\ell_1} P_{\ell_2} P_{\ell_3} u(\tilde{r}_1, \tilde{r}_2, \tilde{t}) \frac{d\tilde{r}_1}{\tilde{r}_1} \frac{d\tilde{r}_2}{\tilde{r}_2} \frac{d\tilde{t}}{\tilde{t}},
\end{aligned}$$

with sufficiently large value of $|\mu|$, where we have replaced the $L_{cl}^s(S^2 \times S^2 \times S^2; \mathbb{R}_\mu)$ part of the operator acting on the S^2 cone bases by spectral resolutions with respect to the corresponding Laplace-Beltrami operators. For the case of $s \geq 0$ we refer to (3.17) and the corresponding discussion.

Finally we want to remark that the expression (3.34) can be further separated by using the expansion (3.21), taking

$$\begin{aligned} u &= z_{\ell_1, \ell_2, \ell_3}(r_1, r_2) |\mathbf{u}(r_1, r_2, t) - \tilde{\mathbf{u}}(r_1, r_2, \tilde{r}_1, \tilde{r}_2, \tilde{t})|, \\ v &= z_{\ell_1, \ell_2, \ell_3}(r_1, r_2) |\tilde{\mathbf{u}}(r_1, r_2, \tilde{r}_1, \tilde{r}_2, \tilde{t})|, \\ w &= z_{\ell_1, \ell_2, \ell_3}(r_1, r_2) |\mathbf{u}(r_1, r_2, t)|, \end{aligned}$$

with

$$\mathbf{u}(r_1, r_2, t) := \begin{pmatrix} \ln(r_1) \\ r_1^{-1} \ln(r_2) \\ r_1^{-1} r_2^{-1} \ln(t) \end{pmatrix}, \quad \tilde{\mathbf{u}}(r_1, r_2, \tilde{r}_1, \tilde{r}_2, \tilde{t}) := \begin{pmatrix} \ln(\tilde{r}_1) \\ \tilde{r}_1^{-1} \ln(\tilde{r}_2) \\ \tilde{r}_1^{-1} \tilde{r}_2^{-1} \ln(\tilde{t}) \end{pmatrix},$$

and

$$\cos(\varphi) = \frac{\mathbf{u}(r_1, r_2, t) \cdot \tilde{\mathbf{u}}(r_1, r_2, \tilde{r}_1, \tilde{r}_2, \tilde{t})}{|\mathbf{u}(r_1, r_2, t)| |\tilde{\mathbf{u}}(\tilde{r}_1, \tilde{r}_2, \tilde{t})|}.$$

By this, we have separated the t and $\tilde{t}$ variables as well as the $\ln(r_i)$ and $\ln(\tilde{r}_i)$, $i = 1, 2$, terms. Such kind of expressions are useful for explicit asymptotic calculations.

4 Summary and outlook

The geometrical structure of a configuration space with its stratification is quite intricate and requires a subtle resolution of singularities. This has been achieved by an appropriate choice of hyperspherical coordinates which are compatible with the singular pseudo-differential calculus. An alternative approach uses techniques from algebraic geometry [2, 16, 27], where a compactification of configuration space¹³ is obtained by a sequence of blow ups along the strata. It turns out that our approach based on hyperspherical coordinates is closely related to the algebraic approach and can be considered as a special realization of the latter. We will elaborate on this connection in a forthcoming paper.

The present work sets the stage for the asymptotic construction of parametrices for Hamilton operators of many-particle Coulomb systems in the case of more than two particles. First of all, one has to establish ellipticity conditions on the hierarchy of symbols corresponding to the underlying stratification. The ellipticity conditions for these symbols provide isomorphisms between appropriate function space on the strata which are required for the parametrix construction, cf. [9, 12] for previous work in this direction. After ellipticity conditions have been established, parametrices and corresponding Green operators can be constructed which provide explicit asymptotic information concerning the eigenfunctions of Hamilton operators [10, 11, 13]. Finally, the constructed parametrices can be further modified to yield classical Green's functions on configuration space [14], which provides insight into the singular structure of Green's functions in quantum many-particle theory [15].

Acknowledgments

The authors HJF and MG were supported by the *Hausdorff Center for Mathematics* (HCM) in Bonn, funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under

¹³Compactification is appropriate for compact sets X , in our context completion of configuration space is more appropriate, cf. [27]

Appendices

A Equivalent norms of non-direct sums of Hilbert spaces.

The scenario we deal with consists of two complex Hilbert spaces H_1 and H_2 merged by a non-direct sum into a new space $H := H_1 \oplus H_2 / \Delta$ with $\Delta := \{(w, -w) : w \in H_1 \cap H_2\}$. Again, the space H is a Hilbert space with scalar product $\langle \cdot | \cdot \rangle_H$ taken on $H_1 \oplus H_2$ orthogonal to Δ , see e.g., the monograph [19] [Definition 2.1.4, Remark 2.1.5, Proposition 2.4.8] for more details. The induced scalar product defines a norm which has the following equivalent expression.

Lemma 2. *The norm defined by the induced scalar product $\langle \cdot | \cdot \rangle_H$ on the non-direct sum H satisfies the norm equivalence*

$$\langle \cdot | \cdot \rangle_H \simeq \min \{ \|u_1\|_{H_1} + \|u_2\|_{H_2} \mid u = u_1 + u_2, u_1 \in H_1, u_2 \in H_2 \}.$$

Proof. $\implies$: For a decomposition $u = u_1 + u_2$ with $u_1 \in H_1, u_2 \in H_2$, to be orthogonal to Δ , the scalar product of the direct sum $H_1 \oplus H_2$ has to satisfy

$$\left\langle \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} \middle| \begin{pmatrix} w \\ -w \end{pmatrix} \right\rangle_{H_1 \oplus H_2} = 0 \iff \langle u_1 | w \rangle_{H_1} - \langle u_2 | w \rangle_{H_2} = 0, \text{ for all } w \in H_1 \cap H_2.$$

Any other equivalent representation satisfies the inequality

$$\left\langle \begin{pmatrix} u_1 + w \\ u_2 - w \end{pmatrix} \middle| \begin{pmatrix} u_1 + w \\ u_2 - w \end{pmatrix} \right\rangle_{H_1 \oplus H_2} = \langle u_1 | u_1 \rangle_{H_1} + \langle u_2 | u_2 \rangle_{H_2} + \langle w | w \rangle_{H_1} + \langle w | w \rangle_{H_2} > 0,$$

for all $w \neq 0 \in H_1 \cap H_2$.

$\impliedby$: Suppose we have given a decomposition $u = u_1 + u_2$ with $u_1 \in H_1, u_2 \in H_2$, such that

$$\left\langle \begin{pmatrix} u_1 + w \\ u_2 - w \end{pmatrix} \middle| \begin{pmatrix} u_1 + w \\ u_2 - w \end{pmatrix} \right\rangle_{H_1 \oplus H_2} \geq \left\langle \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} \middle| \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} \right\rangle_{H_1 \oplus H_2},$$

for all $w \in H_1 \cap H_2$. By scaling w with $\lambda \in \mathbb{R}$, i.e., $w \rightarrow \lambda w$, we get

$$\lambda(2 \operatorname{Re} \langle u_1 | u_1 \rangle_{H_1} - 2 \operatorname{Re} \langle u_2 | u_2 \rangle_{H_2}) + \lambda^2 (\langle w | w \rangle_{H_1} + \langle w | w \rangle_{H_2}) \geq 0,$$

which yields the following limits

$$\lambda \searrow 0 : \operatorname{Re} \langle u_1 | w \rangle_{H_1} - \operatorname{Re} \langle u_2 | w \rangle_{H_2} \geq 0,$$

$$\lambda \nearrow 0 : \operatorname{Re} \langle u_1 | w \rangle_{H_1} - \operatorname{Re} \langle u_2 | w \rangle_{H_2} \leq 0,$$

and therefore $\operatorname{Re} \langle u_1 | w \rangle_{H_1} - \operatorname{Re} \langle u_2 | w \rangle_{H_2} = 0$. A similar argument, using the scaling $w \rightarrow i\lambda w$, gives $\operatorname{Im} \langle u_1 | w \rangle_{H_1} - \operatorname{Im} \langle u_2 | w \rangle_{H_2} = 0$. $\square$

The non-direct sums of Hilbert spaces that we consider in the following are of a specific generic form and can be related to an ordinary L_2 scalar product on a function space. In particular, let us assume that the scalar products have the form

$$\langle u | v \rangle_{H(\Omega)} = \sum_{i=1}^n \int_{\Omega} \mathcal{D}_i u \overline{\mathcal{D}_i v} w_i d\mu, \quad (\text{A.1})$$

with $\mathcal{D}_i$ some differential operators, w_i appropriate weights, and $d\mu$ a Lebesgue measure on $\Omega \subset \mathbb{R}^d$. We are interested in non-direct sums of Hilbert spaces of the form

$$H = \omega H_1 + (1 - \omega) H_2, \quad (\text{A.2})$$

where H_1, H_2 represent function spaces on a domain Ω with scalar products of the form (A.1). For a cut-off function $\omega \in C_0^\infty(\mathbb{R}_+)$, chosen such that $\omega(|x|) = 1$ in a neighbourhood of $|x| = 0$, we decompose Ω as

$$\Omega = \Omega_1 \cup \Omega_2 \cup \Omega_3,$$

where

$$\begin{aligned} \Omega_1 &:= \{x \in \Omega \mid \omega(|x|) = 1\}, \\ \Omega_2 &:= \{x \in \Omega \mid \omega(|x|)(1 - \omega(|x|)) \neq 0\}, \\ \Omega_3 &:= \{x \in \Omega \mid \omega(|x|) = 0\}. \end{aligned}$$

With respect to this decomposition, we require that the norms induced by the scalar products, e.g.,

$$\|\cdot\|_{H_i(\Omega)}^2 := \langle \cdot | \cdot \rangle_{H_i(\Omega)}, \quad i = 1, 2,$$

satisfy two consistency conditions,¹⁴ namely

- norm equivalence in the subdomain Ω_2 , i.e.,

$$\|u\|_{H_1(\Omega_2)} \simeq \|u\|_{H_2(\Omega_2)}, \quad (\text{A.3})$$

- boundedness of the cut-off function, i.e.,

$$\|\omega u\|_{H_i(\Omega_k)} \lesssim \|u\|_{H_i(\Omega_k)}, \quad i = 1, 2, \quad k = 1, 2, 3. \quad (\text{A.4})$$

Lemma 3. *The scalar product of the non-direct sum (A.2) of the two Hilbert spaces H_1, H_2 , satisfying the consistency conditions (A.3), (A.4), induces a norm which is equivalent to the norm*

$$\|u\|_{\min}^2 := \min\{\|\omega u_1\|_{H_1(\Omega)}^2 + \|(1 - \omega)u_2\|_{H_2(\Omega)}^2 \mid u = \omega u_1 + (1 - \omega)u_2, \quad u_1 \in H_1, \quad u_2 \in H_2\}.$$

Furthermore, we have norm equivalence

$$\|u\|_{\min} \simeq \|u\|_{\omega},$$

with

$$\|u\|_{\omega}^2 := \|\omega u\|_{H_1(\Omega)}^2 + \|(1 - \omega)u\|_{H_2(\Omega)}^2.$$

Proof. The first part of the lemma follows from Lemma 2. In the second part, the inequality $\|u\|_{\min} \leq \|u\|_{\omega}$ is obvious. Given a representation $u = \omega \tilde{u}_1 + (1 - \omega) \tilde{u}_2$, $\tilde{u}_1 \in H_1, \tilde{u}_2 \in H_2$, such that

$$\|u\|_{\min}^2 = \|\omega \tilde{u}_1\|_{H_1(\Omega)}^2 + \|(1 - \omega) \tilde{u}_2\|_{H_2(\Omega)}^2,$$

¹⁴Norms on subdomains, i.e., $\|\cdot\|_{H_i(\Omega_k)}, i = 1, 2, k = 1, 2, 3$, are given by restricting the integral in (A.1) to the corresponding subdomain Ω_k .

we get the estimates

$$\begin{aligned}
\|u\|_{\min}^2 &= \|u\|_{H_1(\Omega_1)}^2 + \|\omega \tilde{u}_1\|_{H_1(\Omega_2)}^2 + \|(1-\omega)\tilde{u}_2\|_{H_2(\Omega_2)}^2 + \|u\|_{H_2(\Omega_3)}^2 \\
&\gtrsim \|u\|_{H_1(\Omega_1)}^2 + \|\omega \tilde{u}_1\|_{H_1(\Omega_2)}^2 + \|(1-\omega)\tilde{u}_2\|_{H_1(\Omega_2)}^2 \\
&\quad + \|\omega \tilde{u}_1\|_{H_2(\Omega_2)}^2 + \|(1-\omega)\tilde{u}_2\|_{H_2(\Omega_2)}^2 + \|u\|_{H_2(\Omega_3)}^2 \\
&\gtrsim \|u\|_{H_1(\Omega_1 \cup \Omega_2)}^2 + \|u\|_{H_1(\Omega_2 \cup \Omega_3)}^2 \\
&\gtrsim \|\omega u\|_{H_1(\Omega)}^2 + \|(1-\omega)u\|_{H_1(\Omega)}^2,
\end{aligned}$$

where we have used in the second line the general norm property

$$\|v + w\|^2 \leq (\|v\| + \|w\|)^2 \leq 2(\|v\|^2 + \|w\|^2),$$

and in the second to last line the estimate (A.4). $\square$

B Further terms and definitions from singular analysis

In this appendix, we recall some well known facts and definitions from singular analysis. In particular, we want to discuss Kegel spaces with a smooth bases X in more detail. These spaces are at the bottom of the recursive construction of Kegel spaces for higher order singularities and deserve a careful discussion. Let us consider the Kegel space $\mathcal{K}^{s,\gamma}(X^\wedge)$ with smooth base manifold X of dimension n , for example S^n . It is defined as a non-direct sum

$$\mathcal{K}^{s,\gamma}(X^\wedge) := \omega \mathcal{H}^{s,\gamma}(X^\wedge) + (1-\omega)H_{\text{cone}}^s(X^\wedge) \quad (\text{B.1})$$

for a given cutoff function ω , i.e. $\omega \in C_0^\infty(\overline{\mathbb{R}_+})$ such that $\omega(r) = 1$ near $r = 0$. It should be mentioned that the norms are chosen in such a way that the topology of the spaces do not depend on the particular choice of ω . Let U_i be an open, locally finite covering of X and χ_i an underlying partition of unity. The charts of an atlas of X are given by homeomorphisms $h_i : U_i \rightarrow V_i$ into open subsets $V_i \subset \mathbb{R}^n$. For a function $u : \mathbb{R}_+ \times X \rightarrow \mathbb{R}$, let us consider local push forwards $u|_{U_i} \rightarrow \mathbb{R}_+ \times \mathbb{R}^n$ via

$$\chi_i u \rightarrow \sum_i (\text{id}_{\mathbb{R}_+} \times h_i^{-1})_* (\chi_i u),$$

where $\text{id}_{\mathbb{R}_+}$ is the identity map on $\mathbb{R}_+$. The weighted Sobolev space $\mathcal{H}^{s,\gamma}(X^\wedge)$ is the completion of $C_0^\infty(\mathbb{R}_+ \times X)$ with respect to the norm

$$\|u\|_{\mathcal{H}^{s,\gamma}(X^\wedge)} := \sum_i \|(\text{id}_{\mathbb{R}_+} \times h_i^{-1})_* (\chi_i u)\|_{\mathcal{H}^{s,\gamma}(\mathbb{R}_+ \times \mathbb{R}^n)},$$

where the weighted Sobolev space $\mathcal{H}^{s,\gamma}(\mathbb{R}_+ \times \mathbb{R}^n)$ in turn is the completion of $C_0^\infty(\mathbb{R}_+ \times \mathbb{R}^n)$ with respect to the norm

$$\left\{ \int_{\mathbb{R}^n} \int_{\Gamma_{\frac{n+1}{2}-\gamma}} \langle w, \eta \rangle^{2s} |M_{\gamma-\frac{n}{2}, r \rightarrow w} F_{y \rightarrow \eta}(u)(w, \eta)|^2 dw d\eta \right\}^{\frac{1}{2}}.$$

For practical purposes these rather elaborate definitions can be simplified for $s \in \mathbb{N}_0$ where $\mathcal{H}^{s,\gamma}(X^\wedge) = r^\gamma \mathcal{H}^{s,0}(X^\wedge)$ and $\mathcal{H}^{s,0}(X^\wedge)$ is defined as the set of all $u(r, x) \in r^{-1}L^2(\mathbb{R}_+ \times X)$ such that $(r\partial_r)^j Du \in r^{-1}L^2(\mathbb{R}_+ \times X)$ for all $D \in \text{Diff}^{s-j}(X)$, $0 \leq j \leq s$. The definition for $s \in \mathbb{R}$ follows by duality and complex interpolation. For a precise definition of $H_{\text{cone}}^s(X^\wedge)$ we refer to [24] [Remark 2.1.56]. Here let us just mention that, beyond a certain distance from the singularity, $\mathcal{K}^{s,\gamma}(X^\wedge)$ spaces become

ordinary Sobolev spaces, which means that, for $u \in \mathcal{K}^{s,\gamma}(X^\wedge)$, the part $(1 - \omega)u$ belongs, after back-transformation from polar to Cartesian coordinates, to the ordinary Sobolev space $H^s(\mathbb{R}^{n+1})$.

The Hilbert space structures on $\mathcal{H}^{s,\gamma}$ and $H_{\text{cone}}^s(X^\wedge)$ induce a Hilbert space structure on the non direct sum $\mathcal{H}^{s,\gamma} + H_{\text{cone}}^s(X^\wedge)$, cf. [19] [Definition 2.1.4, Remark 2.1.5, Proposition 2.4.8] for further details, and therefore on the Kegel space $\mathcal{K}^{s,\gamma}(X^\wedge)$. This Hilbert space structure on $\mathcal{K}^{s,\gamma}(X^\wedge)$ is compatible with equivalent scalar products

$$\langle \cdot, \cdot \rangle_{\mathcal{K}^{0,0}(X^\wedge)} \equiv \langle \cdot, \cdot \rangle_{\mathcal{H}^{0,0}(X^\wedge)} \equiv \langle \cdot, \cdot \rangle_{H_{\text{cone}}^0(X^\wedge)} \equiv \langle \cdot, \cdot \rangle_{r^{-\frac{n}{2}}L(\mathbb{R}_+ \times X)}. \quad (\text{B.2})$$

By means of order reducing operators, it is possible to relate the scalar products of $\mathcal{K}^{s,\gamma}(X^\wedge)$ spaces to the common reference $\langle \cdot, \cdot \rangle_{\mathcal{K}^{0,0}(X^\wedge)}$, a concept that has been systematically employed in [3, 4]. For $s \in \mathbb{N}_0$ it is obvious from the previous discussion that Lemma 3 can be applied to (B.1) which yields the norm equivalence

$$\|u\|_{\mathcal{K}^{s,\gamma}(X^\wedge)} \simeq \|\omega u\|_{\mathcal{H}^{s,\gamma}} + \|(1 - \omega)u\|_{H_{\text{cone}}^s(X^\wedge)}.$$

C Norms on Kegel spaces with higher order singularities

In Subsection 3.1, we referred to norms of various Kegel spaces with higher order singularities, i.e.,

$$\|\cdot\|_{\mathcal{K}^{s,\gamma_1,\gamma_2,\gamma_3}(B_2^\wedge)}, \quad \|\cdot\|_{\mathcal{K}^{s,\gamma_1,\gamma_2}(B_1^\wedge)}, \quad \|\cdot\|_{\mathcal{K}^{s,\gamma_1}(C^\wedge)},$$

which again have to be defined in a recursive manner. It has been already mentioned that the composite Kegel spaces (3.3) and (3.9) can be considered as non-direct sums of Frechet spaces. These Frechet spaces have however a natural embedding into their corresponding Hilbert spaces. To get these Hilbert spaces one just has to mimic [3] and to repeat our previous recursive construction by replacing the Kegel spaces with asymptotics by their counterparts without specific asymptotic behaviour. Such kind of construction yields the Kegel spaces $\mathcal{K}^{0,\tilde{\gamma}_1,\tilde{\gamma}_2,\tilde{\gamma}_3}(B_2^\wedge)$, $\mathcal{K}^{0,\tilde{\gamma}_1,\tilde{\gamma}_2}(B_1^\wedge)$ and $\mathcal{K}^{0,\tilde{\gamma}_1}(C^\wedge)$, which represent non-direct sums of Hilbert spaces with simple L_2 -type scalar products, cf. [3] for details. Using the same order reducing operators (3.2), (3.8) as before, one finally obtains the Kegel spaces

$$\begin{aligned} \mathcal{K}^{s,\gamma_1,\gamma_2,\gamma_3}(B_2^\wedge) &:= R_3^{-s} \mathcal{K}^{0,\tilde{\gamma}_1-s,\tilde{\gamma}_2-s,\tilde{\gamma}_3-s}(B_2^\wedge) \\ \mathcal{K}^{s,\gamma_1,\gamma_2}(B_1^\wedge) &:= R_2^{-s} \mathcal{K}^{0,\tilde{\gamma}_1-s,\tilde{\gamma}_2-s}(B_1^\wedge) \end{aligned}$$

which are Hilbert spaces with the corresponding induced scalar products, e.g.,

$$\langle u_1, u_2 \rangle_{\mathcal{K}^{s,\gamma_1,\gamma_2,\gamma_3}(B_2^\wedge)} = \langle v_1, v_2 \rangle_{\mathcal{K}^{0,\tilde{\gamma}_1-s,\tilde{\gamma}_2-s,\tilde{\gamma}_3-s}(B_2^\wedge)},$$

for $u_i = R_3^{-s}v_i$, $i = 1, 2$. Further details concerning the non-direct sums of Hilbert spaces have already been given in Appendix A.

Note that instead of induced Hilbert space norms on Kegel spaces, it is sometimes more convenient to use equivalent Banach space norms. This becomes possible due to the construction of non-direct sums using cut-off functions in (3.3) and (3.9). Thanks to norm equivalences in the overlapping regions it is possible to derive equivalent norms, cf. Lemma 3 in Appendix A. Starting on the lowest level, we have the norm equivalence

$$\|u\|_{\mathcal{K}^{s,\gamma}(C^\wedge)} \simeq \|\omega v\|_{\mathcal{H}^{0,\gamma}} + \|(1 - \omega)v\|_{H_{\text{cone}}^0(C^\wedge)}, \quad \text{with } u = R_1^{-s}v. \quad (\text{C.1})$$

At the next higher level, we require the norm $\|\cdot\|_{\mathcal{K}^{s,\gamma_1,\gamma_2}(B_1^\wedge)}$ which can be defined with (3.9) in an analogous manner, i.e.,

$$\begin{aligned} \|u\|_{\mathcal{K}^{s,\gamma_1,\gamma_2}(B_1^\wedge)} &:= \|\omega_2 \omega_1 v\|_{\mathcal{H}^{0,\gamma_2-s}(\mathbb{R}_+ \times S^2, \mathcal{K}^{0,\gamma_1-s}(C^\wedge))} + \|(1 - \omega_2) \omega_1 v\|_{\mathcal{H}^{0,0}(\mathbb{R}_+ \times S^2, \mathcal{K}^{0,\gamma_1-s}(C^\wedge))} \\ &\quad + \|\omega_2 (1 - \omega_1) v\|_{\mathcal{K}^{0,\gamma_2-s}((2\mathbb{B}_1)^\wedge)} + \|(1 - \omega_2)(1 - \omega_1) v\|_{\mathcal{K}^{0,0}((2\mathbb{B}_1)^\wedge)}, \end{aligned} \quad (\text{C.2})$$

with $u = R_2^{-s}v$ according to definition (3.8). Finally at the highest level, we require the norm $\|\cdot\|_{\mathcal{K}^{0,\gamma_1,\gamma_2,\gamma_3}(B_2^\wedge)}$ which can be derived from the decomposition (3.3) as

$$\begin{aligned} \|u\|_{\mathcal{K}^{s,\gamma_1,\gamma_2,\gamma_3}(B_2^\wedge)} &:= \|\omega_3\omega_2v\|_{\mathcal{H}^{0,0}(\mathbb{R}_+\times S^2,\mathcal{K}^{0,\gamma_1-s,\gamma_2-s}(B_1^\wedge))} \\ &\quad + \|(1-\omega_3)\omega_2v\|_{\mathcal{H}^{0,\gamma_3-s}(\mathbb{R}_+\times S^2,\mathcal{K}^{0,\gamma_1-s,\gamma_2-s}(B_1^\wedge))} \\ &\quad + \|\omega_3(1-\omega_2)v\|_{\mathcal{K}^{0,\gamma_1-s,\gamma_3-s}((2\mathbb{B}_2)^\wedge)} \\ &\quad + \|(1-\omega_3)(1-\omega_2)v\|_{\mathcal{K}^{0,\gamma_1-s,0}((2\mathbb{B}_2)^\wedge)}, \end{aligned} \tag{C.3}$$

with $u = R_3^{-s}v$ according to definition (3.2).

References

- [1] Abramowitz M. and Stegun I. A. *Handbook of Mathematical Functions*. National Bureau of Standards, Applied Mathematics Series - 55, 1972.
- [2] Axelrod S. and Singer I. M.. Chern-Simons perturbation theory. II *J. Diff. Geom.* **39**, 173–213 (1994).
- [3] Chang D. C. and Schulze B.-W. Calculus on spaces with higher singularities. *J. Pseudo-Differ. Oper. Appl.* **8**, 585–622 (2017).
- [4] Chang D. C. and Schulze B.-W. Ellipticity on spaces with higher singularities. *J. Sci. China Math.* **60**, 2053–2076 (2017).
- [5] NIST Digital Library of Mathematical Functions. <https://dlmf.nist.gov/>, Release 1.1.11 of 2023-09-15. Olver F. W. J., Olde Daalhuis A. B., Lozier D. W., Schneider B. I., Boisvert R. F., Clark C. W., Miller B. R., Saunders B. V., Cohl H. S., and McClain M. A., eds.
- [6] Egorov Y. V. and Schulze B.-W. *Pseudo-Differential Operators, Singularities, Applications*. Birkhäuser, Basel, 1997.
- [7] Erdélyi A., Oberhettinger F. and Tricomi F. G.. *Higher Transcendental Functions, Vol. II* McGraw-Hill, New York, 1953.
- [8] Fadell E. R. and Husseini S. Y.. *Geometry and Topology of Configuration Spaces*. Springer, Berlin, 2001.
- [9] Flad H.-J. and Harutyunyan G. Ellipticity of quantum mechanical Hamiltonians in the edge algebra. *Discrete and continuous dynamical systems, Supplement* 2011, 420–429.
- [10] Flad H.-J., Harutyunyan G., Schneider R. and Schulze B.-W. Explicit Green operators for quantum mechanical Hamiltonians. I. The hydrogen atom. *manuscripta math.* **135**, 497-519 (2011).
- [11] Flad H.-J., Harutyunyan G. and Schulze B.-W. Asymptotic parametrices of elliptic edge operators. *J. Pseudo-Differ. Oper. Appl.* **7**, 321–363 (2016).
- [12] Flad H.-J., Flad-Harutyunyan G. and Schulze B.-W. Ellipticity of quantum mechanical Hamiltonians: Corner singularity of the helium atom. *J. Pseudo-Differ. Oper. Appl.* **9**, 451–467 (2018).

- [13] Flad H.-J., Flad-Harutyunyan G. and Schulze B.-W. Explicit Green operators for quantum mechanical Hamiltonians. II. Edge-type singularities of the helium atom. *Asian-Eur. J. Math.* **13**, 2050122 (2020), pp. 64.
- [14] Flad H.-J. and Flad-Harutyunyan G. Fundamental solutions and Green's functions for certain elliptic differential operators from a pseudo-differential algebra. *Math. Methods Appl. Sci.* **48**, 12654-12674 (2025).
- [15] Flad H.-J. and Griebel M. Small distance behavior of one-particle Green's functions in electronic structure theory. *J. Phys. A: Math. Theor.* **58**, 295203 (2025), pp. 36.
- [16] Fulton W. and MacPherson R. A compactification of configuration spaces. *Ann. of Math.* **139**, 183–225 (1994).
- [17] Gradshteyn I. S. and Ryzhik I. M. *Table of Integrals, Series, and Products, Seventh Edition* A. Jeffrey, D. Zwillinger, Editors, Academic Press, San Diego, 2007.
- [18] Granzow K. D. N -dimensional total orbital angular-momentum operator. *J. Math. Phys.* **4**, 897–900 (1963).
- [19] Harutyunyan G. and Schulze B.-W. *Elliptic Mixed, Transmission and Singular Crack Problems*. European Math. Soc., Zürich, 2008.
- [20] Jeanquartier P. Transformation de Mellin et developements asymptotiques. *L'Enseign. Math.* **25**, 285-308 (1979).
- [21] Mott N. F. and Massey H. S. W. *The Theory of Atomic Collisions*, 3rd. ed., Oxford University Press, Oxford, 1965.
- [22] Schlichtkrull H., Trapa P. and Vogan Jr D. A. Laplacians on spheres. *Sao Paulo Journal of Mathematical Sciences* **12**, 295–358 (2018).
- [23] Schulze B.-W. *Pseudo-Differential Operators on Manifolds with Singularities*. North Holland, Amsterdam, 1991.
- [24] Schulze B.-W. *Boundary Value Problems and Singular Pseudo-Differential Operators*. Wiley, New York, 1998.
- [25] Schulze B.-W. Operators with symbol hierarchies and iterated asymptotics. *Publ. RIMS, Kyoto Univ.* **38**, 735–802 (2002).
- [26] Simon B. *Quantum Mechanics for Hamiltonians Defined as Quadratic Forms*. Princeton University Press, San Diego, 1979.
- [27] Sinha D. P. Manifold-theoretic compactifications of configuration spaces. *Sel. math., New ser.* **10**, 391–428 (2004).
- [28] Watson G. N. *A Treatise on the Theory of Bessel Functions, 2nd Ed.* Cambridge University Press, 1941.