Explicit Green operators for quantum mechanical Hamiltonians. II. Edge type singularities of the helium atom

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Abstract

We extend our approach of asymptotic parametrix construction for Hamiltonian operators from conical to edge-type singularities which is applicable to coalescence points of two particles of the helium atom and related two electron systems including the hydrogen molecule. Up to second order we have calculated the symbols of an asymptotic parametrix of the nonrelativistic Hamiltonian of the helium atom within the Born-Oppenheimer approximation and provide explicit formulas for the corresponding Green operators which encode the asymptotic behaviour of the eigenfunctions near an edge.

1 Introduction

1.1 Singular analysis meets quantum chemistry

In a reductionistic approach to chemistry it is the primary goal to explain chemical phenomena in terms of underlying fundamental physical principles. Here a key role has electronic structure theory, where properties of molecules and solids are derived from “first principles” by solving Schrödinger’s equation for many-particle systems interacting via Coulomb potentials. Apparent singularities of Coulomb potentials at coalescence points of particles are reflected by the regularity properties of these solutions. Concerning their global regularity, Kato showed that solutions of an $N$ particle Schrödinger equation belong to the Sobolev space $H^2(\mathbb{R}^{3N})$. Their maximal Sobolev regularity is not much higher, actually it is not difficult to see that already for a hydrogen atom the corresponding solutions are in $H^s(\mathbb{R}^3)$ for $s < 5/2$ only. An alternative measure of global regularity are Sobolev spaces with mixed partial derivatives which are of particular significance with respect to numerical analysis. Basic results for such spaces have been recently obtained by Yserentant [40, 41].

Besides global regularity it is rewarding to study in detail the asymptotic behaviour of solutions near coalescence points of particles. This approach, pioneered by Kato [29], led already to a fairly detailed picture of asymptotic properties of eigenfunctions of many-particle Hamiltonians, mainly due to the work of M. and T. Hoffmann-Ostenhof and coworkers [24, 25, 26, 14, 15]. Their most recent result concerning two-particle singularities has important consequences concerning the present work and will be discussed below.

In our research we pursue the strategy to apply a general operator calculus from singular analysis [7, 39, 22] in order to get a detailed picture concerning the asymptotic behaviour near coalescence points of particles for both the original Schrödinger equation and other many-particle models commonly used in quantum chemistry and solid state physics. The basic idea is to construct an asymptotic parametrix for a Hamiltonian which encodes all the required asymptotic information. Details concerning the general concept of an asymptotic parametrix has been presented elsewhere [11], and
a first application to the Hamiltonian of the hydrogen atom was given in [9]. In the present work, we want to establish an explicit construction of an asymptotic local parametrix for the Hamiltonian of two-electron systems, in particular the helium series and hydrogen molecule, near coalescence points of two particles, i.e., two electrons or an electron and a nucleus. Despite their simplicity, two-electron systems represent an important benchmark problem in quantum chemistry. Furthermore, two-electron subsystems represent the dominant contribution in many-particle models, like coupled cluster theory. Let us just mention that the results of the present work can be applied to these models with minor modifications. For further details and first applications we refer to [10]. There are other approaches in singular analysis which have been applied to electronic structure theory as well, see e.g. the work of Mazzeo, Nistor and collaborators, cf. [2], [3], [27].

In the following we consider the stationary nonrelativistic Schrödinger equation within the Born-Oppenheimer approximation, i.e.,

$$
\left(-\frac{1}{2}(\Delta_1 + \Delta_2) - \frac{Z}{|x_1|} - \frac{Z}{|x_2|} + \frac{1}{|x_1 - x_2|}\right)\Psi(x_1, x_2) = E\Psi(x_1, x_2) \quad (1.1)
$$

for the helium atom ($Z = 2$) and isoelectronic negatively ($Z = 1$) or positively ($Z > 2$) charged ions. Possible modifications of the formalism outlined below for other two electron systems, i.e., the hydrogen molecule, are straightforward and will be discussed in the text where appropriate. Depending on the total spin of the electrons, eigenfunctions $\Psi(x_1, x_2) \in H^2(\mathbb{R}^6)$ must be symmetric (singlet state) or antisymmetric (triplet state). Very accurate approximate solutions of (1.1) have been reported in the literature [28, 37, 16, 17]. Moreover, Fock outlined a recursive approach [13] which has been conjectured to provide an exact solution. Presently a complete proof of his conjecture is still missing, see, however, the work of Morgan [34] and Leray [30, 31, 32]. Higher order terms of the Fock expansion have been studied in the literature, cf. [1, 19, 20]. Furthermore, there exist suggestions how to generalize the Fock expansion to systems with more than two electrons, cf. [4, 5, 6]. There is, however, an essential difference between Fock’s expansion and the present work. We do not attempt to provide a complete solution for the helium atom, instead our approach focuses on the asymptotic behaviour of the solution near coalescence points of particles. Within the present work no ad hoc assumptions concerning the form of asymptotic expansions are involved. Instead we extract these properties in the course of the asymptotic parametrix construction. Nevertheless it is possible to compare our results with corresponding terms in the Fock expansion, cf. [1, 19, 20]. For such comparison it seems, however, to be desirable to incorporate the corner type singularity at the coalescence point of all three particles in the asymptotic analysis. Therefore, we leave this topic for our future work.

### 1.2 Differential operators and function spaces on stratified manifolds

In the following we want to consider a singular operator calculus applied on the configuration space of particles interacting via Coulomb potentials. Owing to the singularities of Coulomb potentials at coalescence points of particles it is convenient to regard the configuration space as a stratified manifold, where strata are classified according to the number of merging particles.

Let us consider a Coulomb system consisting of $N$ electrons and $K$ nuclei in the Born-Oppenheimer approximation, where nuclei are kept fixed and the configuration space restricts to electronic degrees of freedom. First of all, the physical configuration space $\mathcal{M}$ of $N$ electrons can be identified with $\mathbb{R}^{3N}$. We define the subset $\mathcal{M}_0 \subset \mathcal{M}$ of all possible coalescence points of particles including any number of electrons and nuclei. With it, $\mathcal{M} \setminus \mathcal{M}_0$ can be considered as an open smooth manifold or,

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1. We do not consider spin degrees of freedom or equivalent permutational symmetries of the electron coordinates in our discussion.

2. The manifold $\mathcal{M} \setminus \mathcal{M}_0$ actually corresponds to the mathematical notion of a configuration space of $N$ ordered particles in $\mathbb{R}^3$. 

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more generally, as the inner part of an open smooth manifold with boundary. Next, let us consider the subset \( M_1 \subset M_0 \) of all coalescence points of more than two particles. The stratum \( M_0 \setminus M_1 \) is an open smooth manifold representing edges of \( M \). Correspondingly, we denote \( M \setminus M_1 \) as a singular manifold with edges. Higher order strata can be constructed along the same lines, e.g., let \( M_2 \subset M_1 \) denote the set of coalescence points of more than three particles. Again the stratum \( M_1 \setminus M_2 \) is an open smooth manifold representing the lowest order type of corners in \( M \). Therefore, \( M \setminus M_2 \) is a singular manifold with edges and corners. In this way the configuration space can be decomposed into its strata, i.e.,

\[
M = M \setminus M_0 \cup M_0 \setminus M_1 \cup M_1 \setminus M_2 \cdots .
\]

The singular operator calculus associates classes of degenerate differential operators to the singular manifolds \( M \setminus M_i, \ i = 0, 1, \ldots, \) and a corresponding hierarchy of symbols to the strata.

Within the present work we want to study edge singularities corresponding to coalescence points of two particles, i.e., two electrons or an electron and a nucleus. Higher order corner singularities are subject of our future work.

Near an edge, \( M \setminus M_1 \) is identified with a wedge

\[
W = X^\Delta \times Y \quad \text{with } X^\Delta := (\mathbb{R}_+ \times X)/\{0\} \times X
\]

with smooth base \( X \), homeomorphic to \( S^2 \), the unit sphere, and edge \( Y \).

The class \( \text{Diff}^\mu_{deg}(\mathcal{W}) \) of edge-degenerate Fuchs-type differential operators of order \( \mu \in \mathbb{N} \)

\[
A := r^{-\mu} \sum_{j+|\alpha| \leq \mu} a_{j\alpha}(r,y)(-r\partial_r)^j(rD_y)^\alpha
\]

is defined on the associated open stretched wedge

\[
\mathcal{W} = X^\wedge \times Y \quad \text{with } X^\wedge := \mathbb{R}_+ \times X.
\]

Here \( r \in \mathbb{R}_+ \) denotes the distance to the open edge \( Y \subset \mathbb{R}^q \) and \( y \) is a \( q \)-dimensional variable, varying on \( Y \) (for a Coulomb system consisting of \( N \) electrons the dimension \( q \) of \( Y \) equals \( 3N - 3 \)). The coefficients \( a_{j\alpha}(r,y) \) take values in differential operators of order \( \mu - (j + |\alpha|) \) on the base \( X \) of the cone and are smooth in the respective variables up to \( r = 0 \).

On an open stretched wedge it is the distance variable \( r \in \mathbb{R}_+ \) which carries the asymptotic information. In order to incorporate asymptotics into Sobolev spaces let us proceed in a recursive manner. Weighted Sobolev spaces \( \mathcal{K}^{s,\gamma}(X^\wedge) \) on an open stretched cone with base \( X \) are defined with respect to the corresponding polar coordinates \( \tilde{x} \to (r,x) \) via

\[
\mathcal{K}^{s,\gamma}(X^\wedge) := \omega \mathcal{H}^{s,\gamma}(X^\wedge) + (1-\omega)H^s(\mathbb{R}^3),
\]

for a cut-off function \( \omega \), i.e., \( \omega \in C_0^\infty(\mathbb{R}_+) \) such that \( \omega(r) = 1 \) near \( r = 0 \). Here \( \mathcal{H}^{s,\gamma}(X^\wedge) = r^\gamma \mathcal{H}^{s,0}(X^\wedge) \), and \( \mathcal{H}^{s,0}(X^\wedge) \) for \( s \in \mathbb{N}_0 \) is defined to be the set of all \( u(r,x) \in r^{-\frac{1}{2}}L^2(\mathbb{R}_+ \times X) \) such that \( (r\partial_r)^j Du \in r^{-\frac{j}{2}}L^2(\mathbb{R}_+ \times X) \) for all \( D \in \text{Diff}^{-j}(X), \ 0 \leq j \leq s \). The definition for \( s \in \mathbb{R} \) in general follows by duality and complex interpolation. Weighted Sobolev spaces with asymptotics are subspaces of \( \mathcal{K}^{s,\gamma} \) spaces which are defined as direct sums

\[
\mathcal{K}_Q^{s,\gamma}(X^\wedge) := \mathcal{E}^\gamma_Q(X^\wedge) + \mathcal{K}^{s,\gamma}_Q(\mathbb{R}^3),
\]

of flattened weighted cone Sobolev spaces

\[
\mathcal{K}^{s,\gamma}_Q(\mathbb{R}^3) := \bigcap_{\epsilon > 0} \mathcal{K}^{s,\gamma-\theta-\epsilon}(X^\wedge)
\]

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\(^3\)It is not our intention to keep the notation as general as possible, instead we fix certain quantities inherent to the problem, like the basis of the cone and its dimension, from the very beginning.
with $\Theta = (\vartheta, 0)$, $-\infty \leq \vartheta < 0$, and asymptotic spaces

$$\mathcal{E}_Q^\gamma(X^\wedge) := \left\{ \omega(r) \sum_{j} \sum_{k=0}^{m_j} c_{jk}(x) r^{-q_j} \ln^k r \right\}.$$  

The asymptotic space $\mathcal{E}_Q^\gamma(X^\wedge)$ is characterized by a sequence $q_j \in \mathbb{C}$ which is taken from a strip of the complex plane, i.e.,

$$q_j \in \left\{ z : \frac{3}{2} - \gamma + \vartheta < \Re z < \frac{3}{2} - \gamma \right\},$$

where the width and location of this strip are determined by its weight data $(\gamma, \Theta)$ with $\Theta = (\vartheta, 0)$ and $-\infty \leq \vartheta < 0$. Each substrip of finite width contains only a finite number of $q_j$. Furthermore, the coefficients $c_{jk}$ belong to finite dimensional subspaces $L_j \subset C^\infty(X)$. The asymptotics of $\mathcal{E}_Q^\gamma(X^\wedge)$ is therefore completely characterized by the asymptotic type $Q := \{(q_j, m_j)\}_{j \in \mathbb{Z}_+}$. In the following, we employ the asymptotic subspaces

$$\mathcal{S}_Q^\gamma(X^\wedge) := \left\{ u \in \mathcal{K}_Q^{\infty, \gamma}(X^\wedge) : (1 - \omega) u \in \mathcal{S}(\mathbb{R}, C^\infty(X)) |_{\mathbb{R}_+ \times X} \right\}$$

with Schwartz class behaviour for exit $r \to \infty$. The spaces $\mathcal{K}_Q^{\infty, \gamma}(X^\wedge)$ and $\mathcal{S}_Q^\gamma(X^\wedge)$ are Fréchet spaces equipped with natural semi-norms according to the decomposition \cite{13}; we refer to \cite{7, 39} for further details.

Weighted wedge Sobolev spaces on $\mathcal{W} := X^\wedge \times Y$ can be defined as functions $Y \to \mathcal{K}_{(Q)}^{s, \gamma}(X^\wedge)$, where a subscript $(Q)$ optionally denotes cone spaces with and without asymptotics. Let us first consider the case $Y = \mathbb{R}^q$ and corresponding wedge Sobolev spaces

$$\mathcal{W}^s(\mathbb{R}^q, \mathcal{K}_{(Q)}^{s, \gamma}(X^\wedge)) := \left\{ u : \mathbb{R}^q \to \mathcal{K}_{(Q)}^{s, \gamma}(X^\wedge) | u \in \mathcal{S}(\mathbb{R}^q, \mathcal{K}_{(Q)}^{s, \gamma}(X^\wedge)) \right\}$$

with $s, \gamma \in \mathbb{R}$ and norm closure w.r.t. the norm

$$\|u\|_{\mathcal{W}^s(\mathbb{R}^q, \mathcal{K}_{(Q)}^{s, \gamma}(X^\wedge))} := \int [\eta]^{2s} \|\kappa_{[\eta]}^{-1}(F_{y \to \eta} u)(\eta)\|_{\mathcal{K}_{(Q)}^{s, \gamma}(X^\wedge)}^2 d\eta.$$  

Here $F_{y \to \eta}$ denotes the Fourier transform in $\mathbb{R}^q$ and $\{\kappa_\lambda\}_{\lambda \in \mathbb{R}_+}$ a strongly continuous group of isomorphisms $\kappa_\lambda : \mathcal{K}_{(Q)}^{s, \gamma}(X^\wedge) \to \mathcal{K}_{(Q)}^{s, \gamma}(X^\wedge)$ defined by

$$\kappa_\lambda u(r, x, y) := \lambda^{\frac{3}{2}} u(\lambda r, x, y).$$

The function $[\eta]$ involved in the norm is given by a strictly positive $C^\infty(\mathbb{R}^3)$ function of the co-variables $\eta$ such that $[\eta] = |\eta|$ for $|\eta| \geq \epsilon > 0$. The motivation behind this group action is the twisted homogeneity of principal edge symbols discussed below. For $Y \subset \mathbb{R}^q$ an open subset, we define

$$\mathcal{W}_{\text{comp}}^s(Y, \mathcal{K}_{(Q)}^{s, \gamma}(X^\wedge)) := \left\{ u \in \mathcal{W}^s(\mathbb{R}^q, \mathcal{K}_{(Q)}^{s, \gamma}(X^\wedge)) : \text{supp } u \subset Y \text{ compact} \right\},$$

and

$$\mathcal{W}_{\text{loc}}^s(Y, \mathcal{K}_{(Q)}^{s, \gamma}(X^\wedge)) := \left\{ u \in \mathcal{D}'(Y, \mathcal{K}_{(Q)}^{s, \gamma}(X^\wedge)) : \varphi u \in \mathcal{W}_{\text{comp}}^s(\mathbb{R}^q, \mathcal{K}_{(Q)}^{s, \gamma}(X^\wedge)) \text{ for each } \varphi \in C^\infty(\mathbb{R}_+ Y) \right\}.$$  

The class $\text{Diff}_{\text{deg}}^\mu(\mathcal{W})$ of edge-degenerate differential operators represents bounded operators

$$A : \mathcal{W}_{\text{comp(loc)}}^s(Y, \mathcal{K}_{(Q)}^{s, \gamma}(X^\wedge)) \longrightarrow \mathcal{W}_{\text{comp(loc)}}^{s-\mu}(Y, \mathcal{K}_{(Q)}^{s-\mu, \gamma-\mu}(X^\wedge))$$

between appropriate wedge Sobolev spaces. For a compact edge $Y$ both spaces (1.4) and (1.5) become equivalent.
1.3 Pseudo-differential operators on manifolds with edge singularities

The basic idea of the present work is to construct an “approximate inverse”, i.e., a parametrix, for edge-degenerate differential operators \([1,2]\) and their corresponding function spaces. First of all, one has to extend the operator space under consideration from differential to pseudo-differential operators. Furthermore, it requires an appropriate notion of ellipticity, which implies existence of a parametrix for an elliptic operator. For the sake of a concise presentation, we will state in the following only some basic notations and refer to \([11]\) as well as the monographs \([39]\) for further details.

A pseudo-differential operator \(P\), in the edge-degenerate operator class \(L^\mu(Y \times \mathbb{R}^3, g)\), for weight data \(g = (\gamma, \gamma - \mu, \Theta)\), \(\gamma, \mu \in \mathbb{R}\), is given in the general form

\[
P = \sigma' \text{Op}_p(p)\tilde{\sigma}' + (1 - \sigma')P_{\text{int}}(1 - \tilde{\sigma}')
\]  

(1.7)

with cut-off functions \(\tilde{\sigma}' < \sigma' < \tilde{\sigma}'\), i.e., \(\tilde{\sigma}' = \sigma'\) and \(\sigma'\tilde{\sigma}' = \sigma'\). The edge amplitude function \(p\) belongs to the space of operator functions \(R^\mu(Y \times \mathbb{R}^3, g)\) which in turn are of the form

\[
p(y, \eta) = \omega_{1,\eta}^{-\mu} \text{op}_M^{-1}(\omega_{0,\eta})(1 - \omega_{2,\eta}) + \omega_{0,\eta} + \omega_{1,\eta} + \omega_{2,\eta} + m(y, \eta) + g(y, \eta),
\]  

(1.8)

cf. \([11]\) Section 2.1, with cut-off functions \(\omega_{2,\omega_{1,\omega_{0}},\omega_{0}}\) satisfying \(\omega_{2} < \omega_{1} < \omega_{0}\), where we write here and in the following \(\omega_{\eta}(r) := \omega([\eta]r)\). The first and second term of the operator function \(1.8\) correspond to a Mellin and an inner Fourier pseudo-differential operator, respectively. Let us just mention, that the operator-valued Mellin symbol can be defined according to

\[
p_M(r, y, w, \eta) := \tilde{p}_M(r, y, w, \eta)
\]  

(1.9)

with respect to a symbol \(\tilde{p}_M(r, y, w, \eta) \in C^\infty(\mathbb{R}_+ \times \Omega, M^\mu_{\ell}(X, \mathbb{R}^3))\), see e.g. \([11]\) for further details. Here, \(M^\mu_{\ell}(X, \mathbb{R}^3)\) is the set of all holomorphic Mellin symbols with values in \(L^\mu_{\ell}(X, \mathbb{R}^3)\), the space of classical parameter-dependent pseudo differential operators on the base \(X\). Moreover, \(M^-_{\infty}(X)\), for an asymptotic type \(Q\), is the set of all meromorphic Mellin Symbols with values in \(L^{-\infty}(X)\), cf. \([11]\) Section 1.1.

Finally, the last two terms of \(1.8\) represent Green and smoothing Mellin operators, which belong to the subspaces \(R^\mu_{\ell}(Y \times \mathbb{R}^3, g)\) and \(R^\mu_{\ell+G}(Y \times \mathbb{R}^3, g)\) of operator functions, respectively, cf. \([11]\) Section 2.1 for further details. The smoothing Mellin operators in \(R^\mu_{\ell+G}(Y \times \mathbb{R}^3, g)\) have symbols in \(M^-_{\infty}(X)\), which corresponds to the space of meromorphic functions with values in \(L^{-\infty}(X)\), cf. \([11]\) Section 1.1. For further reference let us also define the extended symbol space

\[
M^\mu_{\omega}(X) := M^\mu_{\ell}(X) + M^-_{\infty}(X).
\]

Within the present work we want to construct asymptotic parametrices in local neighbourhoods of the edges separated from the corner singularity at the tip of the cone. Such parametrices exist provided that the Hamiltonian corresponds to an elliptic operator in the edge degenerate sense. Ellipticity of a pseudo-differential operator on a manifold with edge singularity is characterized by a pair of symbols \((\sigma_0, \sigma_1)\), where \(\sigma_0\) is the usual homogeneous principal symbol of a classical pseudo-differential operator in the interior and \(\sigma_1\) denotes the so-called principal edge symbol, which is twisted homogeneous in the sense

\[
\sigma_1(P)(y, \lambda \eta) = \lambda^\mu \kappa_{\lambda} \sigma_1(P)(y, \eta) \kappa_{\lambda}^{-1}
\]

for all \(\lambda \in \mathbb{R}_+\). The principal edge symbol is defined as

\[
\sigma_1(P)(y, \eta) := r^{-\mu} \text{op}_M^{-1}(h_{\text{M}})(y, \eta) + \sigma_1(m + g)(y, \eta),
\]
for \( h_M(r, y, w, \eta) := \tilde{p}_M(0, y, w, r\eta) \), cf. (1.14), and corresponds to a parameter-dependent operator family in the cone algebra. The smoothing Mellin and Green part of the symbol is given by

\[
\eta R \ \text{manner on the subspace}
\]

with \( \eta \neq 0 \), \( \omega_{\eta}(r) := \omega(r|\eta|) \), where \( g(y, \eta) \) is the twisted homogeneous principal symbol of \( g \) as a classical operator-valued symbol of order \( \mu \). Concerning the Mellin part, in particular, the meaning of the Mellin symbols \( f_{j\alpha} \), we refer to [11, Eq. 2.32].

In the particular case of a differential operator (1.2), the principal edge symbol is given by

\[
\sigma_1(A)(y, \eta) := r^{-\mu} \sum_{j+|\alpha| \leq \mu} a_{j\alpha}(0, y)(-r\partial_r)^j(\eta\eta)\alpha.
\]

Ellipticity requires that \( \sigma_1 \) represents Fredholm operators between weighted Sobolev spaces

\[
\sigma_1(P)(y, \eta) : \mathcal{K}^{s, \gamma}(X^\gamma) \to \mathcal{K}^{s-\mu, \gamma-\mu}(X^\gamma).
\]

In the general ellipticity theory developed in [22] or [39], the mapping (1.10) extends to an isomorphism. From a physical point of view, such an extension looks artificial. Therefore, it seems natural to expect values of \( \gamma \) for which \( \sigma_1 \) actually represents isomorphisms between the corresponding Kegel spaces. That such values of \( \gamma \) actually exist is essential for our particular application and will be discussed in the following section. For a detailed discussion of the concept of ellipticity and corresponding symbolic structures, we refer to the monographs [22] and [39].

In order to define asymptotic parametrices for elliptic operators, we have to go one step further in the symbolic hierarchy and consider conormal symbols \( \sigma_c^{\mu-j}(p)(y, w, \eta) \), \( j = 0, \ldots, k \), for parameter dependent operator functions \( p(y, \eta) \) in \( R^\mu(Y \times \mathbb{R}^3, \mathbf{g}) \) of asymptotic type \( \mathbf{g} := (\gamma, \gamma - \mu, \Theta) \), \( \Theta = (-k, 1, 0) \). These conormal symbols are polynomials in \( \eta \) of order \( j \) with coefficients in \( C^\infty(Y, M^j_R(X)) \) for certain Mellin asymptotic types \( R \) and are explicitly given by

\[
\sigma_c^{\mu-j}(p)(y, w, \eta) := \frac{1}{j!}(\partial^j_p M)(0, y, w, \eta) + \sum_{|\alpha|=j} f_{j\alpha}(y)\eta^\alpha.
\]

Conormal symbols can be used to define a filtration of operator function spaces \( R^\mu(Y \times \mathbb{R}^3, \mathbf{g}) \). Let us set

\[
R^{\mu,j}(Y \times \mathbb{R}^3, \mathbf{g}) := R^\mu(Y \times \mathbb{R}^3, \mathbf{g})
\]

and define, for \( 1 \leq j \leq k + 1 \), the sequence

\[
R^{\mu,j}(Y \times \mathbb{R}^3, \mathbf{g}) := \{ p \in R^{\mu,j-1}(Y \times \mathbb{R}^3, \mathbf{g}) : \sigma_c^{\mu-(j-1)}(p) = 0 \}.
\]

Furthermore, let us introduce the filtration \( R^{\mu,j}(\Omega \times \mathbb{R}^3, \mathbf{g}) \), which is defined in an analogous manner on the subspace \( R^{\mu,j}_G(Y \times \mathbb{R}^3, \mathbf{g}) \). With this filtration at hand, we can define the corresponding filtration for classes of edge-degenerate pseudo-differential operators \( L^\mu(M, \mathbf{g}) \) by taking \( L^{\mu,j}(M, \mathbf{g}) \) for \( \mathbf{g} = (\gamma, \gamma - \mu, \Theta) \), \( \Theta = (-k+1, 0) \), as the set of all \( P \in L^\mu(M, \mathbf{g}) \) such that the local edge amplitude functions \( p(y, \eta) \) occurring in (1.7) belong to \( R^{\mu,j}(\Omega \times \mathbb{R}^3, \mathbf{g}) \). This filtration provides the basis for the definition of asymptotic expansions of pseudo-differential operators discussed below.

### 1.4 The Hamiltonian of the helium atom in its edge-degenerate form

In the following, we consider the configuration space \( \mathbb{R}^6 \) of two electrons of the helium atom as a stratified manifold with embedded edge and corner singularities. For this purpose let us introduce polar coordinates in \( \mathbb{R}^6 \) with radial variable

\[
t := \sqrt{x_1^2 + x_2^2 + x_3^2 + x_4^2 + x_5^2 + x_6^2}.
\]
In such coordinates $\mathbb{R}^6$ can be formally considered as a conical manifold with base $S^5$ and embedded conical singularity at the origin, i.e.,

$$\mathbb{R}^6 \equiv (S^5)^\Delta := (\mathbb{R}_+ \times S^5)/\{0\} \times S^5.$$ 

Here, the origin represents the coalescence point of both electrons with the nucleus and all Coulomb potentials in the Hamiltonian become singular. Removal of this singular point defines an open stretched cone

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$$|x_1| = 0, \quad |x_2| = 0, \quad |x_1 - x_2| = 0;$$

each subset of configuration space corresponds to a closed embedded submanifold $Y_i$, $i = 1, 2, 3$, on the base $S^5$. These disjoint submanifolds are homeomorphic to $S^2$ and for any of them there exists a local neighbourhood $U_i$, $i = 1, 2, 3$, on $S^5$ which is homeomorphic to a wedge

$$W_i = X_i^\Delta \times Y_i \quad \text{with} \quad X_i^\Delta := (\mathbb{R}_+ \times X_i)/\{0\} \times X_i,$$

where the base $X_i$ of the wedge is again homeomorphic to $S^2$. The associated open stretched wedges are

$$\mathbb{W}_i = X_i^\wedge \times Y_i \quad \text{with} \quad X_i^\wedge := \mathbb{R}_+ \times X_i, i = 1, 2, 3.$$ 

Globally, the conical manifold $(S^5)^\Delta$ with local wedges on its basis $S^5$ becomes a manifold with corner singularity at the origin.

After these general considerations it remains to explicitly specify local coordinates in neighbourhoods of the edges which provide representations of the Hamiltonian in the class of edge-degenerate differential operators. Fortunately, appropriate hyperspherical coordinates were already known in the physics literature, cf. the monographs [35, pp. 1730ff] and [36, pp. 398ff]. Furthermore, Granzow’s paper [21] provides some useful facts related to these coordinates in spectral and differential geometry.

In a local neighbourhood $U_1$ of the $e - n$ singularity $|x_1| = 0$ let us define hyperspherical coordinates

$$\tilde{x}_1 = \sin r_1 \sin \theta_1 \cos \phi_1, \quad \tilde{x}_2 = \sin r_1 \sin \theta_1 \sin \phi_1, \quad \tilde{x}_3 = \sin r_1 \cos \theta_1, \quad (1.13)$$

$$\tilde{x}_4 = \cos r_1 \sin \theta_2 \cos \phi_2, \quad \tilde{x}_5 = \cos r_1 \sin \theta_2 \sin \phi_2, \quad \tilde{x}_6 = \cos r_1 \cos \theta_2 \quad (1.14)$$

with respect to the projective coordinates $\tilde{x}_i = x_i/t$, $i = 1, \ldots, 6$, on $S^5$. One can consider $\{1.13\}$ as polar coordinates on the stretched cone $X_1^\wedge$ with $r_1 \in (0, \frac{\pi}{2}]$, $\theta_1 \in (0, \pi)$, $\phi_1 \in [0, 2\pi)$. The remaining two angular variables in $\{1.14\}$ with $\theta_2 \in (0, \pi)$, $\phi_2 \in [0, 2\pi)$ provide a spherical coordinate system on $Y_1$. Similar local coordinates can be constructed in a local neighbourhood $U_2$ of the $e - n$ singularity $|x_2| = 0$.

The Hamiltonian of the helium atom is represented in these coordinates by an edge-degenerate differential operator, e.g., in a tubular neighbourhood $U_1$ by

$$H_{\text{edge}} := H|_{\text{tub } U_1} = r_1^{-2} \left[ -\frac{1}{2t^2} (-r_1 \partial_{r_1})^2 - \frac{\hbar}{2t^2} (-r_1 \partial_{r_1}) - \frac{1}{2} (r_1 \partial_t)^2 - \frac{5r_1}{2t} (r_1 \partial_t) \right.$$

$$\left. - \frac{1}{2t^2 \cos^2 r_1} (r_1 \partial_{\theta_2})^2 - \frac{r_1 \tan \theta_2}{2t^2 \cos^2 r_1} (r_1 \partial_{\theta_2}) - \frac{1}{2t^2 \sin^2 \theta_2 \cos^2 r_1} (r_1 \partial_{\theta_2})^2 \right.$$ 

$$\left. - \frac{r_1^2}{2t^2 \sin^2 r_1} \Delta x_1 + \frac{r_1}{t} v_{e-n} \right] \quad (1.15)$$
with
\[ h := 1 + 2r_1 \tan r_1 - 2r_1 \cot r_1 \]
and
\[ v_{e-n} := -\frac{Zr_1}{\sin r_1} - \frac{Zr_1}{\cos r_1} + \frac{r_1}{\sqrt{1 - \sin(2r_1)[\cos \theta_1 \cos \theta_2 + \sin \theta_1 \sin \theta_2 \cos(\phi_1 - \phi_2)]}}. \]

For the singular calculus it is important to note that \( h \) and \( v_{e-n} \) are smooth with respect to \( r_1 \) up to \( r_1 = 0 \).

The arguments are analogous in the case of \(|x_2| = 0\).

In the remaining case of the \( e - e \) edge singularity it is convenient to define center of mass coordinates
\[
\begin{align*}
z_1 &= \frac{1}{\sqrt{2}}(x_1 - x_4), \quad z_2 = \frac{1}{\sqrt{2}}(x_2 - x_5), \quad z_3 = \frac{1}{\sqrt{2}}(x_3 - x_6), \\
z_4 &= \frac{1}{\sqrt{2}}(x_1 + x_4), \quad z_5 = \frac{1}{\sqrt{2}}(x_2 + x_5), \quad z_6 = \frac{1}{\sqrt{2}}(x_3 + x_6)
\end{align*}
\]
in a neighbourhood \( U_3 \) with
\[
\sum_{i=1}^{6} z_i^2 = \sum_{i=1}^{6} x_i^2.
\]

The hyperspherical coordinates can now be introduced in a completely analogous manner. In such a neighbourhood of the \( (e - e) \) edge, the Coulomb potentials can be written in the form
\[
-\frac{Z}{|x_1|} - \frac{Z}{|x_2|} + \frac{1}{|x_1 - x_2|} = \frac{1}{tr_{12}} v_{e-e}(r_{12}, \theta_1, \phi_1, \theta_2, \phi_2)
\]
with
\[
v_{e-e} = -\frac{\sqrt{2}Zr_{12}}{\sqrt{1 + \sin(2r_{12})[\cos \theta_1 \cos \theta_2 + \sin \theta_1 \sin \theta_2 \cos(\phi_1 - \phi_2)]}} - \frac{\sqrt{2}Zr_{12}}{\sqrt{1 - \sin(2r_{12})[\cos \theta_1 \cos \theta_2 + \sin \theta_1 \sin \theta_2 \cos(\phi_1 - \phi_2)]}} + \frac{1}{\sqrt{2}j_0(r_{12})},
\]
where again \( v_{e-e} \) is smooth with respect to \( r_{12} \) up to \( r_{12} = 0 \).

**Remark 1.** The following two properties of the Hamiltonian are essential for our applications.

(i) The Hamiltonian of the helium atom \( H_{\text{edge}} \) corresponds to a bounded edge-degenerate operator
\[
H_{\text{edge}} : W_{\text{comp}(\text{loc})}^{s}(Y, K_{(Q)}^{s,\gamma}(X^{\wedge})) \rightarrow W_{\text{comp}(\text{loc})}^{s-2}(Y, K_{(P)}^{s-2,\gamma-2}(X^{\wedge})) \quad (1.16)
\]
for any \( s, \gamma \in \mathbb{R} \).

(ii) It has been shown in Ref. [8] that \( H_{\text{edge}} \) satisfies the ellipticity conditions of the edge-degenerate calculus for
\[
\frac{1}{2} < \gamma < \frac{3}{2}.
\]

Therefore, there exists a parametrix of \( H_{\text{edge}} \) in the corresponding pseudo-differential operator algebra, cf. [7], [22], [39].
The second part of the previous remark is essentially based on the following lemma, cf. [8] for a proof, which specifies the weights, where the principal edge symbols actually represent isomorphisms between the corresponding Kegel spaces.

**Lemma 1.** The principal edge symbols $\sigma_i(H_{\text{edge}}|_U)$, $i = 1, 2, 3$, represent Fredholm operators

$$\sigma_i(H_{\text{edge}}|_U)(t, (\theta_2, \phi_2), \tau, (\Theta_2, \Phi_2)) : K^{s, \gamma}((S^2)^\wedge) \to K^{s-2, \gamma-2}((S^2)^\wedge)$$

for $\gamma \not\in \mathbb{Z} + \frac{1}{2}$, for all $(t, (\theta_2, \phi_2)) \in \Omega \times S^2$ and all $(\tau, (\Theta_2, \Phi_2)) \neq 0$. Furthermore, they correspond to isomorphisms for any $\gamma$ with $\frac{1}{2} < \gamma < \frac{3}{2}$.

It is worth mentioning that the interval $\gamma$ with $\frac{1}{2} < \gamma < \frac{3}{2}$ actually corresponds to the physically relevant weights for eigenfunctions of the Hamiltonian; we refer to [8] for further discussions.

## 2 Asymptotic parametrices for Hamiltonian operators

### 2.1 Outline of our approach

The underlying theory for the construction of asymptotic parametrices in the edge algebra has been presented in a previous paper [11] of the authors. For the convenience of the reader we give a brief outline of some basic ideas.

(i) **Existence of an asymptotic parametrix:**

Every pseudo-differential operator in $L^p$ can be written in the form

$$P = \sum_{i=0}^{N} r^i P_i$$

modulo Green operators for any $N \in \mathbb{N}$ and for suitable $P_i \in L^\mu$, $i = 0, 1, \ldots, N$. The individual summands $r^i P_i$ belong to $L^\mu \cap L^{\mu+1}(M, g)$, $0 \leq i \leq N-1$, and $r^N P_N \in L^{\mu; N}(M, g)$.

In particular, $r^i P_i$ is flat of order $i$, i.e., in the edge algebra

$$r^i P_i : \mathcal{W}_{\text{comp}}^{s, \gamma}(Y, K^{s, \gamma}(\Theta)) \to \mathcal{W}^{s-\mu, \gamma}(Y, K^{s, \gamma}(\Theta)).$$

There exists an $N \in \mathbb{N}$ such that for $i \geq N$ the operator $r^i P_i$ maps on the flat part $K_\Theta$ of $K_P$, cf. [1,3]. Therefore, for our purposes it is sufficient to consider finite expansions for the Hamiltonian and of the corresponding parametrix.

(ii) **Recursive construction of asymptotic parametrices:**

Let us start with a differential operator $A \in \text{Diff}^\mu_{\text{deg}}(\mathcal{M})$ in the form (2.1) and represent the corresponding parametrix in the same form. Then we have

$$\left( \sum_{i=0}^{N} r^i P_i \right) \left( \sum_{i=0}^{N} r^i A_i \right) \sim I, \quad \left( \sum_{i=0}^{N} r^i A_i \right) \left( \sum_{i=0}^{N} r^i P_i \right) \sim I$$

modulo Green operators and flat remainders $F$, i.e., $r^{-(N+1)} F \in L^0(M)$. From this ansatz we can derive the following recursion scheme for the construction of an asymptotic parametrix.

- Initial step: $P_0 A_0 = I \mod L^0_G + L^0_{\text{flat}}$.
- First recursion: $r^1 P_1 A_0 + P_0 r^1 A_1 = 0 \mod L^0_G + L^0_{\text{flat}}$.

In general an operator $O \in L^\mu(M)$ satisfies a commutator relation

$$O r^\beta - r^\beta O_\beta = G_\beta$$

with an $O_\beta \in L^\mu(M)$ and an Green operator $G_\beta$. Then we have

$$r P_1 \xrightarrow{\text{mod } G} -P_0 r A_1 P_0 \xrightarrow{\text{mod } G} -r P_{0,1} A_1 P_0.$$
– Second recursion: $r^2 P_2 A_0 + r P_1 r A_1 + P_0 r^2 A_2 = 0 \mod L_0^0 + L_0^0$. Again one has to commute powers of $r$ to the left in order to get the recursion relation
\[
r^2 P_2 \equiv G - r P_1 r A_1 P_0 - P_0 r^2 A_2 P_0 = r^2 (P_{0,1,1} A_{0,1,1} P_0 - P_{0,2} A_2 P_0).
\]

– Higher recursions can be performed in a similar manner.

(iii) Calculation of Green operators and the asymptotic behaviour of eigenfunctions:

The parametrix construction of the previous step has been given modulo certain Green operators which carry asymptotic information. In order to get the asymptotic behaviour of eigenfunctions of the Hamiltonian operator, it is essential to keep track of all of these Green operators and to calculate them order by order in the asymptotic expansion. A large part of the present work is actually devoted to the details of their calculation.

Let us define the shifted Hamiltonian operator
\[
A_{\text{edge}} := H_{\text{edge}} - E
\]
with $E$ an eigenvalue of the Hamiltonian and consider the equation $A_{\text{edge}} u = 0$. Now let us apply a parametrix from the left, i.e.,
\[
P A_{\text{edge}} u = u + Gu = 0,
\]
which means that $u$ is an eigenfunction of the Green operator $G$, too. From our calculations, we obtain an asymptotic expansion of the operator valued symbol of the Green operator
\[
g(y, \eta) \sim g_0(y, \eta) + r g_1(y, \eta) + r^2 g(y, \eta) + \cdots
\]
with $r^i g_i(y, \eta) \in \mathcal{R}_G^{0,i}(Y \times \mathbb{R}^3, g) \setminus \mathcal{R}_G^{0,i+1}(Y \times \mathbb{R}^3, g)$, $i = 0, 1, 2, \ldots$, and mapping property
\[
r^i g_i(y, \eta) : \mathcal{K}^{s,\gamma}(X^\wedge) \to \mathcal{S}^{s+i}_q(X^\wedge),
\]
for specific asymptotic types $Q_i$. Therefore, according to equation (2.2), the asymptotic behaviour of an eigenfunction $u$ is completely determined by the asymptotic types $Q_i$ of the asymptotic expansion of the Green operator $G$.

2.2 Asymptotic representation of the Hamiltonian

Let us perform an asymptotic expansion of shifted Hamiltonian operator $A_{\text{edge}}$ in the cone variable
\[
A_{\text{edge}} = \sum_{i=0}^{N} r^i A_i + A_N.
\]
In order to calculate the asymptotic terms from (1.15) some auxiliary Taylor series are required, i.e.,
\[
h(r) = -1 + \frac{8}{3} r^2 + \frac{32}{45} r^3 + O(r^6),
\]
\[
\frac{r^2}{\sin^2 r} = 1 + \frac{1}{3} r^2 + \frac{1}{15} r^4 + O(r^6), \quad \frac{1}{\cos^2 r} = 1 + r^2 + \frac{2}{3} r^4 + O(r^6).
\]
Depending on the specific edge under consideration, the corresponding Taylor series of the Coulomb potentials are given by
\[
v_{e-n} = -Z + (1 - Z) r + (a - \frac{1}{6} Z) r^2 + \frac{1}{3} (3a^2 - Z) r^3 + \frac{1}{360} (-240a + 900a^3 - 7Z) r^4
\]
\[
+ (-2a^2 + \frac{35}{8} a^4 - \frac{5}{24} Z) r^5 + O(r^6)
\]
and
\[ v_{e-e} = \frac{1}{\sqrt{2}} - 2\sqrt{2}Zr + \frac{1}{6\sqrt{2}}r^2 - 3\sqrt{2}a^2 Z r^3 + \frac{7}{360\sqrt{2}}r^4 + \left(4\sqrt{2}a^2 Z - \frac{35}{2\sqrt{2}}a^4 Z\right)r^5 + O(r^6), \]

with
\[ a := \cos \theta_1 \cos \theta_2 + \sin \theta_1 \sin \theta_2 \cos (\phi_1 - \phi_2). \]

With this the asymptotic terms of the Hamiltonian become
\[
A_0 = r^{-2} \left[ -\frac{1}{2t^2} (-r \partial_r)^2 + \frac{1}{2t^2} (-r \partial_r) - \frac{1}{2} (r \partial_r)^2 - \frac{1}{2t^2 \sin^2 \theta_2} (r \partial_{\phi_2})^2 - \frac{1}{2t^2} (r \partial_{\phi_2})^2 - \frac{1}{2t^2} \Delta X \right];
\]
\[
A_1 = r^{-2} \left[ -\frac{5}{2t} (r \partial_r) - \frac{\text{ctan} \theta_2}{2t^2} (r \partial_{\phi_2}) + \frac{1}{t} \left\{ \frac{1}{\sqrt{2}} \text{ for } v_{e-e}, \right\} \right] ;
\]
\[
A_2 = r^{-2} \left[ -\frac{4}{3t^2} (-r \partial_r) - \frac{1}{2t^2} (r \partial_{\phi_2})^2 - \frac{1}{2t^2 \sin^2 \theta_2} (r \partial_{\phi_2})^2 - \frac{1}{6t^2} \Delta S^2 - E + \frac{1}{t} \left\{ \frac{-2\sqrt{2}Z}{1-Z} \text{ for } v_{e-e}, \right\} \right] ;
\]

\[ \vdots \]

2.3 The initial asymptotic parametrix and corresponding Green operators

The edge-degenerate differential operator \( A_0 \) can be expressed as a Leibniz-Mellin pseudo-differential operator close to the edge. Let \( \sigma, \hat{\sigma}, \tilde{\sigma} \) be cut-off functions such that \( \sigma \prec \hat{\sigma}, \hat{\sigma} \prec \sigma \). It is easy to see that \( A_0 \) can be decomposed into two parts in the following way
\[ A_0 = \sigma A_0 \hat{\sigma} + (1 - \sigma) A_0 (1 - \hat{\sigma}). \]

Next, we introduce a locally finite cover \( \{U_i\}_{i=0,1,\ldots,\infty} \) on the edge \( Y = \mathbb{R}_+ \times S^2 \cong \mathbb{R}^3 \setminus \{0\} \) and a subordinate partition of unity \( \{\varphi_i\}_{i=0,1,\ldots,\infty} \). Furthermore, let \( \{\varphi'_i\}_{i=0,1,\ldots,\infty} \) denote a set of functions with \( \varphi'_i \in C^\infty_0(U_i) \) and \( \varphi_i \varphi'_i = \varphi_i \) for \( i = 0, 1, \ldots, \infty \). Herewith \( A_0 \) can be expressed as a Leibniz-Mellin pseudo-differential operator in the algebra \( L^2(M,g) \), i.e.,
\[
A_0 = \sum_i \sigma \varphi_i \text{Op}_g r^{-2} \text{op}^{-1}_M(a_0) \varphi'_i \hat{\sigma} + (1 - \sigma) A_{\text{int}} (1 - \hat{\sigma}) \quad (2.3)
\]

with holomorphic operator valued symbol
\[
a_0(r, w, \eta) = -\frac{1}{4r^2} (w^2 - w - r^2 C(\eta) + \Delta S^2) \quad (2.4)
\]
and
\[
C(\tau, \Theta_2, \Phi_2) := \tau^2 + \Theta_2^2 + \frac{\Phi_2^2}{\sin^2 \theta_2}.
\]

In the second term \( A_0 \) has been pushed forward in the interior to a standard pseudo-differential operator
\[ A_{\text{int}} := \text{Op}(a_{\text{int}}) \]
with symbol
\[
a_{\text{int}}(\xi, \eta) = \frac{1}{2t^2} \left( \xi_1^2 + \xi_2^2 + \xi_3^2 + C(\eta) \right).
\]

\footnote{Throughout this paper a cut-off function is any real-valued \( \sigma \in C^\infty_0(\mathbb{R}_+) \) such that \( \sigma(r) \equiv 1 \) close to \( r = 0 \).}
Remark 2. A parametrix $P_0$ of the edge-degenerate operator \cite{[33]} can be written in the general form

$$P_0 = \sum_i \sigma' \varphi_i \text{Op}_y(p_0) \varphi'_i \sigma' + (1 - \sigma') P_{\text{int}} (1 - \sigma') \quad (2.5)$$

with $p_0 \in R^{-2}(Y \times \mathbb{R}^3, \mathbf{g})$ and given cut-off functions $\sigma' < \sigma < \sigma'$. We can assume w.l.o.g. $\sigma' < \sigma$. Therefore,

$$P_0 A_0 = \sum_i \sigma' \varphi_i \text{Op}_y(p_0) \varphi'_i \sigma A_0 \sigma + \sum_i \sigma' \varphi_i \text{Op}_y(p_0) \varphi'_i \sigma' (1 - \sigma) A_{\text{int}} (1 - \sigma)$$

$$(1 - \sigma') P_{\text{int}} (1 - \sigma') \sigma A_0 \sigma + (1 - \sigma') P_{\text{int}} (1 - \sigma') (1 - \sigma) A_{\text{int}} (1 - \sigma)$$

and the asymptotic behaviour is completely determined by

$$P_0 A_0 \sim \sum_i \sigma' \varphi_i \text{Op}_y(p_0) \varphi'_i \sigma' \sigma A_0 \sigma. \quad (2.6)$$

The Leibniz-Mellin representation of (2.6) is conveniently performed by the following steps

$$\sum_i \sigma' \varphi_i \text{Op}_y(p_0) \varphi'_i \sigma A_0 \sigma = \sum_i \sigma' \varphi_i \text{Op}_y(p_0) \varphi'_i \sigma A_0 \sigma'$$

$$= \sum_i \sigma' \varphi_i \text{Op}_y(p_0) \varphi'_i \sigma A_0 \sigma' \text{Op}_y r^{-2} \text{Op}_{y}^{-1} (a_0) \sigma' \sigma''$$

$$= \sum_i \sigma' \varphi_i \text{Op}_y(p_0) \sigma' \sigma \text{Op}_y r^{-2} \text{Op}_{y}^{-1} (a_0) \sigma' \sigma''$$

$$- \sum_i \sigma' \varphi_i \text{Op}_y(p_0) (1 - \varphi'_i) \sigma' \sigma \text{Op}_y r^{-2} \text{Op}_{y}^{-1} (a_0) \sigma' \sigma'' \quad (2.7)$$

where $\{\varphi''_i\}_{i=0,1,\ldots,\infty}$ denotes another set of functions with $\varphi''_i \in C^\infty_0(U_i)$ and $\varphi'_i < \varphi''_i$ for $i = 0, 1, \ldots, \infty$. The Green operator character in the last line follows from $\varphi_i (1 - \varphi'_i) = 0$, cf. \cite{[33]} Remark 3.4.51.

Proposition 1. A Green operator of the form

$$\sum_i \sigma' \varphi_i \text{Op}_y (h) \xi_i \sigma'$$

with supp $\varphi_i \cap \text{supp} \xi_i = \emptyset$ and $\varphi_i, \xi_i \in C^\infty_0(U_i), i = 0, 1, \ldots, \infty$, is smoothing, i.e., it belongs to $L^{-\infty}_{\text{smooth}}(M, g)$.

Proof. This follows from the properties of the corresponding Schwartz kernel of the edge-degenerate operator which can be written on a coordinate neighbourhood as

$$\varphi_i (y) r^{-1} k_h ((y', y') / (y, y')) \xi_i (y').$$

According to our assumption, the kernel vanishes for $|y - y'| < \epsilon$ for some $\epsilon > 0$. The standard kernel estimate

$$|\partial_x^\alpha \partial_y^\beta k_h (z, y)| \leq c |z|^{-3 - m - |\alpha| - N}, \quad z \neq 0,$$

for all $N \in \mathbb{N}, z = y - y'$, so that $3 + m + |\alpha| + N > 0$, applied to the edge-degenerate case yields the following estimate

$$|\varphi_i (y) r^{-1} k_h ((y', y') / (y, y')) \xi_i (y')| \leq c r^{2 + m + N},$$

which demonstrates the smoothing property. \hfill \Box
Let us write (2.8) in the form

$$\sum_i \sigma^i \varphi_i \text{Op}_y(p_0)(1 - \varphi_i')\varphi_i'' \sigma^i \text{Op}_y r^{-2} \text{op}^{-1}_M (a_0) \tilde{\sigma} \varphi_i''$$

for a set of functions \(\{\varphi_i''\}_{i=0,1,\ldots,\infty}\) with \(\varphi_i'' \in C_0^\infty(U_i)\) and \(\varphi_i'' \prec \varphi_i'''.\) Then, from Proposition \(\text{I}\) it follows that (2.8) belongs to \(L_0\) smooth \((M, g)\).

In order to calculate the parametrix it is convenient to make the following ansatz

$$p_0(y, \eta) = \omega_1' r^2 \text{op}_M,0(y, \eta) \omega_0' + (1 - \omega_2' r) r^2 \text{op}_M,0(y, \eta) (1 - \omega_2' r)$$

(2.9)

with cut-off functions \(\omega_1', \omega_0'\) satisfying \(\omega_0' \prec \omega_1' \prec \omega_0\), where we write \(\omega_r(r) := \omega(|\eta|r);\) here, \([\eta] = |\eta|\) for \(\eta \geq \epsilon\) for some \(\epsilon > 0.\) By a slight modification of the standard notation we incorporate into \(p_M\) contributions from \(R_{\text{M}+\text{C}}(Y \times \mathbb{R}^3, g)\) and assume a Mellin representation

$$p_{M,0}(y, \eta) := \text{op}_M^{-1/2}(a_0)(y, \eta).$$

(2.10)

Remark 3. The operator \((1 - \omega_1') r^2 \text{op}_M,0(y, \eta) (1 - \omega_2' r)\) does not contribute to the asymptotic behaviour. For a proof see, e.g., [39, Prop. 3.3.38].

According to the previous remark, we ignore the second term of (2.8) in the following considerations. Inserting the ansatz (2.9) into the operator product (2.7) with the parametrix acting from the left, yields the Leibniz product

$$\sigma^i \omega_1' r^2 \text{op}_M^{-3}(a_0)(y, \eta) \omega_0' \tilde{\sigma} \text{#} \# \eta, \gamma^r \text{op}_M^{-1}(a_0) \omega_0, \eta \tilde{\sigma},$$

where an optional parameter dependent cut-off function \(\omega_0, \eta,\) with \(\omega_0, \eta \prec \omega_0, \eta,\) has been multiplied to the right. Actually this does not affect the operator product because \(\text{op}_M^{-1}(a_0)\) represents a local differential operator. It enables us, however, to get rid of the disturbing parameter dependent cut-off function \(\omega_0, \eta\) by adding a further Green operator

$$\sigma^i \omega_1' r^2 \text{op}_M^{-3}(a_0)(1 - \omega_0, \eta) \tilde{\sigma} \text{#} \# \eta, \gamma^r \text{op}_M^{-1}(a_0) \omega_0, \eta \tilde{\sigma},$$

which belongs to \(R_{\text{C}}(Y \times \mathbb{R}^3, g)\), to the Leibniz product. We denote our approach to simplify the construction of the parametrix by adding temporarily an appropriate Green operator and neutralizing it at the end of the calculation via dilation of the cut-off functions as \(\varepsilon\)-regularization. The basic idea and some relevant technical details are given in Appendix A.

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\(^5\)The Green character of this operator actually follows from \(\omega_1' \prec \omega_0, \eta,\) cf. [39, Lemmas 2.3.73, 3.3.27].
With this modification, the Leibniz product becomes

\[
\sigma' \omega_{1,q}^r r^2 \text{op}_{M}^{\gamma} (a_0^{(-1)}) \sigma' \#_{\eta,y} \sigma r^{-2} \text{op}_{M}^{\gamma} (a_0) \omega_{0,\eta} \tilde{\sigma} \mod R_{\text{flat}}^{-\infty}(Y \times \mathbb{R}^3, g)
\]

\[
= \sigma' \sum_{\alpha} \frac{1}{\alpha!} \partial_{\eta}^{\alpha} \left( \omega_{1,q}^r r^2 \text{op}_{M}^{\gamma} (a_0^{(-1)}) \right) \sigma' \sigma r^{-2} \text{op}_{y}^{\gamma} (a_0) \omega_{0,\eta} \tilde{\sigma} \mod R_{\text{flat}}^{0}(Y \times \mathbb{R}^3, g)
\]

\[
= \sigma' \sum_{\alpha} \frac{1}{\alpha!} \partial_{\eta}^{\alpha} \left( \omega_{1,q}^r \text{op}_{M}^{\gamma} (T^2 a_0^{(-1)}) \right) \sigma' \sigma \text{op}_{y}^{\gamma} (a_0) \omega_{0,\eta} \tilde{\sigma} \mod R_{\text{flat}}^{0}(Y \times \mathbb{R}^3, g)
\]

\[
= \sigma' \omega_{1,q}^r \sum_{\alpha} \frac{1}{\alpha!} \partial_{\eta}^{\alpha} \left( \text{op}_{M}^{\gamma} (T^2 a_0^{(-1)}) \right) \sigma' \sigma \text{op}_{y}^{\gamma} (a_0) \omega_{0,\eta} \tilde{\sigma} \mod R_{\text{flat}}^{0}(Y \times \mathbb{R}^3, g)
\]

\[
= \sigma' \omega_{1,q}^r \sum_{\alpha} \frac{1}{\alpha!} \partial_{\eta}^{\alpha} \left( \text{op}_{M}^{\gamma} (T^2 a_0^{(-1)}) \right) \sigma' \sigma \text{op}_{y}^{\gamma} (a_0) \omega_{0,\eta} \tilde{\sigma} \mod R_{\text{flat}}^{0}(Y \times \mathbb{R}^3, g)
\]

Here we used the fact that \( \partial_{\eta}^{\alpha} \omega_{1,q}^r \) for \( |\alpha| > 0 \) generates smoothing operators which do not contribute to the asymptotics according to the same arguments as in Remark 3. For the Green operator character of \( g_1 \) and \( g_2 \), cf. [14] Remark 3.12 and [39] Proposition 2.3.69, respectively. In the following we have to determine the symbol \( a_0^{(-1)} \) such that

\[
\sigma' \sum_{\alpha} \frac{1}{\alpha!} \text{op}_{M}^{\gamma} (D_{y}^{\alpha} (-\frac{1}{2\pi^2} T^2 \partial_{\eta}^{\alpha} a_0^{(-1)})_0) \omega_{0,\eta} \tilde{\sigma} \mod R_{\text{flat}}^{0}(Y \times \mathbb{R}^3, g_1).
\]

For our application, we are particularly interested in the Green operator symbols \( g_1 \) and \( g_2 \) which correspond to the left action of the parametrix on the Hamiltonian. It is, however, obvious that any left parametrix is a right parametrix as well and vice versa. Acting on the right side of the Hamiltonian with the parametrix results in another sequence of Green and flat operator symbols plus the condition

\[
\sigma \sum_{\alpha} \frac{1}{\alpha!} \text{op}_{M}^{\gamma} (\partial_{\eta}^{\alpha} T^{-2} a_0^{(-1)} \#_{r,w} \text{op}_{y}^{\gamma} (a_0^{(-1)})) \tilde{\sigma}' = I \mod R_{\text{flat}}^{0}(Y \times \mathbb{R}^3, g_2),
\]

from which the symbol \( a_0^{(-1)} \) can be derived.

**Remark 4.** Conditions (2.12) and (2.13) are equivalent. Once one has constructed e.g. a right parametrix, where the symbol \( a_0^{(-1)} \) satisfies (2.13), it will also satisfy condition (2.12). This follows
From the fact that the parameter dependent Mellin pseudo-differential operators in conditions (2.12) and (2.13) are equal modulo Green and flat operators. Therefore, both Mellin pseudo-differential operators must have the same sequence of conormal symbols.

2.4 Paving the way for the construction of the asymptotic parametrix

In the previous section we have discussed the general structure of the initial parametrix $P_0$ and derived the equivalent conditions (2.12) and (2.13) which can be used for their actual construction. Furthermore, we have derived for a left parametrix the corresponding Green operators which contribute to the asymptotic behaviour. Next, we want to present an asymptotic ansatz for the parameter dependent symbol of the parametrix which can be used in conditions (2.12) and (2.13) for actual calculations. Here one has to pay attention to the specific symbolic structure of the edge-degenerate calculus.

In our calculations we have chosen condition (2.13) because the Leibniz-Mellin product in the corresponding equation

$$
\sum_\alpha \frac{1}{\alpha!} \partial^{\alpha}_\eta T^{-2} a_0 \#_{r,w} D_y a_0^{(-1)} = \sum_\alpha \sum_k \frac{1}{k!} \partial^k_w \partial^{\alpha}_\eta T^{-2} a_0 (-r \partial_r)^k D_y a_0^{(-1)} \sim 1
$$

(2.14)

is represented by a finite number of terms, since $a_0$ is a second order polynomial in $w$ and $\eta$. The symbol $a_0^{(-1)}$ of the parametrix has an asymptotic expansion, i.e.,

$$
a_0^{(-1)} \sim -2t^2 (q_{0,0} + r q_{0,1} + r^2 q_{0,2} + \cdots),
$$

(2.15)

where individual terms can be computed in a recursive manner. Inserting the ansatz (2.15) into (2.14) one gets at zeroth order

$$
r^0 : \quad T^{-2} a_0 q_{0,0} \partial_w T^{-2} a_0 (-r \partial_r) q_{0,0} + \frac{1}{2} \partial^2_w r T^{-2} a_0 (-r \partial_r)^2 q_{0,0} \sim 1.
$$

(2.16)

In order to obtain $q_{0,0}$ as a solution of (2.16) let us start with some formal considerations motivated by the standard approach to the construction of a parametrix in the non-singular pseudo-differential calculus. It should be mentioned, however, that each individual step requires a thorough justification in the singular edge calculus which will be done in the following. Since $q_{0,0}(r,y,w,\eta) \in C^\infty(\mathbb{R}_+ \times Y, L^2_{cd}(X, \Gamma_\alpha \times \mathbb{R}^3))$ with $\Gamma_\alpha := \{ w \in \mathbb{C} : \text{Re} \ w = \alpha \}$, we can obtain an asymptotic sum

$$
q_{0,0} \sim q'_0,0 + q'_0,1 + q'_0,2 + \cdots
$$

(2.17)

with $q'_{0,k}(r,y,w,\eta) = q'_{0,k}(r,y,w,\eta)$ and $q'_{0,k}(r,y,w,\eta) \in C^\infty(\mathbb{R}_+ \times Y, L^2_{cd}(X, \Gamma_\alpha \times \mathbb{R}^3))$, cf. [11, Section 1.1] for further details and definitions. Let us take

$$
q'_{0,0} = -2t^2 h^{-1},
$$

(2.18)

where

$$
h = (w - 2)^2 - (w - 2) - r^2 C(\eta) + \Delta_{S^2}
$$

corresponds to a holomorphic operator valued symbol acting on the basis $X$.

Remark 5. For (2.18) to make sense it requires $h^{-1} \in C^\infty(\mathbb{R}_+ \times Y, L^2_{cd}(X, \Gamma_\alpha \times \mathbb{R}^3))$ which follows from the spectral invariance of $h$ as a parameter dependent uniformly elliptic differential operator on the base $X$.

Successively solving

$$
\sum_{m+n=k} \frac{1}{m!} \partial_w^m T^{-2} a_0 (-r \partial_r)^m q'_{0,n} = 0 \quad \text{for} \ k = 1, 2, \ldots
$$
yields the recurrence relation

\[ q'_{0,k} = -q'_{0,0} \sum_{m+n=k, \ n<k} \frac{1}{m!} \partial_w T^{-2} a_0(-r \partial_r)^m q'_{0,n}; \]  \hfill (2.19)

here the sum restricts to \( m \leq 2 \) because of (2.3). In order to get an asymptotic sum with respect to powers in \( r \eta \), it is necessary to rearrange the individual terms. This can be done in two separate steps. Let us first reorder the sum in powers of \( r^2 C \). A simple calculation yields

\[ q_{0,0} \sim -2t^2 h^{-1} - 2t^2 (2(2 - 4)h^{-3} + (4z^2 - 16z + 16)h^{-4} + (8z^3 - 48z^2 + 96z - 64)h^{-5} + \ldots) r^2 C + O((r^2 C)^2) \]

\[ \sim -2t^2 h^{-1} - 2t^2 \left( \sum_{n=1}^{\infty} (2z - 4)^n h^{-n} \right) h^{-2} r^2 C + O((r^2 C)^2) \]

\[ \sim -2t^2 h^{-1} - 2t^2 (2z - 4) \left( h - (2z - 4) \right)^{-1} h^{-2} r^2 C + O((r^2 C)^2) \]  \hfill (2.20)

with \( z = 2w - 5 \). The geometric sum is tentatively considered in a purely formal sense. As provisional justification, we observe that the reordered asymptotic expansion (2.20) satisfies (2.16) up to terms of \( O((r^2 C)^2) \).

The edge-degenerate pseudo-differential calculus imposes stringent conditions on the symbol \( a_0^{(-1)} \) of the parametrix. In order to demonstrate that individual terms in our formal sum (2.20) are compatible with the edge-degenerate calculus let us first consider the leading order term \( h^{-1} \) which represents a meromorphic operator valued symbol acting on the basis \( X \). Because of \( r^2 C \) in the denominator, its poles depend on the values of the covariables of the edge and therefore it cannot be directly identified with a symbol in the edge calculus. In order to see how this symbol actually fits into the calculus it is convenient to consider a Lippmann-Schwinger expansion

\[ h^{-1} = h_0^{-1} + h^{-1} [h_0 - h] h_0^{-1} \]

\[ h^{-1} = h_0^{-1} + h_0^{-1} [h_0 - h] h_0^{-1} + h^{-1} [h_0 - h] h_0^{-1} [h_0 - h] h_0^{-1} \]

\[ \vdots \]

with \( h_0 = (w - 2)^2 - (w - 2) + \Delta_{s2} \).

For arbitrary \( N \in \mathbb{N} \) this becomes

\[ h^{-1} = \sum_{n=0}^{N-1} (r^2 C)^n h_0^{-1-n} + (r^2 C)^N h_0^{-1} h_0^{-N}. \]  \hfill (2.21)

Applying the kernel cut-off \( H(\phi) \), with \( \phi \in C_0^\infty(\mathbb{R}_+) \) and \( \phi = 1 \) in a neighbourhood of \( r = 1 \), to \( h^{-1} \in C^\infty(\mathbb{R}_+ \times Y, L_{cl}^{-2}(X, \Gamma_\alpha \times \mathbb{R}^3)) \) one gets

\[ h^{-1} = H(\phi) h^{-1} + (1 - H(\phi)) h^{-1}, \]  \hfill (2.22)

where

\[ H(\phi) h^{-1}(r, y, w, \eta) = H(\phi) h^{-1}(y, w, r \eta) \]

with \( H(\phi) h^{-1} \in C^\infty(\mathbb{R}_+ \times Y, M_{\Gamma_0}^{-2}(X, \mathbb{R}^3)) \), cf. [11] Section 1.1 for further details and definitions. Similarly, one can apply the kernel cut-off to the two terms in the decomposition \( h^{-1} = h_{LS}^{-1} + h_{\text{flat}}^{-1} \).
Therefore, the integration contour $\Gamma_{7}$, separately. The operators corresponding to the holomorphic Mellin symbol $H(\phi)h^{-1}$, $H(\phi)h_{LS}^{-1}$ and $H(\phi)h_{flat}^{-1}$ map
\[
\omega_{7}r^{2} \text{op}^{\gamma-3}_{M}(H(\phi)h_{(LS)}^{-1})^{1/2} : \mathcal{K}^{s,\gamma-2} \rightarrow \mathcal{K}^{s+2,\gamma},
\]
\[
\omega_{7}r^{2} \text{op}^{\gamma-3}_{M}(H(\phi)h_{flat}^{-1})^{1/2} : \mathcal{K}^{s,\gamma-2} \rightarrow \mathcal{K}^{s+2+N,\gamma+N},
\]
respectively.

Inserting the Lippmann-Schwinger expansion [221], the operator corresponding to the second term of (2.22) becomes
\[
\omega_{7}r^{2} \text{op}^{\gamma-3}_{M}((1 - H(\phi))h^{-1})^{1/2} = \sum_{n=0}^{N-1} m_{n} + g_{N},
\]
with
\[
m_{n}(y, \eta) := \omega_{7}r^{2}(r^{2}C)^{n} \text{op}^{\gamma-3}_{M}((1 - H(\phi))h^{-1-\eta})^{1/2} \eta^{n},
\]
and
\[
g_{N}(y, \eta) := \omega_{7}r^{2}(r^{2}C)^{N} \text{op}^{\gamma-3}_{M}((1 - H(\phi))h^{-1}h_{0}^{-N})^{1/2} \eta^{N}.
\]

**Proposition 2.** The parameter dependent operators $m_{n}$, $n = 0, \ldots, N - 1$, represent smoothing Mellin operators
\[
m_{n}(y, \eta) : \mathcal{K}^{s,\gamma-2} \rightarrow \mathcal{K}^{\infty,\gamma+2n},
\]
with $(1 - H(\phi))h_{0}^{-1-n} \in M_{R}^{-\infty}(X)$. For $n$ sufficiently large $m_{n}$ and the remainder $g_{N}$ belong to $R_{G}^{2}(Y \times \mathbb{R}^{3}, g)$ and do not contribute to the asymptotics.

**Proof.** The mapping property for $m_{n}$ follows from [39 Lemma 3.3.22].

Twisted homogeneity for $g_{N}$ can be easily shown, i.e.,
\[
k_{\lambda}g_{N}(y, \eta)k_{\lambda}^{-1}u = k_{\lambda}\omega_{7}r^{2}(r^{2}C)^{N} \text{op}^{\gamma-3}_{M}((1 - H(\phi))h^{-1}h_{0}^{-N})^{1/2} \eta^{N}k_{\lambda}^{-1}u
\]
\[
= \omega_{7}(\lambda r)^{2}(\lambda^{2}r^{2}C)^{N} \int_{\mathbb{R}}^{\infty} \left( \frac{\lambda r}{r'} \right)^{-(\frac{3}{2} - \gamma + i\rho)} \left[ (1 - H(\phi))h^{-1}h_{0}^{-N} \right] \left( \frac{7}{2} - \gamma + i\rho, \lambda \eta \right)
\]
\[
\times \omega_{7}^{N}(\lambda \rho) d\rho \frac{d\rho'}{r'}
\]
\[
= \omega_{7}(\lambda r)^{2}(\lambda^{2}r^{2}C)^{N} \int_{\mathbb{R}}^{\infty} \left( \frac{r}{\bar{r}} \right)^{-(\frac{3}{2} - \gamma + i\rho)} \left[ (1 - H(\phi))h^{-1}h_{0}^{-N} \right] \left( \frac{7}{2} - \gamma + i\rho, \lambda \eta \right)
\]
\[
\times \omega_{7}(\lambda \rho) d\rho \frac{d\rho'}{\bar{r}}
\]
\[
= \lambda^{2}g_{N}(y, \lambda \eta)u.
\]
The poles $w_{0}$ of $h^{-1}(y, \eta)$ are all located outside a strip $\{ w : 2 < |w| < 3 \}$ in the complex plane. Therefore, the integration contour $\Gamma_{\frac{7}{2} - \gamma}$ for $\frac{3}{2} < \gamma < \frac{7}{2}$ is separated from the poles, and for fixed $y, \eta$ it follows from [71 Section 7.2.3, Theorem 9] that
\[
g_{N}(y, \eta) : \mathcal{K}^{s,\gamma-2} \rightarrow \mathcal{S}^{\gamma+2N}.
\]

With respect to the norm of $\mathcal{K}^{s,\gamma}$ spaces one gets
\[
\left\| \kappa_{[\theta]}^{-1} \omega_{7}r^{2}(r^{2}C(\eta)^{N} \text{op}^{\gamma-3}_{M}((1 - H(\phi))h^{-1}h_{0}^{-N})^{1/2} (y, \eta)w_{7}^{1/2}(\eta) \right\|_{\mathcal{L}(\mathcal{K}^{s,\gamma-2}, \mathcal{K}^{\infty,\gamma+2N})}
\]
\[
= \left\| \omega_{7}^{-1}r^{2}(r^{2}C(\eta)^{1/2} \eta) \text{op}^{\gamma-3}_{M}((1 - H(\phi))h^{-1}h_{0}^{-N})^{1/2} (y, \eta)^{-1} \eta \right\|_{\mathcal{L}(\mathcal{K}^{s,\gamma-2,\mathcal{K}^{\infty,\gamma+2N}}, \eta)^{-1}}\left\| \eta \right\|_{\mathcal{L}(\mathcal{K}^{s,\gamma-2,\mathcal{K}^{\infty,\gamma+2N}})}\eta^{-2},
\]
and for derivatives of the symbol

\[ \| \kappa_{[\eta]}^{-1} D_y^a D_\eta^b \omega_\eta r^2 (r^2 C(\eta)) \|^N_{\mathcal{M}} \| \phi^{-1} - 1 \|^N_{\mathcal{M}} \| (y, \eta) \|_{\mathcal{L}(\mathbb{K}^\infty)} \]

for \( y \in K \subset U \subset Y, \eta \in \mathbb{R}^3 \). Therefore, \( g_N \) belongs to \( S_{cl}^{-2}(U \times \mathbb{R}^3; \mathbb{K}^\infty) \) and \( g_N \in R^{-2}(U \times \mathbb{R}^3, g) \) follows according to Proposition 2. Furthermore, it turns out that for \( h^{-1} \) to more general higher order terms. In summary, we may say that our formal expansion (2.20) fulfills the requirements of the edge-degenerate calculus.

As a matter of principle we can proceed by calculating higher order terms of \( q_0 \) in the asymptotic expansion (2.20) and use an analogous ansatz for the higher order terms \( q_i, i = 1, 2, \ldots, \) of the asymptotic expansion (2.15) of \( a_0^{-1} \). To this end let us reformulate (2.15) by using the Lippmann-Schwinger expansion in the following form

\[
a_0^{-1} \sim -2\pi^2 \sum_{n \geq 0} r^n q_{0,n} \]

\[
= -2\pi^2 \sum_{n \geq 0} r^n \left( H(\phi) q_{0,n} + (1 - H(\phi)) q_{0,n} \right) \]

\[
= -2\pi^2 \sum_{n \geq 0} r^n \left( H(\phi) [q_{0,n}]_{LS} + H(\phi) [q_{0,n}]_{flat} + (1 - H(\phi)) [q_{0,n}]_{LS} + (1 - H(\phi)) [q_{0,n}]_{flat} \right),
\]

where \([q_{0,n}]_{LS}\) and \([q_{0,n}]_{flat}\) for \( q_{0,n} \) have the same meaning as the first and second term of the decomposition (2.21) for \( h^{-1} \), respectively. In the third line we have, like holomorphic symbols, smoothing Mellin symbols \((1 - H(\phi)) [q_{0,n}]_{LS}\) and flat Green remainders \((1 - H(\phi)) [q_{0,n}]_{flat}\). The latter can be neglected in our considerations according to Proposition 2. Furthermore, it turns out that holomorphic symbols \( H(\phi) [q_{0,n}]_{LS} \) and \( H(\phi) [q_{0,n}]_{flat} \) do not contribute to the Green operators \( g_{1,1} \) and \( g_{2,2} \), i.e., only the \((1 - H(\phi)) [q_{0,n}]_{LS}\) term actually contributes. Furthermore, according to (2.23), the operator corresponding to the holomorphic symbol \( H(\phi) [q_{0,n}]_{flat} \) does not even contribute to the asymptotic parametrix. Therefore, in the following we consider in the asymptotic expansion of \( a_0^{-1} \) only the terms \([q_{0,n}]_{LS}\). For the latter we take the asymptotic ansatz

\[
[q_{0,n}]_{LS} \sim -2\pi^2 \sum_{n \geq 0} d_{n,j}^{(0)}(w, r\eta), \quad (2.24)
\]

where \( d_{n,j} \) denotes a homogeneous polynomial of order \( j \) in the degenerate covariables \( r\eta \), i.e., \( d_{n,j}(\lambda r\eta) = \lambda^j d_{n,j}^{(0)}(r\eta) \) with coefficients depending on the operator valued symbol \( h_0 \).

Summarising our previous discussion, we have derived for the symbol \( a_0^{-1} \) of the initial parametrix \( P_0 \) the asymptotic expansion

\[
a_0^{-1} \sim -2\pi^2 \left( [q_{0,0}]_{LS} + r[q_{0,1}]_{LS} + r^2[q_{0,2}]_{LS} + \cdots \right) \quad (2.25)
\]

\[
\sim -2\pi^2 \sum_{n \geq 0} \sum_{j \geq 0} r^n d_{n,j}^{(0)}(w, r\eta).
\]

For the sake of notational simplicity, we skip the subscript LS in the following, notwithstanding that all asymptotic expansions of the type (2.25), here and in the following, refer to the \([\cdot]_{LS}\) part of the.
the Lippmann-Schwinger decomposition. In order to show, that the asymptotic expansion (2.25) is actually consistent with the symbolic structure of asymptotic parametrices in the edge degenerate calculus, cf. Section 2.1, let us first reveal its relation to the conormal symbols of the parametrix.

**Proposition 3.** The asymptotic expansion (2.25) is equivalent modulo flat remainders to an asymptotic expansion of 

\[ a_0^{(-1)} \] 

via the conormal symbols of \( p_{M,0} \), cf. (2.9),

\[
a_0^{(-1)} \sim \sum_{j \geq 0} r^j \sigma_M^{-2-j} (p_{M,0})(y, \eta)
\]

with

\[
\sigma_M^{-2-j} (p_{M,0})(y, \eta) = \frac{1}{j!} \frac{\partial^j}{\partial r^j} a_{0,h}^{(-1)} |_{r=0} + \sigma_M^{-2-j} (m_0)(y, \eta),
\]

where \( a_{0,h}^{(-1)} \in M_0^{-2}(X, \mathbb{R}^3) \) denotes the holomorphic Mellin symbol and \( m_0 \in R_{M+G}^{-2}(Y \times \mathbb{R}^3, g) \) refers to the smoothing Mellin operator part of \( p_0 \).

**Proof.** Conormal symbols are polynomials in the edge covariable \( \eta \). In order to represent \( d^{(0)}_{n,j} (w, r\eta) \) by conormal symbols one can decompose the latter into their homogeneous components, i.e.,

\[
\sigma_M^{-2-j} (p_{M,0})(y, \eta) = \sum_{k=0}^{j} Q_{k,j}^{(0)}(\eta) \quad \text{with} \quad Q_{k,j}^{(0)}(\lambda \eta) = \lambda^k Q_{k,j}^{(0)}(\eta).
\]

The asymptotic expansion (2.26) becomes

\[
a_0^{(-1)} \sim \sum_{j \geq 0} \sum_{k=0}^{j} Q_{k,j}^{(0)}(\eta)
\]

\[
\sim \sum_{k \geq 0} \sum_{j \geq k} r^j Q_{k,j}^{(0)}(r\eta)
\]

\[
\sim \sum_{m \geq 0} r^m \sum_{k \geq 0} Q_{k,m+k}^{(0)}(r\eta),
\]

and a comparison with (2.25) shows

\[
Q_{k,m+k}^{(0)}(r\eta) = -2t^2 d_{m,k}^{(0)}(r\eta).
\]

**Remark 6.** The asymptotic expansion (2.25) does not depend on the details of the parametrix construction. In particular it does not matter whether it refers to a left or right parametrix. This is an immediate consequence of Proposition 3 and the fact that two edge-degenerate pseudo-differential operators which agree modulo Green and flat operators have the same conormal symbols.

It is obvious that the same type of asymptotic expansion can be as well applied in the subsequent steps of the asymptotic parametrix construction.

The actual calculation of individual terms and corresponding contributions to Green operators, is rather involved. Therefore, in the following section, we first want to present our main result and some of its immediate consequences for the sake of the reader who is not interested in the details of the calculations. The proof and all technical details are given in Section 4.

## 3 Asymptotics of the Green operator

### 3.1 Main result

Before we present our main theorem, we give a few remarks.
i) In Section 2, we have derived an asymptotic parametrix modulo Green operators in \( L^0_\mathfrak{G}(M, g) \). This actually represents the penultimate step in the asymptotic parametrix construction discussed in Ref. [11], cf. Corollary 2.24 and Theorem 2.26 therein. For our purposes it is sufficient to stop at this point because it already provides us with the desired insight into the asymptotic behaviour of solutions to Schrödinger’s equation near edge type singularities.

ii) According to our discussion in Section 2.3, we have applied the \( \varepsilon \)-regularization technique, cf. Appendix A, for the construction of the parametrix and Green operator. This is justified by the fact that we apply the Green operator to an eigenfunction of the Hamiltonian \( u \) which according to standard regularity theory, cf. [39], belongs to \( W^\infty_{\text{loc}}(Y, K^{\infty, \gamma}(\Lambda_2)) \). Therefore, \( u \) is \( \varepsilon \)-regularizable, cf. Lemma 2 below.

iii) It should be mentioned that the spectral resolution of the Laplace-Beltrami operator acting on the base of the cone \( S^2 \) is a pleasant feature of our approach which relates the relative angular momentum of a pair of particles to its radial correlation.

iv) The subsequent formula for the asymptotic expansion of the symbol of the Green operator seems to be rather complicated. In particular, terms depending on edge variables and covariables are rather involved. It is therefore desirable to provide an independent check of its correctness. Such a check has been performed in Appendix B, where we apply the corresponding Green operator to eigenfunctions of a Hamiltonian without \( e-e \) interaction potential. These eigenfunctions are explicitly known for different angular momenta and can be used to verify the essential relation \( G\hat{u} = -u \), cf. (2.2), via explicit calculations.

**Theorem 1.** The Green operator \( g \in \mathcal{R}^0_\mathfrak{G}(Y_i \times \mathbb{R}^3, g) \) \((i = 1, 2, 3)\) for \( \frac{1}{2} \leq \gamma \leq \frac{3}{2} \) has a leading order asymptotic expansion of the form

\[
g\hat{u}(y, \eta) = \sigma' 2 t^2 \left[ \left( 1 + rtZ_1 + r^2 \left( -2 + \frac{1}{3}(tZ_1)^2 + \frac{1}{3}(tZ_2) \right) \right) P_0 Q_{0,1}(\hat{u})(y, \eta)
+ \frac{1}{6} r^2 P_0 Q_{0,2}(\hat{u})(y, \eta) + \left( \frac{4}{3}r + \frac{1}{6}tZ_1r^2 \right) P_1 Q_{1,1}(\hat{u})(y, \eta)
+ \frac{1}{6} r^2 P_2 Q_{2,1}(\hat{u})(y, \eta) - \frac{1}{30} r^2 P_2 Q_{2,2}(\hat{u})(y, \eta) \right] + O(r^3)
\]

with

\[
Z_1 := \begin{cases} 
\frac{1}{\sqrt{2}} & \text{for } v_{\varepsilon-e} \\
-Z & \text{for } v_{\varepsilon-n}
\end{cases}, \quad Z_2 := -tE + \begin{cases} 
-2\sqrt{Z} & \text{for } v_{\varepsilon-e} \\
1-Z & \text{for } v_{\varepsilon-n}
\end{cases}
\]

where \( \varphi_i u \in W^\infty_{\text{comp}}(Y_i, K^{\infty, \gamma}((S^2)\wedge)) \) and \( \hat{u}(r, \varphi_1, \theta_1, \eta) := F_{y\rightarrow\eta}\varphi_i u(r, \varphi_1, \theta_1, y) \). Here, \( P_l, l = 0, 1, 2, \ldots, \) denote projection operators on subspaces which belong to eigenvalues \( -l(l+1) \) of the Laplace-Beltrami operator on \( S^2 \). For terms depending on edge variables and covariables, we have
used the following notations
$$Q_{0,1}(\tilde{u}) := M((\delta \sigma - 1) \, op_M^{\gamma-1}(a) \tilde{\sigma} \tilde{u})(0) + M(\frac{1}{27r} \, r^2 C_0 \tilde{\sigma} \tilde{u})(0) + M(op_M^{\gamma-1}(rs_1) \tilde{\sigma} \tilde{u})(0)$$

$$Q_{0,2}(\tilde{u}) := M((\delta \sigma - 1) \, op_M^{\gamma-1}(\sum_\alpha \frac{1}{\alpha!} \partial^{\alpha}_\eta \tilde{C}_1 D^{\alpha}_y a) \tilde{\sigma} \tilde{u})(0)$$

$$Q_{1,1}(\tilde{u}) := M((\delta \sigma - 1) \, op_M^{\gamma-1}(a) \tilde{\sigma} \tilde{u})(-1) + M(\frac{1}{27r} \, r^2 C_0 \tilde{\sigma} \tilde{u})(-1)$$

$$Q_{2,1}(\tilde{u}) := M((\delta \sigma - 1) \, op_M^{\gamma-1}(\sum_\alpha \frac{1}{\alpha!} \partial^{\alpha}_\eta \tilde{C}_1 D^{\alpha}_y a) \tilde{\sigma} \tilde{u})(0) + M(\frac{1}{27r} \, r^2 C_0 \tilde{\sigma} \tilde{u})(0) + M(op_M^{\gamma-1}(rs_1) \tilde{\sigma} \tilde{u})(0)$$

$$Q_{2,2}(\tilde{u}) := M((\delta \sigma - 1) \, op_M^{\gamma-1}(a) \tilde{\sigma} \tilde{u})(-2) + M(\frac{1}{27r} \, r^4 C_2 \tilde{\sigma} \tilde{u})(-2) + M(op_M^{\gamma-1}(r^3 s_3) \tilde{\sigma} \tilde{u})(-2)$$

with

$$C_1 := -5t \tau - \cot \theta \Theta_2, \quad \tilde{C}_1 := C_0 - 4i \eta \tau + iC_1$$

$$rs_1 := a - a_0, \quad r^2 s_2 := a - a_0 - ra_1;$$

$$a_0 := -\frac{1}{27r} T^2 h_0 + \frac{1}{27r} r^2 C_0, \quad a_1 := \frac{1}{27r} r C_1 + \frac{1}{27r} \tilde{C}_1, \quad a_2 := -\frac{1}{27r} w - \frac{1}{27r} \Delta s^2 + \frac{1}{27r} r^2 C_2 + \frac{1}{27r} \tilde{C}_2$$

$$h_1^{(l)} := \frac{1}{27r} (w^2 - w - l(l + 1)), \quad h_2^{(l)} := \frac{1}{27r} (w^2 - w - l(l + 1) - 2rtZ_1),$$

$$h_3^{(l)} := \frac{1}{27r} (w^2 - w - l(l + 1) + \frac{1}{3r^2} w - r^2 C_0 - ir^2 C_1 - 2rtZ_1 - 2r^2 - 2r^2 t Z_2).$$
3.2 Leading order asymptotic behaviour of helium and the hydrogen molecule

Let us first consider the asymptotic behaviour near the $e-e$ edge. The euclidean distance between two electrons expressed in hyperspherical coordinates is

$$|x_1 - x_2| = \sqrt{2t} \sin r_{12} = \sqrt{2t}(r_{12} + O(r_{12}^2)).$$

With this the asymptotic behaviour on the subspace of $l = 0$ relative angular momentum, defined by $P_0$, becomes

$$GP_0 u \sim \left(1 + \frac{1}{2}|x_1 - x_2|\right)w_0(y) + \cdots$$

which is equivalent to Kato’s famous “cusp” condition

$$\frac{1}{4\pi} \left. \frac{\partial}{\partial x_{12}} \int \int_{S^2} u(x_{12}, \omega_{12}, y) d\omega_{12} \right|_{x_{12} = 0} = \frac{1}{2}u(0,0,y), \quad x_{12} := |x_1 - x_2|, \quad y := \frac{1}{2}(x_1 + x_2) \neq 0,$$

because asymptotic contributions from subspaces $P_n$, $n = 1, 2, \ldots$, vanish in the spherical average. For the subspace of $l = 1$ relative angular momentum, defined by $P_1$, one gets

$$GP_1 u \sim r \left(1 + \frac{1}{4}\sqrt{2t}r\right)w_1(y) + \cdots \sim r \left(1 + \frac{1}{4}|x_1 - x_2|\right)w_1(y) + \cdots.$$ 

The subspace is antisymmetric with respect to the interchange of the electrons, and according to Pauli’s principle it must correspond to a triplet state with respect to the total spin of the wavefunction. This is also reflected by the fact that triplet wavefunctions vanish at the $e-e$ edge.

The leading order asymptotic behaviour in the $l = 0$ case near one of the two $e-n$ edges gives

$$GP_0 u \sim \left(1 - Z|x_1|\right)w_0(y) + \cdots,$$

which is again equivalent to the corresponding variant of Kato’s “cusp” condition

$$\frac{1}{4\pi} \left. \frac{\partial}{\partial x_1} \int \int_{S^2} u(x_1, \omega_1, x_2) d\omega_1 \right|_{x_1 = 0} = -Zu(0,0,x_2), \quad x_1 := |x_1|, \quad x_2 \neq 0.$$

The corresponding asymptotic expression in the $l = 1$ case becomes

$$GP_1 u \sim r \left(1 - \frac{1}{Z}Z|x_1|\right)w_1(y) + \cdots.$$ 

In the limit $t \to \infty$ one electron approaches the nucleus whereas the other electron is far apart of it. This situation resembles to the single electron case and the asymptotic behaviour can be compared with the hydrogen series. For the subspace $l = 0$ one gets

$$GP_0 u \sim \left(1 - Z|x_1| + \frac{1}{3}|x_1|^2(Z^2 - E + \frac{1}{2}\partial_t^2)\right)\tilde{w}_0(y) + \cdots \quad \text{for} \ t \to \infty.$$

This is formally equivalent to the asymptotic expansion of the Green operator for the hydrogen series, cf. [9]. However, let us mention that the second order term for $l = 0$ depends on the eigenvalue of the energy which is different for bound states in the helium and hydrogen series. Only in the limiting case of highly excited states in the helium series the energies approach the ionization threshold, i.e., the ground state energy of the corresponding ion. The additional differential operator $\frac{1}{2}\partial_t^2$ acts as a correction term which can be seen by considering the case of two noninteracting electrons, cf. Appendix refestical.

Let us first consider a system consisting of two electrons and two nuclei $A, B$ with charges $Z_a, Z_b$. For simplicity, the nuclei are arranged at distance $R$ along the $z$-axis at positions $\frac{1}{2}Re_z$ and $-\frac{1}{2}Re_z$, respectively. We introduce the local distance variables

$$r_1 := x_1 - \frac{1}{2}Re_z, \quad r_2 := x_2 + \frac{1}{2}Re_z.$$
and express $r_1, r_2$ in terms of hyperspherical coordinates. With this the potential becomes

$$v_{e-n} := \frac{Z_a r}{\sin r} - \frac{Z_b r}{\cos r} + \frac{Z_a Z_b r t}{R} \sqrt{\frac{Z_b r}{\cos^2 r + \left(\frac{R}{r}\right)^2}} - \frac{Z_a r}{\sqrt{\cos^2 r - 2 \cos r \cos \theta_1 \frac{R}{r} + \left(\frac{R}{r}\right)^2}}$$

The asymptotic expansion becomes

$$v_{e-n} \sim -Z_a + \left[-Z_b + \frac{Z_a Z_b t}{R} + \frac{Z_b t}{R} \frac{Z_a}{\sqrt{1 - 2 \cos \theta_2 \frac{R}{r} + \left(\frac{R}{r}\right)^2}} + \frac{1}{\sqrt{1 - 2 \cos \theta_2 \frac{R}{r} + \left(\frac{R}{r}\right)^2}}\right] r + O(r^2),$$

where $R > t$ has been assumed. For the special case of the hydrogen molecule, i.e., $Z_a = Z_b = 1$, one gets

$$v_{e-n} \sim -1 - r + O(r^2),$$

and

$$Z_2 = -tE - 1 = -t(2E_0 + E_{V,dW}) - 1,$$

where we have decomposed the total energy $E$ into a noninteracting part $E_0$ and the Van der Waals energy $E_{V,dW}$. This shows that the Van der Waals interaction of a distant atom enters already in the second order term of the asymptotic expansion of the wavefunction at a nucleus.

### 3.3 Absence of logarithmic terms in the asymptotics of eigenfunctions near edges

The qualitative behaviour of eigenfunctions of Hamiltonian operators near edges of the stratified configuration space, i.e., at coalescence points of two particles, can be easily derived from a fundamental theorem of Fournais et al. [15], already mentioned in the introduction. There it has been shown in a neighbourhood of a coalescence point of two particles, with respective coordinates $x_i, x_j \in \mathbb{R}^3$ in configuration space, that the wavefunction can be represented in the form $\Psi = \Psi_1 + |x_i - x_j|\Psi_2$ with $\Psi_1$ and $\Psi_2$ real analytic functions of the particle coordinates. This result implies an asymptotic expansion in terms of non negative integer powers of the interparticle distance. In particular there can be no logarithmic terms, which show up in the neighbourhood of coalescence points of three and more particles, cf. Fock’s expansion of eigenfunctions of the helium atom.

Within the present work the asymptotic type is encoded in the meromorphic Mellin symbol of the paramatrix. The location of its poles and corresponding multiplicities determines the asymptotic behaviour. In particular, the absence of logarithmic terms requires that no multiple zeros appear in the denominator of asymptotic symbols $d^u_{k,j}$, with $j,k,n \in \mathbb{N}_0$. We do not want to prove this property in full generality, instead we restrict ourselves to look at those symbols which have been already evaluated in the course of our calculation. In Appendix C we have summarized our state of knowledge concerning the location and multiplicities of poles of some asymptotic symbols. It is interesting to see that multiple poles appear in these symbols at values $u = 3, 4$, however, their location in the complex plane is to the right of the integration contour $\Gamma_{\frac{3}{2}, -\gamma}$ of the inverse Mellin transformation which enters into the Mellin pseudo-differential operator part of the paramatrix. In our particular application, the integration contour $\Gamma_{\frac{3}{2}, -\gamma}$ restricts to the strip of the complex plane \( \{ z \in \mathbb{C} : 2 < |z| < 3 \} \). This is because we consider the Hamiltonian as an unbounded essentially self-adjoint operator on $L_2(\mathbb{R}^6)$, which has its natural domain $H^2(\mathbb{R}^6)$, cf. [16]. Therefore, all eigenfunctions are bounded and $\gamma$ can be restricted to the interval of ellipticity, i.e., $\frac{1}{2} < \gamma < \frac{3}{2}$, cf. Remark [1].
4 Proof of the main result

4.1 Calculation of the asymptotic parametrix up to second order

Let us take the ansatz (2.1) for the construction of the asymptotic parametrix, where the pseudo-differential operator structure of \( P_i \) for \( i > 0 \) is completely analogous to \( P_0 \) given by (2.5), (2.9) and (2.10), respectively. Therefore, we accordingly define the parameter dependent Mellin part by

\[ p_{M,i}(y, \eta) := r^i \text{op}^\gamma_{-3} (a_i^{(-1)})(y, \eta) \text{ for } i = 0, 1, 2, \ldots, \]

where the Mellin symbols \( a_i^{(-1)} \), \( i = 0, 1, 2, \ldots \), have asymptotic expansions of the form

\[ a_i^{(-1)}(y, \eta) \sim -2t^2 \left( q_{i,0} + rq_{i,1} + r^2 q_{i,2} + \cdots \right) \]

\[ \sim -2t^2 \sum_{n \geq 0} \sum_{j \geq 0} r^nd_{i,n,j}(w, r\eta). \]  

(4.1)

It is easy to see, that this particular expansion satisfies the formal requirements of an asymptotic parametrix construction outlined in Section 2.1. Let us just mention the conormal symbols which satisfy

\[ \sigma_c^{-2-j}(p_{M,i})(y, \eta) = 0, \quad j = 0, 1, \ldots, i - 1 \]

and

\[ \sigma_c^{-2-i}(p_{M,i})(y, \eta) = -2t^2 d_{0,0}^{(i)}(w, \eta) \neq 0. \]

Like in Proposition 3 we can express Mellin symbols via an asymptotic expansion in terms of conormal symbols, i.e.,

\[ r^i a_i^{(-1)}(y, \eta) \sim \sum_{j \geq i} t^j \sigma_c^{-2-j}(p_{M,i})(y, \eta), \]

and vice versa conormal symbols via our homogeneous symbols, i.e.,

\[ \sigma_c^{-2-j}(p_{M,i})(y, \eta) = -2t^2 \sum_{k=0}^{j-i} d_{j-i-k,k}^{(i)}(w, \eta). \]

(4.2)

It has been already mentioned in the remark following Proposition 3 that the asymptotic expansion (4.1) does not depend on the details of the parametrix construction. In the following we therefore calculate all symbols of the asymptotic parametrix by applying it from the right side to the Hamiltonian operator.

4.1.1 Initial parametrix \( P_0 \)

In the initial step of the parametrix construction we consider the equation \( P_0 A_0 = I \) modulo Green operators. The symbol \( a_0^{-1} \) of the initial parametrix \( P_0 \) has itself an asymptotic expansion (2.25) and the corresponding zeroth order equation (2.16), derived from (2.14), has been already given. Let us start the actual calculations by inserting the asymptotic expansion \[ q_{0,0} = -2t^2 (d_{0,0}^{(0)} + d_{0,1}^{(0)} + \cdots) \]

(4.2)

into the zeroth order equation (2.16). A simple calculation yields

\[ d_{0,2j}^{(0)} = (r^2 C_0)^j b_j \text{ and } d_{0,2j+1}^{(0)} = 0, \quad j = 0, 1, \ldots, \]

A simple calculation yields

\[ d_{0,2j}^{(0)} = (r^2 C_0)^j b_j \text{ and } d_{0,2j+1}^{(0)} = 0, \quad j = 0, 1, \ldots, \]
with
\[
\begin{aligned}
&b_0 = h_0^{-1}, \\
&b_1 = b_0/(h_0 - 2(2w - 7)), \\
&\vdots \\
&b_n = b_{n-1}/(h_0 - 2n(2w - 5 - 2n)), \\
&\vdots 
\end{aligned}
\]  
(4.3)

The first order equation, derived from (2.14), becomes
\[
\begin{aligned}
r^1: \quad &T^{-2}a_0rq_{0,1} + \partial_w T^{-2}a_0(-r \partial_r)rq_{0,1} + \frac{1}{2} \partial_w^2 T^{-2}a_0(-r \partial_r)^2rq_{0,1} \\
&+ \partial_r T^{-2}a_0D_t q_{0,0} + \partial_{\Theta_2} T^{-2}a_0D_{\Theta_2} q_{0,0} = 0.
\end{aligned}
\]

Inserting the asymptotic expansion
\[
q_{0,1} = -2t^2\left(a_{1,0}^{(0)} + d_{1,1}^{(0)} + \cdots \right)
\]  
(4.4)

as well as (4.2) yields after a simple calculation
\[
\begin{aligned}
d_{1,2j}^{(0)} &= 0 \quad \text{for } j = 0, 1, \ldots, \\
&d_{1,2j+1}^{(0)} = -\sum_{k=0}^{j} (r^2 C)^{j-k} P_{1,2k+1} b_{j+1} \quad \text{for } j = 0, 1, \ldots
\end{aligned}
\]  
(4.5)

with polynomials
\[
P_{1,2j+1} := 4i \left[ t(\tau r)(r^2 C)^j + j \left( t^3(\tau r)^3 - (r \Theta_2)(r \Phi_2)^2 \cot \Theta_2 \sin^2 \theta_2 \right) (r^2 C)^j - 1 \right]
\]

which are homogeneous of order $2j + 1$ in the edge covariables.

The recursive calculation can be carried out to any order, what remains to be done for our purpose is to consider the second order equation, derived from (2.14), which becomes
\[
\begin{aligned}
r^2: \quad &T^{-2}a_0r^2q_{0,2} + \partial_w T^{-2}a_0(-r \partial_r)r^2q_{0,2} + \frac{1}{2} \partial_w^2 T^{-2}a_0(-r \partial_r)^2r^2q_{0,2} \\
&+ \partial_r T^{-2}a_0D_t q_{0,1} + \partial_{\Theta_2} T^{-2}a_0D_{\Theta_2} q_{0,1} + \frac{1}{2} \partial_w^2 T^{-2}a_0D_t^2 q_{0,0} + \frac{1}{2} \partial_{\Theta_2}^2 T^{-2}a_0D_{\Theta_2}^2 q_{0,0} = 0,
\end{aligned}
\]

from which $q_{0,2}$ can be calculated. In particular, we get
\[
\begin{aligned}
d_{2,2j+1}^{(0)} &= 0 \quad \text{for } j = 0, 1, \ldots, \\
&d_{2,0}^{(0)} = -2b_1 \\
&d_{2,2}^{(0)} = -P_{2,2} b_1/(h_0 - 4(2w - 9)) \\
&\vdots
\end{aligned}
\]  
(4.6)

with
\[
P_{2,2} := 34t^2(\tau r)^2 + \frac{2(1+2\cos^2 \theta_2)}{\sin^2 \theta_2}(r \Phi_2)^2 + 4r^2 C_0.
\]
4.1.2 First order parametrix \( P_1 \)

Once we have calculated the symbol of the initial parametrix up to second order in the asymptotic expansion, it can be used in the first recursion step to construct the symbol of the first order parametrix \( P_1 \) from the equation

\[
\sum_{\alpha} \frac{1}{\alpha!} r^{-2} \partial_{\eta}^\alpha \left( \text{op}_M^\gamma (a_0) \right) r^{3} D_y^\alpha \left( \text{op}_M^\gamma (a_1(-1)) \right) + \sum_{\alpha} \frac{1}{\alpha!} r^{-1} \partial_{\eta}^\alpha \left( \text{op}_M^\gamma (a_1) \right) r^{2} D_y^\alpha \left( \text{op}_M^\gamma (a_0(-1)) \right)
\]

\[
= \sum_{\alpha} \frac{1}{\alpha!} \text{op}_M^\gamma \left( \partial_{\eta}^\alpha \text{T}^{-2} a_0 \# r \partial_{\eta} D_y^\alpha a_1(-1) \right) + \sum_{\alpha} \frac{1}{\alpha!} \text{op}_M^\gamma \left( r \partial_{\eta}^\alpha \text{T}^{-2} a_1 \# r \partial_{\eta} D_y^\alpha a_0(-1) \right)
\]

\[
= 0 \mod R^0_{\text{flat}}(Y \times \mathbb{R}^3, \mathbf{g}_r).
\]

From this equation we can derive the first order equation of the corresponding symbol

\[
\begin{align*}
\bar{r} \colon & T^{-2} a_0 q_{1,0} + \partial_{\alpha} T^{-2} a_0 (-r \partial_{\alpha}) (r q_{1,0}) + \frac{1}{2} \partial_{\alpha}^2 T^{-2} a_0 (-r \partial_{\alpha})^2 (r q_{1,0}) \\
& + r T^{-2} a_1 q_{0,0} + r \partial_{\alpha} T^{-2} a_1 (-r \partial_{\alpha}) q_{0,0} \sim 0.
\end{align*}
\]

Inserting the asymptotic expansions

\[
q_{1,0} = -2 t^2 (d_{0,0}^{(1)} + d_{0,1}^{(1)} + \cdots), \quad (4.8)
\]

and \((4.2)\) which has been already calculated up to second order in the previous subsection, one gets the asymptotic equation

\[
(h_0 - r^2 C_0 - (2w - 6)) \sum_{j \geq 0} d_{0,j}^{(1)} - (2w - 7) \sum_{j \geq 1} j d_{0,j}^{(1)} + \sum_{j \geq 1} j^2 d_{0,j}^{(1)} - (irC_1 + 2tZ_1) \sum_{j \geq 0} d_{0,j}^{(0)} \sim 0,
\]

from which we obtain, with respect to powers of \( r \eta \), in zeroth order

\[
(r \eta)^0 \colon d_{0,0}^{(1)} = \frac{2tZ_1}{h_0(h_0 - (2w - 6))}
\]

and first order

\[
(r \eta)^1 \colon d_{0,1}^{(1)} = \frac{irC_1}{h_0(h_0 - 2(2w - 7))},
\]

respectively.

The second order asymptotic parametrix requires one more term which can be obtained from the second order contribution to Eq. \((4.7)\), i.e.,

\[
\begin{align*}
r \colon & T^{-2} a_0 r^2 q_{1,1} + \partial_{\alpha} T^{-2} a_0 (-r \partial_{\alpha}) (r^2 q_{1,1}) + \frac{1}{2} \partial_{\alpha}^2 T^{-2} a_0 (-r \partial_{\alpha})^2 (r^2 q_{1,1}) \\
& + r T^{-2} a_1 r q_{0,1} + r \partial_{\alpha} T^{-2} a_1 (-r \partial_{\alpha}) (r q_{0,1}) + \partial_{\alpha} T^{-2} a_0 D_y (r q_{1,0}) + r \partial_{\alpha} T^{-2} a_1 D_y q_{0,0} \sim 0.
\end{align*}
\]

Inserting the asymptotic expansion

\[
q_{1,1} = -2 t^2 (d_{1,0}^{(1)} + d_{1,1}^{(1)} + \cdots) \quad (4.9)
\]
as well as the already previously considered asymptotic expansions (4.2), (4.4) and (4.8), we get

\[
(h_0 - r^2 C_0 - 2(2w - 7)) \sum_{j \geq 0} d^{(1)}_{0,j} - (2w - 9) \sum_{j \geq 1} j d^{(1)}_{1,j} + \sum_{j \geq 1} j^2 d^{(1)}_{2,j}
\]

\[
-(irC_1 + 2tZ_1) \sum_{j \geq 0} d^{(0)}_{0,j} + r \tau \sum_{j \geq 0} D_t(-2t^2 d^{(1)}_{0,j})
\]

\[
-2r\Theta \sum_{j \geq 0} D_{\theta_2} d^{(1)}_{0,j} - 2r\Phi \frac{1}{\sin^2 \theta_2} \sum_{j \geq 0} D_{\phi_2} d^{(1)}_{0,j} - \frac{i\pi}{2t} \sum_{j \geq 0} D_t(-2t^2 d^{(0)}_{0,j})
\]

\[+ i \cot \theta_2 \sum_{j \geq 0} D_{\theta_2} d^{(0)}_{0,j} \sim 0,
\]

from which we obtain, with respect to powers of \( r\eta \), in zeroth order

\[
(r\eta)^0 : d^{(1)}_{1,0} = -\frac{10}{h_0(h_0 - 2(2w - 7))}.
\]

4.1.3 Second order parametrix \( P_2 \)

Finally, we want to use the symbols of the initial and first order parametrix to calculate in the second recursion step, the remaining symbol of the second order parametrix \( P_2 \) from the equation

\[
\sum_{\alpha} \frac{1}{\alpha!} r^{-2} \partial^\alpha \eta (\text{op}_M \gamma^{-1}(a_0)) r^4 D_y (\text{op}_M \gamma^{-3}(a_2^{(-1)}))
\]

\[
+ \sum_{\alpha} \frac{1}{\alpha!} r^{-1} \partial^\alpha \eta (\text{op}_M \gamma^{-1}(a_1)) r^3 D_y (\text{op}_M \gamma^{-3}(a_1^{(-1)}))
\]

\[
+ \sum_{\alpha} \frac{1}{\alpha!} \partial^\alpha \eta (\text{op}_M \gamma^{-1}(a_2)) r^2 D_y (\text{op}_M \gamma^{-3}(a_0^{(-1)}))
\]

\[
= \sum_{\alpha} \frac{1}{\alpha!} \text{op}_M \gamma^{-3}(\partial^\alpha \eta T^{-2} a_0 \# r, w r^2 D_y a_2^{(-1)})
\]

\[
+ \sum_{\alpha} \frac{1}{\alpha!} \text{op}_M \gamma^{-3}(r \partial^\alpha \eta T^{-2} a_1 \# r, w D_y a_1^{(-1)})
\]

\[
+ \sum_{\alpha} \frac{1}{\alpha!} \text{op}_M \gamma^{-3}(r^2 \partial^\alpha \eta T^{-2} a_2 \# r, w D_y a_0^{(-1)})
\]

\[= 0 \mod \mathcal{P}_{\text{flat}}^0(Y \times \mathbb{R}^3, g_r).
\]

Like before, we derive from it the second order equation of the corresponding symbol

\[
r^2 : T^{-2} a_0 r^2 q_{2,0} + \partial_w T^{-2} a_0 (-r \partial_r)(r^2 q_{2,0}) + \frac{1}{\alpha!} \partial^\alpha \eta T^{-2} a_0 (-r \partial_r)^2 (r^2 q_{2,0})
\]

\[+ r T^{-2} a_1 r q_{1,0} + r \partial_w T^{-2} a_1 (-r \partial_r)(r q_{1,0}) + r^2 T^{-2} a_2 q_{0,0} + r^2 \partial_w T^{-2} a_2 (-r \partial_r) q_{0,0} \sim 0.
\]

Inserting the asymptotic expansion

\[q_{2,0} = -2t^2 (d^{(2)}_{0,0} + d^{(2)}_{0,1} + \cdots) \quad (4.10)
\]

as well as the already previously considered asymptotic expansions (4.2) and (4.8), we get

\[
(h_0 - r^2 C_0 - 2(2w - 7)) \sum_{j \geq 0} d^{(2)}_{0,j} - (2w - 9) \sum_{j \geq 1} j d^{(2)}_{1,j} + \sum_{j \geq 1} j^2 d^{(2)}_{2,j}
\]

\[
-(irC_1 + 2tZ_1) \sum_{j \geq 0} d^{(1)}_{0,j} + \left(\frac{8}{3}(w - 2) + \frac{1}{3} \Delta S^2 - r^2 C_2 - 2tZ_2\right) \sum_{j \geq 0} d^{(0)}_{0,j} - \frac{8}{3} \sum_{j \geq 1} j d^{(0)}_{0,j} \sim 0,
\]
from which we obtain, with respect to powers of \( r\eta \), in zeroth order

\[
(r\eta)^0 : \quad d_{0,0}^{(2)} = \frac{(2tZ_1)^2}{(h_0 - 2(2w - 7))(h_0 - (2w - 6))h_0} - \frac{1}{3} \frac{8(w - 2) + \Delta_{S^2} - 6tZ_2}{(h_0 - 2(2w - 7))h_0}.
\]

### 4.1.4 Asymptotic expansion of the Mellin symbols up to second order

Summing up the asymptotic terms of the previous calculations up to second order leads to the following explicit expressions for the Mellin symbols of the parametrix

\[
a_0^{(-1)} \sim q_{0,0} + rq_{0,1} + r^2 q_{0,2} + \cdots
\]

\[
\sim -2t^2 \left( d_{0,0}^{(0)} + d_{0,1}^{(0)} + rd_{1,1}^{(0)} + r^2 d_{2,0}^{(0)} + \cdots \right)
\]

\[
\sim -2t^2 \left( \frac{1}{h_0} + \frac{r^2C_0}{h_0(h_0 - 2(2w - 7))} - \frac{rP_{1,1}}{h_0(h_0 - 2(2w - 7))} - \frac{2}{h_0(h_0 - 2(2w - 7))} + \cdots \right),
\]

\[
a_1^{(-1)} \sim q_{1,0} + rq_{1,1} + \cdots
\]

\[
\sim -2t^2 \left( d_{0,0}^{(1)} + d_{0,1}^{(1)} + rd_{1,1}^{(1)} + \cdots \right)
\]

\[
\sim -2t^2 \left( \frac{2tZ_1}{h_0(h_0 - (2w - 6))} + \frac{irC_1}{h_0(h_0 - 2(2w - 7))} - \frac{10}{h_0(h_0 - 2(2w - 7))} + \cdots \right),
\]

\[
a_2^{(-1)} \sim q_{2,0} + \cdots
\]

\[
\sim -2t^2 \left( d_{0,0}^{(2)} + \cdots \right)
\]

\[
\sim -2t^2 \left( \frac{(2tZ_1)^2}{(h_0 - 2(2w - 7))(h_0 - (2w - 6))h_0} - \frac{1}{3} \frac{8(w - 2) + \Delta_{S^2} - 6tZ_2}{(h_0 - 2(2w - 7))h_0} + \cdots \right).
\]

### 4.2 Calculation of left Green operators up to second order

In Section 2.3, we have discussed the construction of the initial parametrix and derived the corresponding Green operators. The recursive construction of higher order parametrices proceeds in a similar manner leading to the same types of Green operator which can be grouped in two classes. Let us first consider the class of type-\( a \) Green operator symbols which are of the general form

\[
g_a := \sigma' \omega_{1,0}^l r^{k+l} \sum \frac{1}{\alpha!} \partial_{\eta}^\alpha \left( \text{op}_M^{\gamma_l-1}(a_{k}^{(-1)}) \right) \left( \hat{\sigma}' \sigma - 1 \right) D_y^{\alpha} \left( \text{op}_M^{\gamma_l-1}(a_l) \right) \omega_{0,0} \tilde{\sigma}, \quad k, l = 0, 1, 2, \ldots ,
\]

and belong to \( R_G^{-\infty}(Y \times \mathbb{R}^3, \mathbf{g}) \). The second class of type-\( b \) Green operator symbols are of the general form

\[
g_b := \sigma' \omega_{1,0}^l r^{k+l} \sum \frac{1}{\alpha!} D_y^{\alpha} \left( \frac{C_{22}}{22} \right) \partial_{\eta}^\alpha \left( \text{op}_M^{\gamma_l-3}(a_{k}^{(-1)}) - \text{op}_M^{\gamma_l-1}(a_{k}^{(-1)}) \right) \omega_{0,0} \tilde{\sigma},
\]

and belong to \( R_G^{0}(Y \times \mathbb{R}^3, \mathbf{g}) \). They arise from the commutation of a \( r^l \) term, which belongs to a homogeneous polynomial in the covariables \( C_i(\eta) \), \( i = 0, 1, \ldots \), from the right to the left, cf. our discussion in Section 2.4.
4.2.1 Green operators from initial step of the parametrix construction

According to the calculations in Section 2.3 we get a type-$a$ Green operator symbol, cf. (2.11), which after insertion of the corresponding asymptotic symbol of the initial parametrix becomes

$$g_{0,1} = \sigma' \omega_{1,\eta} \sum_{\alpha} \frac{1}{\alpha!} \text{op}_M^{-1} \left( \left( (-2t^2) T^2 \partial_{\eta}^\alpha (d_{0,0}^{(0)} + d_{0,2}^{(0)} + r d_{1,1}^{(0)} + r^2 d_{2,0}^{(0)}) \right) (\bar{\sigma}' \sigma - 1) \text{op}_M^{-1} (D_y^\alpha a_0) \bar{\sigma} \right).$$

For the type-$b$ Green operator symbol, cf. (2.11), we get the explicit formula

$$g_{0,2} = \sigma' \omega_{1,\eta} \sum_{\alpha} \frac{1}{\alpha!} D_y^\alpha \left( \frac{r^2 C_\alpha}{2t^2} \right) \left[ \text{op}_M^{-3} \left( (-2t^2) \partial_{\eta}^\alpha (d_{0,0}^{(0)} + d_{0,2}^{(0)} + r d_{1,1}^{(0)} + r^2 d_{2,0}^{(0)}) \right) - \text{op}_M^{-1} \left( (-2t^2) \partial_{\eta}^\alpha (d_{0,0}^{(0)} + d_{0,2}^{(0)} + r d_{1,1}^{(0)} + r^2 d_{2,0}^{(0)}) \right) \right] \bar{\sigma}$$

$$= -2t^2 \sigma' \omega_{1,\eta} \left[ r \text{Res}(d_{0,0}^{(0)}, 1) M \left( \frac{C_\alpha}{2t^2} \tilde{\sigma} (\cdot) \right) (1) + \text{Res}(d_{0,0}^{(0)}, 2) M \left( \frac{C_\alpha}{2t^2} \tilde{\sigma} (\cdot) \right) (2) \right.$$  

$$+ \sum_{\alpha} \frac{1}{\alpha!} \text{Res}(\partial_{\eta}^\alpha d_{0,2}^{(0)}, 2) + r \text{Res}(\partial_{\eta}^\alpha d_{1,1}^{(0)}, 2) + r^2 \text{Res}(\partial_{\eta}^\alpha d_{2,0}^{(0)}, 2) M \left( D_y^\alpha \left( \frac{C_\alpha}{2t^2} \tilde{\sigma} (\cdot) \right) (2) + O(r^3) \right),$$

where we applied Cauchy’s residue theorem in order to get an explicit formula. Here and in the following $\text{Res}(f, w_0)$ denotes the residuum of the meromorphic function $f$ at its pole $w_0$.

4.2.2 Green operators from first recursion step of the parametrix construction

The first order contribution to the asymptotic parametrix from the left side is given by

$$\sigma' \omega_{1,\eta} r \sum_{\alpha} \frac{1}{\alpha!} \partial_{\eta}^\alpha \left( \text{op}_M^{-1} (T^2 a_{1}^{(-1)}) \right) \bar{\sigma}' \sigma D_y^\alpha \left( \text{op}_M^{-1} (a_0) \right) \bar{\sigma}$$

$$+ \sigma' \omega_{1,\eta} r \sum_{\alpha} \frac{1}{\alpha!} \partial_{\eta}^\alpha \left( \text{op}_M^{-2} (T a_{0}^{(-1)}) \right) \bar{\sigma}' \sigma D_y^\alpha \left( \text{op}_M^{-1} (a_1) \right) \bar{\sigma}$$

$$= \sigma' \omega_{1,\eta} r \sum_{\alpha} \frac{1}{\alpha!} \text{op}_M^{-1} \left( D_y^\alpha (-\frac{1}{2t^2}) T^2 \partial_{\eta}^\alpha (a_{1}^{(-1)} h_0) + D_y^\alpha \left( \frac{r^2 C_{\alpha}}{2t^2} \right) \partial_{\eta}^\alpha (a_{1}^{(-1)}) \right)$$

$$+ T \partial_{\eta}^\alpha (a_{0}^{(-1)}) D_y^\alpha \left( \frac{1}{t} Z_1 \right) + D_y^\alpha \left( \frac{r C_{\alpha}}{2t^2} \right) \partial_{\eta}^\alpha (a_{0}^{(-1)}) \bar{\sigma} + g_{1,1} + g_{1,2},$$

which has been converted into a single Mellin operator symbol modulo a type-$a$ and $b$ Green operator symbol, in the same manner as it has been discussed for the initial left parametrix in Section 2.3. After insertion of the corresponding asymptotic symbols of the initial and first order parametrix, the type-$a$ Green operator symbol becomes

$$g_{1,1} = \sigma' \omega_{1,\eta} r \sum_{\alpha} \frac{1}{\alpha!} \text{op}_M^{-1} \left( \left( (-2t^2) T^2 \partial_{\eta}^\alpha (d_{0,0}^{(1)} + d_{0,2}^{(1)} + r d_{1,1}^{(1)} + r^2 d_{2,0}^{(1)}) \right) (\bar{\sigma}' \sigma - 1) \text{op}_M^{-1} (D_y^\alpha a_0) \bar{\sigma} \right)$$

$$+ \sigma' \omega_{1,\eta} \sum_{\alpha} \frac{1}{\alpha!} \text{op}_M^{-1} \left( \left( (-2t^2) T^2 \partial_{\eta}^\alpha (d_{0,0}^{(0)} + d_{0,2}^{(0)} + r d_{1,1}^{(0)} + r^2 d_{2,0}^{(0)}) \right) (\bar{\sigma}' \sigma - 1) \text{op}_M^{-1} (r' D_y^\alpha a_1) \bar{\sigma} \right).$$
The corresponding type-\(b\) Green operator symbol is given by

\[
g_{1,2} = \sigma' \omega'_{1,\eta} r \sum_{\alpha} \frac{1}{a^{\alpha}} D_{y}^\alpha \left( r^2 C_{y} \right) \left[ \text{op}_{M} \gamma^{-3} \left( (-2t^2) \partial_y^\alpha (d_{0,0}^{(1)} + d_{0,1}^{(1)} + r d_{1,0}^{(1)}) \right) \right.
\]
\[
- \text{op}_{M}^{-1} \left( (-2t^2) \partial_y^\alpha (d_{0,0}^{(1)} + d_{0,1}^{(1)} + r d_{1,0}^{(1)}) \right) \]
\[
+ \sigma' \omega'_{1,\eta} r \sum_{\alpha} \frac{1}{a^{\alpha}} \left[ \text{op}_{M}^{-1} \left( (-2t^2) T \partial_y^\alpha (d_{0,0}^{(0)} + d_{0,2}^{(0)} + r d_{1,1}^{(0)} + r^2 d_{2,0}^{(0)}) \right) \right.
\]
\[
- \text{op}_{M}^{-1} \left( (-2t^2) T \partial_y^\alpha (d_{0,0}^{(0)} + d_{0,2}^{(0)} + r d_{1,1}^{(0)} + r^2 d_{2,0}^{(0)}) \right) \]
\[
+ \sigma' \omega'_{1,\eta} r \sum_{\alpha} \frac{1}{a^{\alpha}} D_{y}^\alpha \left( \text{irC}_{y} \right) \left[ \text{op}_{M}^{-1} \left( (-2t^2) \partial_y^\alpha (d_{0,0}^{(0)} + d_{0,2}^{(0)} + r d_{1,1}^{(0)} + r^2 d_{2,0}^{(0)}) \right) \right.
\]
\[
- \text{op}_{M}^{-1} \left( (-2t^2) \partial_y^\alpha (d_{0,0}^{(0)} + d_{0,2}^{(0)} + r d_{1,1}^{(0)} + r^2 d_{2,0}^{(0)}) \right) \]
\[
\right]
\]
\[
= -2t^2 \sigma' \omega'_{1,\eta} \left[ r^2 \text{Res}(d_{0,0}^{(1)}, 1) M \left( \frac{C_{y}}{2t^2} \sigma(\cdot) \right) (1) + r \text{Res}(d_{0,0}^{(1)}, 2) M \left( \frac{C_{y}}{2t^2} \sigma(\cdot) \right) (2) \right.
\]
\[
+ \sum_{\alpha} \frac{1}{a^{\alpha}} \left( r \text{Res}(\partial_y^\alpha d_{0,1}^{(1)}, 2) + r^2 \text{Res}(\partial_y^\alpha d_{1,0}^{(1)}, 2) \right) M \left( D_{y}^\alpha \left( \frac{C_{y}}{2t^2} \sigma(\cdot) \right) (2) \right.
\]
\[
+ \text{Res}(T d_{0,0}^{(0)}, 1) M \left( \frac{1}{t} Z_1 \sigma(\cdot) \right) (1) + \sum_{\alpha} \frac{1}{a^{\alpha}} \left( \text{Res}(\partial_y^\alpha d_{0,2}^{(0)}, 1) \right.
\]
\[
+ r \text{Res}(T \partial_y^\alpha d_{1,1}^{(0)}, 1) + r^2 \text{Res}(T \partial_y^\alpha d_{2,0}^{(0)}, 1) \right) M \left( D_{y}^\alpha \left( \frac{1}{t} Z_1 \sigma(\cdot) \right) (2) \right.
\]
\[
+ r \text{Res}(d_{0,0}^{(0)}, 1) M \left( \frac{\text{irC}_{y}}{2t^2} \sigma(\cdot) \right) (1) + \text{Res}(d_{0,0}^{(0)}, 2) M \left( \frac{\text{irC}_{y}}{2t^2} \sigma(\cdot) \right) (2) \right.
\]
\[
+ \sum_{\alpha} \frac{1}{a^{\alpha}} \left( \text{Res}(\partial_y^\alpha d_{0,2}^{(0)}, 2) + r \text{Res}(\partial_y^\alpha d_{1,1}^{(0)}, 2) + r^2 \text{Res}(\partial_y^\alpha d_{2,0}^{(0)}, 2) \right) M \left( D_{y}^\alpha \left( \frac{\text{irC}_{y}}{2t^2} \sigma(\cdot) \right) (2) + O(r^3) \right]
\]
\]

where in the second step Cauchy's residue theorem has been applied.

### 4.2.3 Green operators from second recursion step of the parametrix construction

The second order contribution to the asymptotic parametrix from the left side is given by

\[
\sigma' \omega'_{1,\eta} r^2 \sum_{\alpha} \frac{1}{a^{\alpha}} \partial_y^\alpha \left( \text{op}_{M}^{-1} \left( T^2 a_2^{(-1)} \right) \right) \sigma' \sigma D_{y}^\alpha \left( \text{op}_{M}^{-1} (a_0) \right) \]
\[
+ \sigma' \omega'_{1,\eta} r^2 \sum_{\alpha} \frac{1}{a^{\alpha}} \partial_y^\alpha \left( \text{op}_{M}^{-2} \left( T a_1^{(-1)} \right) \right) \sigma' \sigma D_{y}^\alpha \left( \text{op}_{M}^{-1} (a_1) \right) \]
\[
+ \sigma' \omega'_{1,\eta} r^2 \sum_{\alpha} \frac{1}{a^{\alpha}} \partial_y^\alpha \left( \text{op}_{M}^{-3} (a_0^{(-1)}) \right) \sigma' \sigma D_{y}^\alpha \left( \text{op}_{M}^{-1} (a_2) \right) \]
\[
= \sigma' \omega'_{1,\eta} r^2 \sum_{\alpha} \frac{1}{a^{\alpha}} \text{op}_{M}^{-1} \left( D_{y} \left( -\frac{1}{2t^2} \right) T^2 \partial_y^\alpha (a_2^{(-1)} h_0) + D_{y} \left( \frac{\text{irC}_{y}}{2t^2} \right) \partial_y^\alpha a_2^{(-1)} \right.
\]
\[
+ T \partial_y^\alpha a_1^{(-1)} D_{y} \left( \frac{1}{t} Z_1 \right) D_{y} \left( \frac{\text{irC}_{y}}{2t^2} \right) \partial_y^\alpha a_1^{(-1)} + \partial_y^\alpha a_0^{(-1)} D_{y} \left( -\frac{1}{2t^2} \right) w - \frac{1}{6t^2} \Delta_s^2 + \frac{1}{t} Z_2 \right)
\]
\[
+ D_{y} \left( \frac{\text{irC}_{y}}{2t^2} \right) T^2 \partial_y^\alpha a_0^{(-1)} \left. \right) \sigma + g_{2,1} + g_{2,2},
\]

which has been converted into a single Mellin operator symbol modulo a type-\(a\) and \(b\) Green operator symbol, similar to the previous recursion steps. After insertion of the corresponding asymptotic
symbols of the initial, first and second order parametrix, the type-\(a\) Green operator symbol becomes
\[
g_{2,1} = \sigma' \omega_{1,\eta} r^2 \sum_{\alpha} \frac{1}{\alpha!} \text{op}^{-1} \left( \frac{-2t^2 \sigma^a}{\sigma} \partial^a_{\eta} \partial_{d_{0,0}}^l \right) \left( \sigma' \sigma - 1 \right) \text{op}^{-1} \left( D_y^a a_0 \right) \tilde{\sigma} \\
+ \sigma' \omega_{1,\eta} r^2 \sum_{\alpha} \frac{1}{\alpha!} \text{op}^{-1} \left( \frac{-2t^2 \sigma^a}{\sigma} \partial^a_{\eta} \left( d_{0,0}^{(0)} + d_{0,1}^{(0)} + r d_{1,0}^{(1)} \right) \left( \sigma' \sigma - 1 \right) \text{op}^{-1} \left( r'^2 D_y^{a} a_1 \right) \tilde{\sigma} \\
+ \sigma' \omega_{1,\eta} r^2 \sum_{\alpha} \frac{1}{\alpha!} \text{op}^{-1} \left( \frac{-2t^2 \sigma^a}{\sigma} \partial^a_{\eta} \left( d_{0,0}^{(0)} + d_{0,2}^{(0)} + r d_{1,1}^{(0)} + r^2 d_{2,0}^{(0)} \right) \left( \sigma' \sigma - 1 \right) \text{op}^{-1} \left( r'^2 D_y^{a} a_2 \right) \tilde{\sigma} \\
\]
The corresponding type-\(b\) Green operator symbol is given by
\[
g_{2,2} = \sigma' \omega_{1,\eta} r^2 \sum_{\alpha} \frac{1}{\alpha!} \left[ \text{op}^{-3} \left( \frac{-2t^2 \sigma^a}{\sigma} \partial^a_{\eta} \left( d_{0,0}^{(0)} + d_{0,2}^{(0)} + r d_{1,1}^{(1)} + r^2 d_{2,0}^{(0)} \right) \right) \right. \\
- \text{op}^{-1} \left( \frac{-2t^2 \sigma^a}{\sigma} \partial^a_{\eta} \left( d_{0,0}^{(0)} + d_{0,2}^{(0)} + r d_{1,1}^{(1)} + r^2 d_{2,0}^{(0)} \right) \right] \text{op}^{-1} \left( D_y^a \left( \frac{4 \sigma^a T}{\sigma^2} \right) \right) \tilde{\sigma} \\
+ \sigma' \omega_{1,\eta} r^2 \sum_{\alpha} \frac{1}{\alpha!} \left[ \text{op}^{-2} \left( \frac{-2t^2 \sigma^a}{\sigma} \partial^a_{\eta} \left( d_{0,0}^{(0)} + d_{0,1}^{(1)} + r d_{1,0}^{(1)} \right) \right) \right. \\
- \text{op}^{-1} \left( \frac{-2t^2 \sigma^a}{\sigma} \partial^a_{\eta} \left( d_{0,0}^{(0)} + d_{0,1}^{(1)} + r d_{1,0}^{(1)} \right) \right] \text{op}^{-1} \left( D_y^a \left( \frac{4 \sigma^a Z_1}{\sigma^2} \right) \right) \tilde{\sigma} \\
+ \sigma' \omega_{1,\eta} r^2 \sum_{\alpha} \frac{1}{\alpha!} \left[ \text{op}^{-3} \left( \frac{-2t^2 \sigma^a}{\sigma} \partial^a_{\eta} \left( d_{0,0}^{(2)} \right) \right) \right. \\
- \text{op}^{-1} \left( \frac{-2t^2 \sigma^a}{\sigma} \partial^a_{\eta} \left( d_{0,0}^{(2)} \right) \right] \tilde{\sigma} \\
= -2t^2 \sigma' \omega_{1,\eta} \left[ \left. r \text{Res} \left( d_{0,0}^{(0)}, 1 \right) M \left( \text{op}^{-1} \left( \frac{-4 \sigma^a T}{\sigma^2} \right) \right) \left( \sigma' \sigma - 1 \right) \right. \text{op}^{-1} \left( D_y^a \left( \frac{4 \sigma^a Z_1}{\sigma^2} \right) \right) \tilde{\sigma} \right] \right] (1) \\
+ \text{Res} \left( d_{0,0}^{(0)}, 2 \right) M \left( \text{op}^{-1} \left( \frac{-4 \sigma^a T}{\sigma^2} \right) \right) \left( \sigma' \sigma - 1 \right) \text{op}^{-1} \left( D_y^a \left( \frac{4 \sigma^a Z_1}{\sigma^2} \right) \right) \tilde{\sigma} \right] (2) \\
+ \left( \text{Res} \left( \partial^a_{\eta} d_{0,0}^{(0)}, 2 \right) + r \text{Res} \left( \partial^a_{\eta} d_{0,1}^{(1)}, 2 \right) + r^2 \text{Res} \left( \partial^a_{\eta} d_{2,0}^{(2)}, 2 \right) \right) M \left( \text{op}^{-1} \left( D_y^a \left( \frac{4 \sigma^a T}{\sigma^2} \right) \right) \right) \tilde{\sigma} \right] (3) \\
+ r^2 \text{Res} \left( T^{-2} d_{0,0}^{(0)}, 2 \right) \text{Res} \left( \text{op}^{-1} \left( D_y^a \left( \frac{4 \sigma^a Z_1}{\sigma^2} \right) \right) \right) \tilde{\sigma} \right] (4) \\
+ \left( \text{Res} \left( \partial^a_{\eta} d_{0,2}^{(0)}, 4 \right) + r \text{Res} \left( T^{-2} \partial^a_{\eta} d_{0,1}^{(1)}, 4 \right) + r^2 \text{Res} \left( T^{-2} \partial^a_{\eta} d_{2,0}^{(2)}, 4 \right) \right) M \left( \text{op}^{-1} \left( D_y^a \left( \frac{4 \sigma^a Z_1}{\sigma^2} \right) \right) \right) \tilde{\sigma} \right] (5) \\
+ r \text{Res} \left( T d_{0,0}^{(1)}, 1 \right) M \left( \text{op}^{-1} \left( D_y^a \left( \frac{4 \sigma^a Z_1}{\sigma^2} \right) \right) \right) \tilde{\sigma} \right] (6) \\
+ \left( \text{Res} \left( d_{0,0}^{(1)}, 1 \right) + \text{Res} \left( d_{0,2}^{(0)}, 2 \right) \right) M \left( \text{op}^{-1} \left( D_y^a \left( \frac{4 \sigma^a Z_1}{\sigma^2} \right) \right) \right) \tilde{\sigma} \right] (7) \\
+ \left( \text{Res} \left( \partial^a_{\eta} d_{0,1}^{(1)}, 2 \right) + r \text{Res} \left( \partial^a_{\eta} d_{1,0}^{(1)}, 2 \right) \right) M \left( \text{op}^{-1} \left( D_y^a \left( \frac{4 \sigma^a Z_1}{\sigma^2} \right) \right) \right) \tilde{\sigma} \right] (8) \\
+ r^2 \text{Res} \left( d_{0,0}^{(0)}, 2 \right) M \left( \text{op}^{-1} \left( D_y^a \left( \frac{4 \sigma^a Z_1}{\sigma^2} \right) \right) \right) \tilde{\sigma} \right] + O(r^3) \right] (9) \right] \\
\]
where again in the second step Cauchy’s residue theorem has been applied.

### 4.2.4 Green operators from remainders

In our application, we want to apply the asymptotic parametrix up to second order, i.e., \( P \sim P_0 + r P_1 + r^2 P_2 + \cdots \), from the left to the shifted Hamiltonian \( \tilde{A} \). In the previous paragraphs, however, this has been done only up to second order in the asymptotic expansion of the shifted Hamiltonian, i.e., \( \tilde{A} \sim A_0 + r A_1 + r^2 A_2 + \cdots \). Therefore, certain Green operators of second and lower order are still missing which originate from higher order equations in the asymptotic parametrix construction.

Let us first consider contributions from \( P_0 \), which can be derived from the third order equation

\[
P_0 r^3 S_3 = 0 \mod L_G^0 + L_{flat}^0 \quad \text{with } r^3 S_3 := r^3 A_3 + r^4 A_4 + \cdots.
\]

In terms of operator valued symbols this corresponds to

\[
\sigma' \omega_{1,\eta}^{-1} r^3 \sum_{\alpha} \frac{1}{\alpha!} \partial^\alpha \left( (a_{0}^{-1}(a_0^{-1})(\sigma_D^{\alpha}(a_0^{-1}(a_0^{-1}(\sigma_D^{\alpha}(a_0^{-1}(a_0^{-1})))))) \right) \sigma' \sigma' D_y^\alpha \left( \sigma_D^{\alpha}(a_0^{-1}(a_0^{-1}(\sigma_D^{\alpha}(a_0^{-1}(a_0^{-1}(\sigma_D^{\alpha}(a_0^{-1}(a_0^{-1}))))))) \right) = g_{0,3} + g_{0,4} \mod L_{flat}^0,
\]

where the operator valued Green symbols \( g_{0,3} \) and \( g_{0,4} \) can be obtained along the same line of arguments as presented in the previous paragraphs. Let us first consider the type-\( b \) Green operator symbol

\[
g_{0,3} = \sigma' \omega_{1,\eta}^{-1} r^3 \sum_{\alpha} \frac{1}{\alpha!} \partial^\alpha \left( (a_{0}^{-1}(a_0^{-1}(a_0^{-1}(\sigma_D^{\alpha}(a_0^{-1}(a_0^{-1}(\sigma_D^{\alpha}(a_0^{-1}(a_0^{-1}))))))) \right) \sigma' \sigma' D_y^\alpha \left( \sigma_D^{\alpha}(a_0^{-1}(a_0^{-1}(\sigma_D^{\alpha}(a_0^{-1}(a_0^{-1}(\sigma_D^{\alpha}(a_0^{-1}(a_0^{-1}))))))) \right).
\]

where once again Cauchy’s residue theorem has been applied. Similarly, the type-\( a \) Green operator symbol also follows from this calculation, i.e.,

\[
g_{0,4} = \sigma' \omega_{1,\eta}^{-1} r^3 \sum_{\alpha} \frac{1}{\alpha!} \partial^\alpha \left( (a_{0}^{-1}(a_0^{-1}(a_0^{-1}(\sigma_D^{\alpha}(a_0^{-1}(a_0^{-1}(\sigma_D^{\alpha}(a_0^{-1}(a_0^{-1}))))))) \right) \sigma' \sigma' D_y^\alpha \left( \sigma_D^{\alpha}(a_0^{-1}(a_0^{-1}(\sigma_D^{\alpha}(a_0^{-1}(a_0^{-1}(\sigma_D^{\alpha}(a_0^{-1}(a_0^{-1}))))))) \right) (\sigma' \sigma - 1) \sigma_D^{\alpha}(a_0^{-1}(a_0^{-1}(\sigma_D^{\alpha}(a_0^{-1}(a_0^{-1}(\sigma_D^{\alpha}(a_0^{-1}(a_0^{-1})))))))) \sigma.
\]

Actually, as already mentioned before, these type-\( a \) and \( b \) Green operator symbols are of second and lower order.

Next, let us consider the additional Green operators originating from \( P_1 \), which can be obtained from the third order equation

\[
r P_1 r^2 S_2 = 0 \mod L_G^0 + L_{flat}^0 \quad \text{with } r^2 S_2 := r^2 A_2 + r^3 A_3 + \cdots.
\]

In terms of operator valued symbols this corresponds to

\[
\sigma' \omega_{1,\eta}^{-1} r^3 \sum_{\alpha} \frac{1}{\alpha!} \partial^\alpha \left( (a_{0}^{-1}(a_0^{-1}(a_0^{-1}(\sigma_D^{\alpha}(a_0^{-1}(a_0^{-1}(\sigma_D^{\alpha}(a_0^{-1}(a_0^{-1}))))))) \right) \sigma' \sigma' D_y^\alpha \left( \sigma_D^{\alpha}(a_0^{-1}(a_0^{-1}(\sigma_D^{\alpha}(a_0^{-1}(a_0^{-1}(\sigma_D^{\alpha}(a_0^{-1}(a_0^{-1}))))))) \right) \sigma = g_{1,3} + g_{1,4} \mod L_{flat}^0.
\]
Like before let us first consider the type-$b$ Green operator symbol

\[ g_{1,3} = \sigma' \omega_{1,\eta} r^3 \sum_{\alpha} \frac{1}{\alpha!} \left[ \text{op}_M^{\gamma-3}((-2t^2)\partial_{\eta}^\alpha(d_{0,0}^{(1)} + d_{0,1}^{(1)} + rd_{1,0}^{(1)})) \right. \\
\left. - \text{op}_M^{\gamma-1}(((-2t^2)\partial_{\eta}^\alpha(d_{0,0}^{(1)} + d_{0,1}^{(1)} + rd_{1,0}^{(1)})) \right] \text{op}_M^{\gamma-1}(D_y^\alpha s_2) \tilde{\sigma} \]

\[ = -2t^2 \sigma' \omega_{1,\eta} \left[ r^2 \text{Res}(d_{0,0}^{(1)}, 1) M(\text{op}_M^{\gamma-1}(s_2) \tilde{\sigma}(\cdot))(1) + r \text{Res}(d_{0,0}^{(1)}, 2) M(\text{op}_M^{\gamma-1}(s_2) \tilde{\sigma}(\cdot))(2) \right. \\
\left. + \sum_{\alpha} \frac{1}{\alpha!} \left( r \text{Res}(\partial_{\eta}^\alpha d_{0,1}^{(1)}, 2) + r^2 \text{Res}(\partial_{\eta}^\alpha d_{1,0}^{(1)}, 2) \right) M(\text{op}_M^{\gamma-1}(D_y^\alpha s_2) \tilde{\sigma}(\cdot))(2) + \mathcal{O}(r^3) \right] \]

and subsequently the type-$a$ Green operator symbol

\[ g_{1,4} = \sigma' \omega_{1,\eta} r^4 \sum_{\alpha} \frac{1}{\alpha!} \text{op}_M^{\gamma-1}((-2t^2)T^2 \partial_{\eta}^\alpha(d_{0,0}^{(1)} + d_{0,1}^{(1)} + rd_{1,0}^{(1)})) (\tilde{\sigma}' \sigma - 1) \text{op}_M^{\gamma-1}(r^2 D_y^\alpha s_2) \tilde{\sigma}. \]

Finally, let us consider the additional Green operators originating from $P_2$, which can be obtained from the third order equation

\[ r^2 P_2 r S_1 = 0 \mod L_G^0 + L_{\text{flat}}^0 \quad \text{with} \quad r S_1 := r A_1 + r^2 A_2 + \cdots. \]

In terms of operator valued symbols this corresponds to

\[ \sigma' \omega_{1,\eta} r^4 \sum_{\alpha} \frac{1}{\alpha!} \partial_{\eta}^\alpha (\text{op}_M^{\gamma-3}(s_2^{(-1)})) \tilde{\sigma}' \sigma r^{-1} D_y^\alpha (\text{op}_M^{\gamma-1}(s_1)) \tilde{\sigma} = g_{2,3} + g_{2,4} \mod L_{\text{flat}}^0. \]

The type-$b$ Green operator symbol is given by

\[ g_{2,3} = \sigma' \omega_{1,\eta} r^3 \left[ \text{op}_M^{\gamma-2}((-2t^2)T d_{0,0}^{(2)}) - \text{op}_M^{\gamma-1}((-2t^2)T d_{0,0}^{(2)}) \right] \text{op}_M^{\gamma-1}(s_1) \tilde{\sigma} \]

\[ = -2t^2 \sigma' \omega_{1,\eta} \left[ r^2 \text{Res}(T d_{0,0}^{(2)}, 1) M(\text{op}_M^{\gamma-1}(s_1) \tilde{\sigma}(\cdot))(1) + \mathcal{O}(r^3) \right] \]

and the type-$a$ Green operator symbol by

\[ g_{2,4} = \sigma' \omega_{1,\eta} r^2 \text{op}_M^{\gamma-1}((-2t^2)T^2 d_{0,0}^{(2)})(\tilde{\sigma}' \sigma - 1) \text{op}_M^{\gamma-1}(r s_1) \tilde{\sigma}. \]

### 4.2.5 Summing up the $a$-type Green operator symbols

So far, we have applied Cauchy’s residue theorem only to type-$b$ Green operator symbols in order to fully exploit the formulas for these operators. It is the purpose of this paragraph to perform these calculations for type-$a$ Green operator symbols as well. Before applying Cauchy’s residue theorem, it is, however, convenient to first sum up all $a$-type Green operator symbols into a single operator,
\[ g_a := g_{0.1} + g_{0.4} + g_{1.1} + g_{1.4} + g_{2.1} + g_{2.4} \]
\[ = \sigma' \omega_{1.\eta} \sum_{\alpha} \frac{1}{\alpha!} \text{op}_{M}^{-1}((-2t^{2})T^{2} \partial_{\eta}^{\alpha}(d_{0,0}^{(0)} + d_{0,2}^{(0)} + r d_{1,0}^{(0)} + r^{2} d_{2,0}^{(0)}) \]
\[ + r(d_{0,0}^{(1)} + d_{0,1}^{(1)} + r d_{1,0}^{(1)} + r^{2} d_{2,0}^{(2)})(\sigma' - 1) \text{op}_{M}^{-1}(D_{y}^{\alpha} a) \sigma) \]
\[ = -2t^{2} \sigma' \omega_{1.\eta} \left[ \text{Res}(T^{2} d_{0,0}^{(0)}, 0) M((\sigma' - 1) \text{op}_{M}^{-1}(a) \sigma)(0) \right] \]
\[ + r \text{Res}(T^{2} d_{0,0}^{(0)}, -1) M((\sigma' - 1) \text{op}_{M}^{-1}(a) \sigma)(-1) \]
\[ + r^{2} \text{Res}(T^{2} d_{0,0}^{(0)}, -2) M((\sigma' - 1) \text{op}_{M}^{-1}(a) \sigma)(-2) \]
\[ + \sum_{\alpha} \frac{1}{\alpha!} \left( \text{Res}(T^{2} \partial_{\eta}^{\alpha} d_{0,2}^{(0)}, 0) + r \text{Res}(T^{2} \partial_{\eta}^{\alpha} d_{1,1}^{(0)}, 0) \right) \]
\[ + r^{2} \text{Res}(T^{2} \partial_{\eta}^{\alpha} d_{0,2}^{(0)}, 0) M((\sigma' - 1) \text{op}_{M}^{-1}(D_{y}^{\alpha} a) \sigma)(0) \]
\[ + r \text{Res}(T^{2} d_{0,0}^{(1)}, 0) M((\sigma' - 1) \text{op}_{M}^{-1}(a) \sigma)(0) \]
\[ + r^{2} \text{Res}(T^{2} d_{0,0}^{(1)}, -1) M((\sigma' - 1) \text{op}_{M}^{-1}(a) \sigma)(-1) \]
\[ + \sum_{\alpha} \frac{1}{\alpha!} \left( r \text{Res}(T^{2} \partial_{\eta}^{\alpha} d_{1,1}^{(1)}, 0) + r^{2} \text{Res}(T^{2} \partial_{\eta}^{\alpha} d_{1,1}^{(1)}, 0) \right) \]
\[ + r^{2} \text{Res}(T^{2} \partial_{\eta}^{\alpha} d_{0,2}^{(2)}, 0) M((\sigma' - 1) \text{op}_{M}^{-1}(D_{y}^{\alpha} a) \sigma)(0) + \mathcal{O}(r^{3}) \].

4.2.6 Calculation of the residues

Up to this point, we have obtained explicit formulas for all Green operator symbols which contribute up to second order in the asymptotics. What is only missing are the actual values of residues \( \text{Res}(T^{m} d_{n,j}^{(k)}, w_{0}) \) at certain poles \( w_{0} \) of the shifted meromorphic operator valued symbols \( T^{m} d_{n,j}^{(k)} \) of the asymptotic parametrix. The calculation of these residues is rather straightforward. However, for the convenience of the reader and in order to improve the comprehensibility of our calculations, we list values of all required residues in Appendix D.

4.3 Contributions of specific angular momenta to Green operators

It is a particularly pleasant feature of our asymptotic expansion to provide a resolution of the wavefunction near an edge not only with respect to the distance variable \( r \) but also with respect to the relative angular momentum of the coalescing particles. There is a well known constraint, cf. [25], on the relative angular momentum \( l \) of two particles with respect to the asymptotic order, i.e., only angular momenta \( l \leq k \) contribute to the \( r^{k} \)-term of the asymptotic expansion. This constraint is also an immediate consequence of our calculations and it is convenient to extract from our formulas of the Green operators, contributions of specific angular momenta.

Within the present work we consider the asymptotic expansion up to second order. Therefore, one can derive asymptotic information for angular momenta \( l = 0, 1, 2 \) with corresponding projection operators \( P_{0}, P_{1} \) and \( P_{2} \). For the entire \( a \)-type Green operator, defined in Section 4.2.5, the
individual angular momentum contributions are given by

\[
P_{0g_a} = 2t^2 \sigma' \omega'_{1,0} \left[ (1 + rtZ_1 + r^2 (-2 + (tZ_1)^2 + \frac{tZ_2}{3})) M((\sigma' \sigma - 1) \text{op}_{M}^{\gamma^{-1}}(a)\tilde{\sigma}(\cdot))(0) \right. \\
+ \frac{1}{6} t^2 \sum_{\alpha} \frac{1}{\alpha!} \partial_{\eta}^{\alpha} (C_0 - 4i t \tau + i C_1) M((\sigma' \sigma - 1) \text{op}_{M}^{\gamma^{-1}}(D_y^a)\tilde{\sigma}(\cdot))(0) \bigg] + \mathcal{O}(r^3),
\]

\[
P_{1g_a} = 2t^2 \sigma' \omega'_{1,0} \left[ \frac{1}{2} t^2 \left[ M((\sigma' \sigma - 1) \text{op}_{M}^{\gamma^{-1}}(a)\tilde{\sigma}(\cdot))(-1) - tZ_1 M((\sigma' \sigma - 1) \text{op}_{M}^{\gamma^{-1}}(a)\tilde{\sigma}(\cdot))(0) \right] + \mathcal{O}(r^3),
\]

\[
P_{2g_a} = 2t^2 \sigma' \omega'_{1,0} \left[ \frac{1}{2} t^2 \left[ M((\sigma' \sigma - 1) \text{op}_{M}^{\gamma^{-1}}(a)\tilde{\sigma}(\cdot))(-1) - tZ_1 M((\sigma' \sigma - 1) \text{op}_{M}^{\gamma^{-1}}(a)\tilde{\sigma}(\cdot))(0) \right] + \mathcal{O}(r^3),
\]

The remaining \(b\)-type Green operators are treated separately, with individual angular momentum contributions given by

\[
P_{0g_{0,2}} = 2t^2 \sigma' \omega'_{1,0} \left[ \left( 1 - \frac{1}{3} t^2 \right) M(\text{op}_{M}^{\gamma^{-1}}(r^3s_3)\tilde{\sigma}(\cdot))(0) \right. \\
+ \frac{1}{6} t^2 \sum_{\alpha} \frac{1}{\alpha!} \partial_{\eta}^{\alpha} (C_0 - 4i t \tau) M(D_y^a(r^3s_3)\tilde{\sigma}(\cdot))(0) \bigg] + \mathcal{O}(r^3),
\]

\[
P_{1g_{0,2}} = 2t^2 \sigma' \omega'_{1,0} \left[ \frac{1}{15} t^2 M(\frac{r^2 C_a}{2t^2} \tilde{\sigma}(\cdot))(0) + \mathcal{O}(r^3),
\]

\[
P_{2g_{0,2}} = 2t^2 \sigma' \omega'_{1,0} \left[ \frac{1}{15} t^2 M(\frac{r^2 C_a}{2t^2} \tilde{\sigma}(\cdot))(0) \\
- \frac{1}{30} t^2 \sum_{\alpha} \frac{1}{\alpha!} \partial_{\eta}^{\alpha} (C_0 - 4i t \tau) M(D_y^a(r^3s_3)\tilde{\sigma}(\cdot))(0) \bigg] + \mathcal{O}(r^3),
\]

\[
P_{0g_{0,3}} = 2t^2 \sigma' \omega'_{1,0} \left[ \left( 1 - \frac{1}{3} t^2 \right) M(\text{op}_{M}^{\gamma^{-1}}(r^3s_3)\tilde{\sigma}(\cdot))(0) \right. \\
+ \frac{1}{6} t^2 \sum_{\alpha} \frac{1}{\alpha!} \partial_{\eta}^{\alpha} (C_0 - 4i t \tau) M(\text{op}_{M}^{\gamma^{-1}}(r^3s_3)\tilde{\sigma}(\cdot))(0) \bigg] + \mathcal{O}(r^3),
\]

\[
P_{1g_{0,3}} = 2t^2 \sigma' \omega'_{1,0} \left[ \frac{1}{15} t^2 M(\text{op}_{M}^{\gamma^{-1}}(r^3s_3)\tilde{\sigma}(\cdot))(0) + \mathcal{O}(r^3),
\]

\[
P_{2g_{0,3}} = 2t^2 \sigma' \omega'_{1,0} \left[ \frac{1}{15} t^2 M(\text{op}_{M}^{\gamma^{-1}}(r^3s_3)\tilde{\sigma}(\cdot))(0) \\
- \frac{1}{30} t^2 \sum_{\alpha} \frac{1}{\alpha!} \partial_{\eta}^{\alpha} (C_0 - 4i t \tau) M(\text{op}_{M}^{\gamma^{-1}}(r^3s_3)\tilde{\sigma}(\cdot))(0) \bigg] + \mathcal{O}(r^3),
\]

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\[ \mathcal{P}_{0g_{1,2}} = 2t^2 \sigma' \omega'_{1,q} \left[ \left( rtZ_1 - \frac{5}{3} r^2 \right) M \left( \frac{r^2 \gamma_{1,2}^t}{2 \pi^2} \tilde{\sigma} \right)(0) \right. \\
+ \left( 1 - \frac{1}{3} r^2 \right) M (\text{op}_{M} \gamma_{1,2}^{-1} (ra_1) \tilde{\sigma} \cdot (0)) + \frac{1}{6} r^2 \sum_{\alpha} \frac{1}{\alpha} i \partial^\alpha_{\eta} C_1 M (D_{y}^\alpha \left( \frac{r^2 \gamma_{1,2}^t}{2 \pi^2} \tilde{\sigma} \right)(0) \right. \\
+ \left( 1 - \frac{1}{3} r^2 \right) M (\text{op}_{M} \gamma_{1,2}^{-1} (ra_1) \tilde{\sigma} \cdot (0)) + \frac{1}{6} r^2 \sum_{\alpha} \frac{1}{\alpha} i \partial^\alpha_{\eta} C_1 M (D_{y}^\alpha \left( \frac{r^2 \gamma_{1,2}^t}{2 \pi^2} \tilde{\sigma} \right)(0) \\
+ \left. \mathcal{O}(r^3) \right) , \\
\mathcal{P}_{0g_{1,2}} = 2t^2 \sigma' \omega'_{1,q} \left[ \frac{1}{6} t^2 Z_1 M \left( \frac{r^2 \gamma_{1,2}^{-1} (ra_1) \tilde{\sigma} \cdot (0) \right) \right. \\
+ \left( 1 - \frac{1}{3} r^2 \right) M (\text{op}_{M} \gamma_{1,2}^{-1} (ra_1) \tilde{\sigma} \cdot (0)) + \frac{1}{6} r^2 \sum_{\alpha} \frac{1}{\alpha} i \partial^\alpha_{\eta} C_1 M (D_{y}^\alpha \left( \frac{r^2 \gamma_{1,2}^t}{2 \pi^2} \tilde{\sigma} \right)(0) \\
+ \left. \mathcal{O}(r^3) \right) , \\
\mathcal{P}_{0g_{1,2}} = 2t^2 \sigma' \omega'_{1,q} \left[ \frac{1}{6} t^2 Z_1 M \left( \frac{r^2 \gamma_{1,2}^{-1} (ra_1) \tilde{\sigma} \cdot (0) \right) \right. \\
+ \left( 1 - \frac{1}{3} r^2 \right) M (\text{op}_{M} \gamma_{1,2}^{-1} (ra_1) \tilde{\sigma} \cdot (0)) + \frac{1}{6} r^2 \sum_{\alpha} \frac{1}{\alpha} i \partial^\alpha_{\eta} C_1 M (D_{y}^\alpha \left( \frac{r^2 \gamma_{1,2}^t}{2 \pi^2} \tilde{\sigma} \right)(0) \\
+ \left. \mathcal{O}(r^3) \right) , \\
\mathcal{P}_{0g_{1,2}} = 2t^2 \sigma' \omega'_{1,q} \left[ \frac{1}{6} t^2 Z_1 M \left( \frac{r^2 \gamma_{1,2}^{-1} (ra_1) \tilde{\sigma} \cdot (0) \right) \right. \\
+ \left( 1 - \frac{1}{3} r^2 \right) M (\text{op}_{M} \gamma_{1,2}^{-1} (ra_1) \tilde{\sigma} \cdot (0)) + \frac{1}{6} r^2 \sum_{\alpha} \frac{1}{\alpha} i \partial^\alpha_{\eta} C_1 M (D_{y}^\alpha \left( \frac{r^2 \gamma_{1,2}^t}{2 \pi^2} \tilde{\sigma} \right)(0) \\
+ \left. \mathcal{O}(r^3) \right) , \\
\mathcal{P}_{0g_{1,2}} = 2t^2 \sigma' \omega'_{1,q} \left[ \frac{1}{6} t^2 Z_1 M \left( \frac{r^2 \gamma_{1,2}^{-1} (ra_1) \tilde{\sigma} \cdot (0) \right) \right. \\
+ \left( 1 - \frac{1}{3} r^2 \right) M (\text{op}_{M} \gamma_{1,2}^{-1} (ra_1) \tilde{\sigma} \cdot (0)) + \frac{1}{6} r^2 \sum_{\alpha} \frac{1}{\alpha} i \partial^\alpha_{\eta} C_1 M (D_{y}^\alpha \left( \frac{r^2 \gamma_{1,2}^t}{2 \pi^2} \tilde{\sigma} \right)(0) \\
+ \left. \mathcal{O}(r^3) \right) , \\
\mathcal{P}_{0g_{1,2}} = 2t^2 \sigma' \omega'_{1,q} \left[ \frac{1}{6} t^2 Z_1 M \left( \frac{r^2 \gamma_{1,2}^{-1} (ra_1) \tilde{\sigma} \cdot (0) \right) \right. \\
+ \left( 1 - \frac{1}{3} r^2 \right) M (\text{op}_{M} \gamma_{1,2}^{-1} (ra_1) \tilde{\sigma} \cdot (0)) + \frac{1}{6} r^2 \sum_{\alpha} \frac{1}{\alpha} i \partial^\alpha_{\eta} C_1 M (D_{y}^\alpha \left( \frac{r^2 \gamma_{1,2}^t}{2 \pi^2} \tilde{\sigma} \right)(0) \\
+ \left. \mathcal{O}(r^3) \right) , \\
\mathcal{P}_{0g_{1,2}} = 2t^2 \sigma' \omega'_{1,q} \left[ \frac{1}{6} t^2 Z_1 M \left( \frac{r^2 \gamma_{1,2}^{-1} (ra_1) \tilde{\sigma} \cdot (0) \right) \right. \\
+ \left( 1 - \frac{1}{3} r^2 \right) M (\text{op}_{M} \gamma_{1,2}^{-1} (ra_1) \tilde{\sigma} \cdot (0)) + \frac{1}{6} r^2 \sum_{\alpha} \frac{1}{\alpha} i \partial^\alpha_{\eta} C_1 M (D_{y}^\alpha \left( \frac{r^2 \gamma_{1,2}^t}{2 \pi^2} \tilde{\sigma} \right)(0) \\
+ \left. \mathcal{O}(r^3) \right) , \\
\mathcal{P}_{0g_{1,2}} = 2t^2 \sigma' \omega'_{1,q} \left[ \frac{1}{6} t^2 Z_1 M \left( \frac{r^2 \gamma_{1,2}^{-1} (ra_1) \tilde{\sigma} \cdot (0) \right) \right. \\
+ \left( 1 - \frac{1}{3} r^2 \right) M (\text{op}_{M} \gamma_{1,2}^{-1} (ra_1) \tilde{\sigma} \cdot (0)) + \frac{1}{6} r^2 \sum_{\alpha} \frac{1}{\alpha} i \partial^\alpha_{\eta} C_1 M (D_{y}^\alpha \left( \frac{r^2 \gamma_{1,2}^t}{2 \pi^2} \tilde{\sigma} \right)(0) \\
+ \left. \mathcal{O}(r^3) \right) , \\
\mathcal{P}_{0g_{1,2}} = 2t^2 \sigma' \omega'_{1,q} \left[ \frac{1}{6} t^2 Z_1 M \left( \frac{r^2 \gamma_{1,2}^{-1} (ra_1) \tilde{\sigma} \cdot (0) \right) \right. \\
+ \left( 1 - \frac{1}{3} r^2 \right) M (\text{op}_{M} \gamma_{1,2}^{-1} (ra_1) \tilde{\sigma} \cdot (0)) + \frac{1}{6} r^2 \sum_{\alpha} \frac{1}{\alpha} i \partial^\alpha_{\eta} C_1 M (D_{y}^\alpha \left( \frac{r^2 \gamma_{1,2}^t}{2 \pi^2} \tilde{\sigma} \right)(0) \\
+ \left. \mathcal{O}(r^3) \right) , \\
\mathcal{P}_{0g_{1,2}} = 2t^2 \sigma' \omega'_{1,q} \left[ \frac{1}{6} t^2 Z_1 M \left( \frac{r^2 \gamma_{1,2}^{-1} (ra_1) \tilde{\sigma} \cdot (0) \right) \right. \\
+ \left( 1 - \frac{1}{3} r^2 \right) M (\text{op}_{M} \gamma_{1,2}^{-1} (ra_1) \tilde{\sigma} \cdot (0)) + \frac{1}{6} r^2 \sum_{\alpha} \frac{1}{\alpha} i \partial^\alpha_{\eta} C_1 M (D_{y}^\alpha \left( \frac{r^2 \gamma_{1,2}^t}{2 \pi^2} \tilde{\sigma} \right)(0) \\
+ \left. \mathcal{O}(r^3) \right) . \\
\]
\[ P_{0g_{2,3}} = 2t^2 \sigma' \omega_{1,\eta}^l \left[ r^2 \left( \frac{1}{3} (tZ_1)^2 + \frac{1}{3} tZ_2 \right) M \left( \text{op}_M^{-1} (r s_1) \tilde{\sigma} (\cdot) \right)(0) + O(r^3) \right], \]

\[ P_{1g_{2,3}} = 2t^2 \sigma' \omega_{1,\eta}^l \left[ -\frac{1}{6} r^2 (tZ_1)^2 M \left( \text{op}_M^{-1} (r s_1) \tilde{\sigma} (\cdot) \right)(0) + O(r^3) \right], \]

\[ P_{2g_{2,3}} = 2t^2 \sigma' \omega_{1,\eta}^l \left[ r^2 \left( \frac{1}{30} (tZ_1)^2 - \frac{1}{15} (1 + tZ_2) \right) M \left( \text{op}_M^{-1} (r s_1) \tilde{\sigma} (\cdot) \right)(0) + O(r^3) \right]. \]

Finally, the individual angular momentum resolved symbols of the Green operators can be arranged together in the form of Theorem 1, thus finishing its proof.

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Appendix

A \( \varepsilon \)-regularization of parametrix and Green operator

The motivation for this regularization procedure is to simplify the construction and evaluation of the asymptotic parametrix and corresponding Green operators. This can be achieved by attaching a scaling parameter \( \varepsilon \) to certain cut-off functions and by adding an appropriate Green operator to the equation for the parametrix. Let us first outline the basic idea in an informal manner for an eigenvalue problem of the general form \( A u_i = 0 \), where \( A = H - E_i \) corresponds to a Hamiltonian shifted by one of its eigenvalues. We want to recall, that the left parametrix equation

\[ PAu = (1 + G) u \]

yields the asymptotic behaviour of the eigenfunction via \( u_i = -Gu_i \). Now we add a parameter dependent Green operator \( G_\varepsilon^0 \), which in a certain weak sense (to be specified below) vanishes for \( \varepsilon \to 0 \), to the left hand side of the parametrix equation and introduce scaling parameters in certain cut-off functions which results in a modified equation

\[ P_\varepsilon Au + G_\varepsilon^0 u = (1 + G_\varepsilon) u, \tag{A.1} \]

where a parameter dependent parametrix \( P_\varepsilon \) appears on the left and a modified Green operator \( G_\varepsilon \) on the right hand side of the equation. With these modifications, the asymptotic behaviour follows from

\[ u_i = (G_\varepsilon^0 - G_\varepsilon) u_i. \tag{A.2} \]

In the generic case, it is not possible to perform the limit \( \varepsilon \to 0 \) in Eq. (A.1) with respect to a given norm \( \| \cdot \| \). However we are only interested in some particular functions \( u \), i.e., eigenfunctions which have special regularity and decay properties. In these particular cases it is actually possible to perform the limit \( \varepsilon \to 0 \) with respect to the norm \( \| \cdot \|_{W^{s,\gamma}} \) and to get a limiting equation of the form

\[ P_0 Au = (1 + G_0) u, \tag{A.3} \]

with

\[ P_0 Au := \lim_{\varepsilon \to 0} P_\varepsilon Au \quad \text{and} \quad G_0 u := \lim_{\varepsilon \to 0} G_\varepsilon u, \tag{A.4} \]
Lemma 2. Any function discussed before.

Let us consider the specific Proof.

\[ \lim_{\varepsilon \to 0} G_{\varepsilon}^{(0)} u = 0. \]

The asymptotic behaviour of the eigenfunction \( u_i \) can therefore be obtained from the equation

\[ -u_i = G_0 u_i. \]

In our specific applications we consider additional Green operators

\[ G_{\varepsilon}^{(0)} u = \int d\eta e^{i\eta y} g_{\varepsilon}^{(0)}(y, \eta) F_{y \to \eta} u \quad (A.5) \]

with operator valued symbols \( g_{\varepsilon}^{(0)}(y, \eta) \in R_G^{-m}(\mathbb{R}^3, \mathbb{R}) \) for \( m = 0, 1, 2, \ldots \), which are twisted homogeneous of order \( m \), i.e.,

\[ \kappa_{\lambda} g_{\varepsilon}^{(0)}(y, \eta) \kappa_{\lambda}^{-1} u = \lambda^m g_{\varepsilon}^{(0)}(y, \lambda \eta) u. \]

In particular let us assume a Green operator symbol of the following form

\[ g_{\varepsilon}^{(0)}(y, \eta) = \omega_{1, \varepsilon} r^{2+k} \text{op}_M \gamma^3 (d_{k,j})(y, \eta)(1 - \omega_{0, \varepsilon}) a_i(y, \eta) \omega_{0, \varepsilon y}, \quad (A.6) \]

with homogeneous parameter dependent differential operators \( a_i(y, \eta) \in \text{Diff}_{\leq q}(X^\gamma) \), \( i = 0, 1, 2 \), on the right and Mellin pseudo-differential operator with homogeneous parameter dependent symbol \( d_{k,j}(y, \eta) \) of order \( j \) on the left side. Such type of Green operator is twisted homogeneous of order \( m = 2 - i + k \).

Definition 1. Let us denote a particular function \( u \in \mathcal{W}^s(\mathbb{R}^q, K^{s,\gamma}(X^\gamma)) \) to be \( \varepsilon \)-regularizable with respect to \( G_{\varepsilon}^{(0)} \) if

\[ \lim_{\varepsilon \to 0} \| G_{\varepsilon}^{(0)} u \|_{\mathcal{W}^{s,\gamma}} = 0 \]

and the limits \( (A.4) \) exist, where we assume a Green operator symbol, cf. \( (A.5) \), of the type \( (A.6) \) discussed before.

For our purposes, the following lemma is sufficient.

Lemma 2. Any function \( u \in \mathcal{W}_{\text{comp}}^{\infty}(\mathbb{R}^q, K^{s,\gamma}(X^\gamma)) \subset \mathcal{W}^s(\mathbb{R}^q, K^{s,\gamma}(X^\gamma)) \) is \( \varepsilon \)-regularizable.

Proof. Let us consider the specific \( \mathcal{W}^s(\mathbb{R}^q, K^{s,\gamma}(X^\gamma)) \) norm

\[ \| G_{\varepsilon}^{(0)} u \|_{\mathcal{W}^{s,\gamma}}^2 := \int [\eta]^{2s} \kappa_{[\eta]}^{-1} (F_{y \to \eta} G_{\varepsilon}^{(0)} u)(\eta) \|_{K^{s,\gamma}}^2 d\eta. \]

Taking into account \( u \in \mathcal{W}_{\text{comp}}^{\infty}(\mathbb{R}^q, K^{s,\gamma}(X^\gamma)) \), let us perform the following estimate

\[ \| G_{\varepsilon}^{(0)} u \|_{\mathcal{W}^{s,\gamma}}^2 \leq \int [\eta]^{2s} \kappa_{[\eta]}^{-1} (F_{y \to \eta} G_{\varepsilon}^{(0)} u)(\eta) \|_{K^{s,\gamma}}^2 d\eta \]

\[ = \int [\eta]^{2s} \kappa_{[\eta]}^{-1} (F_{y \to \eta} \int d\tilde{\eta} e^{iy\tilde{\eta}} g_{\varepsilon}^{(0)}(y, \tilde{\eta}) F_{y \to \eta} u)(\eta) \|_{K^{s,\gamma}}^2 d\eta \]

\[ = \int [\eta]^{2s} \kappa_{[\eta]}^{-1} (F_{y \to \eta} \int d\tilde{\eta} e^{iy\tilde{\eta}} g_{\varepsilon}^{(0)}(y, \tilde{\eta})(r[\tilde{\eta}])^{-N} (r[\tilde{\eta}])^N F_{y \to \eta} u)(\eta) \|_{K^{s,\gamma}}^2 d\eta \]

\[ \leq \| G_{\varepsilon}^{(-N)} u \|_{\mathcal{W}_{\text{comp}}^{\infty}(\mathbb{R}^q, K^{s,\gamma}(X^\gamma))} \int [\eta]^{2s+2N} \kappa_{[\eta]}^{-1} (F_{y \to \eta} r^N u)(\eta) \|_{K^{s,\gamma}}^2 d\eta \]

with respect to the modified Green operator

\[ G_{\varepsilon}^{(-N)} u = \int d\eta e^{iy\eta} g_{\varepsilon}^{(0)}(y, \eta)(r[\eta])^{-N} F_{y \to \eta} u. \]
For $u \in \mathcal{W}_{\text{comp}}^{\infty}(\mathbb{R}^{q}, \mathcal{K}^{s,\gamma}(X^\wedge))$, the Fourier integral
\[
\int [\eta]^{2s-2N} \kappa_{\{\eta\}}^{-1} \left(F_{y-\eta} r^{N} u(\eta)\right)^{2} \kappa_{\{\eta\}}^{-1} \eta d\eta = \|r^{N} u\|^{2}_{\mathcal{W}_{\infty}^{s+N,\gamma}}
\]
is obviously finite and it remains to show that the operator norm of the modified Green operator vanishes for $\varepsilon \to 0$. According to [39, Theorem 1.3.59], its operator norm can be estimated by
\[
\|G_{\varepsilon}^{(-N)}\|_{\mathcal{L}(\mathcal{W}_{\infty}^{s,\varepsilon}, \mathcal{W}_{\infty}^{s,\varepsilon})} \lesssim \sup_{y \in Y} \sup_{\eta \in \mathbb{R}^{3}} \|\kappa_{\{\eta\}}^{-1} \partial_{y}^{\alpha} g_{\varepsilon}^{(0)}(y, \eta) (r^{N})^{-N} \kappa_{\{\eta\}}\|_{\mathcal{L}(\mathcal{K}^{s,\gamma}, \mathcal{K}^{s,\gamma})}
\]
with $s$ dependent constant $l$. In our particular applications, we consider local edges $Y$ which correspond to bounded open subsets of $\mathbb{R}^{3}$. Taking furthermore into account the smoothness properties of the symbol $g_{\varepsilon}^{(0)}$ it turns out to be sufficient to consider the norm estimate (A.7) pointwise with respect to the edge variables $y$. In order to estimate the operator norm, let us next take into account twisted homogeneity, i.e.,
\[
\|\kappa_{\{\eta\}}^{-1} \partial_{y}^{\alpha} g_{\varepsilon}^{(0)}(y, \eta) (r^{N})^{-N} \kappa_{\{\eta\}}\|_{\mathcal{L}(\mathcal{K}^{s,\gamma}, \mathcal{K}^{s,\gamma})} = [\eta]^{-m} \|\partial_{y}^{\alpha} g_{\varepsilon}^{(0)}(y, \eta/[\eta]) r^{N} \|_{\mathcal{L}(\mathcal{K}^{s,\gamma}, \mathcal{K}^{s,\gamma})}.
\]
Therefore, it is sufficient to consider the norm
\[
\|\partial_{y}^{\alpha} g_{\varepsilon}^{(0)}(y, \eta/[\eta]) r^{N} \|_{\mathcal{L}(\mathcal{K}^{s,\gamma}, \mathcal{K}^{s,\gamma})} = \sup_{v \in \mathcal{K}^{s,\gamma}} \|\partial_{y}^{\alpha} g_{\varepsilon}^{(0)}(y, \eta/[\eta]) r^{N} v\|_{\mathcal{K}^{s,\gamma}}.
\]
A simple calculation shows
\[
\|\partial_{y}^{\alpha} g_{\varepsilon}^{(0)}(y, \eta/[\eta]) r^{N} v\|_{\mathcal{K}^{s,\gamma}} = \varepsilon^{2m-N} \|\partial_{y}^{\alpha} g_{\varepsilon}^{(0)}(y, \eta/[\eta]) r^{N} v(\varepsilon^{-1} \cdot)\|_{\mathcal{K}^{s,\gamma}}.
\]
To proceed, we need to estimate $v(\varepsilon^{-1} \cdot)$ in the $\mathcal{K}^{s,\gamma}$-norm.

**Proposition 4.** For $v \in \mathcal{K}^{s,\gamma}(X^\wedge)$, we get the estimate
\[
\|v(\varepsilon^{-1} \cdot)\|_{\mathcal{K}^{s,\gamma}} \lesssim \varepsilon^{-\gamma-s+3/2} \|v\|_{\mathcal{K}^{s,\gamma}}.
\]

**Proof.** According to the definition, we have
\[
\|v(\varepsilon^{-1} \cdot)\|_{\mathcal{K}^{s,\gamma}} = \|v(\varepsilon^{-1} \cdot)\|_{\mathcal{H}^{s,\gamma}} + \|v(\varepsilon^{-1} \cdot)\|_{(1-\sigma)\mathcal{H}^{s}}.
\]

Let us first consider
\[
\|v(\varepsilon^{-1} \cdot)\|_{\mathcal{H}^{s,\gamma}}^{2} = \sum_{|\beta| \leq s} \int \sigma|x|^{-\gamma+|\beta|} \partial_{x}^{\beta} v(\varepsilon^{-1} \cdot) dx
\]

\[
= \sum_{|\beta| \leq s} \int \sigma(\varepsilon \cdot) |x|^{-\gamma+|\beta|} \partial_{x}^{\beta} v|^{2} \varepsilon^{3} dx
\]

\[
= \sum_{|\beta| \leq s} \varepsilon^{-2\gamma+3} \left[ \int \sigma|x|^{-\gamma+|\beta|} \partial_{x}^{\beta} v|^{2} dx + \int (1-\sigma)\sigma(\varepsilon \cdot) |x|^{-\gamma+|\beta|} \partial_{x}^{\beta} v|^{2} dx \right],
\]

where w.l.o.g. we assume in the last line $\sigma \prec \sigma(\varepsilon \cdot)$ for $\varepsilon$ sufficiently small. In order to estimate the second term, let us first observe
\[
(1-\sigma)|x|^{-2\gamma} \leq C_{1} \quad \text{for } \gamma > 0
\]
and
\[
\sigma(\varepsilon \cdot) \varepsilon|x|^{2|\beta|} \leq C_{2}.
\]
Therefore, we get the estimate
\[
\int (1 - \sigma) \sigma (\epsilon ) \| x |^{-\gamma + |\beta |} \partial_x^\beta v \|^2 dx \lesssim \epsilon^{-2|\beta|} \int (1 - \sigma) | \partial_x^\beta v |^2 dx
\]
which yields
\[
\| v (\epsilon^{-1} \cdot ) \|^2_{H^{s, \gamma}} \lesssim \epsilon^{-2\gamma + 3} \| v \|_{H^{s, \gamma}} + \epsilon^{-2\gamma - 2s + 3} \| v \|_{(1 - \sigma)H^s}
\]
\[
\lesssim \epsilon^{-2\gamma - 2s + 3} \| v \|_{H^{s, \gamma}}.
\]
For the remaining part of (A.8), we get the estimate
\[
\| v (\epsilon^{-1} \cdot ) \|_{(1 - \sigma)H^s} \lesssim \sum_{|\beta| \leq s} \int (1 - \sigma) | \partial_x^\beta v |^2 dx
\]
\[
\lesssim \sum_{|\beta| \leq s} \epsilon^{-2|\beta| + 3} \int (1 - \sigma (\epsilon \cdot )) | \partial_x^\beta v |^2 dx
\]
\[
\lesssim \epsilon^{-2s + 3} \| v \|_{(1 - \sigma)H^s}.
\]
Putting all together, we, finally, get the desired estimate.

We can now estimate the operator norm in the following manner
\[
\| \partial_\alpha y g (0) \|_{L(K^{s, \gamma}, K^{s, \gamma})} \lesssim \epsilon^{-\gamma - s - \frac{1}{2} - m + N} \sup_{v \in K^{s, \gamma}} \| \partial_\alpha g (0) (y, \eta/[\eta]) r^{-N} v (\epsilon^{-1} \cdot ) \|_{K^{s, \gamma}}
\]
\[
\lesssim \epsilon^{-\gamma - s - \frac{1}{2} - m + N} \| \partial_\alpha g (0) (y, \eta/[\eta]) r^{-N} \|_{L(K^{s, \gamma}, K^{s, \gamma})}
\]
and, therefore, for \( N > \gamma + s + \frac{1}{2} + m \), we get
\[
\lim_{\epsilon \to 0} \| \partial_\alpha g (0) (y, \eta/[\eta]) r^{-N} \|_{L(K^{s, \gamma}, K^{s, \gamma})} = 0.
\]

\[\square\]

\section{Some simple calculations in the noninteracting case}

On a first glance, the asymptotic expression for the Green operator (3.1) looks rather awkward concerning the explicit formulas of the coefficients \( Q_{l,n} \) given in terms of Mellin transforms. In this appendix we present some explicit calculations for wavefunctions of two noninteracting electrons, i.e., we consider the equation
\[
\left( -\frac{1}{2} (\Delta_1 + \Delta_2) - \frac{Z}{|x_1|} - \frac{Z}{|x_2|} \right) \Psi(x_1, x_2) = E \Psi(x_1, x_2).
\]
In particular, it provides an independent check for the correctness of our asymptotic Green operator. Obviously it is only the \( e - n \) cusp which can be studied for different angular momenta \( l = 0, 1, 2 \).

Let us start with \( l = 0 \), where the exact ground state wavefunction\( ^6 \) is given in hyperspherical coordinates
\[
u_0(r, t) = e^{-Zt(\sin r + \cos r)}.
\]
\( ^6 \)Here and in the following we disregard proper normalization constants.
The corresponding asymptotic expansion is given by
\[ u_0(r,t) \sim (1 - Ztr + \frac{1}{2}(Zt + (Zt)^2)r^2 \cdots )e^{-Zt}. \]
We want to calculate
\[ Gu_0(r,y) = \int d\eta e^{i\eta y} \tilde{u}_0(y,\eta). \]
Let us first note that
\[ \int d\eta e^{i\eta y} Q_{0,1}(\tilde{u}_0) = \int d\eta e^{i\eta y} M(\text{op}_{M}^{-1}(h_1(0))\tilde{\sigma}\tilde{u}_0)(0), \]
because
\[ \int d\eta e^{i\eta y} M(\sigma'\sigma \text{op}_{M}^{-1}(a)\tilde{\sigma}\tilde{u}_0)(0) = 0, \]
which is due to the fact that the Mellin operator can be expressed as a local Hamiltonian operator, i.e., \( \sigma'\sigma r^2 (H - E_0)\tilde{\sigma} \) with cut-off functions \( \sigma' < \hat{\sigma} \) such that \( Hu_0 = E_0u_0 \) is satisfied on the support of \( \sigma'\sigma \). The remaining term becomes
\[ \int d\eta e^{i\eta y} M(\text{op}_{M}^{-1}(h_1(0))\tilde{\sigma}\tilde{u}_0)(0) \]
\[ = \frac{1}{2t^2}(w^2 - w)M(\tilde{\sigma}u_0)_{w=0} \]
\[ = \frac{1}{2t^2} \int_0^\infty dr e^{-r} \left[ (-r\partial_r)^2(\tilde{\sigma}u_0) - (-r\partial_r)(\tilde{\sigma}u_0) \right] \bigg|_{w=0} \]
\[ = \frac{1}{2t^2} \int_0^\infty dr \left[ \partial_r(r\partial_r(\tilde{\sigma}u_0)) + \partial_r(\tilde{\sigma}u_0) \right] \]
\[ = -\frac{1}{2t^2} u_0(0) \]
\[ = -\frac{1}{2t^2} e^{-Zt}. \]
In order to calculate
\[ \int d\eta e^{i\eta y} Q_{0,2}(\tilde{u}_0) \]
let us replace the product of pseudo-differential operators by a product of the corresponding differential operators and using the same arguments as before we obtain
\[ \int d\eta e^{i\eta y} Q_{0,2}(\tilde{u}_0) = (-t^2\partial_t^2 - 9t\partial_t) \int d\eta e^{i\eta y} M(\text{op}_{M}^{-1}(h_1(0))\tilde{\sigma}\tilde{u}_0)(0) \]
\[ = (-t^2\partial_t^2 - 9t\partial_t)(-\frac{1}{2t^2})e^{-Zt} \]
\[ = (12 + 5Zt - Z^2t^2)(-\frac{1}{2t^2})e^{-Zt}. \]
Putting things together one recovers the required asymptotic identity
\[ Gu_0(r,y) = \int d\eta e^{i\eta y} g\tilde{u}_0(y,\eta) \]
\[ \sim 2t^2 \left[ \left( 1 + rtZ_1 + r^2 (-2 + \frac{1}{3}(tZ_1)^2 + \frac{1}{3}tZ_2) \right) \int d\eta e^{i\eta y} Q_{0,1}(\tilde{u}_0)(y,\eta) \right. \]
\[ + \frac{1}{6}t^2 \int d\eta e^{i\eta y} Q_{0,2}(\tilde{u}_0)(y,\eta) + \cdots \]
\[ \sim -(1 - rtZ - 2r^2 + \frac{2}{3}Z^2(tr)^2 - \frac{ZtZ^2}{3})e^{-Zt} - \frac{1}{6}t^2(12 + 5Zt - Z^2t^2)e^{-Zt} \]
\[ \sim -(1 - rtZ + \frac{1}{3}tZ^2 + \frac{1}{2}Z^2(tr)^2)e^{-Zt} \]
\[ \sim -u_0, \]
where we used $Z_1 = -Z$ and $Z_2 = -tE_0 - Z = t - Z$ in the noninteracting case.

For $l = 1$ let us consider the noninteracting wavefunction

$$u_1(r, t) = t \sin re^{-\frac{Z}{2}t} e^{-Zt\cos r} Y_{1,m}(\theta_1, \phi_1),$$

with asymptotic expansion

$$u_1(r, t) \sim tr(1 - Ztr)e^{-Zt} Y_{1,m}(\theta_1, \phi_1).$$

Once again we want to calculate

$$Gu_1(r, y) = \int d\eta e^{iy\eta} g\hat{u}_1(y, \eta)$$

in the asymptotic limit $r \to 0$. Following the same line of arguments as before we get

$$\int d\eta e^{iym} Q_{1,1}(\hat{u}_1) = \int d\eta e^{iy\eta} M(op_{op}^{-1}(h_{11}(1))\sigma\hat{u}_1)(-1) - tZ_1 \int d\eta e^{iy\eta} M(op_{op}^{-1}(h_{11}(1))\sigma\hat{u}_1)(0)$$

$$= \frac{1}{2\pi^2} \int_0^\infty dr \int_0^\infty d\eta e^{-\frac{Z}{2}t(\sigma\hat{u}_1)(0) - 2\sigma u_1(0)}.$$

Let us now substitute $u_1 = r\hat{u}_1$, from which it follows that the last integral vanishes and one gets

$$\int d\eta e^{iym} Q_{1,1}(\hat{u}_1) = \int d\eta e^{iy\eta} M(op_{op}^{-1}(h_{11}(1))\sigma\hat{u}_1)(-1) - tZ_1 \int d\eta e^{iy\eta} M(op_{op}^{-1}(h_{11}(1))\sigma\hat{u}_1)(0)$$

$$= \frac{1}{2\pi^2} \int_0^\infty dr \int_0^\infty d\eta e^{-\frac{Z}{2}t(\sigma\hat{u}_1)(0) - 2\sigma u_1(0)}.$$

The asymptotic expansion becomes

$$Gu_1(r, y) = \int d\eta e^{iy\eta} g\hat{u}_1(y, \eta) \sim -\frac{1}{2\pi^2} \int_0^\infty dr \int_0^\infty d\eta e^{-\frac{Z}{2}t} (tr - \frac{1}{2}Z(tr)^2)e^{-Zt} Y_{1,m}(\theta_1, \phi_1) \sim -u_1.$$

Finally, for $l = 2$ let us consider the noninteracting wavefunction

$$u_2(r, t) = t^2 \sin^2 re^{-\frac{Z}{3}t\sin r} e^{-Zt\cos r} Y_{2,m}(\theta_1, \phi_1) \sim (tr)^2 e^{-Zt} Y_{2,m}(\theta_1, \phi_1).$$

In this case the corresponding coefficients become

$$\int d\eta e^{iym} Q_{2,1}(\hat{u}_2) = \int \int d\eta e^{iy\eta} M(op_{op}^{-1}(h_{22}(1))\sigma\hat{u}_2)(-1) - \frac{1}{2}tZ_1 \int d\eta e^{iy\eta} M(op_{op}^{-1}(h_{22}(1))\sigma\hat{u}_2)(0)$$

$$+ \frac{1}{2} \int_0^\infty \int d\eta e^{iy\eta} M(op_{op}^{-1}(h_{22}(1))\sigma\hat{u}_2)(0) \int d\eta e^{iy\eta} M(op_{op}^{-1}(h_{22}(1))\sigma\hat{u}_2)(0).$$

$$\int d\eta e^{iym} Q_{2,2}(\hat{u}_2) = \int \int d\eta e^{iy\eta} M(op_{op}^{-1}(h_{22}(1))\sigma\hat{u}_2)(0) \int d\eta e^{iy\eta} M(op_{op}^{-1}(h_{22}(1))\sigma\hat{u}_2)(0).$$
Setting \( u_2 = r^2 \tilde{u}_2 \), explicit calculations yield

\[
\int d\eta e^{i\eta y} M(\text{op}_M \gamma^{-1}(h_1^{(2)}) \tilde{u}_2)(0) = -\frac{1}{2\pi i} \int_0^\infty dr 6r\tilde{u},
\]

\[
\int d\eta e^{i\eta y} M(\text{op}_M \gamma^{-1}(h_2^{(2)}) \tilde{u}_2)(-1) = -\frac{1}{2\pi i} \int_0^\infty dr (4 + 2trZ_1)\tilde{u},
\]

\[
\int d\eta e^{i\eta y} M(\text{op}_M \gamma^{-1}(h_3^{(2)}) \tilde{u}_2)(-2) = \frac{1}{2\pi i} \left( w^2 - w - 6 + \frac{8}{3}r^2w + (rt)^2 \partial_t^2 + 5r^2t\partial_t - 2rtZ_12r^2 - 2r^2tZ_2 \right) \times M(\tilde{\sigma}u_2)|_{w=-2}
\]

\[
= \frac{1}{2\pi i} \int_0^\infty dr \left( 5\partial_r\tilde{u} + rt^2\partial_t^2\tilde{u} + 5rt\partial_t\tilde{u} - 2tZ_1\tilde{u} - 2r\tilde{u} - 2trZ_2\tilde{u} \right).
\]

Summing up, one gets

\[
\int d\eta e^{i\eta y} Q_{1,2}(\tilde{u}_2) = \frac{1}{2\pi i} \int_0^\infty dr \left( 5\partial_r\tilde{u} + rt^2\partial_t^2\tilde{u} + 5rt\partial_t\tilde{u} - 12r\tilde{u} \right),
\]

\[
\int d\eta e^{i\eta y} Q_{2,2}(\tilde{u}_2) = \left( -t^2\partial_t^2 - 9t\partial_t \right) \int d\eta e^{i\eta y} M(\text{op}_M \gamma^{-1}(h_1^{(2)}) \tilde{u}_2)(0)
\]

\[
= \left( -t^2\partial_t^2 - 9t\partial_t \right) \left( -\frac{1}{2\pi i} \right) \int_0^\infty dr 6r\tilde{u}
\]

\[
= \frac{1}{2\pi i} \int_0^\infty dr \left( 6rt^2\partial_t^2\tilde{u} + 30rt\partial_t\tilde{u} - 72r\tilde{u} \right)
\]

and, finally,

\[
Gu_2(r, y) = \int d\eta e^{i\eta y} g\tilde{u}_2(y, \eta)
\]

\[
\sim 2t^2 \left[ \frac{1}{5} r^2 \int d\eta e^{i\eta y} Q_{1,2}(\tilde{u}_2) - \frac{1}{30} r^2 \int d\eta e^{i\eta y} Q_{2,2}(\tilde{u}_2) \cdots \right]
\]

\[
\sim r^2 \int_0^\infty dr \partial_r\tilde{u}
\]

\[
\sim -r^2\tilde{u}_2(0)
\]

\[
\sim -(tr)^2 e^{-Zt}Y_{2,m}(\theta_1, \phi_1)
\]

\[
\sim -u_2.
\]

### C  Location and multiplicity of poles of Mellin type symbols

In Section 3.3 we have discussed the absence of logarithmic terms in the edge asymptotic behaviour of eigenfunctions of the Hamiltonian. Within our approach, this follows from the multiplicity of poles of Mellin type symbols of the parametrix. The present work did not attempt to give a complete description of the location and multiplicity of these poles. Instead we merely want to summarize in this Appendix our findings from the previous calculations.

Let us start with the symbol \( a_0^{-1} \), where our calculations can be subsumed in the following remark which shows that all of its poles are simple.
Remark 7. The poles of the meromorphic operator valued symbols $q_{0,n}$, $n = 0, 1, \ldots$, are determined by the recursive relation (1.3). A simple calculation shows that

$$(h_0 - 2n(2w - 5 - 2n))^{-1}$$

is a meromorphic operator valued symbol with simple poles at $w = 2n + 3 + l$ and $w = 2n + 2 - l$ with $l = 0, 1, \ldots$, which follows from the spectral decomposition of the Laplace-Beltrami operator on $S^2$, i.e., $\Delta_{S^2} = -\sum_{l=0}^{\infty} l(l+1)P_l$. Furthermore, it follows from $2m + 3 + l \neq 2n + 2 - l$, i.e., $2(n - m) \neq 2l + 1$, that $d_{j,n}$, $j, n = 0, 1, \ldots$, are meromorphic operator valued symbols with simple poles at $w \in \mathbb{Z}$.

At next let us consider the operator valued symbol $a_1^{-1}$, where a new type of denominator appears in $d_{0,0}^{(1)}$ which is of the form

$$h_0(h_0 - (2w - 6)).$$

Resolving $\Delta_{S^2}$ like in the previous remark, we get

$$P_l h_0 = (w - 2)^2 - (w - 2) - l(l + 1) = (w - 3 - l)(w - 2 + l)$$

with simple zeros at $w_1 = 3 + l$ and $w_2 = 2 - l$, as well as

$$P_l(h_0 - (2w - 6)) = (w - 4 - l)(w - 3 + l)$$

with simple zeros at $w_3 = 4 + l$ and $w_4 = 3 - l$, respectively. Combining both factors it turns out that only for $l = 0$ a multiple zero appears at $w_1 = w_4 = 3$.

Closing our discussion, we consider the operator valued symbol $a_2^{-1}$, where the denominator of $d_{0,0}^{(2)}$ is of the form

$$h_0(h_0 - (2w - 6)) (h_0 - 2(2w - 7)).$$

The additional factor $(h_0 - 2(2w - 7))$ has simple poles at $w_5 = 5 + l$ and $w_6 = 4 - l$, respectively. Therefore, multiple zeros appear for $l = 0$ at $w_3 = w_6 = 4$ and $w_1 = w_4 = 3$, respectively.

D Calculation of the residues

In this appendix, we provide the necessary residues of the meromorphic operator valued symbols of the asymptotic parametrix up to second order. Let us first list the angular momentum resolved shifted symbols. The two shifted symbols contributing to zero and first order are given by

$$T^n d_{0,0}^{(0)}(w) = \sum_l \frac{P_l}{(w - (l + 3 - n))(w - (2 - l - n))},$$

and

$$T^n d_{0,0}^{(1)}(w) = 2t Z_l \sum_l \frac{P_l}{(w - (l + 3 - n))(w - (2 - l - n))(w - (l + 4 - n))(w - (3 - l - n))},$$

respectively. For the symbols contributing in second order it is convenient to define the meromorphic function

$$h_n(w) := \sum_l \frac{P_l}{(w - (l + 3 - n))(w - (2 - l - n))(w - (l + 5 - n))(w - (4 - l - n))},$$

with it these symbols become

$$\partial_\eta T^n d_{0,2}^{(0)}(w) = r^2 \partial_\eta C_0 h_n(w), \quad \partial_\eta T^n d_{1,1}^{(0)}(w) = -r \partial_\eta (4it\tau) h_n(w), \quad \partial_\eta T^n d_{2,0}^{(0)}(w) = -2h_n(w),$$
\[ T^\alpha d_{0,0}^{(1)}(w) = -10 h_n(w), \quad \partial^\alpha_\eta T^\alpha d_{0,1}^{(1)}(w) = i r \partial^\alpha_\eta C_1 h_n(w), \]

\[ T^n d_{0,0}^{(2)}(w) = \sum_l \left[ \frac{(2tZ_1)^2}{(w-(l+4-n))(w-(3-l-n))} - \frac{1}{3} (8(w - 2 + n) - l(l + 1) - 6tZ_2) \right] h_n(w). \]

The corresponding residues which are required in our calculations for the entire \( a \)-type Green operator, defined in Section 4.2.5, are given by

\[ g_a : \]

\[ \text{Res}(T^2 d_{0,0}^{(0)}, -l) = -\frac{1}{2l+1} \mathcal{P}_l, \]

\[ \text{Res}(T^2 d_{0,0}^{(1)}, -l) \mathcal{P}_l = -\frac{2tZ_1}{2(2l+1)(l+1)} \mathcal{P}_l, \quad (l \geq 0), \]

\[ \text{Res}(T^2 d_{0,0}^{(1)}, 1-l) \mathcal{P}_l = \frac{2tZ_1}{2(2l+1)} \mathcal{P}_l \quad (l \geq 1), \]

\[ \text{Res}(T^2 d_{0,0}^{(1)}, -m) = -\frac{2tZ_1}{2(2m+1)(m+1)} \mathcal{P}_m + \frac{2tZ_1}{2(m+1)(2m+3)} \mathcal{P}_{1+m} \quad (m \geq 0), \]

\[ \text{Res}(T^2 d_{0,0}^{(2)}, 1-l) \mathcal{P}_l = \frac{(2tZ_1)^2}{4(l+1)(l+1)} \mathcal{P}_l \quad (l \geq 1), \]

\[ \text{Res}(T^2 d_{0,0}^{(2)}, -l) \mathcal{P}_l = -\left[ \frac{(2tZ_1)^2}{(l+1)(2l+1)(2l+3)} + \frac{l(l+1)+6tZ_2}{6(2l+1)^2} \right] \mathcal{P}_l \quad (l \geq 0), \]

\[ \text{Res}(T^2 d_{0,0}^{(2)}, 2-l) \mathcal{P}_l = -\left[ \frac{(2tZ_1)^2}{4(l+1)(2l+1)(2l+3)} + \frac{l(l+9)+6tZ_2}{6(2l+1)(2l+1)} \right] \mathcal{P}_l \quad (l \geq 2), \]

\[ \text{Res}(T^2 d_{0,0}^{(2)}, -m) = -\left[ \frac{(2tZ_1)^2}{4(m+1)(2m+3)(2m+3)} + \frac{m(m+9)+6tZ_2}{6(2m+3)(2m+3)} \right] \mathcal{P}_m + \frac{(2tZ_1)^2}{4(m+1)(2m+3)(m+2)} \mathcal{P}_{1+m} \]

\[ + \left[ -\frac{(2tZ_1)^2}{4(m+1)(2m+3)(2m+3)} + \frac{m(m+9)+6tZ_2}{6(2m+3)(2m+3)} \right] \mathcal{P}_{2+m} \quad (m \geq 0), \]

\[ \text{Res}(\partial^\alpha_\eta T^2 d_{0,2}^{(0)}, -l) \mathcal{P}_l = -r^2 \partial^\alpha_\eta C_0 \frac{1}{2(l+1)(2l+3)} \mathcal{P}_l, \quad (l \geq 0), \]

\[ \text{Res}(\partial^\alpha_\eta T^2 d_{0,2}^{(0)}, 2-l) \mathcal{P}_l = r^2 \partial^\alpha_\eta C_0 \frac{1}{2(l+1)(2l+1)} \mathcal{P}_l \quad (l \geq 2), \]

\[ \text{Res}(\partial^\alpha_\eta T^2 d_{0,2}^{(0)}, -m) = r^2 \partial^\alpha_\eta C_0 \left( -\frac{1}{2(2m+1)(2m+3)} \mathcal{P}_m + \frac{1}{2(2m+5)(2m+3)} \mathcal{P}_{2+m} \right) \quad (m \geq 0), \]

\[ \text{Res}(\partial^\alpha_\eta T^2 d_{0,1}^{(1)}, -l) \mathcal{P}_l = -ir \partial^\alpha_\eta C_1 \frac{1}{2(l+1)(2l+3)} \mathcal{P}_l, \quad (l \geq 0), \]

\[ \text{Res}(\partial^\alpha_\eta T^2 d_{0,1}^{(1)}, 2-l) \mathcal{P}_l = ir \partial^\alpha_\eta C_1 \frac{1}{2(l+1)(2l+1)} \mathcal{P}_l \quad (l \geq 2), \]

\[ \text{Res}(\partial^\alpha_\eta T^2 d_{0,1}^{(1)}, -m) = ir \partial^\alpha_\eta C_1 \left( -\frac{1}{2(2m+1)(2m+3)} \mathcal{P}_m + \frac{1}{2(2m+5)(2m+3)} \mathcal{P}_{2+m} \right) \quad (m \geq 0). \]
Finally, the remaining residues corresponding to various $b$-type Green operators are given by

\[
g_{0.2} : \quad \text{Res}(d_{0,0}^{(0)}, 1) = -\frac{1}{3} P_1, \quad \text{Res}(d_{0,0}^{(0)}, 2) = -P_0,
\]
\[
\text{Res}(\partial_\eta^0 d_{0,2}^{(0)}, 1) = r^2 \partial_\eta^0 C_0 \left[ -\frac{4}{35} P_1 + \frac{1}{30} P_3 \right],
\]
\[
\text{Res}(\partial_\eta^0 d_{0,2}^{(0)}, 2) = r^2 \partial_\eta^0 C_0 \left[ -\frac{1}{10} P_0 + \frac{1}{30} P_2 \right],
\]
\[
g_{0.3} : \quad \text{Res}(T^{-1} d_{0,0}^{(0)}, 1) = -\frac{1}{3} P_2, \quad \text{Res}(T^{-1} d_{0,0}^{(0)}, 2) = -\frac{1}{3} P_1, \quad \text{Res}(T^{-1} d_{0,0}^{(0)}, 3) = -P_0,
\]
\[
\text{Res}(T^{-1} \partial_\eta^0 d_{0,2}^{(0)}, 1) = r^2 \partial_\eta^0 C_0 \left[ -\frac{1}{35} P_2 + \frac{1}{120} P_4 \right],
\]
\[
\text{Res}(T^{-1} \partial_\eta^0 d_{0,2}^{(0)}, 2) = r^2 \partial_\eta^0 C_0 \left[ -\frac{1}{35} P_1 + \frac{1}{70} P_3 \right],
\]
\[
\text{Res}(T^{-1} \partial_\eta^0 d_{0,2}^{(0)}, 3) = r^2 \partial_\eta^0 C_0 \left[ -\frac{1}{6} P_0 + \frac{1}{30} P_2 \right],
\]

\[
g_{1.2} : \quad \text{Res}(T d_{0,0}^{(0)}, 1) = -P_0, \quad \text{Res}(d_{0,0}^{(0)}, 1) = -\frac{1}{3} P_1, \quad \text{Res}(d_{0,0}^{(0)}, 2) = -P_0,
\]
\[
\text{Res}(T \partial_\eta^0 d_{0,2}^{(0)}, 1) = r^2 \partial_\eta^0 C_0 \left[ -\frac{1}{6} P_0 + \frac{1}{30} P_2 \right],
\]
\[
\text{Res}(\partial_\eta^0 d_{0,2}^{(0)}, 1) = r^2 \partial_\eta^0 C_0 \left[ -\frac{1}{35} P_1 + \frac{1}{70} P_3 \right],
\]
\[
\text{Res}(\partial_\eta^0 d_{0,2}^{(0)}, 2) = r^2 \partial_\eta^0 C_0 \left[ -\frac{1}{6} P_0 + \frac{1}{30} P_2 \right],
\]
\[
\text{Res}(d_{0,0}^{(1)}, 1) = 2t Z_1 \left[ -\frac{1}{12} P_1 + \frac{1}{20} P_2 \right],
\]
\[
\text{Res}(d_{0,0}^{(1)}, 2) = 2t Z_1 \left[ -\frac{1}{7} P_0 + \frac{1}{6} P_1 \right],
\]
\[
\text{Res}(\partial_\eta^0 d_{0,1}^{(1)}, 1) = i r \partial_\eta^0 C_1 \left[ -\frac{1}{30} P_1 + \frac{1}{70} P_3 \right],
\]
\[
\text{Res}(\partial_\eta^0 d_{0,1}^{(1)}, 2) = i r \partial_\eta^0 C_1 \left[ -\frac{1}{6} P_0 + \frac{1}{30} P_2 \right],
\]

\[
g_{1.3} : \quad \text{Res}(d_{0,0}^{(1)}, 1) = 2t Z_1 \left[ -\frac{1}{12} P_1 + \frac{1}{20} P_2 \right],
\]
\[
\text{Res}(d_{0,0}^{(1)}, 2) = 2t Z_1 \left[ -\frac{1}{7} P_0 + \frac{1}{6} P_1 \right],
\]
\[
\text{Res}(\partial_\eta^0 d_{0,1}^{(1)}, 1) = i r \partial_\eta^0 C_1 \left[ -\frac{1}{30} P_1 + \frac{1}{70} P_3 \right],
\]
\[
\text{Res}(\partial_\eta^0 d_{0,1}^{(1)}, 2) = i r \partial_\eta^0 C_1 \left[ -\frac{1}{6} P_0 + \frac{1}{30} P_2 \right],
\]
\[ g_{2,2} : \]
\[
\text{Res}(d_{0,0}^{(0)}, 1) = -\frac{1}{3} P_1, \quad \text{Res}(d_{0,0}^{(0)}, 2) = -P_0, \quad \text{Res}(T^{-2}d_{0,0}^{(0)}, 1) = -\frac{1}{7} P_3,
\]
\[
\text{Res}(T^{-2}d_{0,0}^{(0)}, 2) = -\frac{1}{5} P_2, \quad \text{Res}(T^{-2}d_{0,0}^{(0)}, 3) = -\frac{1}{3} P_1, \quad \text{Res}(T^{-2}d_{0,0}^{(0)}, 4) = -P_0,
\]
\[
\text{Res}(d_{0,0}^{(2)}, 1) = -\left[\frac{1}{30}(tZ_1)^2 + \frac{1}{15}(5 + 3tZ_2)\right] P_1 + \frac{1}{30}(tZ_1)^2 P_2
\]
\[
+ \left[-\frac{1}{105}(tZ_1)^2 + \frac{1}{105}(10 + 3tZ_2)\right] P_3
\]
\[
\text{Res}(d_{0,0}^{(2)}, 2) = -\left[\frac{1}{3}(tZ_1)^2 + \frac{1}{3} tZ_2\right] P_0 + \frac{1}{6}(tZ_1)^2 P_1
\]
\[
+ \left[-\frac{1}{30}(tZ_1)^2 + \frac{1}{15}(1 + tZ_2)\right] P_2
\]
\[
\text{Res}(Td_{0,0}^{(1)}, 1) = 2tZ_1 \left[-\frac{1}{2} P_0 + \frac{1}{6} P_1\right],
\]
\[
\text{Res}(d_{0,0}^{(1)}, 1) = 2tZ_1 \left[-\frac{1}{12} P_1 + \frac{1}{30} P_2\right],
\]
\[
\text{Res}(d_{0,0}^{(1)}, 2) = 2tZ_1 \left[-\frac{1}{2} P_0 + \frac{1}{6} P_1\right],
\]
\[
\text{Res}(\partial_\eta^\alpha d_{0,2}^{(0)}, 1) = r^2 \partial_\eta^\alpha C_0 \left[-\frac{1}{30} P_1 + \frac{1}{10} P_3\right],
\]
\[
\text{Res}(\partial_\eta^\alpha d_{0,2}^{(0)}, 2) = r^2 \partial_\eta^\alpha C_0 \left[-\frac{1}{6} P_0 + \frac{1}{30} P_2\right],
\]
\[
\text{Res}(T^{-2}\partial_\eta^\alpha d_{0,2}^{(0)}, 1) = r^2 \partial_\eta^\alpha C_0 \left[-\frac{1}{120} P_3 + \frac{1}{198} P_5\right],
\]
\[
\text{Res}(T^{-2}\partial_\eta^\alpha d_{0,2}^{(0)}, 2) = r^2 \partial_\eta^\alpha C_0 \left[-\frac{1}{40} P_2 + \frac{1}{120} P_4\right],
\]
\[
\text{Res}(T^{-2}\partial_\eta^\alpha d_{0,2}^{(0)}, 3) = r^2 \partial_\eta^\alpha C_0 \left[-\frac{1}{30} P_1 + \frac{1}{40} P_3\right],
\]
\[
\text{Res}(T^{-2}\partial_\eta^\alpha d_{0,2}^{(0)}, 4) = r^2 \partial_\eta^\alpha C_0 \left[-\frac{1}{6} P_0 + \frac{1}{30} P_2\right],
\]
\[
\text{Res}(T\partial_\eta^\alpha d_{0,1}^{(1)}, 1) = ir \partial_\eta^\alpha C_1 \left[-\frac{1}{6} P_0 + \frac{1}{30} P_2\right],
\]
\[
\text{Res}(\partial_\eta^\alpha d_{0,1}^{(1)}, 1) = ir \partial_\eta^\alpha C_1 \left[-\frac{1}{30} P_1 + \frac{1}{10} P_3\right],
\]
\[
\text{Res}(\partial_\eta^\alpha d_{0,1}^{(1)}, 2) = ir \partial_\eta^\alpha C_1 \left[-\frac{1}{6} P_0 + \frac{1}{30} P_2\right],
\]
\[ g_{2,3} : \]
\[
\text{Res}(Td_{0,0}^{(2)}, 1) = -\left[\frac{1}{3}(tZ_1)^2 + \frac{1}{3} tZ_2\right] P_0 + \frac{1}{6}(tZ_1)^2 P_1
\]
\[
+ \left[-\frac{1}{30}(tZ_1)^2 + \frac{1}{15}(1 + tZ_2)\right] P_2.
\]
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