SYMMETRIES OF THE HYDROGEN ATOM

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ABSTRACT. We exhibit a new type of symmetry of the Schrödinger equation for the hydrogen atom that uses algebraic families of groups. We prove that the regular solutions of the Schrödinger equation carry the structure of an algebraic family of Harish-Chandra modules, and we characterize this family. We show that the spectrum of the Schrödinger operator and the spaces of definite energy states, as they are calculated in physics, may be obtained from these families, the latter via a Jantzen filtration. Then we connect these algebraic constructions with analytic techniques from spectral theory and scattering theory. We use the limiting absorption principle to give an explicit description of the family of intertwining operators to which the Jantzen technique is applied and we compare the algebraic family of regular solutions with the measurable family of solutions of the Schrödinger equation that is obtained from Hilbert space spectral theory.

1. INTRODUCTION

It has long been known that, besides its visible rotational symmetries, the Schrödinger equation for the hydrogen atom possesses hidden symmetries that explain the degeneracy of energy eigenspaces, and help determine the eigenvalues and eigenfunctions. The purpose of this paper is to fit all these symmetries into a new algebraic form, called an algebraic family of Harish-Chandra pairs, and then analyze the consequences in detail. We shall determine the spectrum using the family, and then explore further implications for the solutions of the Schrödinger equation, as they are understood both in physics and in spectral theory.

Among other things, we shall develop a new, conceptual and algebraic perspective on results in scattering theory that connect the bound and unbound states of the hydrogen atom. Our approach refines these scattering-theoretic results and eliminates apparent singularities that arise in the transition between positive and negative energies.

The time-independent Schrödinger equation for the hydrogen atom is the eigenvalue equation

\[
H\psi = E\psi,
\]

where \(\psi\) is a function on \(\mathbb{R}^3\), \(E\) is a real number (the energy), and \(H\) is the Schrödinger operator

\[
H = -\frac{\hbar^2}{2\mu} \Delta - \frac{e^2}{r}.
\]

Here \(\mu\) is the reduced mass, \(e^2\) is the square of the electron charge, \(\hbar\) is the reduced Planck’s constant, and \(r\) is the distance in \(\mathbb{R}^3\) from the origin.

In physics, one seeks solutions of (1.0.1) with definite total angular momentum and a definite component of angular momentum along some chosen axis. One
further imposes the condition that $\psi$ be square-integrable, or almost square integrable. The linear span of all such $\psi$, as the angular momenta vary but the energy $E$ is fixed, is what we shall call the physical solution space $\text{PhysSol}(E)$. From the physics point of view, the spectrum of the Schrödinger operator is the set of all real $E$ for which the physical solution space is nonzero. It has the form

$$\text{Spec}(H) = \left\{ -\frac{e^4 \mu}{2\hbar^2 n^2} : n = 1, 2, \ldots \right\} \sqcup [0, \infty).$$

This is one of the fundamental formulas in non-relativistic quantum mechanics.

The orthogonal group $K = O(3)$ acts on each physical solution space. But it was discovered early on that $\text{PhysSol}(E)$ is also acted on by a 6-dimensional Lie algebra that varies with $E$ and extends the Lie algebra $\mathfrak{so}(3)$. This was first done by Pauli [Pau26] in the case where $E$ is negative, whose work was subsequently developed by Fock [Foc35], Bargmann [Bar36] and many others, leading to the discovery of hidden symmetry Lie algebra actions for all $E$, and also unitary Lie group representations on Hilbert space completions of the physical solution spaces.

Roughly speaking, an algebraic family of Harish-Chandra pairs over a complex variety is a collection of complex Lie algebras, together with a collection of complex algebraic groups, that are both parametrized by the points of the variety, and that both vary algebraically from point to point. Our work begins with the construction, directly from the Schrödinger equation, of an algebraic family of Harish-Chandra pairs $(\mathfrak{g}, K)$.

For us, the base variety will be the complex affine line, corresponding to the set of possible complex eigenvalues $E$ in (1.0.1). The family of groups $K$ will be the constant family whose fiber is the complexification of the visible symmetry group $O(3)$. To obtain the family of Lie algebras we examine in Section 2 the centralizer of the Schrödinger operator $H$ in the algebra of differential operators on $\mathbb{R}^3_0$, the complement of the origin in $\mathbb{R}^3$. The first and second order elements in the centralizer determine a Lie algebra $\mathfrak{g}$ over the algebra $\mathcal{O}$ of polynomials in $H$. We view $\mathfrak{g}$ as a family of Lie algebras over the maximal ideal spectrum of $\mathcal{O}$ (namely the affine line).

Because the family $\mathfrak{g}$ is concretely realized as differential operators, it carries a natural complex conjugation operation $\sigma$, also called a real structure, from which we obtain a family $\left(\mathfrak{g}^{\sigma}, K^{\sigma}\right)$ of real Harish-Chandra pairs over the real line. The family of groups $K^{\sigma}$ is the constant family with fiber $O(3)$. The fibers of the real family $\mathfrak{g}^{\sigma}$ are

$$\mathfrak{g}^{\sigma}|_E \cong \begin{cases} \mathfrak{so}(3,1) & E > 0 \\ \mathfrak{so}(3) \ltimes \mathbb{R}^3 & E = 0 \\ \mathfrak{so}(4) & E < 0. \end{cases}$$

These are precisely the Lie algebras that arise in the theory of hidden symmetries. Moreover, it is a simple matter to pass from Lie algebras to Lie groups:

**Theorem** (See Section 2). There is an algebraic family of complex algebraic groups $G$ over the complex affine line, together with a real structure that is compatible with the standard real structure on the complex line, such that the associated algebraic family of Lie
algebras is the family $g$ above, and such that, for every $E \in \mathbb{R}$, the associated real group is
\[
G^\sigma|_E = \begin{cases} 
SO(3, 1) & E > 0 \\
O(3) \ltimes \mathbb{R}^3 & E = 0 \\
SO(4) & E < 0.
\end{cases}
\]

In a previous paper [Sub18], results similar to those above were obtained for the 2-dimensional Schrödinger equation, along with classification results for algebraic families of Harish-Chandra modules in the 2-dimensional case. We shall also consider the classification problem here, in Section 3, and these results will play an important role in our analysis of the 3-dimensional Schrödinger equation here. But then we shall go much further by studying families of solutions of the Schrödinger equation as algebraic families of Harish-Chandra modules over $(g, K)$, and analyzing the close relationship between these and the functional analysis of the Schrödinger equation.

Basic ODE theory provides distinguished regular solutions of the eigenvalue equation (1.0.1) that extend to entire functions of the radial coordinate. They may be characterized as those solutions that are bounded in a neighborhood of the origin in $\mathbb{R}^3$. It is a simple matter to realize the spaces $\text{RegSol}(E)$ as the fibers of an $O$-module $\text{RegSol}$. Our first main result is as follows:

**Theorem** (See Section 5). The module $\text{RegSol}$ carries the structure of an algebraic family of Harish-Chandra modules (as in [BHS18b]) for the given algebraic family $(g, K)$ of Harish-Chandra pairs.

While the method of combining individual solution spaces into an algebraic family of vector spaces is simple and natural, the fact that the resulting algebraic structure is invariant under the action of $g$ is by no means evident. The regular eigenspaces of the Schrödinger operator constitute the first algebraic family of modules found outside of representation theory, and it is interesting to come upon such a family in a context of direct physical relevance.

As we shall soon see, the family $\text{RegSol}$ gives surprisingly algebraic form to constructions in scattering theory, which is another context where families of solutions are encountered. More broadly, it underlines the value of the perspective on symmetries of an eigendifferential equation that we are introducing and studying here, in which the eigenvalue is treated as a geometric coordinate.

Along with the regular solutions there are also singular solutions. We define the space of singular solutions at a given energy $E$ to be the quotient $\text{Sol}(E)/\text{RegSol}(E)$ of the space of all (K-finite) solutions by the regular solutions. Singular solutions do not feature among the solutions considered by the physicists, which are all regular. However the singular solutions carry the structure of an algebraic family of Harish-Chandra modules. In fact the Wronskian form from differential equations identifies the singular and regular solutions as (twisted) duals of one another:

**Theorem** (See Section 5). The Wronskian defines a twisted-equivariant, nondegenerate pairing
\[
\text{Wr}: \text{SingSol} \times \text{RegSol} \longrightarrow O
\]
between the algebraic families of singular and regular solutions, and an isomorphism from $\text{SingSol}$ to the twisted dual of $\text{RegSol}$.
The theorem foreshadows the important role that singular solutions do in fact play in the analysis of regular solutions, and particularly the physical solutions. Here is a first instance. The space of all regular and \( K \)-finite solutions of the Schrödinger equation is infinite-dimensional for every \( E \), real or complex, and it is much larger than the space of all physical solutions, since for some values of \( E \) there are no physical solutions at all, while for others there is only a finite-dimensional space of physical solutions. It is natural to ask how the physical solutions can be extracted from the family \( \text{RegSol} \).

Our answer is that the Jantzen filtration technique from representation theory not only isolates the physical solutions among the regular solutions, but it also determines unitary inner products on the physical solution spaces. To bring the technique into play we study not the duality between singular and regular solutions, but rather intertwining operators between these families.

**Theorem** (See Section 6). There is an essentially unique algebraic intertwining operator from \( \text{SingSol} \) to \( \text{RegSol} \). The spectrum of \( H \) coincides with the set of all \( E \in \mathbb{C} \) for which the fiber \( \text{RegSol}(E) \) has a nonzero infinitesimally unitary Jantzen quotient, and \( \text{PhysSol}(E) \) identifies with this (unique) quotient as a \( (\mathfrak{g}_E, K) \)-module.

So the singular solutions, considered as an algebraic family, play a decisive role in isolating the physical solutions from among all regular solutions. The method relies on studying the family as a whole; it would work awkwardly, if at all, if positive spectral values were considered separately from negative values. This calls to mind similar features of scattering theory, and it is to these analytic issues that we turn next.

It follows from either the Kato-Rellich theorem or the Friedrichs method that the Schrödinger operator for the 3-dimensional hydrogen atom has a natural self-adjoint extension on the Hilbert space of square-integrable functions on \( \mathbb{R}^3 \) (the two approaches give the same result). Henceforth we shall work with this self-adjoint extension.

Fix a value \( E \) that is not in the spectrum of \( H \). A Hilbert space operator-theoretic technique determines a subspace of \( \text{Sol}(E) \) that is precisely complementary to \( \text{RegSol}(E) \). It leads to the construction of an analytic, rather than algebraic, family of solution spaces for the Schrödinger eigenvalue equation, that is defined only over the complement of the spectrum. These are only superficial shortcomings: in the text we shall explain how to simultaneously upgrade the structure from analytic to algebraic, and obtain an algebraic family of Harish-Chandra modules over the whole affine line.

The technique is as follows. The range of the Hilbert space resolvent operator \( (H-E)^{-1} \) is the self-adjoint domain of \( H \), for every \( E \) in the resolvent set. But if the domain of \( (H-E)^{-1} \) is restricted to the \( K \)-finite, smooth and compactly supported functions on \( \mathbb{R}^3 \), then the restricted range varies with \( E \) and determines the required subspace of \( \text{Sol}(E) \): it is the space of those functions in \( \text{Sol}(E) \) that agree near infinity with a function in the restricted range. We shall call this complementary space of eigenfunctions \( \text{Sol}_\infty(E) \); it is invariant under the Lie algebra of hidden symmetries. Under projection it is isomorphic to the space \( \text{SingSol}(E) \).

We can now exploit results of Kodaira [Kod49] that were used by him for closely related purposes in scattering theory, including his confirmation of Heisenberg’s discovery [Hei43a, Hei43b, Hei44] that the negative spectrum of the Schrödinger
operator is determined by scattering data associated to the positive spectrum. In effect, Kodaira showed this:

1.0.4. **Theorem** (See Section 8). Let $G \in \text{SingSol}$, and let $V$ be the unique lifted family of eigenfunctions that is defined over the complement of the spectrum of $H$, as above. If $E > 0$, then the limits

$$
\lim_{\varepsilon \to 0^+} V_{E+i\varepsilon} \quad \text{and} \quad \lim_{\varepsilon \to 0^+} V_{E-i\varepsilon}
$$

both exist. Moreover the difference is a member of $\text{RegSol}(E)$.

This is an instance of the so-called limiting absorption principle in scattering theory. After adjusting by a Wronskian factor $w(E)$ (which will appear in another guise below) the difference of limits in the theorem is not only a member of $\text{RegSol}(E)$, but varies algebraically with $E$, and determines an element of the algebraic family $\text{RegSol}$ of regular solutions. So the theorem determines by purely analytic means an intertwining operator between algebraic families,

$$
\mathcal{A}: \text{SingSol} \to \text{RegSol}.
$$

It is precisely the one to which we applied the Jantzen technique earlier, which we proved to exist by purely algebraic means.

Our result builds a new and unexpected algebraic foundation underneath the scattering-theoretic results of Heisenberg and Kodaira in the case of the hydrogen atom. It also reinforces the idea that the most fruitful approach to the hidden symmetries of the hydrogen atom is to view them together as a family, as we have done in this paper.

The final results in the paper have to do with the measurable families of solution spaces provided by spectral theory, and their relation with algebraic and physical families studied so far. By the spectral theorem, there is a Borel measure $\mu$ on $\text{Spec}(H)$, a measurable field of Hilbert spaces, $\{H_E\}_{E \in \text{Spec}(H)}$, and a unitary isomorphism

$$
L^2(\mathbb{R}^3) \cong \int_{\text{Spec}(H)} H_E \, d\mu(E).
$$

It is easy to arrange compatibility with the group of visible symmetries. That is, one can equip the measurable field with a unitary action of the group $K=\text{O}(3)$ so that the above unitary equivalence is $K$-equivariant.

The Gelfand-Kostyuchenko theory (see for example [Ber88] for a quick introduction), provides, for almost all $E \in \text{Spec}(H)$, a $K$-equivariant, continuous realization morphism, from $H_E$ into the space $C^\infty(\mathbb{R}^3)_E$ of smooth $E$-eigenfunctions on $\mathbb{R}^3$. We shall prove the following result:

**Theorem** (See Section 9). For almost every $E$, the space $\mathcal{H}_{E,\text{fin}}$ of $K$-finite vectors in $\mathcal{H}_E$ carries an action of $U(\mathfrak{g})$ for which the realization map

$$
\mathcal{H}_{E,\text{fin}} \to C^\infty(\mathbb{R}^3)_E,\text{fin}
$$

is an isomorphism of Harish-Chandra modules onto $\text{PhysSol}(E)$.

A last issue is the determination of the measure $\mu$. This was in fact Kodaira’s original objective, following the pioneering work of Weyl [Wey10]. The same Wronskian factor $w(E)$ that we encountered above in the definition of the intertwining operator $\mathcal{A}$ reappears here.
Theorem (See Section 9). If the norms on the spaces $H_E$ are fixed so that nowhere vanishing $K$-fixed sections of $\text{RegSol}$ over $\mathbb{C}$ have constant norms over $(0, \infty)$, then measure $\mu$ is given there by the formula

$$\text{constant} \cdot d\mu(E) = w(E) dE.$$ 

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2. The Family of Harish-Chandra Pairs for the Hydrogen Atom

In this section we shall associate to the Schrödinger operator (1.0.2) an algebraic family of Harish-Chandra pairs that organizes the various hidden symmetries of the Schrödinger equation.

2.1. Rescaled Schrödinger Operator. To streamline formulas we shall work not with the operator $H$ in (1.0.2) but with the rescaled Schrödinger operator

$$(2.1.1) \quad T = \frac{2\mu}{\hbar^2} H.$$ 

It follows from the definition above that $T = -\Delta - \frac{2\gamma}{r}$, where

$$(2.1.2) \quad \gamma = \frac{\mu e^2}{\hbar^2}.$$ 

We shall use $T$ and $\gamma$ throughout the paper (we might have chosen units so that $\gamma = 1$, but we resisted the temptation to do so).

To become a bit more familiar with the new notation, observe that the formula for the spectrum of $H$ given in the introduction is equivalent to

$$\text{Spec}(T) = \left\{ -\frac{\gamma^2}{n^2} : n = 1, 2, \ldots \right\} \cup [0, \infty).$$ 

One of our aims is to understand this formula from a purely representation-theoretic perspective.

2.2. The Infinitesimal Hidden Symmetries. In this subsection we shall consider $T$ as an element in the algebra of linear partial differential operators on the space $\mathbb{R}_0^3 = \mathbb{R}^3 \setminus \{0\}$ with smooth function coefficients. We shall denote by Centralizer($T$) the centralizer of the rescaled Schrödinger operator in this algebra.

Since $T$ is rotation-invariant, the most evident elements in Centralizer($T$) are the infinitesimal rotation operators

$$(2.2.1) \quad L_1 = x_2 \partial_3 - x_3 \partial_2, \quad L_2 = x_3 \partial_1 - x_1 \partial_3 \quad \text{and} \quad L_3 = x_1 \partial_2 - x_2 \partial_1.$$ 

But in addition, the centralizer includes the so-called Runge-Lenz operators

$$(2.2.2) \quad R_1 = \sqrt{-T} \left( L_3 \partial_2 - L_2 \partial_3 - \partial_1 + \frac{\gamma x_1}{r} \right),$$

$$(2.2.2) \quad R_2 = \sqrt{-T} \left( L_1 \partial_3 - L_3 \partial_1 - \partial_2 + \frac{\gamma x_2}{r} \right),$$

$$(2.2.2) \quad R_3 = \sqrt{-T} \left( L_2 \partial_1 - L_1 \partial_2 - \partial_3 + \frac{\gamma x_3}{r} \right),$$

which Pauli obtained by quantizing the similarly-named quantities in the classical Kepler problem (see for example [GS90, Chs. 1&2] or [Hal13, Ch. 18]).
2.2.3. **Definition.** We shall denote by $\mathcal{O}$ the subalgebra of $\text{Centralizer}(T)$ consisting of polynomials in $T$. It is an embedded copy of the algebra of polynomial functions on the line. In addition, we shall denote by $\mathfrak{g}$ the $\mathcal{O}$-linear span of the operators
\[ \{L_1, L_2, L_3\} \quad \text{and} \quad \{R_1, R_2, R_3\} \]
within $\text{Centralizer}(T)$.

2.2.4. **Lemma.** The space $\mathfrak{g}$ is a free $\mathcal{O}$-module on the elements in Definition 2.2.3, and a Lie algebra over $\mathcal{O}$ under the commutator bracket.

**Proof.** By a direct calculation,
\[
[ L_i, L_j ] = -\varepsilon_{ijk} L_k \\
[ R_i, R_j ] = \varepsilon_{ijk} TL_k \\
[ L_i, R_j ] = -\varepsilon_{ijk} R_k,
\]
where $\varepsilon_{ijk}$ is the Levi-Civita symbol (which is 0 if an index is repeated, and the sign of the permutation $(i, j, k)$ otherwise). This shows that $\mathfrak{g}$ is a Lie algebra.

Freeness can be checked by examining leading-order terms (that is, the principal symbols) of the operators $T^kL_i$ and $T^kR_i$. The former have order exactly $2k+1$, and for each $k$ are linearly independent over $\mathbb{C}$; the latter have order exactly $2k+2$, and again for each $k$ they are linearly independent over $\mathbb{C}$. The lemma follows from this. □

Because $\mathfrak{g}$ is finitely generated and free as a module over $\mathcal{O}$, and also a Lie algebra over $\mathcal{O}$, it may be viewed as (the Lie algebra of global sections of) an algebraic family of complex Lie algebras over $\mathbb{C}$, the maximal ideal spectrum of $\mathcal{O}$. The individual fibers of the family are $\mathfrak{g}|_{\lambda} = \mathfrak{g}/I_{\lambda} \cdot \mathfrak{g}$, where $\lambda \in \mathbb{C}$ and where $I_{\lambda} \subseteq \mathcal{O}$ is the ideal generated by $T-\lambda$ (in the text we shall denote typical points on the line by $\lambda$ rather than by $E$ as we did in the introduction).

To better understand these fibers, let us give a concrete realization of the family $\mathfrak{g}$ as an algebraic family of matrix Lie algebras. Define a morphism from the $\mathcal{O}$-module $\mathfrak{g}$ into the $4 \times 4$-matrices over $\mathcal{O}$ by
\[
L_1 \mapsto \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \quad L_2 \mapsto \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix} \quad \text{and} \quad L_3 \mapsto \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}
\]
\[
R_1 \mapsto \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \quad R_2 \mapsto \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad \text{and} \quad R_3 \mapsto \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}.
\]

The image matrices are linearly independent over $\mathcal{O}$, so the morphism is injective. The explicit computations in the proof of Lemma 2.2.4 show that it is also a Lie algebra homomorphism.

The image of $\mathfrak{g}$ is the Lie algebra of all matrices over $\mathcal{O}$ of the form
\[
\begin{bmatrix}
0 & e(T) & f(T) & p(T) \\
-e(T) & 0 & g(T) & q(T) \\
-f(T) & -g(T) & 0 & r(T) \\
T p(T) & T q(T) & T r(T) & 0
\end{bmatrix},
\]
where $e$, $f$, $g$, $p$, $q$ and $r$ are polynomial functions. The fiber Lie algebra $g|_{\lambda}$ is therefore isomorphic to Lie algebra of all matrices of the same form, but with $T$ replaced by $\lambda \in \mathbb{C}$.

When $\lambda = 0$, the fiber is the semidirect product $so(3, \mathbb{C}) \ltimes \mathbb{C}^3$. When $\lambda \neq 0$, it is the complex Lie algebra of infinitesimal symmetries of the symmetric bilinear form

$$S_\lambda = \text{diag}(1, 1, 1, -\lambda).$$

If we fix a complex number $\mu$ such that

$$\mu^2 \lambda = -1 \tag{2.2.7}$$

and if we define

$$L_j^\pm = \frac{1}{2} (L_j \pm \mu R_j), \quad \tag{2.2.8}$$

then

$$[L_i^+, L_j^+] = -\varepsilon_{ijk} L_k^+, \tag{2.2.10}$$

and moreover

$$[L_i^+, L_j^-] = 0.$$

So the elements $L_j^\pm$ determine an isomorphism of complex Lie algebras

$$g|_{\lambda} \cong so(3) \times so(3) \tag{2.2.9}$$

when $\lambda \neq 0$. The isomorphism depends on the choice of $\mu$; the two possible choices lead to isomorphisms that differ from one another by the flip automorphism of the product Lie algebra. Note also that under the isomorphism, the subalgebra of $g|_{\lambda}$ spanned by the elements $L_j$ is mapped to the diagonal subalgebra of the product in (2.2.9).

From the embedding (2.2.6) we see that $g$ is the family of Lie algebras associated to an algebraic family $G$ of groups (that is, a smooth group scheme over the complex line; see [BHS18b, Sec. 2.2]), namely

$$G = \{(W, \lambda) \in \text{GL}(4, \mathbb{C}) \times \mathbb{C} : \det(W) = 1 \text{ and } WS_\lambda W^t = S_\lambda \}. \tag{2.2.10}$$

The fiber groups are isomorphic to

$$\begin{cases} 
O(3, \mathbb{C}) \ltimes \mathbb{C}^3 & \lambda = 0 \\
SO(4, \mathbb{C}) & \lambda \neq 0.
\end{cases}$$

Here the action of $O(3, \mathbb{C})$ on $\mathbb{C}^3$ in the semidirect product is given by

$$A : v \mapsto \det(A)^{-1} Av. \tag{2.2.11}$$

This is, of course, not quite the standard matrix action on $\mathbb{C}^3$. But it and the corresponding action of the compact group $O(3)$ on $\mathbb{R}^3$ will reappear throughout the paper.

2.3. The visible symmetries and Harish-Chandra pairs. The constant family of groups

$$K = O(3, \mathbb{C}) \times \mathbb{C}$$

may be viewed as a subfamily $G$ via the embedding

$$A \mapsto \begin{bmatrix} A & 0 \\ 0 & \det(A)^{-1} \end{bmatrix}.$$
The family $K$ acts on the family $g$ via the isomorphism (2.2.6) and the adjoint action. This makes $(g, K)$ into an algebraic family of Harish-Chandra pairs in the sense of [BHS18b, BHS18c].

Note that in terms of differential operators, the action of $K$ on $g$ is induced from the action of $O(3)$ on $\mathbb{R}^3$ via the formula (2.2.11).

2.4. Real structure. The family $(g, K)$ carries a natural real structure, which is to say a set of compatible conjugate-linear involutions on $O$, $g$ and $K$. See [BHS18b, Sec. 2.5] for details concerning the definition, but the formulas below should make those details clear.

First, we define a complex-conjugate-linear involution

$$\sigma: O \rightarrow O$$

by means of the standard formula $\sigma(p)(z) = \overline{p(z)}$. Here we are viewing elements of $O$ as polynomial functions on the line. Thinking of them as polynomials in $T$, the involution acts by complex-conjugating all the coefficients of the polynomial.

Next, the elements of $g$, being linear partial differential operators on $\mathbb{R}^3$, have formal adjoints. The family $g$ is stable under the formal adjoint operation since $T$ is formally self-adjoint, while each of the operators $L_i$ and $R_i$ in (2.2.1) and (2.2.2) is formally skew-adjoint. Using this fact, we define

$$\sigma_g: g \rightarrow g$$

by $\sigma_g(X) = -X^*$. This preserves the Lie bracket and satisfies

$$\sigma_g(p \cdot X) = \sigma(p) \cdot \sigma_g(X)$$

for all $p \in O$ and all $X \in g$.

Finally we define an involution on $K$ by combining the involution on the base with the antiholomorphic involution

$$k \mapsto (k^*)^{-1}$$

on the fiber $O(3, \mathbb{C})$. The three involutions so-defined constitute a real structure on the algebraic family of Harish-Chandra pairs $(g, K)$.

2.5. Cartan involution. There is a second natural complex-conjugate-linear involution

$$\sigma'_g: g \rightarrow g,$$

which is defined as follows: each element of $g$ is a linear differential operator on $\mathbb{R}^3$, and $\sigma'_g$ replaces each coefficient function in the operator by its complex conjugate. Like the involution $\sigma_g$, it is compatible with the involution on $O$ in the sense of the formula (2.4.2). Moreover $\sigma_g$ and $\sigma'_g$ commute with one another. So the composition

$$\theta = \sigma_g \circ \sigma'_g: g \rightarrow g$$

is an $O$-linear involution of $g$. Its fixed subalgebra is precisely the algebra $\mathfrak{t}$ of visible symmetries, while its $-1$ eigenspace is spanned by the Runge-Lenz operators.

2.5.3. Remark. The symmetries of the Schrödinger equation are related to our involutions as follows: the visible symmetries are those elements of $g$ that are fixed by both $\sigma_g$ and $\theta$, whereas the hidden symmetries are those fixed by $\sigma_g$ alone.
2.6. **Involutions at the group level.** The involutions $\theta$ and $\sigma_g$ assume a simple form under the isomorphism in (2.2.6) from $g$ to a family of $4 \times 4$-matrix Lie algebras. On the matrix fibers, $\sigma_g$ is simply entry-wise complex conjugation, whereas $\theta$ is conjugation by the matrix

$$\Theta = \text{diag}(1, 1, 1, -1).$$

So these involutions lift to the family of groups $G$. To summarize:

2.6.1. **Theorem.** There is an algebraic family of complex algebraic groups $G$ over the complex line, together with a real structure $\sigma$ and a commuting involution $\theta$ such that

(a) The associated algebraic family of Lie algebras is the family $g$.

(b) The family $G$ includes the constant family $K$ with fiber $O(3, \mathbb{C})$ as a subfamily, and the real structure restricts to the standard real structure on this subfamily given by entry-wise complex conjugation.

(c) The induced real structure on $g$ is the involution in (2.4.1), and the fixed groups for the real structure over the points $\lambda \in \mathbb{R}$ are the hidden symmetry groups

$$G|_{\sigma_{\lambda}}^G \cong \begin{cases} 
SO(3, 1) & \lambda > 0 \\
O(3) \ltimes \mathbb{R} & \lambda = 0 \\
SO(4) & \lambda < 0.
\end{cases}$$

(d) The fixed family for the involution $\theta$ is $K$, and the induced action at the Lie algebra level is the involution in (2.5.2). \qed

2.6.2. **Remark.** As explained in [BHS18a], the family $G$ can actually be constructed from the commuting involutions $\sigma$ and $\theta$ on the fiber over $\lambda=1$.

2.7. **The enveloping algebra and its center.** Denote by $U(g)$ the enveloping algebra of the $O$-Lie algebra $g$. See [Bou60, Section 2.7] for general information on enveloping algebras applicable to Lie algebras over commutative rings, including for instance the Poincaré-Birkhoff-Witt theorem, which applies to our case because $g$ is free as a module over $O$.

We shall be especially concerned with the center $Z(g)$ of the enveloping algebra, and we shall give here an analysis of its structure. It follows from the formulas (2.2.5) that the elements

$$RL, \quad TL^2 - R^2$$

belong to the center of the enveloping algebra (we are using standard abbreviated notation, so that $R^2 = R_1^2 + R_2^2 + R_3^2$, and so on). Moreover these elements are $O(3)$-invariant.

2.7.2. **Proposition.** The center of the enveloping algebra $U(g)$ is freely generated, as a commutative $O$-algebra, by $RL$ and $TL^2 - R^2$.

**Proof.** View $U(g)$ as a complex associative algebra, and equip it with the increasing filtration for which

$$\text{order}(L_i) = 0, \quad \text{order}(R_i) = 1 \quad \text{and} \quad \text{order}(T) = 0.$$ 

The associated graded algebra is the tensor product $U(g_0) \otimes_O O$, where $g_0$ is the $6$-dimensional graded complex Lie algebra with basis elements $\ell_1, \ell_2, \ell_3$ in degree $0$ and $r_1, r_2, r_3$ in degree $1$, and relations

$$[\ell_i, \ell_j] = -\epsilon_{ijk} \ell_k, \quad [r_i, r_j] = 0 \quad \text{and} \quad [\ell_i, r_j] = -\epsilon_{ijk} r_k;$$
compare to formulas (2.2.5) earlier.

Now, the center of the associated graded algebra is $Z(g_0) \otimes \mathbb{C} O$, and by an explicit computation $Z(g_0)$ is a free commutative algebra over $\mathbb{C}$ on the elements $r\ell$ and $r^2$. Compare [Gon88, Theorem 2.1]. The proposition follows from this by a standard induction argument on the order of elements in the center of the enveloping algebra.

2.7.5. Remark. The reference [Gon88, Theorem 2.1] actually computes the $O(3)$-invariant part of $Z(g_0)$ for the standard action of $O(3)$ on $\mathbb{C}^3$, not the action (2.2.11). For that action the invariant part is freely generated by $(r\ell)^2$ and $r^2$. The element $r\ell$ is not $O(3)$-invariant for the standard action; instead, it transforms under $A \in O(3)$ as $r\ell \mapsto \det(A) \cdot r\ell$.

But the computation of $Z(g_0)$ is easily reduced to the computation of the standard $O(3)$-invariant part using the formula

$$Z(g_0) = Z(g_0)^{O(3), \text{standard}} \oplus r\ell \cdot Z(g_0)^{O(3), \text{standard}}.$$  

2.8. Realization in differential operators. Because $g$ is defined as a Lie algebra of linear differential operators commuting with the rescaled Schrödinger operator $T$, there is a canonical morphism of $O$-algebras

$$\alpha: U(g) \to \text{Centralizer}(T).$$

We shall briefly examine both the image and the kernel of this morphism.

The algebra $\text{Centralizer}(T)$ is filtered by the usual order of differential operators. The following lemma is proved by a direct computation, which we shall omit:

2.8.2. Lemma. The order 2 part of $\text{Centralizer}(T)$ is spanned by the totality of the elements

(i) $1$ (the identity operator)
(ii) $T$ (the rescaled Schrödinger operator)
(iii) $L_1$, $L_2$ and $L_3$
(iv) $R_1$, $R_2$ and $R_3$
(v) $L_1^2 + L_2^2 + L_3^2$
(vi) $L_1L_2 + L_2L_1$, $L_1L_3 + L_3L_1$, $L_2L_3 + L_3L_2$, $L_1^2 - L_2^2$ and $L_2^2 - L_3^2$.

We grouped the elements into six separate sets because the operators in each span an irreducible representation of the group $O(3)$.

The following formulas for the action of $Z(g)$ under the morphism $\alpha$ will play important roles in the sequel. For the proofs, see for example [Hal13, Prop. 18.11].

2.8.3. Lemma. The images of the central elements $RL$ and $TL^2 - R^2$ in (2.7.1) under the homomorphism $\alpha$ are given by the formulas

$$\alpha(RL) = 0$$

and

$$\alpha(TL^2 - R^2) = T + \gamma^2 I.$$  

2.8.4. Remark. It is evident from Lemma 2.8.2 that the range of (2.8.1) includes the full second-order part of the centralizer. Indeed it is asserted in [DSS96] that the full centralizer is generated by $g$. This is consistent with experience from the study
of classical superintegrable systems, such as the Kepler system, where, in $n$ dimensions there are at most $2n-1$ functionally independent conserved quantities; see for example [MPW13, p.11]. The analogous statement for quantum superintegrable systems is known in some cases and there are no known counterexamples; see [MPW13, p.12].

It also seems likely to us that the kernel of the morphism from $\mathcal{U}(\mathfrak{g})$ into the centralizer is fully described by the relations in Lemma 2.8.3.

3. Families of Harish-Chandra modules

In this section, we shall collect some general information about families of Harish-Chandra modules over the family of Harish-Chandra pairs that we constructed in the previous section, including definitions and a classification theorem. This is in preparation for our representation-theoretic analysis of the solutions of the Schrödinger equation in Section 5.

3.1. Locally finite-dimensional group representations. Let $V$ be a complex vector space that is equipped with a linear representation of the group $K = \text{O}(3, \mathbb{C})$. There is a natural evaluation map

\[(3.1.1) \quad \bigoplus_{\sigma \in \hat{K}} W_\sigma \otimes \text{Hom}_K(W_\sigma, V) \rightarrow V,\]

where the sum is over the equivalence classes of irreducible (finite-dimensional) linear representations of the complex algebraic group $K$, and $W_\sigma$ is a representative of the equivalence class $\sigma$.

The representation $V$ is said to be locally finite-dimensional if the map (3.1.1) is a vector space isomorphism. In any case the image, which we shall denote by $V_{\text{fin}}$, is a locally finite-dimensional representation of $K$ in its own right. The individual images $V_\sigma$ of the summands in (3.1.1) are the isotypical summands of the representation. They are the same for $V$ and $V_{\text{fin}}$.

Denote by $\mathcal{O}(K)$ the space of regular functions on $K$. A locally finite-dimensional representation of $K$ on $V$ determines, and is determined by, the vector space morphism

\[(3.1.2) \quad V \rightarrow \mathcal{O}(K) \otimes_{\mathbb{C}} V\]

for which composition with evaluation at $k \in K$ (a map $\mathcal{O}(K) \rightarrow \mathbb{C}$) gives the action of $k$ on $V$.

A dual form of (3.1.2) may be defined as follows. Given any locally finite-dimensional representation of $K$ on a vector space $V$, let us denote by

\[V^* = \text{Hom}_\mathbb{C}(V, \mathbb{C})_{\text{lin}}\]

the locally finite contragredient representation. From the left translation action of $K$ on $\mathcal{O}(K)$ we obtain in this way

\[R(K) = \mathcal{O}(K)^*.\]

The morphism (3.1.2) then corresponds to a morphism

\[(3.1.3) \quad R(K) \otimes_{\mathbb{C}} V \rightarrow V.\]

Applying this in the case where $V$ is $R(K)$ itself, we get a morphism of vector spaces

\[R(K) \otimes_{\mathbb{C}} R(K) \rightarrow R(K).\]
This is an associative product on $\mathbb{R}(K)$ and (3.1.3) is a module action.\(^1\) In fact a locally finite-dimensional representation of $K$ is exactly the same as a left $\mathbb{R}(K)$-module that is nondegenerate in the sense that $\mathbb{R}(K) \cdot V = V$.

Examining (3.1.3) in the case where $V$ is the direct sum of all irreducible representations of $K$, up to equivalence, we obtain the Peter-Weyl isomorphism of algebras

\[
\mathbb{R}(K) \xrightarrow{\cong} \bigoplus_{\sigma \in \hat{K}} \text{End}(W_{\sigma}).
\]

One consequence of the Peter-Weyl isomorphism is that $\mathbb{R}(K)$ contains many central idempotents, corresponding to the identity operators on the spaces $W_{\sigma}$. The idempotent associated to the trivial representation will be especially important in what follows.

3.1.5. **Definition.** We shall denote by $e \in \mathbb{R}(K)$ the central idempotent that is mapped to the identity operator on the trivial representation under (3.1.4), and is mapped to zero in any other summand of (3.1.4).

Finally, let us establish some notation for later use. Throughout this paper we shall be considering only representations of $K$ for which the element $-1 \in K$ acts trivially. As a result, the irreducible representations where $-1$ acts nontrivially will play no role. The group $K$ is the direct product of its 2-element center, generated by $-1$, and its identity component, which is of course $\text{SO}(3, \mathbb{C})$. So effectively we shall be studying representations of $\text{SO}(3, \mathbb{C})$, and we shall call these the SO(3)-type representations of $K$. They may be listed as

\[
\{ \sigma_\ell : \ell = 0, 1, \ldots \},
\]

where $\sigma_\ell$ has dimension $2\ell+1$. We shall write $W_\ell$ in place of $W_{\sigma_\ell}$.

3.2. **Families of locally finite-dimensional representations.** By an algebraic family of representations of $K$ we shall mean a locally free, and hence in our context free, $\mathcal{O}$-module $\mathcal{F}$ that is equipped with a locally finite-dimensional representation of $K$ by $\mathcal{O}$-module automorphisms.

Each of the isotypical summands of $\mathcal{F}$ is now a free $\mathcal{O}$-module, and we shall say that $\mathcal{F}$ is admissible if all its isotypical summands are finitely generated (and necessarily free) $\mathcal{O}$-modules. Finally the locally finite contragredient of the family is

\[
\mathcal{F}^* = \text{Hom}_\mathcal{O}(\mathcal{F}, \mathcal{O})_{\text{fin}}.
\]

3.3. **Algebraic families of Harish-Chandra modules.** An admissible algebraic family of Harish-Chandra modules for $(\mathfrak{g}, K)$ is an admissible algebraic family of $K$-representations $\mathcal{F}$ that is equipped with an $\mathcal{O}$-linear action of $\mathfrak{g}$,

\[
\mathfrak{g} \otimes_\mathcal{O} \mathcal{F} \longrightarrow \mathcal{F},
\]

that is compatible with the $K$-action in the sense that the action map is $K$-equivariant, and its restriction to $\mathfrak{t} \subseteq \mathfrak{g}$ is the infinitesimal form of the $K$-action.

---

\(^1\)The algebra $\mathbb{R}(K)$ is often called the Hecke algebra of $K$. After fixing a Haar measure on $O(3)$, using which we can identify elements of $\mathbb{R}(K)$ with functions on $O(3)$, the product corresponds to convolution of functions on $O(3)$. The module structure may also be described using convolution. See [KV95].
As was the case with locally finite-dimensional $K$-actions, it is possible to describe $(\mathfrak{g}, K)$-module structures using an appropriate associative algebra. Form the tensor product

$$\mathcal{U}(\mathfrak{g}, K) = \mathcal{U}(\mathfrak{g}) \otimes_{\mathcal{U}(\mathfrak{g})} R(K).$$

The actions of $\mathfrak{g}$ and $K$ on $\mathcal{F}$ determine a morphism

$$\mathcal{U}(\mathfrak{g}, K) \otimes \mathcal{O} \mathcal{F} \rightarrow \mathcal{F}.$$  

(3.3.1)

The $\mathcal{O}$-module $\mathcal{U}(\mathfrak{g}, K)$ itself carries actions of $\mathfrak{g}$ and $K$, the later being the tensor product of the adjoint and left-translation actions, and so we obtain a morphism

$$\mathcal{U}(\mathfrak{g}, K) \otimes \mathcal{O} \mathcal{U}(\mathfrak{g}, K) \rightarrow \mathcal{U}(\mathfrak{g}, K)$$

which is an $\mathcal{O}$-linear associative product on $\mathcal{U}(\mathfrak{g}, K)$. The morphism (3.3.1) gives $\mathcal{F}$ the structure of a $\mathcal{U}(\mathfrak{g}, K)$-module, and in this way algebraic families of Harish-Chandra modules for $(\mathfrak{g}, K)$ correspond exactly to $\mathcal{U}(\mathfrak{g}, K)$-modules that are free as $\mathcal{O}$-modules and nondegenerate in the sense that $\mathcal{U}(\mathfrak{g}, K) \cdot \mathcal{F} = \mathcal{F}$. For all this, see [KV95] (which treats the case of individual Harish-Chandra modules, but families may be handled in the same way).

3.4. The spherical Hecke algebra. In this section we shall classify certain algebraic families of Harish-Chandra modules. Later on we shall use the classification to characterize the families that arise from the solution of the Schrödinger equation (see Sections 5.6 and 6.4) and to prove the existence of intertwining operators between these families (see Section 6.2).

3.4.1. Definition. Let us say that an algebraic family $\mathcal{F}$ of Harish-Chandra modules for $(\mathfrak{g}, K)$ is standard and spherical if

(i) The $K$-isotypical decomposition of $\mathcal{F}$ consists of the full set of $SO(3)$-type representations, each occurring with multiplicity one.

(ii) $\mathcal{F}$ is generated by its spherical vectors (that is, by its $K$-fixed elements) in the sense that $\mathcal{U}(\mathfrak{g}) \cdot \mathcal{F}^0 = \mathcal{F}$, where $\mathcal{F}^0$ is the isotypical subspace for the trivial representation of $K$.

3.4.2. Remark. In most situations involving families of irreducible Harish-Chandra modules, item (i) above is implied by item (ii).

3.4.3. Definition. If $\mathcal{F}$ is standard and spherical, then the element $\mathcal{TL}^2 - R^2 \in \mathcal{Z}(\mathfrak{g})$ acts on $\mathcal{F}^0$, and indeed on $\mathcal{F}$, as multiplication by some polynomial $Q \in \mathcal{O}$. We shall call $Q$ the value of $\mathcal{TL}^2 - R^2$ on $\mathcal{F}$.

3.4.4. Theorem. A standard and spherical family of Harish-Chandra modules for $(\mathfrak{g}, K)$ is determined up to isomorphism by the value in $\mathcal{O}$ of $\mathcal{TL}^2 - R^2$. Moreover any element of $\mathcal{O}$ can arise as the value of $\mathcal{TL}^2 - R^2$ in a standard and spherical family.

We shall prove this by means of the following auxiliary constructions.

3.4.5. Definition. The spherical Hecke algebra for the family $(\mathfrak{g}, K)$ is the following $\mathcal{O}$-algebra:

$$\mathcal{H}(\mathfrak{g}, K) = e \cdot \mathcal{U}(\mathfrak{g}, K) \cdot e.$$ 

Here $e \in R(K)$ is the idempotent in Definition 3.1.5, and we view it as an element of $\mathcal{H}(\mathfrak{g}, K)$ via the embedding $e \mapsto 1 \otimes e$. Let us also define

$$\mathcal{U}\mathcal{H}(\mathfrak{g}, K) = \mathcal{U}(\mathfrak{g}, K) \cdot e$$

This is a $\mathcal{U}(\mathfrak{g}, K)$-$\mathcal{H}(\mathfrak{g}, K)$-bimodule by left and right multiplication.
3.4.6. Proposition. The spherical Hecke algebra \( H(\mathfrak{g}, K) \) is freely generated as an \( \mathcal{O} \)-algebra by the (tensor) product of \( TL^2 - R^2 \in \mathbb{Z}(\mathfrak{g}) \) with \( e \in \mathcal{R}(K) \).

3.4.7. Proposition. The space \( \mathcal{UH}(\mathfrak{g}, K) \) is a free \( \mathcal{H}(\mathfrak{g}, K) \)-module. Moreover there is an isomorphism

\[
\mathcal{UH}(\mathfrak{g}, K) \cong \bigoplus_{\ell \geq 0} W_{\ell} \otimes_{\mathcal{C}} \mathcal{H}(\mathfrak{g}, K),
\]

of \( K \)-modules and \( \mathcal{H}(\mathfrak{g}, K) \)-modules.

We shall prove these results in a moment, but first let us explain how they lead to a proof of Theorem 3.4.4.

If \( \mathcal{F} \) is any algebraic family of Harish-Chandra modules, then the trivial isotypical summand \( e\mathcal{F} = \mathcal{F}^0 \) is an \( \mathcal{H}(\mathfrak{g}, K) \)-module and a free \( \mathcal{O} \)-module. The tensor product

\[
\mathcal{UH}(\mathfrak{g}, K) \otimes_{\mathcal{H}(\mathfrak{g}, K)} \mathcal{F}^0
\]

is a standard and spherical family, and it is determined up to isomorphism by the value of \( TL^2 - R^2 \), since by Proposition 3.4.6 this determines \( \mathcal{F}^0 \) as an \( \mathcal{H}(\mathfrak{g}, K) \)-module, up to isomorphism. Now the formula \( X \otimes f \mapsto Xf \) defines a classifying morphism of families

(3.4.8)

\[
\mathcal{UH}(\mathfrak{g}, K) \otimes_{\mathcal{H}(\mathfrak{g}, K)} \mathcal{F}^0 \longrightarrow \mathcal{F}.
\]

If \( \mathcal{F} \) is itself standard and spherical, then (3.4.8) is surjective, and, by counting dimensions in like isotypical summands using Proposition 3.4.7, we find that it is in fact an isomorphism. So there is at most one standard and spherical family, up to isomorphism, for any given value of \( TL^2 - R^2 \).

In the reverse direction if \( \mathcal{M} \) is any \( \mathcal{H}(\mathfrak{g}, K) \)-module that is free and of rank one as an \( \mathcal{O} \)-module, then the tensor product

(3.4.9)

\[
\mathcal{UH}(\mathfrak{g}, K) \otimes_{\mathcal{H}(\mathfrak{g}, K)} \mathcal{M}
\]

is a standard and spherical family. So using Proposition 3.4.6 again we can construct standard and spherical families with any given value of \( TL^2 - R^2 \).

Let us turn now to the proofs of Propositions 3.4.6 and 3.4.7. The family \( \mathfrak{g} \) may be decomposed as a \( K \)-equivariant direct sum of \( \mathcal{O} \)-modules

\[
\mathfrak{g} = \mathfrak{t} \oplus \mathfrak{s},
\]

where the summand \( \mathfrak{s} \) is freely generated as an \( \mathcal{O} \)-module by the elements \( R_1, R_2 \) and \( R_3 \). It will be convenient to denote by \( \mathfrak{s} \) the \( \mathbb{R} \)-linear span of these three elements, so that

\[
\mathfrak{s} = \mathcal{O} \otimes_{\mathbb{R}} \mathfrak{s}.
\]

The three-dimensional real vector space \( \mathfrak{s} \) carries the action (2.2.11) of the compact group \( O(3) \). It also carries an essentially unique invariant inner product, using which the symmetric and polynomial algebras of \( \mathfrak{s} \) may be identified.

We shall use the following simple and well-known facts concerning the algebra of complex polynomial functions on \( \mathfrak{s} \). First, the \( K \)-invariant polynomials are freely generated by \( R^2 = R_1^2 + R_2^2 + R_3^2 \). Second, the full polynomial algebra is a free module over its \( K \)-invariant subalgebra. To be more precise, if \( Harm(\mathfrak{s}) \) denotes the space of harmonic polynomials on \( \mathfrak{s} \), then the multiplication map

\[
Harm(\mathfrak{s}) \otimes Sym(\mathfrak{s})^K \longrightarrow Sym(\mathfrak{s})
\]
is a complex vector space isomorphism (this is a very special case of a much more general theorem of Kostant [Kos63, BL96]).

The degree $\ell$ harmonic polynomials form a copy of the irreducible $SO(3)$-type representation of dimension $2\ell+1$. So the space $\text{Harm}(s)$ decomposes as a direct sum of precisely one copy of $W_\ell$ for each $\ell = 0, 1, 2, \ldots$.

**Proof of Proposition 3.4.6.** Filter the algebra $\mathcal{U}(\mathfrak{g}, K)$ by means of the filtration (2.7.3) on the enveloping algebra and by deeming $R(K)$ to be of order zero. The spherical Hecke algebra is a filtered subalgebra, and it suffices to show that its associated graded algebra is freely generated as an $\mathcal{O}$-algebra by the symbol of the order 2 element $TL^2 - R^2$, or equivalently by the symbol of $R^2$.

The composition of the symmetrization map from the $K$-invariant part of the symmetric algebra of $s$ into $\mathcal{U}(\mathfrak{g})$ with multiplication with $e \in R(K)$ on both sides is an isomorphism of filtered $\mathcal{O}$-modules

$$\text{Sym}(s)^K \xrightarrow{\cong} \mathcal{H}(\mathfrak{g}, K).$$

This is an algebra isomorphism at the level of associated graded algebras, because the elements in $s \subseteq \mathcal{U}(\mathfrak{g})$ commute with one another up to elements of lower order. Moreover the invariant part of the symmetric algebra is freely generated by $R^2$, as we noted above.

**Proof of Proposition 3.4.7.** Let us use the same filtration of $\mathcal{U}(\mathfrak{g}, K)$ as in the previous proof, which we shall now restrict to $\mathcal{U}\mathcal{H}(\mathfrak{g}, K)$. It suffices to show that the associated graded space is a free module over the associated graded algebra of the spherical Hecke algebra, and to compute that each $K$-type occurs in it with multiplicity one.

The associated graded space is $\text{Sym}(s)$, via the same identifications as in the previous lemma, while associated graded algebra of the spherical Hecke algebra is $\text{Sym}(s)^K$. As we already noted, the former decomposes as $\text{Harm}(s) \otimes \mathcal{C} \mathcal{H}(\mathfrak{g}, K)$ as both a $K$-module and a module over the invariant functions.

### 3.5. Twisted dual families.

The same formula (3.2.1) used for families of representations of $K$ defines the locally finite-dimensional contragredient $\mathcal{F}^*$ of an algebraic family of Harish-Chandra modules. But it will be a bit more relevant in this paper to examine the following variants of the locally finite-dimensional contragradient that involve the involutions introduced in Subsections 2.4 and 2.5.

The $\theta$-twisted dual $\mathcal{F}^{*, \theta}$ is simply $\mathcal{F}^*$ but with the action of $\mathfrak{g}$ twisted by the involution $\theta$: for $\xi \in \mathcal{F}^*$ and $X \in \mathfrak{g}$ we change the action of $X$ on $\xi$ to

$$X: \xi \mapsto \theta(X)\xi.$$

The $\sigma$-twisted dual $\mathcal{F}^{*, \sigma}$ is the complex conjugate space $\overline{\mathcal{F}^*}$, which we consider to be an $\mathcal{O}$-module via the given involution on $\mathcal{O}$:

$$p \cdot \overline{\xi} := \overline{\sigma(p)\xi} \quad \forall p \in \mathcal{O} \quad \forall \xi \in \mathcal{F}.$$ 

It is similarly a $\mathfrak{g}$-module and a $K$-module via the involutions on $\mathfrak{g}$ and $K$. See [BHS18c, Sec. 2.4] for further information.
4. Principal Series Representations

To provide some context for our treatment of families of Harish-Chandra modules in the next section, we shall review here the classification of the irreducible modules of a single Harish-Chandra pair \((g, \lambda, K)\) (see [Wal88, Ch. 3] for basic information concerning Harish-Chandra modules, which will in any case be reviewed in the families context in the next section). We shall focus on the case where \(\lambda \neq 0\), and throughout this section \(\lambda\) will be a fixed nonzero complex number.

4.1. Parabolically induced representations. The group \(K=O(3)\) is disconnected, but it is the direct product of its connected identity component \(K_0=SO(3)\) and the two-element center of \(K\). The center acts trivially on \(g|\lambda\), and so the irreducible representations of the pair \((g|\lambda, K)\) are partitioned into set of those where the center of \(K\) acts trivially, and an otherwise identical set of irreducible representations where it does not. From now on we shall concentrate on the former, which correspond to irreducible \((g|\lambda, K_0)\)-modules.

We have seen that \((g|\lambda, K_0)\) is isomorphic to \((so(3,\mathbb{C})\times so(3,\mathbb{C}), SO(3))\), with \(SO(3)\) acting diagonally. Since the latter is the Harish-Chandra pair associated to the real reductive group \(PSL(2,\mathbb{C})\), we can determine the irreducible representations of \((g|\lambda, K_0)\) by computing the irreducible admissible representations of \(PSL(2,\mathbb{C})\) up to infinitesimal equivalence.

The irreducible admissible representations of \(PSL(2,\mathbb{C})\), or more generally of \(SL(2,\mathbb{C})\), are well known and may be described using parabolic induction from the subgroup of upper triangular matrices. Let \((\sigma, \varphi) \in \mathbb{Z} \times \mathbb{C}\). The parabolically induced representation of \(SL(2,\mathbb{C})\) associated to the character

\[
\begin{bmatrix}
  a & 0 \\
  0 & a^{-1}
\end{bmatrix} \mapsto \text{phase}(a)^\sigma |a|^\varphi
\]

of the diagonal subgroup is either irreducible or has a composition series with two irreducible factors, one finite-dimensional and one infinite-dimensional. In either case, the representations, or irreducible factors, at \((\sigma, \varphi)\) and \((-\sigma, -\varphi)\) are the same. See, for example [Kna86, Chap VIII, Problems 9-14] for details concerning all the above.

Each infinite-dimensional, irreducible, admissible representation of the real reductive group \(SL(2,\mathbb{C})\) arises as a parabolically induced representation, and does so in a unique way, except for the equivalence just mentioned. Moreover each finite-dimensional and irreducible representation of \(SL(2,\mathbb{C})\) arises as a composition factor of a unique reducible parabolically induced representation, again except for the equivalence between the factors associated to \((\sigma, \varphi)\) and \((-\sigma, -\varphi)\). We find, in summary that the admissible dual of \(SL(2,\mathbb{C})\) is parametrized by the set

\[
(Z \times \mathbb{C}) / \mathbb{Z}_2,
\]

where the group \(\mathbb{Z}_2\) acts as the involution \((\sigma, \varphi) \mapsto (-\sigma, -\varphi)\). The irreducible admissible representations of \(SL(2,\mathbb{C})\) that factor through the quotient \(PLS(2,\mathbb{C})\), and so correspond to irreducible Harish-Chandra modules for \((g|\lambda, K_0)\), are those with parameters in the subset

\[
(2Z \times \mathbb{C}) / \mathbb{Z}_2 \subseteq (Z \times \mathbb{C}) / \mathbb{Z}_2.
\]
4.2. **Casimir elements.** In this paragraph we shall compute the action of the central elements $LR$ and $\lambda L^2 - R^2$

in the enveloping algebra of $g|_{\lambda}$, on the principal series representation with parameters $(\sigma, \varphi)$.

First, it is well known that the $so(3)$ Casimir element

$$\Omega = L^2 = L_1^2 + L_2^2 + L_3^2$$

acts as $-\frac{1}{4}n(n+2)$ in the irreducible finite-dimensional representation of $so(3)$ of dimension $n+1$ (this is the representation of highest weight $n$). It follows from this that if $\Omega^\pm$ are the Casimir elements associated to the generators $L^\pm_j$ in (2.2.8), then

$$\frac{1}{\sqrt{-\lambda}} LR = \Omega^+ - \Omega^- = \pm \frac{1}{4}(m(m+2) - n(n+2))$$

and

$$L^2 - \frac{1}{\lambda} R^2 = 2\Omega^+ + 2\Omega^- = -\frac{1}{4}(m(m+2) + n(n+2))$$

in the representation of $g|_{\lambda}$ corresponding under the isomorphism (2.2.9) to the finite-dimensional, irreducible, tensor product representation of the direct product $so(3) \times so(3)$ of highest weight $(m, n)$; the indeterminacy in sign corresponds to the indeterminacy in the choice of square root of $-\lambda$.

Now the above finite-dimensional representation of $(g|_{\lambda}, K_0)$ arises as a quotient of the principal series representation with parameters

$$(4.2.2) \quad \sigma = m - n \quad \text{and} \quad \varphi = 2 + m + n.$$  

Since it follows from (4.2.2) that

$$\sigma \varphi = m(m+2) - n(n+2) \quad \text{and} \quad \sigma^2 + \varphi^2 = 2(m(m+2) + n(n+2)) + 4,$$

we find that in the principal series representation with parameters $(\sigma, \varphi)$ as in (4.2.2), the Casimir elements act as

$$(4.2.3) \quad LR = \pm \sqrt{-\lambda} \frac{\sigma \varphi}{4} \quad \text{and} \quad \lambda L^2 - R^2 = \frac{\lambda}{4} \frac{\sigma^2 - \varphi^2}{4}.$$  

Once again the indeterminacy in sign corresponds to the indeterminacy in the choice of square root, and hence the choice of isomorphism in (2.2.9).\(^2\)

Although we have computed the formulas (4.2.3) for $(\sigma, \varphi)$ satisfying (4.2.2) they must in fact hold for all $(\sigma, \varphi)$ by a Zariski density argument, since both sides are regular in $\varphi$.

4.3. **Spherical representations.** We are particularly interested in representations that include $K_0$-fixed vectors. The lowest $K_0$-type in the principal series representation with parameters $(\sigma, \varphi)$ has highest weight $|\sigma|$, and so the principal series representations that include $K_0$-fixed vectors are precisely those for which $\sigma = 0$. Hence:

4.3.1. **Lemma.** The $K$-types of an irreducible infinite-dimensional representation with parameters $(0, \varphi)$ are the full set of $SO(3)$-types $\ell = 0, 1, 2, \ldots$, and each occurs with multiplicity one.  

\(^2\)The outer automorphism of the pair $(so(3) \times so(3), K_0)$ that flips the two $so(3)$-factors induces the involution $(\sigma, \varphi) \mapsto (-\sigma, \varphi)$ on parameters for irreducible modules.
We shall again use the term standard for representations with the above $K_0$-isotypical structure.

We are also particularly interested in those representations in which the Casimir element $\lambda L^2 - R^2$ acts as the scalar $\lambda + \gamma^2$; compare Lemma 2.8.3.

4.3.2. Lemma. Let $V$ be a standard representation of $(g|_\lambda, K_0)$. If the Casimir element $\lambda L^2 - R^2$ acts on $V$ as the scalar $\lambda + \gamma^2$, then the irreducible quotient of $V$ including the $K_0$-type $\ell = 0$ has classification parameters $\sigma = 0$ and $\varphi^2 = -4\gamma^2/\lambda$.

Proof. It follows from (4.2.3) that
\[
\lambda \cdot \frac{\varphi^2 - 4}{4} + \lambda + \gamma^2 = R^2 - \lambda L^2 + \lambda + \gamma^2 = 0,
\]
or in other words that
\[
\lambda \cdot \frac{\varphi^2}{4} + \gamma^2 = 0.
\]
This implies the result. \qed

4.3.3. Corollary. Let $V$ be a standard representation of $(g|_\lambda, K_0)$ in which the Casimir element $\lambda L^2 - R^2$ acts on $V$ as the scalar $\lambda + \gamma^2$. Unless $-4\gamma^2/\lambda$ is an integer square, $V$ is an irreducible principal series representation.

Proof. The criterion for reducibility of a parabolically induced representation is that $\varphi$ be an integer of the same parity as $n$, with $|\varphi| > |n|$. See [Kna86, Chap VIII, Problems 9-14] again. So if $\varphi$ is non-integral, then any irreducible representation with parameters $(0, \varphi)$ is an irreducible principal series representation. The result now follows from the Lemma 4.3.2. \qed

4.3.4. Remark. In the next section we shall construct families of representations using solutions of the rescaled Schrödinger equation. They will satisfy the hypotheses of the corollary, and as a result for almost all $\lambda$ the fibers will be irreducible principal series representations with parameters $(0, \sqrt{-4\gamma^2/\lambda})$. Among other things our construction will in effect extend the principal series to $\varphi = \infty$, where we will obtain a Harish-Chandra module for $(g|_0, K)$.

5. Solutions of the Schrödinger equation

In this section, we shall associate to every $\lambda \in \mathbb{C}$ a space $\text{RegSol}(\lambda)$ of “regular” solutions of the rescaled Schrödinger equation $T\psi = \lambda \psi$. Then we shall construct a natural algebraic family of Harish-Chandra modules $\text{RegSol}$ whose fibers are the spaces $\text{RegSol}(\lambda)$.

The solutions of the Schrödinger equation that are studied in physics are all regular, but here we shall also examine the “singular” solutions. Contrary to what one might expect, the singular solutions will play a decisive role in our study of the physical solutions of the Schrödinger equation.

5.1. Solutions by separation of variables. In this subsection we shall review the standard approach to the solution of the (rescaled) Schrödinger equation by separation of variables in spherical coordinates.

5.1.1. Definition. For each $\lambda \in \mathbb{C}$ we define
\[
\text{Sol}(\lambda) = \{ \psi \in C^\infty(\mathbb{R}^3_0)_{\text{fin}} : T\psi = \lambda \psi \}.
\]
The Laplacian on $\mathbb{R}^3_0$ may be written as
\[ \Delta = \frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \Omega \]
where $\Omega$ is the Casimir operator (4.2.1) and where $\partial/\partial r$ is differentiation in the radial direction:
\[ \frac{\partial}{\partial r} = \frac{1}{r} \left( x_1 \frac{\partial}{\partial x_1} + x_2 \frac{\partial}{\partial x_2} + x_3 \frac{\partial}{\partial x_3} \right). \]
So the rescaled Schrödinger operator $T$ acts on the $\ell$-isotypical component of the space $\mathcal{C}^\infty(\mathbb{R}^3_0)$ fin as
\[ (5.1.2) \quad T = -\frac{\partial^2}{\partial r^2} - \frac{2}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \ell(\ell + 1) - \frac{2\gamma}{r}. \]
Using the standard diffeomorphism
\[ (5.1.3) \quad \mathbb{R}^3_0 \xrightarrow{\cong} \mathbb{R}_+ \times S^2 \]
\[ x \mapsto (\|x\|, \|x\|^{-1} x), \]
we find that for any $\lambda \in \mathbb{C}$, the $\ell$-isotypical space in $\text{Sol}(\lambda)$ is the tensor product of the two-dimensional space of $\lambda$-eigenfunctions of (5.1.2) in $\mathcal{C}^\infty(\mathbb{R}_+)$ with the $\ell$-isotypical component of the space $\mathcal{C}^\infty(S^2)_{\text{fin}}$. The latter is a single copy of the irreducible $\text{SO}(3)$-type representation $W_\ell$; as noted in Section 3 it consists of the spherical harmonic functions of degree $\ell$, which are the restrictions of harmonic polynomial functions of degree $\ell$ to the sphere. We arrive at the following simple conclusion:

5.1.4. Proposition. For every $\lambda \in \mathbb{C}$ the subspace $\text{Sol}(\lambda) \subseteq \mathcal{C}^\infty(\mathbb{R}^3_0)_{\text{fin}}$ is invariant under the action of the Lie algebra $\mathfrak{g}$. Moreover the action of $\mathfrak{g}$ on $\text{Sol}(\lambda)$ factors through the fiber $\mathfrak{g}_\lambda$, and gives $\text{Sol}(\lambda)$ the structure of an admissible $(\mathfrak{g}_\lambda, K)$-module, with each $\text{SO}(3)$-type representation of $K$ occurring with multiplicity 2. \(\square\)

5.2. Regular solutions of the Schrödinger equation. Let us examine the radial operator (5.1.2), acting on smooth functions of $r > 0$, a little more closely. Its $\lambda$-eigenfunctions are precisely the solutions of the differential equation
\[ (5.2.1) \quad r^2 \frac{d^2 \psi}{dr^2} + 2r \frac{d \psi}{dr} - \ell(\ell + 1) \psi + 2\gamma r \psi + \lambda r^2 \psi = 0. \]
This equation is regular-singular at $r = 0$, with indicial roots $\ell$ and $-(\ell+1)$, and general theory (namely the Frobenius method; see [WW96, Chapter X] or [Tes12, Ch 4]) provides a smooth solution defined on $\mathbb{R}_+$ that in fact extends to an entire function of $r \in \mathbb{C}$ with a zero of order precisely $\ell$ at $r = 0$.

5.2.2. Definition. We shall denote by $F_{\ell,\lambda}$ the unique solution of (5.2.1) that extends to an analytic function of $r \in \mathbb{C}$ and has the Taylor series
\[ (5.2.3) \quad F_{\ell,\lambda}(r) = r^\ell + \text{higher-order terms in } r. \]
General theory also provides a second, linearly independent solution of the form
\[ (5.2.4) \quad G_{\ell,\lambda}(r) = H_{\ell,\lambda}(r) + C_{\ell,\lambda} \log(r) F_{\ell,\lambda}(r), \]
where $H_{\ell,\lambda}$ is a meromorphic function of $r$ with a pole of order $\ell+1$. The constant $C_{\ell,\lambda}$ might be 0. Whether or not that is the case, the scalar multiples of $F_{\ell,\lambda}$ are the only solutions that are bounded near $0 \in \mathbb{R}^3$. 


5.2.5. **Definition.** We shall denote by RegSol(\(\lambda\)) the subspace of Sol(\(\lambda\)) comprised of functions that are bounded near \(0 \in \mathbb{R}^3\). Equivalently, RegSol(\(\lambda\)) is spanned by functions of the form

\[
\mathbb{R}_+ \times S^2 \ni (r, \theta) \mapsto F_{\ell, \lambda}(r)Y_\ell(\theta)
\]

in spherical coordinates (5.1.3), where:

(i) \(F_{\ell, \lambda}\) is the regular solution of the radial equation (5.2.1) with leading coefficient 1, as in (5.2.3), and

(ii) \(Y_\ell\) is any spherical harmonic function of degree \(\ell\).

5.2.6. **Proposition.** The subspace \(\text{RegSol}(\lambda) \subseteq \text{Sol}(\lambda)\) is a \((g|_{\lambda}, K)\)-submodule.

To prove this we shall use the following computation of the Runge-Lenz operators in polar coordinates.

5.2.7. **Lemma.** After applying the diffeomorphism \(\mathbb{R}_0^3 \cong \mathbb{R}_+ \times S^2\) in (5.1.3) each of the Runge-Lenz operators \(\mathcal{R}: C^\infty(\mathbb{R}_0^3) \to C^\infty(\mathbb{R}_0^3)\) assumes the form

\[
\sqrt{-\mathbf{\Gamma}} \cdot \mathcal{R} = C + \frac{1}{r} \cdot \mathbf{D} + \partial_r \cdot \mathbf{E},
\]

where \(C, D\) and \(E\) are linear differential operators on \(S^2\) with real coefficients.

**Proof.** Each coordinate vector field \(\partial_j\) on \(\mathbb{R}_0^3\) has the form

\[
h_j \cdot \partial_r + \frac{1}{r} \cdot X_j,
\]

where \(h_j\) is a smooth function on the 2-sphere and \(X_j\) is a vector field on \(S^2\). The lemma follows from this and the fact that

\[
\sqrt{-\mathbf{\Gamma}} \cdot \mathcal{R}_i = \sum_{j \neq i} \pm L_i \partial_j + \partial_i - \frac{\gamma x_i}{r},
\]

keeping in mind that each \(L_i\) is a vector field on \(S^2\) in spherical coordinates while \(x_i/r\) is a smooth function on \(S^2\).

**Proof of Proposition 5.2.6.** Let \(\psi = F_{\ell, \lambda} \cdot Y_\ell\) be a generating element of the vector space \(\text{RegSol}(\lambda)\), as in Definition 5.2.5. It suffices to show that if \(\mathcal{R}\) is any one of the Runge-Lenz operators, then the function \(\mathcal{R}\psi\) is bounded in a neighbourhood of \(0 \in \mathbb{R}^3\).

When \(\ell \geq 1\), boundedness is clear from the formula for the operator \(\mathcal{R}\) given in Lemma 5.2.7, since \(F_{\ell, \lambda}\) vanishes at \(r=0\). But when \(\ell = 0\), the function \(F_{\ell, \lambda}\) does not vanish at \(r=0\), and the formula in Lemma 5.2.7 suggests that \(\mathcal{R}\psi\) might behave like \(1/r\) at \(r=0\). So a somewhat closer examination is required.

Suppose then that \(\ell = 0\). Denote by \(\langle \mathcal{R}\psi \rangle^k\) the projection of \(\mathcal{R}\psi\) into the \(k\)-isotypical component of \(\text{Sol}(\lambda)\), so that

\[
\mathcal{R}\psi = \sum_{k \geq 0} \langle \mathcal{R}\psi \rangle^k.
\]

The functions \(\langle \mathcal{R}\psi \rangle^k\) for \(k \geq 1\) must be bounded near \(r=0\), since the space \(\text{Sol}(\lambda)^k\) consists of functions that are either bounded near \(r=0\) or have poles of order \(k+1\), and \(k+1 \geq 2\), while \(\mathcal{R}\psi\) behaves at worst like \(1/r\). As for the component \(\langle \mathcal{R}\psi \rangle^0\), it follows from the definitions that

\[
\langle \mathcal{R}\psi \rangle^0 = e \text{Re}\psi,
\]
and we have seen that eRe, like any element of $\mathcal{H}(\mathfrak{g}, K)$, acts on the 0-isotypical component as a polynomial function of $\lambda$, so that $(R\psi)^0$ is a scalar multiple of $\psi$ and is therefore bounded near $r=0$ as required.  

5.3. **The algebraic family of regular solutions.** We shall now assemble the spaces $\text{RegSol}(\lambda)$ into an algebraic family, as follows.

5.3.1. **Definition.** We shall denote by $\mathcal{R}_{\text{RegSol}}$ the complex vector space that is spanned by functions on $\mathbb{C} \times \mathbb{R}_+ \times S^2$ (using spherical coordinates) of the form

$$(\lambda, r, \theta) \mapsto p(\lambda) F_{\ell, \lambda}(r) Y_{\ell}(\theta),$$

where

(i) $p$ is any polynomial function, and
(ii) $F_{\ell, \lambda}$ and $Y_{\ell}$ are as in Definition 5.2.5 above.

We give $\mathcal{R}_{\text{RegSol}}$ the structure of a (free) $O$-module via the natural action of the rescaled Schrödinger operator $T \in O$ on functions, which is in this case of course multiplication by $\lambda$ since the action is on eigenfunctions.

The group $K$ acts on $\mathcal{R}_{\text{RegSol}}$ as $O$-module automorphisms via the action (2.2.11) of $K$ on $\mathbb{R}^3_0$. There are obvious $K$-equivariant isomorphisms

$$(5.3.2) \quad \mathcal{R}_{\text{RegSol}}|_{\lambda} \cong \mathcal{R}_{\text{RegSol}}(\lambda)$$

for all $\lambda \in \mathbb{C}$. We wish to make $\mathcal{R}_{\text{RegSol}}$ a $\mathfrak{g}$-module via the natural action of $\mathfrak{g}$ as differential operators on smooth functions on $\mathbb{R}^3_0$. But we need to prove first that $\mathcal{R}_{\text{RegSol}}$ is invariant under this action. The following is one of our main results:

5.3.3. **Theorem.** The vector space $\mathcal{R}_{\text{RegSol}}$ is invariant under the following action of elements $X \in \mathfrak{g}$:

$$X: (p \cdot F_{\ell, \lambda} \cdot Y_{\ell}) \mapsto \left[ (\lambda, r, \theta) \mapsto p(\lambda)(X(F_{\ell, \lambda}Y_{\ell}))(r, \theta) \right].$$

As a result, $\mathcal{R}_{\text{RegSol}}$ carries the structure of an algebraic family of Harish-Chandra modules.

It is enough to prove that $\mathcal{R}_{\text{RegSol}}$ is invariant under the action of the Runge-Lenz operators, and this is what we shall do in the next several lemmas.

5.3.4. **Lemma.** If $\ell \geq 1$ and if $\psi \in \mathcal{R}_{\text{RegSol}}^\ell$, and if $R$ is any Runge-Lenz operator, then $(R\psi)^{\ell-1} \in \mathcal{R}_{\text{RegSol}}^{\ell-1}$.

**Proof.** Think of $\psi$ as a section $\lambda \mapsto \psi_{\lambda}$ of the family of spaces $\text{RegSol}(\lambda)$. We may assume that $\psi$ is one of the generators of $\mathcal{R}_{\text{RegSol}}$, so that

$$\psi_{\lambda} = p(\lambda) \cdot F_{\ell, \lambda} \cdot Y_{\ell}.$$ 

Using Lemma 5.2.7 we compute that

$$(5.3.5) \quad R\psi_{\lambda} = p(\lambda) \cdot \ell \cdot r^{\ell-1} \cdot DY_{\ell} + p(\lambda) \cdot r^{\ell-1} \cdot EY_{\ell} + \text{higher-order terms in } r.$$

The formula shows that the $(\ell-1)$-component of $R\psi$ belongs to $\mathcal{R}_{\text{RegSol}}$, as required.  

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3In fact one can compute that $eRe=0$ in $\mathcal{H}(\mathfrak{g}, K)$, so that $(R\psi)^0 = 0$. 
It will be convenient now to introduce a somewhat larger space than \( \text{RegSol} \). We shall denote by \( \text{RegSol}_{\text{hol}} \) the space defined in exactly the same way as \( \text{RegSol} \), except that \( p(\lambda) \) is replaced by any entire function \( h(\lambda) \). Since the eigenfunctions \( F_{\ell,\lambda} \) depend analytically on \( \lambda \), the space \( \text{RegSol}_{\text{hol}} \) is certainly invariant under the action of \( g \).

5.3.6. **Lemma.** If \( \varphi \in \text{RegSol}_{\text{hol}} \), and if \( p \cdot \varphi \in \text{RegSol} \) for some nonzero polynomial \( p \), then \( \varphi \in \text{RegSol} \).

**Proof.** This follows from the fact that the only entire rational functions are polynomials. \( \square \)

To proceed, let us make note of a simple fact that will be discussed further in the next section (and in any case the lemma may be proved by direct computation):

5.3.7. **Lemma.** For all but countably many \( \lambda \in \mathbb{C} \) the space \( \text{RegSol}(\lambda) \) is an irreducible \((\mathfrak{g}_\lambda, K)\)-module. \( \square \)

5.3.8. **Lemma.** If \( \ell \geq 1 \), if \( \psi \in \text{RegSol}_{\text{hol}}^t \), and if \( \langle RS\psi \rangle^{\ell - 1} \in \text{RegSol}^{\ell - 1} \) for every Runge-Lenz operator \( R \) and every \( S \in R[K] \), then \( \psi \in \text{RegSol}^t \).

**Proof.** Assume that \( \psi = h \cdot F_{\ell,\lambda} \cdot Y_\ell \), with \( h \) holomorphic. It follows from the explicit formula (5.3.5) that \( \langle RS\psi \rangle^{\ell - 1} \) has the form

\[
h \cdot F_{\ell - 1,\lambda} \cdot Z_{\ell - 1}
\]

for some \( Z_{\ell - 1} \) in the \((\ell - 1)\)-isotypical part of \( C^\infty(S^2) \) that depends on the choices of \( R \) and \( S \).

If \( Y_\ell \) is nonzero, then \( Z_{\ell - 1} \) must be nonzero for some \( R \) and some \( S \), for otherwise the \((\mathfrak{g}_\lambda, K)\)-submodule of \( \text{RegSol}(\lambda) \) generated by \( \psi_\lambda \) would be a proper submodule for every \( \lambda \), contrary to Lemma 5.3.7. In the case where \( Z_{\ell - 1} \) is nonzero, if \( \langle RS\psi \rangle^{\ell - 1} \in \text{RegSol} \), then it follows that \( h \) is in fact a polynomial function, and hence that \( \psi \in \text{RegSol} \), as required. \( \square \)

5.3.9. **Lemma.** If \( X \in \mathcal{U}(\mathfrak{g}, K) \) and if \( \psi \in \text{RegSol}^0 \), then \( X\psi \in \text{RegSol} \).

**Proof.** Fix \( \psi \in \text{RegSol}^0 \). We need to prove that \( \langle X\psi \rangle^\ell \in \text{RegSol} \) for every \( X \) and every \( \ell \geq 0 \). If \( \ell = 0 \), then since

\[
\langle X\psi \rangle^0 = eXe \cdot \psi,
\]

with \( eXe \in \mathcal{H}(\mathfrak{g}, K) \), the required result follows for every \( X \) from Proposition 3.4.6 and Lemma 2.8.3, which together show that \( e \cdot X \cdot e \) acts on \( \text{RegSol}^0 \) as multiplication by a polynomial in \( \lambda \). The cases of higher \( \ell \) are handled by induction on \( \ell \) using Lemma 5.3.8. \( \square \)

5.3.10. **Lemma.** If \( \psi \in \text{RegSol} \), then there exists a nonzero polynomial \( p \), some \( S^0 \in \mathcal{U}(\mathfrak{g}, K) \) and some \( \psi^0 \in \text{RegSol}^0 \), such that \( p \cdot \psi = S^0 \cdot \psi^0 \).

**Proof.** It follows from the Peter-Weyl decomposition (3.1.4) and the \( K \)-isotypical decomposition of \( \text{RegSol} \) that there is a family of pairwise orthogonal idempotents \( f_\alpha \) in \( R[K] \) such that

\[
\text{RegSol} = \bigoplus_\alpha f_\alpha \cdot \text{RegSol}
\]
and such that each summand on the right is a free $\mathcal{O}$-module of rank one. It suffices to prove the lemma for generators of each of these summands, so let $\psi$ be a generator for the $\mathcal{O}$-module $f_\alpha \cdot \text{RegSol}$. Thanks to Lemma 5.3.7 we can write

$$\psi_\lambda = (f_\alpha \cdot \psi)_\lambda = (f_\alpha \cdot S_\alpha \cdot \psi^0)_\lambda$$

for at least one value of $\lambda$, for some $S_\alpha \in \mathcal{U}(\mathfrak{g}, \mathbb{K})$ and for some $\psi^0 \in \text{RegSol}^0$. This means, in particular that $f_\alpha \cdot S_\alpha \cdot \psi^0_\lambda$ is nonzero, and hence that $f_\alpha \cdot S_\alpha \cdot \psi^0$ is nonzero. Since the latter is an element of a free $\mathcal{O}$-module of rank one, of which $\psi$ is a generator, we can write

$$f_\alpha \cdot S_\alpha \cdot \psi^0 = p \cdot \psi$$

for some $p \in \mathcal{O}$, as required. □

**Proof of Theorem 5.3.3.** Given $\psi \in \text{RegSol}$ and $S \in \mathcal{U}(\mathfrak{g}, \mathbb{K})$, we wish to prove that $S\psi \in \text{RegSol}$. As we have already observed, certainly $S\psi \in \text{RegSol}_{\text{hol}}$. But if $p\psi = S^0\psi^0$, as in Lemma 5.3.10, then

$$pS\psi = SS^0\psi^0,$$

and so it follows from Lemma 5.3.9 that $pS\psi \in \text{RegSol}$. Lemma 5.3.6 now implies that $S\psi \in \text{RegSol}$, as required. □

5.4. **An explicit formula for the action.** It is also possible to prove Theorem 5.3.3 by an explicit computation, although the details are surprisingly intricate. Here we give a sketch of the method and at the same time give explicit formulas for a basis of the regular solutions.

To begin, if $\lambda \neq 0$, then it may be shown that

$$(5.4.1) \quad F_{\ell,\lambda}(r) = r^\ell e^{-\sqrt{-\lambda}r} M\left( -\frac{\gamma}{\sqrt{-\lambda}} + \ell + 1, 2\ell + 2, \frac{2}{\sqrt{-\lambda}}r \right),$$

where $M(a, b, z)$ is Kummer’s confluent hypergeometric function. (It follows from Kummer’s formula

$$e^{-z} M(a, b, z) = M(b - a, b, -z)$$

and the fact that Bessel functions of odd order are odd that $F_{\ell,\lambda}$ does not depend on the choice of the square root.) If $\lambda = 0$, then

$$(5.4.2) \quad F_{\ell,\lambda}(r) = \frac{(2\ell + 1)!}{2^{2\ell + 1} \gamma^{2\ell + 1}} J_{2\ell + 1}(\sqrt{8r})$$

where $J_{\nu}(z)$ is the Bessel function of the first kind. See for example [LL58, Section 36].

Next, for $\ell \geq m \geq -\ell$, we define $\psi^\ell_m \in \text{RegSol}$ by

$$\psi^\ell_m = F_{\ell,\lambda} \cdot \gamma^\ell_m,$$

where the functions $\gamma^\ell_m$ are the basis for the spherical harmonic functions of degree $\ell$ from [AWH13, Chap. 15, eq. 15.137]. Now, form the following combination of Runge-Lenz vectors:

$$R_- = -iR_1 - R_2.$$
Then it may be calculated that
\begin{equation}
R_{-}\psi_{\lambda}^{\ell,\ell} = \sqrt{2\ell(2\ell+1)}\ell \psi_{\lambda}^{\ell-1,\ell-1} - \frac{\sqrt{2}}{\sqrt{(2\ell+3)(2\ell+1)}} \gamma^2 + \lambda(\ell + 1)^2 \frac{\psi_{\lambda}^{\ell+1,\ell-1}}{(\ell + 1)(2\ell + 3)}.
\end{equation}

The computation involves the explicit form of the functions $F_{\ell,\lambda}$ along with various identities for hypergeometric, and other, functions.

It can be shown that the entire $g$-action is determined by this family of formulas. The formulas indicate that $R_{-}$ maps $\psi_{\lambda}^{\ell,\ell}$ back into $\text{RegSol}$, and hence $\text{RegSol}$ is invariant under the full action of $g$.

5.5. **Singular solutions and the Wronskian form.** In this subsection we shall examine the quotient

$$\text{SingSol}(\lambda) = \text{Sol}(\lambda) / \text{RegSol}(\lambda)$$

as a $(g|_{\lambda}, K)$-module.

5.5.1. **Definition.** The (modified) Wronskian of two functions $\varphi$ and $\psi$ of $r > 0$ is the function

$$\text{wr}(\varphi, \psi)(r) = r^2 \left( \frac{d\varphi(r)}{dr} \psi(r) - \varphi(r) \frac{d\psi(r)}{dr} \right).$$

The modification ensures that if $\varphi$ and $\psi$ are two solutions of the radial equation (5.2.1) for the same $\lambda$ and the same $\ell$, then $\text{wr}(\varphi, \psi)$ is a constant function of $r$, to see this, differentiate with respect to $r$. Moreover since all solutions are real-analytic functions of $r > 0$, the (modified) Wronskian of two solutions vanishes identically if and only if the solutions are linearly dependent.

Of course the Wronskian pays no attention to the angular coordinates in $S^2$. In order to remedy this, we make the following definition.

5.5.2. **Definition.** The **Wronskian form** on $\text{Sol}(\lambda)$ is the bilinear form

$$\text{Wr}: \text{Sol}(\lambda) \times \text{Sol}(\lambda) \rightarrow \mathbb{C}$$

defined by

$$\text{Wr}(\varphi, \psi) = \frac{1}{4\pi} \int_{S^2} \text{wr}(\varphi, \psi) \ d\text{Area}.$$ 

The integral is a $K$-invariant and nondegenerate bilinear form on each $K$-isotypical subspace of $\text{Sol}(\lambda)$, and moreover distinct isotypical subspaces are orthogonal to one another.

5.5.3. **Lemma.** If $\varphi, \psi \in \text{RegSol}(\lambda)$, then $\text{Wr}(\varphi, \psi) = 0$.

**Proof.** If $\varphi$ and $\psi$ belong to distinct isotypical subspaces, then the integral is zero. If they belong to the same isotypical space, then, both functions being regular solutions, their radial parts are linearly dependent, and so the integrand is zero. \hfill $\square$

Thanks to the lemma, the Wronskian form defines a nondegenerate bilinear form

$$\text{Wr}: \text{SingSol}(\lambda) \times \text{RegSol}(\lambda) \rightarrow \mathbb{C}.$$ 

We shall prove the following result:
5.5.4. **Theorem.** Let $\lambda \in \mathbb{C}$, and let $X \in \mathfrak{g}|_{\lambda}$. If $\varphi \in \text{SingSol}(\lambda)$ and $\psi \in \text{RegSol}(\lambda)$, then
\[
\text{Wr}(X\varphi, \psi) + \text{Wr}(\varphi, \theta(X)\psi) = 0.
\]
As a result, the Wronskian induces an isomorphism of $(\mathfrak{g}|_{\lambda}, K)$-modules from $\text{SingSol}(\lambda)$ to the $\theta$-twisted dual of $\text{RegSol}(\lambda)$.

5.5.5. **Corollary.** If $\lambda \in \mathbb{R}$, then the Wronskian form induces an isomorphism of $(\mathfrak{g}|_{\lambda}, K)$-modules from $\text{SingSol}(\lambda)$ to the $\sigma$-twisted dual of $\text{RegSol}(\lambda)$.

**Proof of the Corollary.** The theorem immediately gives
\[
\text{Wr}(X\varphi, \psi) + \text{Wr}(\varphi, \theta(X)\psi) = 0
\]
for $\varphi \in \text{SingSol}(\lambda)$ and $\psi \in \text{RegSol}(\lambda)$. But this the same as
\[
\text{Wr}(X\varphi, \psi) + \text{Wr}(\varphi, \sigma(X)\psi) = 0,
\]
from which the result follows. □

We shall prove the theorem in a sequence of steps. The first concerns the constituents of the formula
\[
(5.5.6) \quad \sqrt{-R} = C + \frac{1}{r} \cdot D + \partial_r \cdot E
\]
for a Runge-Lenz operator that we obtained in Lemma 5.2.7. We shall use the following notation: if $A$ is a linear operator on a locally finite-dimensional representation space $V$ for $K$, then we shall denote by
\[
A^k_\ell : V^k \longrightarrow V^\ell
\]
the composition of the restriction of $A$ to the $k$-isotypical space of $V$ with the projection onto the $\ell$-isotypical space.

5.5.7. **Lemma.** If $D$ and $E$ are the operators in (5.5.6), acting on smooth functions on $S^2$, and if $\ell \geq 1$, then
\[
E^\ell_{\ell-1} = (1-\ell)D^\ell_{\ell-1}
\]
and
\[
E^{\ell-1}_\ell = (1+\ell)D^{\ell-1}_\ell.
\]

**Proof.** A short computation reveals that
\[
[T, R] = \frac{1}{r^2} \partial_r \cdot (2E - 2D - [\Omega, D]) - \frac{1}{r^2} \cdot (\gamma D + [\Omega, C])
\]
\[
+ \frac{1}{r^3} \cdot (2[\Omega, D] - 2\Omega D - [\Omega, E]).
\]
Since $[T, R] = 0$, each of the three terms in parentheses is zero. Our interest is in the first. Since $\Omega$ acts as $\ell(\ell+1)$ on the $\ell$-isotypical space we obtain
\[
[2E - 2D + \ell(\ell+1)D - D(\ell-1)\ell]^{\ell}_{\ell-1} = 0
\]
and after simplification this becomes
\[
[E - (1-\ell)D]^{\ell}_{\ell-1} = 0
\]
as required for the first identity. The second is handled similarly. □
5.5.8. **Lemma.** If $Y$ and $Z$ are smooth functions on $S^2$, then
\[
\int_{S^2} Y \cdot DZ \, d\text{Area} = -\int_{S^2} DY \cdot Z \, d\text{Area}
\]
and
\[
\int_{S^2} Y \cdot EZ \, d\text{Area} = \int_{S^2} EY \cdot Z \, d\text{Area} - 2\int_{S^2} DY \cdot Z \, d\text{Area}.
\]

**Proof.** The operator $\sqrt{-1}R$ is formally self-adjoint for the usual inner product of functions on $\mathbb{R}^3$. The present lemma follows from the formula for $\sqrt{-1}R$ and from the fact that the formal adjoint of $\partial_r$ is $-\partial_r - 2/r$. $\Box$

5.5.9. **Lemma.** If $\varphi \in \text{SingSol}(\lambda)^{\ell-1}$ and $\psi \in \text{RegSol}(\lambda)^{\ell}$, then
\[
\text{Wr}(R\varphi, \psi) - \text{Wr}(\varphi, R\psi) = 0.
\]

**Proof.** First, we compute that
\[
\text{wr}(R\varphi, \psi) = (2\ell^2 + \ell)r^{\ell} \cdot DY \cdot Z - (2\ell + 1)r^{\ell} \cdot EY \cdot Z + \text{positive-order terms in } r,
\]
for some spherical harmonic functions $Y$ and $Z$ of degrees $\ell-1$ and $\ell$, respectively. Hence
\[
\text{Wr}(R\varphi, \psi) = (2\ell^2 + \ell)\int_{S^2} DY \cdot Z \, d\text{Area} - (2\ell + 1)\int_{S^2} EY \cdot Z \, d\text{Area},
\]
and similarly
\[
\text{Wr}(\varphi, R\psi) = -(2\ell^2 - \ell)\int_{S^2} Y \cdot DZ \, d\text{Area} - (2\ell - 1)\int_{S^2} Y \cdot EZ \, d\text{Area}.
\]
It follows that
\[
\text{Wr}(R\varphi, \psi) - \text{Wr}(\varphi, R\psi) = (2\ell - 2)\int_{S^2} DY \cdot Z \, d\text{Area} - 2\int_{S^2} EY \cdot Z \, d\text{Area},
\]
and to complete the proof we need only apply Lemma 5.5.7. $\Box$

**Proof of Theorem 5.5.4.** The Wronskian pairing determines a $K$-equivariant vector space isomorphism
\[
(5.5.10) \quad \text{SingSol}(\lambda) \longrightarrow \text{RegSol}(\lambda)^{*,0}
\]
(the right-hand side is the $\theta$-twisted dual). Moreover this isomorphism is compatible with the action of the Runge-Lenz operators $R$ from $(\ell-1)$- to $\ell$-isotypical components, for all $\ell > 0$, thanks to Lemma 5.5.9.

Now, for all but countably many $\lambda$, the $(g|_\lambda, K)$-modules in (5.5.10) are irreducible, and moreover they are isomorphic to one another. This follows from the discussion in Section 4. It therefore follows from Schur’s lemma that for such $\lambda$, (5.5.10) can differ from an isomorphism of $(g|_\lambda, K)$-modules only by a multiplicative scalar in each $K$-isotypical component, since these components have multiplicity one. But compatibility with the Runge-Lenz operators, even to the limited extent we have exhibited it, implies that these scalars must all be equal to one another. So (5.5.10) is indeed an isomorphism of $(g|_\lambda, K)$-modules. This proves the lemma when the modules in (5.5.10) are irreducible. The general case follows by a continuity argument. $\Box$
5.6. **The algebraic family of singular solutions.** In view of the preceding section it is natural to organize the modules SingSol(λ) into an algebraic family. Linearly independent solutions to the radial Schrödinger equation are given in (5.2.3) and (5.2.4), and from the formulas it is clear that the coefficient of \( r^{-(\ell+1)} \) in a solution depends only on the class of the solution in SingSol(λ).

5.6.1. **Definition.** We shall denote by SingSol the complex vector space spanned by sections

\[ C \ni \lambda \mapsto \phi_\lambda \in \text{SingSol}(\lambda) \]

that are representable in the form

\[ \psi_\lambda = p(\lambda) G_{\ell,\lambda} \cdot Y_\ell \in \text{Sol}(\lambda) \]

where \( p(\lambda) \) is a polynomial function of \( \lambda \) and where \( G_{\ell,\lambda} \) is as in (5.2.4), with coefficient of \( r^{-(\ell+1)} \) the constant 1.

By repeating computations from the previous two subsections we arrive at the following result.

5.6.2. **Theorem.** The space SingSol is an algebraic family of Harish-Chandra modules for \((g, K)\). The Wronskian form

\[ \text{SingSol} \times \text{RegSol} \longrightarrow \mathcal{O} \]

induces an isomorphism of algebraic families from SingSol to the \( \theta \)-twisted dual of RegSol.

\[ \square \]

5.6.3. **Proposition.** The family SingSol is a standard and spherical family of \((g, K)\)-modules, in the sense of Definition 3.4.1.

**Proof.** We need to check that SingSol is generated by its spherical vectors. It follows from the formula in Lemma 5.2.7 for the Runge-Lenz operators in polar coordinates that if \( \psi_\lambda = G_{\ell,\lambda} Y_\ell \), then

\[ R\psi_\lambda = -(\ell+1) r^{-(\ell+2)} \cdot D Y_\ell + r^{-(\ell+2)} \cdot E Y_\ell + \text{higher-order terms in } r. \]

Thus

\[ \langle R\psi_\lambda \rangle^{\ell+1} = G_{\ell+1,\lambda} Z_{\ell+1} \]

for some spherical harmonic function \( Z_{\ell+1} \). Now for every \( \ell \geq 0 \) there is at least one \( Y_\ell \), as above, for which \( Z_{\ell+1} \) is nonzero, for otherwise every module SingSol(λ) would be reducible. It follows that

\[ \text{SingSol}^{\ell+1} \subseteq \mathcal{U}(g) \cdot \text{SingSol}^\ell, \]

and hence that SingSol is generated by its spherical vectors, as required.

\[ \square \]

The following is an immediate consequence of the classification result in Theorem 3.4.4 and Lemma 2.8.3.

5.6.4. **Theorem.** Up to isomorphism, SingSol is the unique standard and spherical family for which the Casimir element \( TL^2 - R^2 \) acts as \( T + \gamma^2 I \).

\[ \square \]

Of course, this result leads to a characterization of RegSol, since it is the \( \theta \)-twisted dual of SingSol.
6. Physical Solutions and Jantzen Quotients

In this section we shall examine the solution spaces

\[ \text{PhysSol}(\lambda) \subseteq \text{RegSol}(\lambda) \]

for the Schrödinger equation that are used in physics. The physical solutions are characterized within \( \text{RegSol}(\lambda) \) by boundary conditions at infinity in \( \mathbb{R}^3_0 \), which imply that the physical solutions are either square-integrable, or nearly square-integrable. The main purpose of this section is to explain that the physical solutions can also be obtained in a purely representation-theoretic fashion using the Jantzen technique.

6.1. Physical solution spaces. By the \( K \)-finite physical solutions of the (rescaled) Schrödinger equation we mean the solutions computed in physics texts by separation of variables in spherical coordinates. See for example [LL58, Section 36] or Section 5.4.

For a given \( \lambda \in \mathbb{R} \), the space \( \text{PhysSol}(\lambda) \) of physical solutions consists of those functions in \( \text{RegSol}(\lambda) \) that converge to zero at infinity. Computations using explicit formulas show that

(a) \( \text{PhysSol}(-\gamma^2/n^2) \) is the finite-dimensional subspace of \( \text{RegSol}(-\gamma^2/n^2) \) comprised of the \( \text{SO}(3) \)-types \( \ell<n \). It is a Harish-Chandra submodule.

(b) \( \text{PhysSol}(\lambda) = \text{RegSol}(\lambda) \) for all \( \lambda \geq 0 \)

(c) \( \text{PhysSol}(\lambda) = 0 \) otherwise.

Moreover in every case the physical solution space has the structure of an irreducible \( (g|\lambda, K) \)-module and carries an invariant inner product. See for example [Bl66a], [TdCA98] and [Bl66b] for the cases of \( \lambda<0 \), \( \lambda=0 \) and \( \lambda>0 \), respectively.

6.2. An intertwining operator. In this subsection we shall analyze the intertwining operator \( A \) from the algebraic family of singular solutions to the regular of solutions that is characterized by the following diagram:

\[ \begin{CD}
\text{SingSol} @> A >> \text{RegSol} \\
\equiv @> UH(g, K) \otimes H(g, K) \circlearrowleft \end{CD} \]

The tensor product at the bottom is that for which the Casimir \( TL^2 - R^2 \in H(g, K) \) acts as multiplication by \( T + \gamma^2 I \) on \( O \). The diagonal morphisms are the classifying morphisms (3.4.8) for \( \text{SingSol} \) and \( \text{RegSol} \) (we identify the \( \ell=0 \) isotypical parts of these families with \( O \) using any isomorphisms of \( H(g, K) \)-modules). The left classifying morphism is an isomorphism since the \( \sigma \)-twisted dual is standard and spherical; see the proof of Theorem 3.4.4. There is therefore a unique morphism \( A \) that makes the diagram commute.

If \( B : \text{SingSol} \to \text{RegSol} \) is any other intertwining morphism, then since almost all fibers in the families are irreducible, it follows from Schur’s lemma that there are nonzero and relatively prime \( p, q \in O \) for which

\[ p \cdot A = q \cdot B. \]

But the morphism \( A \) is nonzero in each fiber since it is an isomorphism on \( \ell=0 \) isotypical spaces, and as a result \( q \) must be a constant polynomial. So, up to a
nonzero complex scalar multiple, $A$ is the unique intertwining morphism that is nonzero in each fiber.

We can identify all the $\ell$-isotypical space $\text{RegSol}^\ell$ as an $\mathcal{O}$-module and a $K$-module with $\mathcal{O} \otimes_{C} W_{\ell}$, for example by the mapping

$$\text{RegSol}^\ell \ni F_{\ell,\lambda} \cdot Y_{\ell} \mapsto 1 \otimes Y_{\ell} \in \mathcal{O} \otimes_{C} W_{\ell}.$$ 

Compare Definition 5.2.5. We can do the same for the $\ell$-isotypical subspace of $\text{SingSol}$. After making these identifications, it follows from Schur’s lemma that the restriction of $A$ to the $\ell$-isotypical parts of our families is multiplication by a diagonal coefficient polynomial function $A_{\ell}(\lambda)$ that is determined up to multiplication by a nonzero constant. The constant depends on $\ell$, and varies with our choices of identifications.

The diagonal coefficient polynomials may be explicitly computed quite easily by making an explicit calculation with a single Runge-Lenz operator. The result is as follows:

6.2.2. Proposition. The intertwining operator $A$ has diagonal coefficients

$$A_{\ell}(\lambda) = \text{constant}_{\ell} \cdot \prod_{n=1}^{\ell} (\lambda n^2 + \gamma^2),$$

for all $\ell \geq 1$. □

Compare [Sub18, Sec. IV], where essentially the same computation is carried out for the 2-dimensional hydrogen atom.

6.3. Jantzen quotients. We begin with a quick introduction; see [BHS18c, Sec. 4.1] for further details, which are given in precisely the context we are discussing.

An intertwiner $A: F \to H$ between algebraic families of Harish-Chandra modules over $C$ determines $\text{Jantzen filtrations}$ of the fibers of $F$ and $H$, as follows:

(a) For $F$, the filtration is decreasing, and for $p \in \mathbb{Z}$ the space $F_{\lambda}^{(p)}$ is defined to be the image in the fiber $F_{\lambda}$ of all sections $f$ for which $A(f)$ vanishes to order $p$ or more at $\lambda$.

(b) For $H$ the filtration is increasing, and $H_{\lambda}^{(p)}$ is defined to be the image in the fiber $H_{\lambda}$ of the space of all sections $h$ such that $(T-\lambda)^p \cdot h$ belongs to the image of $A$.

The map $f \mapsto (T-\lambda)^{-p} A(f)$ induces an isomorphism of $(g_{\lambda}, K)$-modules

$$A^{(p)}: F_{\lambda}^{(p)} / F_{\lambda}^{(p+1)} \cong H_{\lambda}^{(p)} / H_{\lambda}^{(p-1)}.$$ (6.3.1)

For the specific intertwiner introduced in (6.2.1) it is a simple matter to read off the terms in the Jantzen filtration, and the $\text{Jantzen quotients}$ (6.3.1), from Proposition 6.2.2. We’ll state the results only for the regular solutions; the results for the singular solutions can of course be inferred from the isomorphism in (6.3.1).

6.3.2. Proposition. Let $\lambda \in \mathbb{C}$. The Jantzen filtration of the fiber $\text{RegSol}(\lambda)$ determined by the intertwiner (6.2.1) is as follows:

(a) If $\lambda = -\gamma^2/n^2$, then $\text{RegSol}(\lambda)^{(p)}$ is zero for $p<0$, it is the direct sum of the $\ell$-isotypical subspaces in the range $\ell = 0, 1, 2, \ldots, n-1$ for $p=0$, and it is the full space
RegSol(\lambda) for p \geq 1. There are therefore exactly two nonzero Jantzen quotients. The first is n^2-dimensional with K-types
\ell = 0, 1, 2, \ldots, n-1,
each with multiplicity one. The second is irreducible and infinite-dimensional, with K-types
\ell = n, n+1, n+2, \ldots,
each with multiplicity one.

(b) For other values of \lambda the Jantzen filtration of RegSol(\lambda) is trivial: RegSol(\lambda)^{(p)} is zero for p<0, while it is the full space RegSol(\lambda) for p\geq 0. □

6.3.3. Remark. The term Jantzen quotient is standard, but of course a more accurate term would be Jantzen subquotient. Indeed the Jantzen quotient of most interest in the proposition above, namely the finite-dimensional Jantzen quotient in item (a), is in fact a submodule of RegSol(\lambda).

6.3.4. Corollary. The negative part of the physical spectrum of the rescaled Schrödinger operator T coincides with the set of all \lambda \in \mathbb{C} for which RegSol(\lambda) has a nontrivial Jantzen filtration. □

6.4. Non-degenerate invariant Hermitian forms. Here we shall use the fact that SingSol is isomorphic to the \sigma-twisted dual of RegSol (this follows from Theorem 3.4.4). Intertwiners of the form
A: RegSol^\ast,\sigma \longrightarrow RegSol,
between a family and its \sigma-twisted dual were analyzed in [BHS18c, Sec. 4.2], where it was pointed out that for a suitable c \in \mathbb{C}^\ast the formula
\langle A^{(p)}[\alpha], [\varphi] \rangle = c \cdot \left( (T - \lambda)^{-p} \cdot \alpha(\varphi) \right) \bigg|_{\lambda}
determines an invariant and nondegenerate hermitian form on the p’th Jantzen quotient. Here \alpha and \varphi determine elements in the p’th parts of the Jantzen filtrations, as in Subsection 6.3, and [\alpha] and [\varphi] are the corresponding elements in the Jantzen quotients. The term on the right is a polynomial in T, and in the formula we take its value at \lambda.

The Hermitian forms, like the Jantzen quotients themselves, are easy to compute using Proposition 6.2.2. Compare [BHS18c, Sec. 5] or [Sub18, Sec. IV]. Doing so, one obtains the following:

6.4.1. Proposition. For \lambda \in \mathbb{R} the above Hermitian form is definite precisely on the following Jantzen quotients:
(a) The unique Jantzen quotient when \lambda \geq 0.
(b) The finite-dimensional Jantzen quotient when \lambda = -\gamma^2/n^2, for some natural number n \geq 1. □

We arrive at the following theorem, which completely recovers both the physical spectrum of the rescaled Schrödinger operator and the physical solution spaces themselves from the algebraic family RegSol.

6.4.2. Theorem. The physical spectrum of the rescaled Schrödinger operator T coincides with the set of all \lambda \in \mathbb{R} for which RegSol(\lambda) has a nonzero infinitesimally unitary Jantzen quotient. There is in this case a unique infinitesimally unitary Jantzen quotient, and it is the submodule PhysSol(\lambda) of RegSol(\lambda). □
7. The Schrödinger Operator as a Self-Adjoint Operator

In this section we shall begin an examination of the Schrödinger operator from the point of view of Hilbert space spectral theory by reviewing how one can obtain a self-adjoint operator (in the technical sense of unbounded operator theory) from the rescaled Schrödinger operator

\[(7.0.1) \quad T = -\Delta - \frac{2\gamma}{r}.\]

There are two well-known approaches, both leading to the same self-adjoint operator, and we shall need to make use of both of them in what follows.

7.1. The Kato-Rellich theorem. The function \(-2\gamma/r\) is locally square-integrable on \(\mathbb{R}^3\), and therefore the operator (7.0.1) is well-defined as map from \(C^\infty_c(\mathbb{R}^3)\) into \(L^2(\mathbb{R}^3)\). Initially, we shall view \(T\) as a symmetric operator with this domain. The domain can then be extended, as follows. Denote by \(H^2(\mathbb{R}^3)\) the completion of \(C^\infty_c(\mathbb{R}^3)\) in the norm

\[\|f\|^2_{H^2(\mathbb{R}^3)} = \|\Delta f\|^2 + \|f\|^2,
\]

where—here and below—the unlabelled norms and inner products are to be taken in \(L^2(\mathbb{R}^3)\). This is a standard Sobolev space, of course. The inclusion of \(C^\infty_c(\mathbb{R}^3)\) into \(H^2(\mathbb{R}^3)\) extends to a continuous inclusion of \(H^2(\mathbb{R}^3)\) into \(L^2(\mathbb{R}^3)\). Moreover:

7.1.1. Lemma. The inclusion of \(C^\infty_c(\mathbb{R}^3)\) into \(L^\infty(\mathbb{R}^3)\) extends to a continuous inclusion of \(H^2(\mathbb{R}^3)\) into \(L^\infty(\mathbb{R}^3)\).

This is a special case of the Sobolev embedding theorem. As a result of the lemma, the operator (7.0.1) is in fact well-defined as a bounded linear operator from \(H^2(\mathbb{R}^3)\) into \(L^2(\mathbb{R}^3)\). The following result is well known; see for example [Kat76, Chap. V, Thm. 5.4] for a proof.

7.1.2. Theorem. The rescaled Schrödinger operator \(T\) for the 3-dimensional hydrogen atom is essentially self-adjoint and bounded below on the domain \(C^\infty(\mathbb{R}^3)\). The domain of the unique self-adjoint extension is the Sobolev space \(H^2(\mathbb{R}^3)\subseteq L^2(\mathbb{R}^3)\).

7.1.3. Remark. Recall for later that to say that \(T\) is bounded below on \(H^2(\mathbb{R}^3)\) is to say that there is a constant \(C_0 \geq 0\) such that

\[\langle T f, f \rangle \geq -C_0 \langle f, f \rangle\]

for every \(f \in H^2(\mathbb{R}^3)\). Equivalently, the spectrum of the self-adjoint operator \(T\) is bounded below by \(-C_0\).

Theorem 7.1.2 is the archetypical application of the Kato-Rellich theorem, [Kat76, Chap. 5, Thm 4.4], and accordingly we shall call the self-adjoint operator it provides the Kato-Rellich extension of (7.0.1).

7.1.4. Theorem. The spectrum of the Kato-Rellich extension of \(T\) consists of the nonnegative reals \([0, \infty)\) together with a countable discrete subset of \((\infty, 0)\), each element of which is an eigenvalue of finite multiplicity.

This is proved by arguing that the potential term \(-2\gamma/r\) in the rescaled Schrödinger operator is a relatively compact perturbation of the kinetic term; see for example [Kat76, Chap. V, Thm. 5.7].

By elliptic regularity, the negative energy eigenfunctions for the Kato-Rellich extension are smooth functions on the open set \(\mathbb{R}^3_0 \subseteq \mathbb{R}^3\). They are, of course
eigenfunctions, in the ordinary sense there, and they are square-integrable. Conversely, the space of all such square-integrable eigenfunctions may be determined explicitly, as we indicated in Section 6.1, and by Theorem 7.1.2 they all belong to the domain of the Kato-Rellich extension. So after these explicit computations we arrive at the following:

7.1.5. **Theorem.** The spectrum of the Kato-Rellich extension of the rescaled Schrödinger operator $T$ is the set

$$\{ -\frac{\gamma^2}{n^2} : n = 1, 2, \ldots \} \cup [0, \infty).$$

7.2. **The Friedrichs extension.** In this section we shall review the Friedrichs extension of $T$. See for instance [Kat76, Chap. VI, Sec. 3] for full details.

We have already seen that $T$ is bounded below on $C^\infty_c(\mathbb{R}^3_0)$ (and indeed on a larger domain). Choose a constant $C_0 > 0$ so that

$$\langle Tf, f \rangle + C_0 \langle f, f \rangle \geq 0$$

for every $f \in C^\infty_c(\mathbb{R}^3_0)$, and then choose $C > C_0$. Using this choice of $C$, denote by $F(\mathbb{R}^3)$ the Hilbert space completion of $C^\infty_c(\mathbb{R}^3_0)$ in the norm associated to the inner product

$$(7.2.1) \quad \langle f, g \rangle_{F(\mathbb{R}^3)} = \langle (T + C)f, g \rangle_{L^2(\mathbb{R}^3)}.$$

There is a bounded linear map

$$F(\mathbb{R}^3) \rightarrow L^2(\mathbb{R}^3)$$

that extends the inclusion of $C^\infty_c(\mathbb{R}^3_0)$ into $L^2(\mathbb{R}^3)$. The extended map is an inclusion, too, and we can therefore regard $F(\mathbb{R}^3)$ as a dense linear subspace of $L^2(\mathbb{R}^3)$ as well as a Hilbert space in its own right.

7.2.2. **Theorem.** There is a unique extension of the operator $(7.0.1)$ with domain $C^\infty_c(\mathbb{R}^3_0)$ to a self-adjoint operator on a domain that is included within the subspace $F(\mathbb{R}^3) \subseteq L^2(\mathbb{R}^3)$. The extension is characterized by the formula

$$\langle (T + C)^{-1}f, g \rangle_{F(\mathbb{R}^3)} = \langle f, g \rangle_{L^2(\mathbb{R}^3)}$$

for all $f \in L^2(\mathbb{R}^3)$ and all $g \in F(\mathbb{R}^3)$.

This is the Friedrichs extension of the rescaled Schrödinger operator $T$ from the initial domain $C^\infty_c(\mathbb{R}^3_0)$ to a self-adjoint operator that is bounded below; see for example [Kat76, Chap. VI, Thm 2.11].

7.2.3. **Theorem.** The Friedrichs extension of the Schrödinger operator from Theorem 7.2.2 coincides with the Kato-Rellich extension from Theorem 7.1.2.

**Proof.** Thanks to the uniqueness assertion in Theorem 7.2.2, it suffices to prove that

$$H^2(\mathbb{R}^3) \subseteq F(\mathbb{R}^3) \subseteq L^2(\mathbb{R}^3).$$

We shall use the Sobolev space $H^1(\mathbb{R}^3)$, which is the completion of $C^\infty_c(\mathbb{R}^3)$ in the norm associated to the inner product

$$(f, f)_{H^1(\mathbb{R}^3)} = -\langle \Delta f, f \rangle + \langle f, f \rangle.$$

As with $H^2(\mathbb{R}^3)$ and $F(\mathbb{R}^3)$, the natural map from $H^1(\mathbb{R}^3)$ into $L^2(\mathbb{R}^3)$ is an inclusion, and moreover

$$H^2(\mathbb{R}^3) \subseteq H^1(\mathbb{R}^3) \subseteq L^2(\mathbb{R}^3).$$
Now it may be shown without difficulty that \( C_c^\infty(\mathbb{R}^3) \) is dense in \( \mathcal{H}^1(\mathbb{R}^3) \), and since it is clear from (7.2.1) that
\[
\langle f, f \rangle_{\mathcal{F}(\mathbb{R}^3)} \leq \text{constant} \cdot \langle f, f \rangle_{\mathcal{H}^1(\mathbb{R}^3)}
\]
for all \( f \in C_c^\infty(\mathbb{R}^3) \), the space \( \mathcal{H}^1(\mathbb{R}^3) \) is included within \( \mathcal{F}(\mathbb{R}^3) \). We see therefore that
\[
\mathcal{H}^2(\mathbb{R}^3) \subseteq \mathcal{H}^1(\mathbb{R}^3) \subseteq \mathcal{F}(\mathbb{R}^3),
\]
which proves the theorem. \( \square \)

8. Resolvents of the Schrödinger Operator

In this section we shall work with the self-adjoint rescaled Schrödinger operator \( T \), with \( \text{dom}(T)=\mathcal{H}^2(\mathbb{R}^3) \), as in Section 7. We shall use the resolvent operators \( (T-\lambda)^{-1} \) to construct new families of eigenfunctions for \( T \). Using these we shall give an explicit construction of the intertwining operator between the algebraic families of singular and regular solutions that we examined in Section 6.

8.1. Resolvents and solutions of the Schrödinger equation.

8.1.1. Definition. A smooth function \( \sigma: \mathbb{R}^3 \rightarrow \mathbb{C} \) is a cutoff at \( 0 \) if it is compactly supported and if it is identically equal to 1 in some neighborhood of 0. A smooth function \( \sigma: \mathbb{R}^3 \rightarrow \mathbb{C} \) is a cutoff at \( \infty \) if it is identically equal to 1 in the complement of some compact set.

In the following definition \( \text{dom}(T) \) will refer to the self-adjoint domain of \( T \) constructed in Section 7.

8.1.2. Definition. We shall write
\[
\text{dom}_0(T) = \{ f: \mathbb{R}^3 \rightarrow \mathbb{C} : \sigma f \in \text{dom}(T) \text{ for some cutoff } \sigma \text{ at } 0 \}
\]
and
\[
\text{dom}_\infty(T) = \{ f: \mathbb{R}^3 \rightarrow \mathbb{C} : \sigma f \in \text{dom}(T) \text{ for some cutoff } \sigma \text{ at } \infty \}.
\]

8.1.3. Remark. Note that \( \text{dom}(T) \) is closed under pointwise multiplication by smooth functions on \( \mathbb{R}^3 \) that are constant outside of a compact set. It follows that \( \text{dom}(T) \) is included in both \( \text{dom}_0(T) \) and \( \text{dom}_\infty(T) \).

8.1.4. Definition. We shall write
\[
\text{Sol}_0(\lambda) = \text{Sol}(\lambda) \cap \text{dom}_0(T) \text{ and } \text{Sol}_\infty(\lambda) = \text{Sol}(\lambda) \cap \text{dom}_\infty(T).
\]
We shall be most concerned with \( \text{Sol}_\infty(\lambda) \), which according to the definition consists of those \( K \)-finite smooth \( \lambda \)-eigenfunctions of the rescaled Schrödinger operator \( T \) that coincide with elements of \( \text{dom}(T) \) near infinity in \( \mathbb{R}^3 \). Here is its most important property, as far as we are concerned:

8.1.5. Theorem. Suppose that \( \lambda \notin \text{Spec}(T) \). For every \( G \in \text{SingSol}(\lambda) \) there is a unique \( V \in \text{Sol}_\infty(\lambda) \) such that
\[
\text{Wr}(G, F) = \text{Wr}(V, F) \quad \forall F \in \text{RegSol}(\lambda).
\]

Proof. First we shall prove existence, and for this it suffices to consider each \( \ell \)-isotypical component of \( \text{SingSol}(\lambda) \) individually. Suppose that \( G \in \text{SingSol}(\lambda) \) is represented by the product of a \( \lambda \)-eigenfunction \( G_{\ell, \lambda} \) of the radial operator (5.1.2) and a spherical harmonic function \( Y_\ell \) of degree \( \ell \). Let \( f \) be a smooth, compactly
supported function on \( \mathbb{R}^3_0 \) of the form \( \varphi \cdot Y_\ell \), where \( \varphi \) is a smooth, compactly supported function of \( r \in (0, \infty) \). The function

\[
U = (T - \lambda)^{-1} f
\]

is smooth on \( \mathbb{R}^3_0 \) thanks to elliptic regularity, and has the form

\[
U = \psi \cdot Y_\ell
\]

for some smooth function \( \psi \) of \( r \) (which is not necessarily compactly supported) thanks to the K-equivariance of the rescaled Schrödinger operator. From the equation

\[
TU = \lambda U + f
\]

we see that \( U \) is a \( \lambda \)-eigenfunction for \( T \) outside of the compact set where \( f \) is supported, and so \( \psi \) is a \( \lambda \)-eigenfunction for the radial operator (5.1.2) outside of a compact subset of \( (0, \infty) \).

Now every solution of the eigenvalue equation (5.2.1) that is defined on a subinterval of \( (0, \infty) \) may be extended to a solution on \( (0, \infty) \). So there are \( \lambda \)-eigenfunctions \( \psi_0 \) and \( \psi_\infty \) that agree with \( \psi \) near 0 and near \( \infty \), respectively. The corresponding functions

\[
U_0 = \psi_0 \cdot Y_\ell \quad \text{and} \quad U_\infty = \psi_\infty \cdot Y_\ell
\]

belong to \( \text{Sol}_0(\lambda) \) and \( \text{Sol}_\infty(\lambda) \), respectively. Note that since \( (T - \lambda)^{-1} \) has dense range, there is at least one \( \psi \) for which \( U_0 \) and \( U_\infty \) are nonzero.

The functions \( \psi_0 \) and \( \psi_\infty \) cannot be linearly dependent, because if they were, then after adjusting one by a multiplicative scalar the two functions would glue together to determine a \( \lambda \)-eigenfunction in \( \text{dom}(T) \). This would contradict the assumption that \( \lambda \notin \text{Spec}(T) \). So \( \psi_0 \) and \( \psi_\infty \) must span the two-dimensional space of \( \lambda \)-eigenfunctions of the radial operator (5.1.2).

Let \( F_{\ell, \lambda} \) be the regular radial eigenfunction in (5.2.3), and let \( G_{\ell, \lambda} \) the eigenfunction from (5.2.4), normalized so that \( \text{Wr}(F_{\ell, \lambda}, G_{\ell, \lambda}) = 1 \). From the above we can write

\[
F_{\ell, \lambda} \cdot Y_\ell = a \cdot U_0 + b \cdot U_\infty \quad \text{and} \quad G_{\ell, \lambda} \cdot Y_\ell = c \cdot U_0 + d \cdot U_\infty,
\]

for suitable constants \( a, b, c, d \). The scalar \( d \) must be nonzero because \( G_{\ell, \lambda} \) is unbounded near 0, and is therefore not an element of \( \text{dom}_0(T) \); compare Lemma 7.1.1. It therefore follows from the second equation that \( U_\infty \) is unbounded near 0, and from this it follows from the first equation that the scalar \( b \) must be zero. This implies that \( a \) is nonzero, and so we can write

\[
d \cdot U_\infty = G_{\ell, \lambda} \cdot Y_\ell - c \cdot U_0 = G_{\ell, \lambda} \cdot Y_\ell - c/a \cdot F_{\ell, \lambda} \cdot Y_\ell.
\]

It follows that we can take \( V = d \cdot U_\infty \). This completes the proof of existence.

To prove uniqueness, note first that the above argument shows \( F_{\ell, \lambda} \cdot Y_\ell \in \text{Sol}_0(\lambda) \), and therefore \( \text{RegSol}(\lambda) \subseteq \text{Sol}_0(\lambda) \). Now it suffices to show that if \( V \in \text{Sol}_\infty(\lambda) \), and if \( \text{Wr}(V, F) = 0 \) for all \( F \in \text{RegSol}(\lambda) \), then \( V = 0 \). But if the Wronskians are all 0, then \( V \in \text{RegSol}(\lambda) \), and hence \( V \in \text{Sol}_0(\lambda) \), so that in fact \( V \in \text{dom}(T) \). This again contradicts the assumption that \( \lambda \notin \text{Spec}(T) \). \( \square \)

8.1.6. Remark. The proof shows that if \( \lambda \notin \text{Spec}(T) \), then

\[
\text{Sol}_0(\lambda) = \text{RegSol}(\lambda) \quad \text{and} \quad \text{Sol}(\lambda) = \text{Sol}_0(\lambda) \oplus \text{Sol}_\infty(\lambda).
\]
8.2. The family of Kodaira-type solutions. In this subsection we shall use the solutions in Theorem 8.1.5 to create an algebraic family of \((g, K)\)-modules. We shall name the family after Kodaira, in recognition of his fundamental results from [Kod49] that we shall review in the next subsection.

8.2.1. Theorem. If \(\lambda \notin \text{Spec}(T)\), if \(V \in \text{Sol}_\infty(\lambda)\), and if \(R\) is any Runge-Lenz operator, then \(RV \in \text{Sol}_\infty(\lambda)\).

Proof. The only issue is whether or not \(RV \in \text{dom}_\infty(T)\). The smooth, \(K\)-finite function \(V\) is in the Sobolev space \(H^2(\mathbb{R}^3)\) near infinity (that is, \(\sigma V \in H^2(\mathbb{R}^3)\) for a suitable cutoff \(\sigma\) at infinity). But \(V\) is also an eigenfunction for \(T\), so the function \(TV = -\Delta V - 2\gamma/r V\) is in the Sobolev space \(H^2(\mathbb{R}^3)\) near infinity. Since the Coulomb potential has bounded derivatives away from zero, it follows from elliptic regularity that \(V\) lies in the Sobolev space \(H^4(\mathbb{R}^3)\) near infinity.

Now the Runge-Lenz operators have the form
\[
(8.2.2) \quad -\sqrt{-1} R_i = \frac{\gamma x_i}{r} - \partial_i + \sum_{j \neq i} \pm \partial_j L_j.
\]
Each \(L_j\) acts as a bounded operator on any \(\ell\)-isotypical part of \(H^4(\mathbb{R}^3)\). The partial derivatives map \(H^4(\mathbb{R}^3)\) into \(H^3(\mathbb{R}^3)\), and so into \(H^2(\mathbb{R}^3)\), and \(\gamma x_i/r\) maps \(H^4(\mathbb{R}^3)\) into itself near infinity. \(\square\)

8.2.3. Definition. We shall denote by \(\text{KodairaSol}\) the complex vector space spanned by functions \([\mathbb{C} \setminus \text{Spec}(T)] \times \mathbb{R}^3_0 \rightarrow \mathbb{C}\) of the form \((\lambda, x) \mapsto V_\lambda(x)\), where

(i) \(V_\lambda \in \text{Sol}_\infty(\lambda)\), and
(ii) if \(F \in \text{RegSol}\), then \(\text{Wr}(F_\lambda, V_\lambda)\) is a polynomial function of \(\lambda\) on the complement of \(\text{Spec}(T)\).

We give \(\text{KodairaSol}\) the structure of an \(O\)-module via pointwise multiplication by polynomial functions in \(\lambda\), and the structure of a \(K\)-module via the actions of \(K\) on the \(K\)-finite solution spaces \(\text{Sol}(\lambda)\).

8.2.4. Lemma. The usual action of differential operators on functions gives the \(O\)-module the structure of a \((g, K)\)-module.

Proof. In view of Theorem 8.2.1 it only needs to be shown that if \(V \in \text{KodairaSol}\), and if \(R \in g\) is a Runge-Lenz operator, then \(\text{Wr}(F_\lambda, RV_\lambda)\) is a polynomial function of \(\lambda\). But this follows from Theorem 5.5.4. \(\square\)

The following result shows that the family of Kodaira solutions carries the structure of an algebraic family of Harish-Chandra modules over \((g, K)\), despite being initially defined only over the complement of the spectrum of \(T\).

8.2.5. Theorem. The \(O\)-module morphism
\[
\text{SingSol} \rightarrow \text{KodairaSol}
\]
that maps each \(G \in \text{SingSol}\) to the unique \(V \in \text{KodairaSol}\) such that
\[
\text{Wr}(G_\lambda, F_\lambda) = \text{Wr}(V_\lambda, F_\lambda) \quad \forall F \in \text{RegSol} \quad \forall \lambda \notin \text{Spec}(T)
\]
is an isomorphism of \((g, K)\)-modules.
8.2.6. Remark. By definition, if \( G \in \text{SingSol} \), then \( \text{Wr}(G, F) \) is a polynomial function of \( \lambda \). So the function \( V \) defined above is indeed an element of \( \text{KodairaSol} \).

**Proof.** The \( g \)-equivariance of the morphism follows from Theorem 5.5.4. The \( K \)-equivariance is clear. The fact that the morphism is an isomorphism follows from Theorem 5.6.2. \( \square \)

8.3. **The limiting absorption principle.** The title of this subsection refers to the idea that physical solutions of the Schrödinger equation for the real eigenvalue \( \lambda \) should be expressible as limits, as \( \varepsilon \to 0 \), of rapidly decaying \( (\lambda \pm \varepsilon) \)-eigenfunctions (classically these correspond to solutions of equations with damping terms added).

In mathematics the term has come to refer to the convergence of resolvent operators \( (T - \lambda)^{-1} \) in some topology as \( \lambda \) converges to the spectrum, but here we shall keep close to the original meaning. We shall use some decisive contributions of Kodaira [Kod49] on the limiting absorption principle to obtain an explicit intertwining operator from singular to regular solutions of the rescaled Schrödinger equation. Later, in Theorem 9.6.3, we shall use the same techniques to fully determine the spectral theory of the rescaled Schrödinger operator; this was one of Kodaira's original purposes.

The starting point is the following theorem of Kodaira concerning eigenfunctions for the rescaled Schrödinger operator associated to non-real eigenvalues.

8.3.1. **Theorem** (See [Kod49, Theorem 5.1]). If \( \text{Im}(k) \geq 0 \) and \( k \neq 0 \), then there is a unique \( K \)-invariant eigenfunction \( U_k \) for the eigenvalue \( k^2 \) with

\[
U_k(r) - \frac{1}{r} \exp\left(\sqrt{-1}kr + \frac{\gamma \sqrt{-1}k}{k} \log(r)\right) \quad \text{as} \quad r \to \infty.
\]

As \( k \) varies, the functions \( U_k \) vary continuously in the topology of uniform convergence of smooth functions and all their derivatives on compact subsets of \( \mathbb{R}^3_0 \).

In the numerator in the display is the constant \( \gamma \) from (2.1.2). Observe that if \( \text{Im}(k) > 0 \), then \( U_k \in \text{dom}_\infty(T) \).

8.3.2. **Lemma.** If \( k > 0 \), then \( \text{Wr}(U_k, U_{-k}) = 2ik \). In particular, \( U_k \) and \( U_{-k} \) are linearly independent.

**Proof.** Kodaira shows in [Kod49, Theorem 5.1] that differentiating both sides of the asymptotic equivalence in Theorem 8.3.1 with respect to \( r \) preserves the asymptotic equivalence. The result follows. \( \square \)

Now define a continuous function in the region \( \text{Im}(k) \geq 0 \) by

\[ a(k) = \text{Wr}(F_{0, \lambda}, U_k), \]

where \( \lambda = k^2 \).

8.3.3. **Lemma.** If \( k > 0 \), and if \( \lambda = k^2 \), then

\[ F_{0, \lambda} = \frac{1}{2\pi i} (a(-k)U_k - a(k)U_{-k}). \]

**Proof.** It suffices to compute that the Wronskians of both sides of the asserted equality with \( U_k \) and \( U_{-k} \) are equal, since by Lemma 8.3.2 these two functions span the spherical \( \lambda \)-eigenfunctions. \( \square \)

8.3.5. **Lemma.** If \( \text{Im}(k) > 0 \) and \( a(k) = 0 \), then \( k^2 \in \text{Spec}(T) \).
Proof. Let $\lambda = k^2$. We can write
\[ U_k = a(k)G_{0,\lambda} + b(k)F_{0,\lambda}, \]
where $F_{0,\lambda}$ and $G_{0,\lambda}$ are as in the proof of Theorem 8.1.5, except that we view them here as $K$-invariant functions on $\mathbb{R}^3_0$, and $b(k)$ is some scalar. If $a(k) = 0$, then $F_{0,\lambda}$ is a multiple of $U_k$, and hence belongs to $\text{dom}_\infty(T)$. It then follows from Remark 8.1.6 that $\lambda \in \text{Spec}(T)$. □

8.3.6. Lemma. If $k > 0$, then $a(-k) = a(k)$ and $a(k) \neq 0$.

Proof. It follows from the uniqueness statement in Theorem 8.3.1 that if $k > 0$ then $U_k = U_{-k}$. Since $F_{0,\lambda}$ is real-valued when $\lambda$ is real, it follows from Lemma 8.3.4 that $a(-k) = a(k)$. This shows that $a(k)$ must be nonzero, for otherwise $F_{0,\lambda}$ would be identically zero. □

8.3.7. Theorem. Let $V_0 \in \text{KodairaSol}$ be the family of $K$-invariant Kodaira-type eigenfunctions such that
\[ \text{Wr}(V_{0,\lambda}, F_{0,\lambda}) = 1 \]
for every $\lambda \not\in \text{Spec}(T)$. For every $\lambda > 0$ the limits
\[ V_{0,\lambda}^+ = \lim_{\varepsilon \to 0^+} V_{0,\lambda + i\varepsilon} \quad \text{and} \quad V_{0,\lambda}^- = \lim_{\varepsilon \to 0^+} V_{0,\lambda - i\varepsilon} \]
exist in the standard topology on $C^\infty(\mathbb{R}^3_0)$, of uniform convergence on compact sets of functions and all their derivatives. The limits are $\lambda$-eigenfunctions, and moreover
\[ V_{0,\lambda}^+ - V_{0,\lambda}^- = \text{Wr}(V_{0,\lambda}^+, V_{0,\lambda}^-) \cdot F_{0,\lambda} \]
for every $\lambda > 0$.

Proof. To begin, suppose that $\lambda \not\in \text{Spec}(T)$. Choose $k \in \mathbb{C}$ such that $\text{Im}(k) > 0$ and $k^2 = \lambda$. By Lemma 8.3.5, $a(k)$ is nonzero. As we already noted, $U_k \in \text{Sol}_\infty(\lambda)$. Therefore $V_{0,\lambda}$ and $U_k$ are multiples of one another, since the space of $K$-invariant functions in $\text{Sol}_\infty(\lambda)$ is one-dimensional. In fact it follows from (8.3.3) and the Wronskian condition in the statement of the theorem that
\[ V_{0,\lambda} = \frac{1}{a(k)}U_k \]
(8.3.8)
Once again, this formula holds for $\lambda \not\in \text{Spec}(T)$ and $\text{Im}(k) > 0$ with $k^2 = \lambda$.

Now suppose that $\lambda > 0$. The existence of the limits in the statement of the theorem follows from the continuity properties of $U_k$ as a function of $k$, and from Lemmas 8.3.5 and 8.3.6. In fact
\[ V_{0,\lambda}^+ = \frac{1}{a(\sqrt{\lambda})}U_{\sqrt{\lambda}} \quad \text{and} \quad V_{0,\lambda}^- = \frac{1}{a(-\sqrt{\lambda})}U_{-\sqrt{\lambda}}, \]
where in both cases we used the positive square root of $\lambda$. The final formula in the statement of the theorem is a consequence of Lemma 8.3.4. □

For $\lambda > 0$ let us now define
\[ w(\lambda) = \text{Wr}(V_{0,\lambda}^+, V_{0,\lambda}^-) = \frac{2i\sqrt{\lambda}}{|a(\sqrt{\lambda})|^2} \]
(8.3.9)
as in Theorem 8.3.7.
8.3.10. **Theorem.** For every \( V \in \text{KodairaSol} \) and for every \( \lambda > 0 \) the limits
\[
V_{\lambda}^+ = \lim_{\epsilon \to 0^+} V_{\lambda + i \epsilon} \quad \text{and} \quad V_{\lambda}^- = \lim_{\epsilon \to 0^-} V_{\lambda - i \epsilon}
\]
exist in the standard topology on \( C^\infty(\mathbb{R}^3) \) of uniform convergence on compact sets of functions and all their derivatives. The limits are \( \lambda \)-eigenfunctions, and moreover
\[
V_{\lambda}^+ - V_{\lambda}^- \in \text{RegSol}(\lambda).
\]
In fact there is a unique \( F \in \text{RegSol} \) such that
\[
V_{\lambda}^+ - V_{\lambda}^- = w(\lambda) \cdot F
\]
for every \( \lambda > 0 \).

**Proof.** The case where \( V \) is spherical is covered by Theorem 8.3.7. Because the limits there exist in the \( C^\infty \) topology, if \( X \in \mathcal{U}(\mathfrak{g}) \), then in addition the limits
\[
(XV_{0,\lambda})^+ = \lim_{\epsilon \to 0^+} XV_{0,\lambda + i \epsilon} \quad \text{and} \quad (XV_{0,\lambda})^- = \lim_{\epsilon \to 0^-} XV_{0,\lambda - i \epsilon}
\]
exist, and if \( \lambda > 0 \), then
\[
(XV_{0,\lambda})^+ - (XV_{0,\lambda})^- = w(\lambda) \cdot XF_{0,\lambda}
\]
This proves the theorem because \( \text{KodairaSol} \) is generated by its spherical isotypical component.

We come now to one of the main results in this paper, which recovers the algebraic intertwining operator of Section 6 from analysis and the limiting absorption principle.

8.3.11. **Theorem.** Define a morphism of \( \mathcal{O} \)-modules
\[
\mathcal{A}: \text{KodairaSol} \longrightarrow \text{RegSol}
\]
by mapping \( V \in \text{KodairaSol} \) to the unique \( F \in \text{RegSol} \) for which
\[
F_\lambda = \frac{1}{w(\lambda)} (V_{\lambda}^+ - V_{\lambda}^-) \quad \forall \lambda > 0,
\]
as in Theorem 8.3.10. This is a morphism of algebraic families of \( (\mathfrak{g}, K) \)-modules, and an isomorphism on \( \ell = 0 \) isotypical components.

Using the isomorphism in Theorem 8.2.5 we obtain from Theorem 8.3.11 an intertwining operator from \( \text{SingSol} \) to \( \text{RegSol} \). It agrees with the intertwiner analyzed in Subsection 6.2 up to an overall complex multiplicative factor, because up to a scalar factor there is a unique intertwiner that is an isomorphism on \( \ell = 0 \) isotypical components.

9. **The Spectral Decomposition of the Schrödinger Operator**

The spectral theorem for unbounded self-adjoint operators provides a measurable family of solution spaces parametrized by the values in the spectrum of the Schrödinger operator. These spaces, \( \mathcal{H}_\lambda \), which are Hilbert spaces, carry actions of the visible symmetry group \( K \). We shall prove that for almost every \( \lambda \) in the spectrum, the space of \( K \)-finite vectors in \( \mathcal{H}_\lambda \) carries a natural action of the hidden symmetry Lie algebra \( \mathfrak{g}|_{\lambda} \), and that the \( (\mathfrak{g} |_{\lambda}, K) \)-module so-obtained coincides with the physical solution space for \( \lambda \).
9.1. **Direct integral decomposition.** From now on we shall denote by $T$ the Kato-Rellich extension of the rescaled operator (7.0.1). Since $T$ is self-adjoint, general theory provides a spectral decomposition of the underlying Hilbert space $L^2(\mathbb{R}^3)$, as in the following theorem. See for example [Dix82, A.69] for the terminology and [Dix82, A.84] for the result.

9.1.1. **Theorem.** There is a fully-supported Borel measure $\mu$ on $\text{Spec}(T)$, a $\mu$-measurable field of Hilbert spaces $\{H_\lambda\}_{\lambda \in \text{Spec}(T)}$, and a unitary isomorphism

$$L^2(\mathbb{R}^3) \xrightarrow{\cong} \int_{\text{spec}(T)} H_\lambda \, d\mu(\lambda),$$

from $L^2(\mathbb{R}^3)$ to the space of $\mu$-square-integrable sections of the measurable field, such that if $f \in L^2(\mathbb{R}^3)$, then

$$[(T \pm iI)^{-1} f]_\lambda = (\lambda \pm iI)^{-1}[f]_\lambda$$

for almost every $\lambda$ (we are writing $\lambda \mapsto [f]_\lambda$ for the measurable, square-integrable section of $\{H_\lambda\}_{\lambda \in \text{Spec}(T)}$ that is attached to $f \in L^2(\mathbb{R}^3)$ by the unitary isomorphism).

The Hilbert spaces $H_\lambda$ for $\lambda < 0$ identify with the $\lambda$-eigenspaces for $T$ in $L^2(\mathbb{R}^3)$ via the isomorphism in the theorem, and so are easily analyzed. The situation for $\lambda \geq 0$ is more complicated; it will be explained in the following subsections.

9.2. **Visible symmetries.** For the sequel, we shall fix a measure $\mu$ and a $\mu$-measurable field as in Theorem 9.1.1. Our ultimate aim is to equip the fibers of the field with hidden symmetries, but we shall start here with the easier visible symmetries.

In the following theorem, by a measurable family of unitary actions of $K$ on the measurable field $\{H_\lambda\}$ we shall mean a family of unitary group actions, one on each of the fibers $H_\lambda$, that maps measurable sections to measurable sections.

9.2.1. **Theorem.** There is a measurable family of unitary $K$-actions on the measurable field $\{H_\lambda\}$ such that

$$[g \cdot f]_\lambda = g \cdot [f]_\lambda$$

for every $g \in K$ and almost every $\lambda$.

This is a consequence of the fact that the $K$-action on $L^2(\mathbb{R}^3)$ maps the domain of the self-adjoint operator $T$ into itself, and fixes $T$. See [Dix82, 8.3.1, 18.7.6, A.80].

9.3. **Hidden symmetries.** Our aim in this subsection is to decompose the Runge-Lenz operators

$$R : C^\infty_c(\mathbb{R}^3_0) \to C^\infty_c(\mathbb{R}^3_0),$$

into families of operators acting on the Hilbert spaces $H_\lambda$ in Theorem 9.1.1, although actually it will be necessary to consider only the $K$-finite vectors in $H_\lambda$. We shall prove the following result:

9.3.1. **Theorem.** There are operators

$$R_\lambda : H_{\lambda,\text{fin}} \to H_{\lambda,\text{fin}}$$

with the following properties:

(a) if $\{f_\lambda\}$ is a measurable section of $\{H_\sigma^*\}$ for some $\sigma \in \tilde{K}$, then $\{R_\lambda f_\lambda\}$ is a measurable section of $\{H_\lambda\}$; and

(b) if $g \in C^\infty_c(\mathbb{R}^3_0)_{\text{fin}}$, then $[Rg]_\lambda = R_\lambda[g]_\lambda$ for $\mu$-almost every $\lambda$. 
Well-known examples show that care must be taken when attempting to decompose one unbounded operator with respect to a direct integral decomposition of another; see for example [Nel59, Sec. 10]. So we shall proceed cautiously, following a sequence of small steps.

9.3.2. Lemma. Each of the Runge-Lenz operators on $C_c^\infty(\mathbb{R}_0^3)$ extending to a continuous linear operator from $\mathcal{F}(\mathbb{R}^3)_\text{fin}$ into $\mathcal{L}^2(\mathbb{R}^3)_\text{fin}$ (the operator is bounded on each isotypical subspace, but not uniformly bounded over all isotypical subspaces). The extension maps the subspace $\mathcal{H}^2(\mathbb{R}^3)_\text{fin} \subseteq \mathcal{F}(\mathbb{R}^3)_\text{fin}$ into $\mathcal{F}(\mathbb{R}^3)_\text{fin}$.

Proof. From (2.7.1) and Lemma 2.8.3

\[
TL^2 - R^2 = T + \gamma^2 I
\]

on $C_c^\infty(\mathbb{R}_0^3)_\text{fin}$. The operator $L^2$ in this formula is the Casimir for $K$, and on each isotypical component of $C_c^\infty(\mathbb{R}_0^3)_\text{fin}$ it acts as a scalar. Therefore on any such component we have

\[
(9.3.3) \quad -\langle R^2 f, f \rangle = \text{constant} \cdot \langle T f, f \rangle + \text{constant} \cdot \langle f, f \rangle.
\]

But recall that when viewed as unbounded operators on $L^2(\mathbb{R}^3)$ with domain $C_c^\infty(\mathbb{R}_0^3)$, the Runge-Lenz operators are skew-symmetric. So it follows from (9.3.3) that

\[
\| R_1 f \|^2 + \| R_2 f \|^2 + \| R_3 f \|^2 \leq \text{constant} \cdot \| f \|^2_{L^2(\mathbb{R}^3)}.
\]

This proves the first assertion in the lemma.

To prove the second assertion, recall the formula (8.2.2) for $R_i$. The operators $L_i$ map each isotypical component of $\mathcal{H}^2(\mathbb{R}^3)$ boundedly into itself. The operators $\delta_1, \delta_j$ are bounded as operators from $\mathcal{H}^2(\mathbb{R}^3)$ into $\mathcal{H}^1(\mathbb{R}^3)$, and hence as operators from $\mathcal{H}^2(\mathbb{R}^3)$ into $\mathcal{L}(\mathbb{R}^3)$; see the proof of Theorem 7.2.3. Finally, $\gamma x_i/r$ maps $\mathcal{H}^2(\mathbb{R}^3)$ continuously into $\mathcal{H}^1(\mathbb{R}^3)$, and hence into $\mathcal{F}(\mathbb{R}^3)$. This is a simple direct computation using Lemma 7.1.1.

\[ \square \]

9.3.4. Lemma. If $h \in \mathcal{F}(\mathbb{R}^3)$ and $g \in C_c^\infty(\mathbb{R}^3)$, then

\[
\langle h, g \rangle_{\mathcal{F}(\mathbb{R}^3)} = \langle h, (T + C)g \rangle_{L^1(\mathbb{R}^3)}.
\]

Proof. In the special case where $h \in C_c^\infty(\mathbb{R}_0^3)$, the only difference between the right-hand side of the formula in the lemma and the definition (7.2.1) of the inner product on $\mathcal{F}(\mathbb{R}^3)$ is the choice of factor in the inner product to which $T+C$ is applied. So the lemma follows in this special case from the symmetry of $T$ on $C_c^\infty(\mathbb{R}_0^3) \subseteq L^2(\mathbb{R}^3)$. Since both sides of the formula are continuous in $h \in \mathcal{F}(\mathbb{R}^3)$, the general case follows from the special case.

\[ \square \]

9.3.5. Lemma. If $h \in \mathcal{F}(\mathbb{R}^3)_\text{fin}$ and $g \in C_c^\infty(\mathbb{R}^3)_\text{fin}$, then

\[
\langle R_i h, g \rangle_{L^2(\mathbb{R}^3)} = -\langle h, R_i g \rangle_{L^2(\mathbb{R}^3)}.
\]

Proof. This is obvious for $h \in C_c^\infty(\mathbb{R}_0^3)$ and follows in general by continuity of the left-hand and right-hand sides in $h \in \mathcal{F}(\mathbb{R}^3)_\text{fin}$.

\[ \square \]

9.3.6. Lemma. The restriction of the operator

\[
R_i (T + C)^{-1} : L^2(\mathbb{R}^3)_\text{fin} \longrightarrow \mathcal{F}(\mathbb{R}^3)_\text{fin}
\]

to $\mathcal{F}(\mathbb{R}^3)_\text{fin} \subseteq L^2(\mathbb{R}^3)_\text{fin}$ is equal to $(T+C)^{-1} R_i$.
Proof. It suffices to prove that
\[
\langle R_i(T + C)^{-1}f, g \rangle_{\mathcal{F}(\mathbb{R}^3)} = \langle (T + C)^{-1}R_if, g \rangle_{\mathcal{F}(\mathbb{R}^3)}
\]
for all \( f, g \in C_\infty^c(\mathbb{R}_3^0) \). Using Lemmas 9.3.4 and 9.3.5 we compute that
\[
\langle R_i(T + C)^{-1}f, g \rangle_{\mathcal{F}(\mathbb{R}^3)} = \langle R_i(T + C)^{-1}f, (T + C)g \rangle_{L^2(\mathbb{R}^3)}
\]
\[
= -\langle (T + C)^{-1}f, R_i(T + C)g \rangle_{L^2(\mathbb{R}^3)}
\]
\[
= -\langle (T + C)^{-1}f, (T + C)R_ig \rangle_{L^2(\mathbb{R}^3)}
\]
\[
= -\langle f, R_ig \rangle_{L^2(\mathbb{R}^3)}
\]
\[
= \langle R_if, g \rangle_{L^2(\mathbb{R}^3)}.
\]

The proof is finished by using the characterization in Theorem 7.2.2. \( \square \)

Proof of Theorem 9.3.1. The operators
\[
S_i = R_i(T + C)^{-1}
\]
are defined on \( L^2(\mathbb{R}^3)_{\text{fin}} \) and are bounded on each isotypical component. Moreover it follows immediately from Lemma 9.3.6 that these operators commute with the resolvent operator \( (T + C)^{-1} \). It follows that each \( S_i \) decomposes as a bounded measurable family \( \{ S_i, \lambda \} \) on each isotypical part of the measurable family \( \{ H_\lambda \} \).

The operators \( S_i, \lambda \) have the property that if \( f \in L^2(\mathbb{R}^3)_{\text{fin}} \), then
\[
[S_if]_\lambda = S_i,\lambda[f]_\lambda
\]
for \( \mu \)-almost every \( \lambda \). Now we define
\[
R_i,\lambda = (\lambda + C)S_i,\lambda : H_\lambda_{\text{fin}} \to H_\lambda_{\text{fin}}.
\]
If \( g \in C_\infty^c(\mathbb{R}_3^0) \), and if \( f = (T + C)g \), then (9.3.7) implies that
\[
[R_ig]_\lambda = R_i,\lambda[g]_\lambda,
\]
for \( \mu \)-almost every \( \lambda \), as required. \( \square \)

9.4. Gelfand-Kostyuchenko method. The abstract direct integral decomposition in Theorem 9.1.1 can be made more concrete using the theory of distributions. The technique, which sometimes called the Gelfand-Kostyuchenko method, is as follows.

9.4.1. Theorem. There is a family of continuous linear maps
\[
\varepsilon_\lambda : C_\infty^c(\mathbb{R}_3^0) \to H_\lambda \quad (\lambda \in \text{Spec}(T))
\]
such that
(a) for every \( f \in C_\infty^c(\mathbb{R}_3^0) \) the family \( \{ \varepsilon_\lambda(f) \} \) is a measurable and square-integrable section of the field \( \{ H_\lambda \} \);
(b) for every \( f \in C_\infty^c(\mathbb{R}_3^0) \), the sections \( \{ f \}_\lambda \) and \( \{ \varepsilon_\lambda(f) \} \) are equal, almost everywhere; and
(c) for almost every \( \lambda \) the map \( \varepsilon_\lambda \) has dense range.

See [Ber88, Sec. 1] for an account of this result that is especially well suited to our purposes.
9.4.2. Lemma. The evaluation morphisms in Theorem 9.4.1 may be chosen so that they are $K$-equivariant, and in addition so that

$$
\varepsilon_\lambda(Tf) = \lambda \varepsilon_\lambda(f) \quad \text{and} \quad \varepsilon_\lambda(R_i f) = R_i \varepsilon_\lambda(f)
$$

for all $f \in C^\infty_c(\mathbb{R}^3)$ and all $i = 1, 2, 3$.

Proof. Fix a countable dense set in $C^\infty_c(\mathbb{R}^3)$. For any element of this set, the displayed equations hold almost everywhere. So by redefining $\varepsilon_\lambda$ to be zero on a suitable nullset of values $\lambda$, we can arrange for the equations to hold for all $\lambda$ and all elements of our countable dense set. The equations now hold for all $f$ by continuity. The property of $K$-equivariance is handled in the same way. □

Now let us denote by $D'(\mathbb{R}^3_0)$ the space of distributions on $\mathbb{R}^3_0$; it is of course the topological dual space of $C^\infty_c(\mathbb{R}^3_0)$. It acquires by duality an action of the group $K$ and the Lie algebra $\mathfrak{g}$.

9.4.3. Definition. For decomposition $\{H_\lambda\}$ as in Theorem 9.1.1 and a family of evaluation maps $\{\varepsilon_\lambda\}$ as in Theorem 9.4.1 and Lemma 9.4.2, the realization morphisms

$$
\rho_\lambda : H_\lambda \longrightarrow D'(\mathbb{R}^3_0)
$$

are the complex conjugates of the adjoints of the morphisms $\varepsilon_\lambda$, and hence are characterized by

$$
\langle \varepsilon_\lambda(f), v_\lambda \rangle_{H_\lambda} = \int_{\mathbb{R}^3_0} T \cdot \rho_\lambda(v_\lambda),
$$

where the integral on the right denotes the natural pairing between distributions on $\mathbb{R}^3_0$ and test functions.

9.4.4. Lemma. For almost every $\lambda \in \text{Spec}(T)$, the realization map

$$
\rho_\lambda : H_\lambda \longrightarrow D'(\mathbb{R}^3_0)
$$

is injective. For every $\lambda$ the map $\rho_\lambda$ is $K$-equivariant, and its image lies within the space of $\lambda$-eigendistributions of the Schrödinger operator.

Proof. Injectivity of $\rho_\lambda$ follows from the density of the image of $\varepsilon_\lambda$. Equivariance and the eigendistribution property follow from the equivariance of $\varepsilon_\lambda$ and compatibility of $\varepsilon_\lambda$ with $T$, as in Lemma 9.4.2. □

9.5. Comparison with the physical solution spaces. It is a consequence of elliptic regularity and Lemma 9.4.4 above that the range of the realization morphism in Definition 9.4.3 in fact lies in the space of smooth $\lambda$-eigenfunctions for $T$ on $\mathbb{R}^3_0$, which we shall denote by $C^\infty(\mathbb{R}^3_0)_\lambda$. Of course this space was studied in detail in Section 5, and we shall use some of the information presented there to compute the $K$-equivariant map

$$
\rho_\lambda : H_{\lambda, \text{fin}} \longrightarrow C^\infty(\mathbb{R}^3_0)_{\lambda, \text{fin}}
$$

9.5.1. Theorem. For almost every $\lambda$ there is an action of $\mathfrak{g}|_\lambda$ on the space $H_{\lambda, \text{fin}}$ such that

(a) the $\mathfrak{g}|_\lambda$-action on $H_{\lambda, \text{fin}}$, together with the $K$-action, gives $H_{\lambda, \text{fin}}$ the structure of a $(\mathfrak{g}|_\lambda, K)$-module; and

(b) the realization map $\rho_\lambda : H_{\lambda, \text{fin}} \rightarrow C^\infty(\mathbb{R}^3_0)_{\lambda, \text{fin}}$ is an injective morphism of $(\mathfrak{g}|_\lambda, K)$-modules.
Proof. The K-action and Theorem 9.3.1 give actions of the individual generators $L_i$ and $R_i$ of $\mathfrak{g}|_{\lambda}$ on $\mathcal{H}_{\lambda,\text{fin}}$. It follows from Lemma 9.4.2 that these actions commute with the morphism $\varepsilon_{\lambda}$, and hence also with $\rho_{\lambda}$. It follows from the injectivity of $\rho_{\lambda}$ that the actions of the individual generators constitute an action of $\mathfrak{g}|_{\lambda}$, and indeed a $(\mathfrak{g}|_{\lambda},K)$-module structure. \hfill\qed

9.5.2. Theorem. For almost every $\lambda \in \text{Spec}(T)$ the realization morphism

$$\rho_{\lambda} : \mathcal{H}_{\lambda,\text{fin}} \longrightarrow C^\infty(\mathbb{R}_0^3)_{\lambda,\text{fin}}$$

is an isomorphism of $\mathfrak{g}|_{\lambda}$-modules onto the physical solution space $\text{PhysSol}(\lambda)$.

Proof. When $\lambda < 0$ the theorem follows from the discussion preceding Theorem 7.1.5. The singleton set $\{\lambda=0\}$ has $\mu$-measure zero since there is no $\lambda=0$ eigenfunction that is square-integrable. So we can concentrate on the case where $\lambda > 0$.

We have seen that $C^\infty(\mathbb{R}_0^3)_{\lambda,\text{fin}}$ is an extension

$$0 \longrightarrow \text{PhysSol}(\lambda) \longrightarrow C^\infty(\mathbb{R}_0^3)_{\lambda,\text{fin}} \longrightarrow C^\infty(\mathbb{R}_0^3)_{\lambda,\text{fin}}/\text{PhysSol}(\lambda) \longrightarrow 0$$

of one irreducible $(\mathfrak{g}|_{\lambda},K)$-module by a second (which is a copy of the first). We shall show that the composition

$$(9.5.3) \quad \mathcal{H}_{\lambda,\text{fin}} \longrightarrow C^\infty(\mathbb{R}_0^3)_{\lambda,\text{fin}} \longrightarrow C^\infty(\mathbb{R}_0^3)_{\lambda,\text{fin}}/\text{PhysSol}(\lambda)$$

is zero for almost every $\lambda$. This will show that the realization morphism maps the $(\mathfrak{g}|_{\lambda},K)$-module $\mathcal{H}_{\lambda,\text{fin}}$ injectively into a submodule of $\text{PhysSol}(\lambda)$ for almost every $\lambda$. Since the physical solution space is irreducible, when the realization morphism is injective the only possibilities are that the map is an isomorphism, or that $\mathcal{H}_{\lambda,\text{fin}}$ is zero. But since the spectrum of $T$ includes the full half line $(0,\infty)$, the space $\mathcal{H}_{\lambda,\text{fin}}$ and hence $\mathcal{H}_{\lambda}$ can be zero only for a measure zero set of positive energy values. So if we can show that $(9.5.3)$ is zero, then the proof will be complete.

To prove that $(9.5.3)$ is zero, since the quotient $(\mathfrak{g}|_{\lambda},K)$-module is irreducible it suffices to show that the restriction

$$\mathcal{H}_{\lambda}^\ell \longrightarrow C^\infty(\mathbb{R}_0^3)^0_{\lambda,\ell} \longrightarrow C^\infty(\mathbb{R}_0^3)^0_{\lambda}/\text{PhysSol}(\lambda)^0$$

to the trivial $K$-isotypical part (that is, the $\ell=0$ part) is zero. This is what we shall now do.

The space $\text{Sol}(\lambda)^0=\text{C}^\infty(\mathbb{R}_0^3)^0_\lambda$ is spanned by the regular solution $F_{0,\lambda}$ in (5.2.3), which spans $\text{PhysSol}(\lambda)^0$, and the solution $G_{0,\lambda}$ in (5.2.4). If $\{v_\lambda\}$ is a measurable section of $\{\mathcal{H}_{\lambda}^\ell\}$ then we may write

$$\rho_{\lambda}(v_\lambda) = a_\lambda F_{0,\lambda} + b_\lambda G_{0,\lambda}$$

where $a$ and $b$ are measurable scalar functions of $\lambda$. We must show that $b_\lambda = 0$ for almost every $\lambda$.

Suppose that for some section $\{v_\lambda\}$ the function $b$ is not zero almost everywhere. After multiplying the section by a suitable scalar function of $\lambda$, we may assume that $b_\lambda \geq 0$ for all $\lambda$; that $v_\lambda$ is square-integrable; that $v_\lambda$ vanishes outside a compact set in $(0,\infty)$; that $a$ and $b$ are bounded functions; but still $b$ is not zero almost everywhere. The square-integrable section $\{v_\lambda\}$ corresponds to a function $g \in L^2(\mathbb{R}^3)$. In fact the function $g$ lies in the domain $\mathcal{H}^2(\mathbb{R}^3)$ of the self-adjoint
operator $T$ because the section $\{ \lambda \cdot v_\lambda \}$ is square-integrable. But if $f \in C^\infty_c(\mathbb{R}^3_0)$, then

$$\int_{\mathbb{R}^3} \overline{f(x)} \cdot g(x) \, dx = \int_{\text{Spec}(T)} \langle \varepsilon_\lambda(f), v_\lambda \rangle \, d\mu(\lambda)$$

$$= \int_{\text{Spec}(T)} \left( \int_{\mathbb{R}^3} \overline{f(x)} \cdot (a_\lambda F_{0,\lambda}(x) + b_\lambda G_{0,\lambda}(x)) \, dx \right) \, d\mu(\lambda)$$

$$= \int_{\mathbb{R}^3} f(x) \cdot \left( \int_{\text{Spec}(T)} (a_\lambda F_{0,\lambda}(x) + b_\lambda G_{0,\lambda}(x)) \, d\mu(\lambda) \right) \, dx.$$ 

This shows that the function $g$ is equal almost everywhere to the function

$$x \mapsto \int_{\text{Spec}(T)} (a_\lambda F_{0,\lambda}(x) + b_\lambda G_{0,\lambda}(x)) \, d\mu(\lambda).$$

But this is not an $L^\infty$-function on $\mathbb{R}^3$, which contradicts Lemma 7.1.1. 

9.6. The spectral measure. We conclude by recalling for completeness Kodaira’s method [Kod49] for computing the measure $\mu$ in the direct integral of Theorem 9.1.1. We shall be brief; see the appendix of [HT20] for a more leisurely summary.

The starting point is the following formula of Kodaira and Titchmarsh for the spectral projection associated to any self-adjoint operator $T$ and any suitable interval $(\alpha, \beta) \subseteq \mathbb{R}$.

$$P_{(\alpha, \beta)} = \lim_{\varepsilon \to 0^+} \frac{1}{2\pi i} \int_\alpha^\beta (T - \lambda - i\varepsilon)^{-1} - (T - \lambda + i\varepsilon)^{-1} \, d\lambda.$$ 

This is valid as long as neither $\alpha$ nor $\beta$ are eigenvalues of $T$. The limit may be computed in our case using the following formula, which uses Kodaira’s eigenfunctions $U_k$ from Theorem 8.3.1:

$$\text{Wr}(F_{0,\lambda}, U_k) \cdot \left( (T - \lambda)^{-1} f \right)(r)$$

$$= F_{0,\lambda}(r) \int_r^\infty U_k(s) f(s) \, ds + U_k(r) \int_0^r F_{0,\lambda}(s) f(s) \, ds.$$ 

Proof. If we denote by $(K_\lambda f)(r)$ the right-hand side of the formula in the statement of the lemma, then the formula defines a linear operator $K_\lambda$ from smooth compactly supported functions on $(0, \infty)$ to the vector space of smooth functions in $\text{dom}(T)$. We compute directly from the definition of the Wronskian that

$$(T - \lambda)K_\lambda f = \text{Wr}(F_{0,\lambda}, U_k) f,$$

It follows that $K_\lambda f = \text{Wr}(F_{0,\lambda}, U_k) \cdot (T - \lambda)^{-1} f$, as required. 

□
Now we apply the lemma with $\lambda \pm i \varepsilon$ in place of $\lambda$, with $\lambda > 0$. Using our previous notation $a(k)$ for the Wronskian in Lemma 9.6.2 we obtain
\[
\lim_{\varepsilon \to 0^+} \left((T - \lambda - i \varepsilon)^{-1} f - (T - \lambda + i \varepsilon)^{-1} f\right) = F_{0, \lambda}(r) \int_{r}^{\infty} \frac{1}{a(k)} U_{k}(s) f(s) \, ds + \frac{1}{a(k)} \int_{0}^{r} F_{0, \lambda}(s) f(s) \, ds + \frac{1}{a(k)} \int_{0}^{r} F_{0, \lambda}(s) f(s) \, ds,
\]
where $k$ is the positive square root of $\lambda$. Taking into account Lemma 8.3.4 we obtain
\[
\lim_{\varepsilon \to 0^+} \left((T - \lambda - i \varepsilon)^{-1} f - (T - \lambda + i \varepsilon)^{-1} f\right) = \frac{2i\sqrt{\lambda}}{|a(\sqrt{\lambda})|^2} F_{0, \lambda}(r) \int_{0}^{\infty} F_{0, \lambda}(s) f(s) \, ds.
\]
We find that on spherical functions that are smooth and compactly supported in $\mathbb{R}^3_0$,
\[
(P_{\alpha, \beta}) f(r) = \frac{1}{\pi} \int_{\alpha}^{\beta} \int_{0}^{\infty} F_{0, \lambda}(r) F_{0, \lambda}(s) f(s) \, ds \frac{\sqrt{\lambda}}{|a(\sqrt{\lambda})|^2} \, d\lambda.
\]
This computation is equivalent to the following result:

9.6.3. **Theorem** (Compare [Kod49, Theorem 4.1]). *If the Hilbert spaces $H_{\lambda}$ in Theorem 9.1.1 are normed so that $\|F_{0, \lambda}\| = 1$ for all $\lambda \in \text{Spec}(T)$, then on $(0, \infty)$ the measure $\mu$ in Theorem 9.1.1 is given by the formula
\[
2\pi i \cdot d\mu(\lambda) = w(\lambda) \, d\lambda,
\]
with $w(\lambda)$ as in (8.3.9). \qed

9.6.4. **Remark.** It is possible to compute $w(\lambda)$ by determining the asymptotic behavior of the solutions $F_{0, \lambda}$; compare [LL58, (36.27) & (36.28)]. The result is
\[
w(\lambda) = 4\pi i \gamma (1 - e^{2\pi \gamma / \sqrt{\lambda}})^{-1} \quad (\lambda > 0).
\]
Observe this has singularities when $\lambda$ is one of the discrete spectral values $-\gamma^2 / n^2$ for $T$. The singularities come from zeros of $a(\sqrt{\lambda})$, as predicted by a formula discovered by Heisenberg and proved by Kodaira in [Kod49, Sec. 6]. Compare Lemma 8.3.5. There is a further essential singularity at 0, even when $w$ is considered as a function of $k = \sqrt{\lambda}$. This seems to be an inescapable feature in scattering theory, and so it is interesting that in the algebraic approach there is no kind of singularity at 0 at all.

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