

FAMILIES OF SYMMETRIES AND THE HYDROGEN ATOM

NIGEL HIGSON AND EYAL SUBAG

ABSTRACT. We study a new type of symmetry for the hydrogen atom involving algebraic families of groups parametrized by the energy value in the time-independent Schrödinger equation. We construct an algebraic family of Harish-Chandra modules from the solutions of the Schrödinger equation, and we characterize this family. We show that the subspaces of physical states may be obtained from our algebraic family using a Jantzen filtration, and we relate our algebraic methods with spectral theory and scattering theory using the limiting absorption principle.

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 [Pau26, Foc35, Bar36]. These larger symmetry groups vary from energy to energy, although the groups attached to all positive energies, and separately those attached to all negative energies, may be—and usually are—identified with one another.

In this paper we shall develop a different approach. We shall organize the various symmetry groups into an algebraic family, and analyze the consequences. We shall determine the physical states of the hydrogen atom algebraically, using the Jantzen filtration. We shall explain how our algebraic account is parallel to early analytic work in scattering theory by Heisenberg [Hei43a, Hei43b, Hei44] and Kodaira [Kod49]. In fact we shall directly connect the limiting absorption principle in scattering theory to algebraic families. Along the way we shall prove a classification result for representations of the kinds of algebraic families introduced here, give a complete analysis of the Hilbert space spectral decomposition of the Schrödinger operator from the point of view of representation theory, and prove a variety of other results.

In physics, one seeks solutions of the time-independent Schrödinger equation for the hydrogen atom, $H\psi = E\psi$, with definite total angular momentum. One further imposes the condition that ψ be square-integrable, or almost square integrable. The linear span of all such ψ , as the angular momentum varies but the energy E is fixed, is what we shall call in this paper the physical solution space, and denote by $\text{PhysSol}(E)$. 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. In simplified units it has the form

$$\text{Spec}(H) = \left\{ -\frac{1}{n^2} : n = 1, 2, \dots \right\} \cup [0, 1).$$

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

The orthogonal group $K=O(3)$ acts on each of the spaces $\text{PhysSol}(E)$, because the Schrödinger operator H is $O(3)$ -invariant. But $\text{PhysSol}(E)$ is also acted on by a 6-dimensional Lie algebra

$$g_E = \begin{cases} \mathfrak{so}(3; 1) & E > 0 \\ \mathfrak{so}(3) \ltimes \mathbb{R}^3 & E = 0 \\ \mathfrak{so}(4) & E < 0: \end{cases}$$

This was first discovered by Pauli [Pau26] in the case $E < 0$, and then developed further by Fock [Foc35], Bargmann [Bar36] and many others.

Instead of making the identifications in the display above, we shall view the Lie algebras g_E as (the real forms of) some of the fibers of an algebraic family of Lie algebras defined over the complex affine line. The space of algebraic sections of this family is a finite-dimensional Lie algebra g over the algebra \mathcal{O} of complex polynomial functions on the line, and it is concretely realized as differential operators on \mathbb{R}^3 . Putting it together with the constant family K whose fiber is the visible symmetry group $O(3)$, we obtain an algebraic family $(g; K)$ of Harish-Chandra pairs [BHS20a].

We shall study the solutions of the Schrödinger equation using representation theory for the family $(g; K)$. Basic ODE theory provides regular solutions that extend to entire functions of the radial coordinate. It is a simple matter to realize the spaces $\text{RegSol}(E)$ of regular solutions as the fibers of an \mathcal{O} -module RegSol . The visible symmetry group K acts on RegSol , with each isotypical part being a free and finitely generated \mathcal{O} -module. Our launching point is the following result, which is by no means evident:

Theorem (See Section 5). The module RegSol carries the structure of an algebraic family of Harish-Chandra modules (as in [BHS20a]) for $(g; K)$.

We shall also define a family of spaces of singular solutions (meaning only not regular, rather than actually singular in any particular way) by taking the quotient of all solutions by the regular solutions:

$$\text{SingSol}(E) = \text{Sol}(E) = \text{RegSol}(E) \quad (E \in \mathbb{C}):$$

These spaces, too, are the fibers of an algebraic family of Harish-Chandra modules, which we shall denote by SingSol .

Theorem (See Section 5). The Wronskian bilinear form (from elementary differential equations) defines a twisted-equivariant and nondegenerate pairing

$$\text{Wr}: \text{SingSol} \otimes \text{RegSol} \rightarrow \mathcal{O}:$$

It follows that the Wronskian induces an isomorphism from the \mathcal{O} -twisted dual of the family RegSol to the family SingSol (the type of twisting that is involved here is explained in Section 3.5). We shall also prove the following result, using representation theory techniques and without reference to the Wronskian or differential equations:

Theorem (See Section 6). There is an essentially unique, generically invertible, algebraic intertwining operator from the family SingSol to the family RegSol .

Now the space of all regular solutions of the Schrödinger equation is infinite-dimensional for every energy E , real or complex. It is often 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. One can therefore ask how the physical solutions can be extracted from the family RegSol .

Our answer is that the Jantzen filtration technique from representation theory, used as in [BHS20b], not only isolates the physical solutions among the regular solutions, but it also determines unitary inner products on the physical solution spaces. The technique applies whenever one is given a generically invertible, algebraic family of intertwining operators acting between a family and its dual, as is the case here thanks to the previous two theorems.

Theorem (See Section 6). The physical spectrum of hydrogen atom coincides with the set of all energies $E \in \mathbb{C}$ for which the fiber $\text{RegSol}(E)$ has a nonzero infinitesimally unitary Jantzen quotient. This quotient is unique, and it identifies with $\text{PhysSol}(E)$ as a unitary $(\mathfrak{g}_E; K)$ -module.

This theorem, which spotlights the role that the algebraic family as a whole plays in determining the spectrum, calls to mind similar features of scattering theory, and it is to these analytic issues that we turn next.

The Schrödinger operator for the hydrogen atom has a natural self-adjoint extension on the Hilbert space of square-integrable functions on \mathbb{R}^3 . We shall give a complete analysis of the spectral decomposition of the Schrödinger operator from the perspective of unitary representation theory, and show that the spectral subspaces are the irreducible unitary representations obtained by completing the physical solution spaces. We shall also compute the spectral measure. See Section 9. But here we shall focus on a single issue that relates the Jantzen technique to scattering theory.

Fix a value E that is not in the spectrum of the self-adjoint Schrödinger operator H , and define

$$\text{Sol}_0(E); \text{Sol}_1(E) \subset \text{Sol}(E)$$

to be the spaces of all those $(K$ -finite) solutions of the time-independent Schrödinger equation whose restrictions to neighborhoods of 0 , respectively 1 , coincide with the restrictions of functions in the self-adjoint domain of H . As a result of the assumption that E is not in the self-adjoint spectrum of H , these are complementary within the space of all solutions:

$$\text{Sol}(E) = \text{Sol}_0(E) \oplus \text{Sol}_1(E):$$

Moreover it follows from a simple analysis of the self-adjoint domain of H that

$$\text{Sol}(E)_0 = \text{RegSol}(E):$$

Now, let us say that a family $\{v_E\}_{E \in \mathbb{C} \setminus \text{Spec}(H)}$ of eigenfunctions in the spaces $\text{Sol}_1(E)$ is of Kodaira type if its Wronskian pairing with any algebraic section of RegSol is polynomial in E . Such a family determines, and is determined by, an algebraic section of the family SingSol .

The following is a variation on a result used by Kodaira [Kod49] to confirm Heisenberg's discovery [Hei43a, Hei43b, Hei44] that the negative spectrum of the Schrödinger operator is determined by scattering data associated to the positive spectrum. Kodaira's result is an instance of the limiting absorption principle in scattering theory.

Theorem (See Section 8). If $fV_{E \in \text{Spec}(H)}$ is a Kodaira-type family in the spaces $\text{Sol}_1(E)$, then for every $E > 0$ the limits

$$\lim_{\epsilon \rightarrow 0^+} V_{E+\epsilon} \quad \text{and} \quad \lim_{\epsilon \rightarrow 0^+} V_{E-\epsilon}$$

both exist.

Now, our result relating the Jantzen filtration to the physical spectrum of the hydrogen atom is very much in the same spirit as Heisenberg's discovery. The following theorem makes an explicit connection between algebraic families and scattering theory.

Theorem (See Section 8). The difference of the limits in the theorem above is a member of $\text{RegSol}(E)$. After adjusting by a Wronskian factor, the difference varies algebraically with E , and the morphism

$$A: \text{SingSol} \rightarrow \text{RegSol}$$

that is determined in this way is the unique generically invertible intertwining operator between algebraic families of Harish-Chandra modules for $(g; K)$ (from which the physical states of the hydrogen atom may be obtained using the Jantzen technique).

We believe that this unexpected bridge back to algebra from analysis makes it apparent that the approach to hidden symmetries via algebraic families, particularly algebraic families of solutions, merits close attention.

Acknowledgments. The late Joseph Birman drew the authors' attention to the hydrogen atom system, and suggested that scattering phenomena there should be investigated further. The authors are also grateful to Joseph Bernstein for many useful remarks.

2. THE FAMILY OF HARISH-CHANDRA PAIRS FOR THE HYDROGEN ATOM

In this section we shall associate to the Schrödinger operator (2.1.2) an algebraic family of Harish-Chandra pairs that organizes the various hidden symmetries of the Schrödinger equation.

2.1. Rescaled Schrödinger operator. The time-independent Schrödinger equation for the hydrogen atom is the eigenvalue equation

$$(2.1.1) \quad H \psi = E \psi;$$

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

$$(2.1.2) \quad H = -\frac{\hbar^2}{2m} \Delta - \frac{e^2}{r}.$$

Here \hbar is the reduced Planck's constant, m is the reduced mass, e is the electron charge and r is the distance in \mathbb{R}^3 from the origin. To streamline formulas we shall work not with the operator H in (2.1.2) but with the rescaled Schrödinger operator

$$(2.1.3) \quad T = \frac{2}{\hbar^2} H;$$

It follows from the definition above that $T = -\frac{1}{2} \Delta - \frac{2}{r}$, where

$$(2.1.4) \quad = -\frac{1}{2} \Delta - \frac{2}{r}.$$

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

To familiarize the reader with the new notation, we note that the computation of the spectrum of H mentioned in the introduction is equivalent to the formula

$$\text{Spec}(T) = \left\{ -\frac{2}{n^2} : n = 1; 2; \dots; t \in [0; 1) \right\}$$

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 $R^3 = {}_0R^3$ with smooth function coefficients. We shall denote by $\text{Centralizer}(T)$ the centralizer of the rescaled Schrodinger operator in this algebra.

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

$$(2.2.1) \quad L_1 = x_2 @_3 - x_3 @_2; \quad L_2 = x_3 @_1 - x_1 @_3 \quad \text{and} \quad L_3 = x_1 @_2 - x_2 @_1;$$

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

$$(2.2.2) \quad \begin{aligned} R_1 &= \frac{1}{r} (x_2 @_3 - x_3 @_2) - L_2 @_3 - L_3 @_2 + \frac{x_1}{r}; \\ R_2 &= \frac{1}{r} (x_3 @_1 - x_1 @_3) - L_3 @_1 - L_1 @_3 + \frac{x_2}{r}; \\ R_3 &= \frac{1}{r} (x_1 @_2 - x_2 @_1) - L_1 @_2 - L_2 @_1 + \frac{x_3}{r}; \end{aligned}$$

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 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 g the O -linear span of the operators

$$fL_1; L_2; L_3g \quad \text{and} \quad fR_1; R_2; R_3g$$

within $\text{Centralizer}(T)$.

2.2.4. Lemma. The space g is a free O -module on the elements in Definition 2.2.3, and a Lie algebra over O under the commutator bracket.

Proof. By a direct calculation,

$$(2.2.5) \quad \begin{aligned} [L_i; L_j] &= -\epsilon_{ijk} L_k \\ [R_i; R_j] &= -\epsilon_{ijk} R_k \\ [\epsilon_{ijk} L_k; R_j] &= -\epsilon_{ijk} R_k; \end{aligned}$$

where ϵ_{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 g is a Lie algebra. Freeness can be checked by examining leading-order terms (that is, the principal symbols) of the operators $T^k L_i$ and $T^k R_i$. The former have order exactly $2k+1$, and for each k are linearly independent over C ; the latter have order exactly $2k+2$, and again for each k they are linearly independent over C . The lemma follows from this.

Because g is finitely generated and free as a module over O , and also a Lie algebra over 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 the complex Lie algebras

$$\mathfrak{g}_j = \mathfrak{g} + \mathfrak{l}_j \mathfrak{g};$$

where $\lambda \in \mathbb{C}$ and where $\mathfrak{l}_j \mathfrak{O}$ is the ideal generated by $T - \lambda$ (in the text we shall denote typical points on the line by λ 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 44 -matrices over \mathcal{O} by

$$(2.2.6) \quad \begin{aligned} L_1 &= \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}; & L_2 &= \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} & \text{and} & L_3 &= \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \\ R_1 &= \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}; & R_2 &= \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix} & \text{and} & R_3 &= \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix} : \end{aligned}$$

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

$$\begin{pmatrix} \lambda & 0 & e(T) & f(T) & p(T) \\ 6-e(T) & \lambda & g(T) & q(T) & 7 \\ 4-f(T) & -g(T) & \lambda & r(T) & 5 \\ Tp(T) & Tq(T) & Tr(T) & \lambda & 0 \end{pmatrix};$$

where e, f, g, p, q and r are polynomial functions. The fiber Lie algebra \mathfrak{g}_λ 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 $\mathfrak{so}(3; \mathbb{C}) \ltimes \mathbb{C}^3$. When $\lambda \neq 0$, it is the complex Lie algebra of infinitesimal symmetries of the symmetric bilinear form

$$S = \text{diag}(1; 1; 1; -);$$

If we fix a complex number λ such that

$$(2.2.7) \quad \lambda^2 = -1$$

and if we define

$$(2.2.8) \quad L_j = \frac{1}{2} (L_j + R_j);$$

then

$$[L_i, L_j] = -\epsilon_{ijk} L_k;$$

and moreover

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

So the elements L_j determine an isomorphism of complex Lie algebras

$$(2.2.9) \quad \mathfrak{g}_\lambda \cong \mathfrak{so}(3) \oplus \mathfrak{so}(3)$$

when $\lambda \neq 0$. The isomorphism depends on the choice of λ ; 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 \mathfrak{g}_λ 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 \mathfrak{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 [BHS20a, Sec. 2.2]), namely

$$(2.2.10) \quad G = (W;) \subset GL(4; \mathbb{C})/\mathbb{C} : \det(W) = 1 \text{ and } WSW^t = S :$$

The fiber groups are isomorphic to

$$\begin{aligned} O(3; \mathbb{C}) \ltimes \mathbb{C}^3 &= 0 \\ SO(4; \mathbb{C}) &= 0: \end{aligned}$$

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

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

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

$$K = O(3; \mathbb{C})/\mathbb{C}$$

may be viewed as a subfamily G via the embedding

$$\begin{pmatrix} A & 0 \\ 0 & \det(A)^{-1} \end{pmatrix} : \mathbb{C}^3 \rightarrow \mathbb{C}^3$$

The family K acts on the family \mathfrak{g} via the isomorphism (2.2.6) and the adjoint action. This makes $(\mathfrak{g}; K)$ into an algebraic family of Harish-Chandra pairs in the sense of [BHS20a, BHS20b].

Note that in terms of differential operators, the action of K on \mathfrak{g} is induced from the action of $O(3)$ on \mathbb{R}_0^3 via the formula (2.2.11).

2.4. Real structure. The family $(\mathfrak{g}; K)$ carries a natural real structure, which is to say a set of compatible conjugate-linear involutions on O , \mathfrak{g} and K . See [BHS20a, 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

$$: O \rightarrow O$$

by means of the standard formula $(p)(z) = \overline{p(\bar{z})}$. 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 \mathfrak{g} , being linear partial differential operators on \mathbb{R}_0^3 , have formal adjoints. The family \mathfrak{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

$$(2.4.1) \quad \mathfrak{g} : \mathfrak{g} \rightarrow \mathfrak{g}$$

by $\mathfrak{g}(X) = -X^*$. This preserves the Lie bracket and satisfies

$$(2.4.2) \quad \mathfrak{g}(p \cdot X) = (p) \cdot \mathfrak{g}(X)$$

for all $p \in O$ and all $X \in \mathfrak{g}$.

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

$$(2.5.1) \quad {}^c_g : g \rightarrow g;$$

which is defined as follows: each element of g is a linear differential operator on \mathbb{R}^3_0 , and c_g replaces each coefficient function in the operator by its complex conjugate. Like the involution g , it is compatible with the involution on O in the sense of the formula (2.4.2). Moreover g and c_g commute with one another. So the composition

$$(2.5.2) \quad = g \circ g : g \rightarrow g$$

is an O -linear involution of g . Its fixed subalgebra is precisely the algebra k 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 g and c_g , whereas the hidden symmetries are those fixed by g alone.

2.6. Involutions at the group level. The involutions g and c_g assume a simple form under the isomorphism in (2.2.6) from g to a family of 44-matrix Lie algebras. On the matrix fibers, g is simply entry-wise complex conjugation, whereas c_g is conjugation by the matrix

$$= \text{diag}(1; 1; 1; -1):$$

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 and a commuting involution 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 $z \in \mathbb{R}$ are the hidden symmetry groups

$$G_z = \begin{cases} \text{SO}(3; 1) & z > 0 \\ O(3) \ltimes \mathbb{R}^3 & z = 0 \\ \text{SO}(4) & z < 0: \end{cases}$$

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

2.6.2. Remark. As explained in [BHS18], the whole family G can actually be constructed from the commuting involutions g and c_g on the fiber over $z=1$.

2.6.3. Remark. Starting from Fock's work [Foc35], a substantial literature has developed from the fact that the symmetry groups described in the theorem above are isomorphic to one another for all negative λ , and also for all positive λ . One remarkable development, with ramifications that continue to be explored, has been the realization of all the physical solutions of the time-dependent Schrödinger equation associated to all λ inside a single irreducible unitary representation of a larger group, namely the minimal representation of (the connected component of the identity of) $O(4; 2)$, called the dynamical symmetry group. See [KO03a, KO03b, KO03c] for a comprehensive mathematical treatment of the minimal representation in this case, and see [Mac20] or [MZ11, Men10] for recent accounts from the physics perspective.

The approach to the symmetries of the hydrogen atom via the minimal representation of $O(4; 2)$ is rather different from our aims here, which are to view the Schrödinger operator as a sort of Casimir operator for an algebraic family of groups, and then understand how the eigenspaces vary algebraically as individual irreducible representations of the groups in this family. But it is interesting to consider possible connections between the two.

To list one such possibility, away from $\lambda = 0$, the isomorphisms in Theorem 2.6.1 lead to an embedding of the family of groups studied in this paper into the constant family with fiber (the complexification of) $O(4; 2)$. The embedding becomes algebraic if one extends O by adjoining a square root of T . (Another way to understand the embedding is to note that our family, away from $\lambda = 0$, is naturally a subfamily of the family of orthogonal groups preserving the forms

$$Q = \text{diag } 1; 1; 1; \dots; -1; \dots; -1 \quad (\lambda \neq 0);$$

while conjugation by

$$A = \text{diag } 1; 1; 1; \dots; 1^{1=2}; 1; \dots; 1^{-1=2}$$

transforms these orthogonal groups into the standard group $O(4; 2)$.) The embedding of groups is compatible with the embedding of the solutions of the Schrödinger equation into the minimal representation. It therefore becomes an interesting problem to construct the algebraic families of solutions analyzed in this paper by starting from the minimal representation. We hope to take up this issue elsewhere, and are obliged to the referee for suggesting this type of investigation.

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

$$(2.7.1) \quad RL \quad \text{and} \quad TL^2 - R^2$$

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

$$(2.7.3) \quad \text{order}(L_i) = 0; \quad \text{order}(R_i) = 1 \quad \text{and} \quad \text{order}(T) = 0:$$

The associated graded algebra is the tensor product $U(g_0) \otimes_{\mathbb{C}} O$; where g_0 is the 6-dimensional graded complex Lie algebra with basis elements r'_1, r'_2, r'_3 in degree 0 and r_1, r_2, r_3 in degree 1, and relations

$$(2.7.4) \quad [r'_i, r'_j] = -\epsilon_{ijk} r'_k; \quad [r_i, r_j] = 0 \quad \text{and} \quad [r'_i, r_j] = -\epsilon_{ijk} r_k;$$

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'_i 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 $(r')^2$ and r^2 . The element r' is not $O(3)$ -invariant for the standard action; instead, it transforms under $A_2 O(3)$ as

$$r' \mapsto \det(A) r';$$

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

$$Z(g_0) = Z(g_0)^{O(3); \text{standard}} \otimes_{\mathbb{C}} r' Z(g_0)^{O(3); \text{standard}}.$$

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

$$(2.8.1) \quad \text{Centralizer}(T) \rightarrow U(g)$$

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) I (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) $L_1 L_2 + L_2 L_1, L_1 L_3 + L_3 L_1, L_2 L_3 + L_3 L_2, L_1^2 - L_2^2$ 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 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 are given by the formulas

$$(RL) = 0$$

and

$$(TL^2 - R^2) = T + 2I:$$

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 $U(g)$ 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 $K = O(3; \mathbb{C})$. There is a natural evaluation map

$$(3.1.1) \quad \sum_{k \in K/b} \text{Hom}_K(W; V) \rightarrow V;$$

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

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_{fin} , is a locally finite-dimensional representation of K in its own right. The individual images V of the summands in (3.1.1) are the isotypical summands of the representation. They are the same for V and V_{fin} .

Denote by $O(K)$ 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

$$(3.1.2) \quad \rho_V : O(K) \rightarrow \text{Hom}_{\mathbb{C}}(V, V)$$

for which composition with evaluation at $k \in K$ (a map $O(K) \rightarrow \mathbb{C}$) 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

$$V^* = \text{Hom}_{\mathbb{C}}(V, \mathbb{C})_{\text{fin}}$$

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

$$R(K) = O(K):$$

The morphism (3.1.2) then corresponds to a morphism

$$(3.1.3) \quad R(K) \rightarrow \text{Hom}(V, V):$$

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

$$R(K) \rightarrow \text{Hom}(R(K), R(K)):$$

This is an associative product on $R(K)$ 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 $R(K)$ -module that is nondegenerate in the sense that $R(K) \cdot V = V$.

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

$$(3.1.4) \quad R(K) \cong \bigoplus_{\lambda \in \hat{K}} \text{End}(W_\lambda)$$

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

3.1.5. Definition. We shall denote by $e \in R(K)$ 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 $SO(3; \mathbb{C})$. So effectively we shall be studying representations of $SO(3; \mathbb{C})$, and we shall call these the $SO(3)$ -type representations of K . They may be listed as

$$\lambda = 0, 1, 2, \dots;$$

where λ has dimension $2\lambda+1$. We shall write W_λ in place of W .

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, O -module F that is equipped with a locally finite-dimensional representation of K by O -module automorphisms.

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

$$(3.2.1) \quad F^\vee = \text{Hom}_O(F, O)_{\text{fin}}$$

¹The algebra $R(K)$ is often called the Hecke algebra of K . After fixing a Haar measure on $O(3)$, using which we can identify elements of $R(K)$ 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].

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

$$\begin{array}{c} g \\ \circ F \end{array} \rightarrow F;$$

that is compatible with the K -action in the sense that the action map is K -equivariant, and its restriction to k is the infinitesimal form of the K -action.

As was the case with locally finite-dimensional K -actions, it is possible to describe $(g; K)$ -module structures using an appropriate associative algebra. Form the tensor product

$$\begin{array}{c} U(g; K) = U(g) \\ \otimes_{U(k)} R(K): \end{array}$$

The actions of g and K on F determine a morphism

$$(3.3.1) \quad \begin{array}{c} U(g; K) \\ \otimes F \end{array} \rightarrow F;$$

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

$$\begin{array}{c} U(g; K) \\ \otimes U(g; K) \end{array} \rightarrow U(g; K)$$

which is an O -linear associative product on $U(g; K)$. The morphism (3.3.1) gives F the structure of a $U(g; K)$ -module, and in this way algebraic families of Harish-Chandra modules for $(g; K)$ correspond exactly to $U(g; K)$ -modules that are free as O -modules and nondegenerate in the sense that $U(g; K) \otimes F = F$. 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 F of Harish-Chandra modules for $(g; K)$ is standard and spherical if

- (i) The K -isotypical decomposition of F consists of the full set of $SO(3)$ -type representations, each occurring with multiplicity one.
- (ii) F is generated by its spherical vectors (that is, by its K -fixed elements) in the sense that $U(g) \otimes F^0 = F$, where 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 F is standard and spherical, then the element $TL^2 - R^2 \in Z(g)$ acts on F^0 , and indeed on F , as multiplication by some polynomial $Q \in O$. We shall call Q the value of $TL^2 - R^2$ on F .

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

$$H(g; K) = e U(g; K) e$$

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

$$U H(g; K) = U(g; K) e$$

This is a $U(g; K)$ - $H(g; K)$ -bimodule by left and right multiplication.

3.4.6. Proposition. The spherical Hecke algebra $H(g; K)$ is freely generated as an \mathcal{O} -algebra by the (tensor) product of $TL^2 - R^2 \otimes Z(g)$ with $e \in R(K)$.

3.4.7. Proposition. The space $U H(g; K)$ is a free $H(g; K)$ -module. Moreover there is an isomorphism

$$U H(g; K) \cong \bigoplus_{\substack{M \\ \subset H(g; K); \text{ free}}} W_M$$

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

$$U H(g; K) \otimes_{H(g; K)} F^0$$

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 F^0 as an $H(g; K)$ -module, up to isomorphism. Now the formula $X \mapsto Xf$ defines a classifying morphism of families

$$(3.4.8) \quad U H(g; K) \otimes_{H(g; K)} F^0 \xrightarrow{\sim} F$$

If 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 M is any $H(g; K)$ -module that is free and of rank one as an \mathcal{O} -module, then the tensor product

$$(3.4.9) \quad U H(g; K) \otimes_{H(g; K)} M$$

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 g may be decomposed as a K -equivariant direct sum of \mathcal{O} -modules

$$g = \bigoplus_k s_k$$

where the summand 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 s the R -linear span of these three elements, so that

$$s = \bigoplus_{R \in S} R s_i$$

The three-dimensional real vector space 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 s may be identified.

We shall use the following simple and well-known facts concerning the algebra of complex polynomial functions on 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 $\text{Harm}(s)$ denotes the space of harmonic polynomials on s , then the multiplication map

$$\begin{array}{c} \text{Harm}(s) \\ \text{Sym}(s)^K \rightarrow \text{Sym}(s) \end{array}$$

is a complex vector space isomorphism (this is a very special case of a much more general theorem of Kostant [Kos63, BL96]).

The degree ℓ 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_ℓ for each $\ell = 0; 1; 2; \dots$.

Proof of Proposition 3.4.6. Filter the algebra $U(\mathfrak{g}; K)$ 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 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 $U(\mathfrak{g})$ with multiplication with $e_2 R(K)$ on both sides is an isomorphism of filtered O -modules

$$\text{Sym}(s)^K \xrightarrow{\sim} H(\mathfrak{g}; K):$$

This is an algebra isomorphism at the level of associated graded algebras, because the elements in $s \subset U(\mathfrak{g})$ 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 $U(\mathfrak{g}; K)$ as in the previous proof, which we shall now restrict to $UH(\mathfrak{g}; K)$. 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 $\text{Harm}(s) \subset H(\mathfrak{g}; K)$ 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 F^\vee 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 contragredient that involve the involutions introduced in Subsections 2.4 and 2.5.

The τ -twisted dual F^\vee is simply F but with the action of \mathfrak{g} twisted by the involution τ : for $X \in \mathfrak{g}$ and $f \in F$ we change the action of X on f to

$$X \cdot f = -\tau(X)f$$

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

$$p \cdot \bar{q} := \overline{(p \cdot q)} \quad \text{for } p, q \in F.$$

It is similarly a g -module and a K -module via the involutions on g and K . See [BHS20b, 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 $(g; K)$ (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 $\epsilon = 0$, and throughout this section λ 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 , and so the irreducible representations of the pair $(g; K)$ 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 $(g; K_0)$ -modules.

We have seen that $(g; K_0)$ is isomorphic to $(\mathfrak{so}(3; \mathbb{C})\mathfrak{so}(3; \mathbb{C}); SO(3))$, 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 $(g; K_0)$ 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 $(\lambda; \mu) \in \mathbb{Z} \times \mathbb{C}$. The parabolically induced representation of $SL(2; \mathbb{C})$ associated to the character

$$\begin{pmatrix} a & 0 \\ 0 & a^{-1} \end{pmatrix} \mapsto \text{phase}(a)|a|^\lambda$$

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 $(\lambda; \mu)$ and $(-\lambda; -\mu)$ 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 $(\lambda; \mu)$ and $(-\lambda; -\mu)$. We find, in summary that the admissible dual of $SL(2; \mathbb{C})$ is parametrized by the set

$$(\mathbb{Z} \times \mathbb{C})/\mathbb{Z}_2;$$

where the group Z_2 acts as the involution $(;') \mapsto (-; -')$. 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 $(\mathfrak{g}_j; K_0)$, are those with parameters in the subset

$$(2\mathbb{Z} \times \mathbb{C}) \times Z_2 \times (2\mathbb{Z} \times \mathbb{C}) \times Z_2:$$

4.2. Casimir elements. In this paragraph we shall compute the action of the central elements

$$LR \quad \text{and} \quad L^2 - R^2$$

in the enveloping algebra of \mathfrak{g}_j on the principal series representation with parameters $(;')$.

First, it is well known that the $\mathfrak{so}(3)$ Casimir element

$$(4.2.1) \quad L^2 = L_1^2 + L_2^2 + L_3^2$$

acts as $-\frac{1}{4}n(n+2)$ in the irreducible finite-dimensional representation of $\mathfrak{so}(3)$ of dimension $n+1$ (this is the representation of highest weight n). It follows from this that

if L_j are the Casimir elements associated to the generators L_j in (2.2.8), then

$$\begin{aligned} \frac{1}{2}LR &= \frac{1}{2} \\ &+ \dots \\ &= \frac{1}{4}m(m+2) - \frac{1}{4}n(n+2) \text{ and } \frac{1}{2} \\ L^2 - R^2 &= 2 \\ &+ 2 \\ &= -\frac{1}{2}m(m+2) + n(n+2) \end{aligned}$$

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

Now the above finite-dimensional representation of $(\mathfrak{g}_j; K_0)$ arises as a quotient of the principal series representation with parameters

$$(4.2.2) \quad = m - n \quad \text{and} \quad ' = 2 + m + n:$$

Since it follows from (4.2.2) that

$$' = m(m+2) - n(n+2) \quad \text{and} \quad ^2 + ' ^2 = 2m(m+2) + n(n+2) + 4;$$

we find that in the principal series representation with parameters $(;')$ as in (4.2.2), the Casimir elements act as

$$(4.2.3) \quad LR = \frac{p}{4} - \frac{' }{4} \quad \text{and} \quad L^2 - R^2 = \frac{4 - ^2 - ' ^2}{4}.$$

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 $(;')$ satisfying (4.2.2) they must in fact hold for all $(;')$ by a Zariski density argument, since both sides are regular in $'$.

²The outer automorphism of the pair $(\mathfrak{so}(3)\mathfrak{so}(3); K_0)$ that flips the two $\mathfrak{so}(3)$ -factors induces the involution $(;') \mapsto (-; -')$ on parameters for irreducible modules.

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 $(\lambda; \mu)$ has highest weight $j\mu$, and so the principal series representations that include K_0 -fixed vectors are precisely those for which $\mu = 0$. Hence:

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

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 $L^2 - R^2$ acts as the scalar μ^2 ; compare Lemma 2.8.3.

4.3.2. Lemma. Let V be a standard representation of $(\mathfrak{g}_j; K_0)$. If the Casimir element $L^2 - R^2$ acts on V as the scalar μ^2 , then the irreducible quotient of V including the K_0 -type $\mu = 0$ has classification parameters $\mu = 0$ and $\mu^2 = -4^2 = -16$.

Proof. It follows from (4.2.3) that

$$\frac{\mu^2 - 4}{4} + \mu^2 = R^2 - L^2 + \mu^2 = 0;$$

or in other words that

$$\frac{\mu^2 - 4}{4} = 0:$$

This implies the result.

4.3.3. Corollary. Let V be a standard representation of $(\mathfrak{g}_j; K_0)$ in which the Casimir element $L^2 - R^2$ acts on V as the scalar μ^2 . Unless $-4^2 = -16$ is a integer square, V is an irreducible principal series representation.

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

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 μ the fibers will be irreducible principal series representations with parameters $(0; \mu^2)$. Among other things our construction will in effect extend the principal series to $\mu = 1$, where we will obtain a Harish-Chandra module for $(\mathfrak{g}_0; K)$.

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 $Tf = \lambda f$. Then we shall construct a natural algebraic family of Harish-Chandra modules 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 $\ell \in \mathbb{C}$ we define

$$\text{Sol}(\ell) = \{ \psi \in C^1(\mathbb{R}^3)_{\text{fin}} : T\psi = \ell\psi \}.$$

The Laplacian on \mathbb{R}^3 may be written as

$$\Delta = \frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \Delta_{\mathbb{S}^2}$$

where

$\Delta_{\mathbb{S}^2}$ is the Casimir operator (4.2.1) and where $\frac{\partial}{\partial r}$ is differentiation in the radial direction:

$$\frac{\partial}{\partial r} = \frac{1}{r} (x_1 \frac{\partial}{\partial x_1} + x_2 \frac{\partial}{\partial x_2} + x_3 \frac{\partial}{\partial x_3})$$

So the rescaled Schrödinger operator T acts on the ℓ -isotypical component of the space $C^1(\mathbb{R}^3)_{\text{fin}}$ as

$$(5.1.2) \quad T = -\frac{\partial^2}{\partial r^2} - \frac{2}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} (\ell(\ell+1) - \frac{2}{r}).$$

Using the standard diffeomorphism

$$(5.1.3) \quad \begin{aligned} \mathbb{R}_0^+ &\xrightarrow{\sim} \mathbb{R}_+ \times \mathbb{S}^2 \\ x &\mapsto (|x|, x/|x|); \quad |x| \in \mathbb{R}_+, x \in \mathbb{R}^3 \end{aligned}$$

we find that for any $\ell \in \mathbb{C}$, the ℓ -isotypical space in $\text{Sol}(\ell)$ is the tensor product of the two-dimensional space of ℓ -eigenfunctions of (5.1.2) in $C^1(\mathbb{R}_+)$ with the ℓ -isotypical component of the space $C^1(\mathbb{S}^2)_{\text{fin}}$. The latter is a single copy of the irreducible $\text{SO}(3)$ -type representation W_ℓ ; as noted in Section 3 it consists of the spherical harmonic functions of degree ℓ , which are the restrictions of harmonic polynomial functions of degree ℓ to the sphere. We arrive at the following simple conclusion:

5.1.4. Proposition. For every $\ell \in \mathbb{C}$ the subspace $\text{Sol}(\ell) \subset C^1(\mathbb{R}^3)_{\text{fin}}$ is invariant under the action of the Lie algebra \mathfrak{g} . Moreover the action of \mathfrak{g} on $\text{Sol}(\ell)$ factors through the fiber gj and gives $\text{Sol}(\ell)$ the structure of an admissible $(\text{gj}; K)$ -module, with each $\text{SO}(3)$ -type representation of K occurring with multiplicity 2.

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 ℓ -eigenfunctions are precisely the solutions of the differential equation

$$(5.2.1) \quad r^2 \frac{d^2}{dr^2} + 2r \frac{d}{dr} - (\ell(\ell+1) + 2r + r^2) = 0:$$

This equation is regular-singular at $r = 0$, with indicial roots ℓ 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 ℓ at $r = 0$.

5.2.2. Definition. We shall denote by F_{ℓ} the unique solution of (5.2.1) that extends to an analytic function of $r \in \mathbb{C}$ and has the Taylor series

$$(5.2.3) \quad F_{\ell}(r) = r^{\ell} + \text{higher-order terms in } r;$$

General theory also provides a second, linearly independent solution of the form

$$(5.2.4) \quad G_{\ell}(r) = H_{\ell}(r) + C_{\ell} \log(r) F_{\ell}(r);$$

where H_{ℓ} is a meromorphic function of r with a pole of order $\ell+1$. The constant C_{ℓ} might be 0. Whether or not that is the case, the scalar multiples of F_{ℓ} are the only solutions that are bounded near $0 \in \mathbb{R}^3$.

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

$$R_+ S^2 \ni (r, \cdot) \mapsto F_{\ell}(r) Y_{\ell}(\cdot)$$

in spherical coordinates (5.1.3), where:

- (i) F_{ℓ} is the regular solution of the radial equation (5.2.1) with leading coefficient 1, as in (5.2.3), and
- (ii) Y_{ℓ} is any spherical harmonic function of degree ℓ .

5.2.6. Proposition. The subspace $\text{RegSol}()$ of $\text{Sol}()$ is a $(g; K)$ -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 $\mathbb{R}^3 \xrightarrow{0} \mathbb{R} + S^2$ in (5.1.3) each of the Runge-Lenz operators $R: C^1(\mathbb{R}^3) \rightarrow C^1(\mathbb{R}^3)$ assumes the form

$$p \text{-} \overline{1} \quad R = C + \frac{1}{r} D + @_r E;$$

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

Proof. Each coordinate vector field $@_j$ on \mathbb{R}_0^3 has the form

$$h_j @_r + \frac{1}{r} X_j;$$

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

$$p \text{-} \overline{1} \quad R_i = \sum_{j=i}^X L_i @_j + @_i - \frac{x_i}{r};$$

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

When $\ell=1$, boundedness is clear from the formula for the operator R given in Lemma 5.2.7, since F_{ℓ} vanishes at $r=0$. But when $\ell=0$, the function F_{ℓ} does not

vanish at $r=0$, and the formula in Lemma 5.2.7 suggests that R might behave like $1=r$ at $r=0$. So a somewhat closer examination is required.

Suppose then that $\ell=0$. Denote by hR_{i^k} the projection of R into the k -isotypical component of $\text{Sol}()$, so that

$$R = \sum_{k=0}^{\infty} hR_{i^k}.$$

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

$$hR_{i^0} = eRe;$$

and we have seen that eRe , like any element of $H(g; K)$, acts on the 0-isotypical component as a polynomial function of r , so that hR_{i^0} is a scalar multiple of r and is therefore bounded near $r=0$ as required.³

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

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

$$(r; \zeta) \mapsto p(r) F_{\zeta}(r) Y_{\ell}(\zeta);$$

where

- (i) p is any polynomial function, and
- (ii) F_{ζ} and Y_{ℓ} are as in Definition 5.2.5 above.

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

The group K acts on RegSol as \mathcal{O} -module automorphisms via the action (2.2.11) of K on R_0^3 . There are obvious K -equivariant isomorphisms

$$(5.3.2) \quad \text{RegSol}[j] = \text{RegSol}()$$

for all $j \in \mathbb{Z}$. We wish to make RegSol a g -module via the natural action of g as differential operators on smooth functions on R_0^3 . But we need to prove first that RegSol is invariant under this action. The following is one of our main results:

5.3.3. Theorem. The vector space RegSol is invariant under the following action of elements $X \in g$:

$$X: p F_{\zeta} Y_{\ell} \mapsto (r; \zeta) \mapsto p(r) X(F_{\zeta} Y_{\ell})(r; \zeta).$$

As a result, RegSol carries the structure of an algebraic family of Harish-Chandra modules.

It is enough to prove that RegSol is invariant under the action of the Runge-Lenz operators, and this is what we shall do in the next several lemmas.

³In fact one can compute that $eRe=0$ in $H(g; K)$, so that $hR_{i^0} = 0$.

5.3.4. Lemma. If $\ell' \geq 1$ and if $\ell \geq 2$ RegSol' , and if R is any Runge-Lenz operator, then $hR \ell'^{-1} \geq 2$ $\text{RegSol}'^{\ell-1}$.

Proof. Think of ℓ as a section ℓ of the family of spaces $\text{RegSol}()$. We may assume that ℓ is one of the generators of RegSol , so that

$$\ell = p(\ell) F_{\ell}; Y_{\ell}$$

Using Lemma 5.2.7 we compute that

$$(5.3.5) \quad R \ell = p(\ell) \ell' \ell'^{-1} D Y_{\ell} + p(\ell) \ell' \ell'^{-1} E Y_{\ell} + \text{higher-order terms in } \ell;$$

The formula shows that the $(\ell'-1)$ -component of $R \ell$ belongs to RegSol , as required.

It will be convenient now to introduce a somewhat larger space than RegSol . We shall denote by $\text{RegSol}_{\text{hol}}$ the space defined in exactly the same way as RegSol , except that $p(\ell)$ is replaced by any entire function $h(\ell)$. Since the eigenfunctions $F_{\ell};$ depend analytically on ℓ , the space $\text{RegSol}_{\text{hol}}$ is certainly invariant under the action of g .

5.3.6. Lemma. If $\ell' \geq 2$ $\text{RegSol}_{\text{hol}}$, and if $p \ell' \geq 2$ RegSol for some nonzero polynomial p , then $\ell' \geq 2$ RegSol .

Proof. This follows from the fact that the only entire rational functions are polynomials.

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 $\ell \in \mathbb{C}$ the space $\text{RegSol}(\ell)$ is an irreducible $(\mathfrak{g}; K)$ -module.

5.3.8. Lemma. If $\ell' \geq 1$, if $\ell \geq 2$ $\text{RegSol}'_{|\ell|}$, and if $hR \ell'^{-1} \geq 2$ $\text{RegSol}'^{\ell-1}$ for every Runge-Lenz operator R and every $S \in R(K)$, then $\ell \geq 2$ RegSol' .

Proof. Assume that $\ell = h F_{\ell}; Y_{\ell}$, with h holomorphic. It follows from the explicit formula (5.3.5) that $hR \ell'^{-1}$ has the form

$$h F_{\ell'-1}; Z_{\ell'-1}$$

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

If Y_{ℓ} is nonzero, then $Z_{\ell'-1}$ must be nonzero for some R and some S , for otherwise the $(\mathfrak{g}; K)$ -submodule of $\text{RegSol}(\ell)$ generated by ℓ would be a proper submodule for every ℓ , contrary to Lemma 5.3.7. In the case where $Z_{\ell'-1}$ is nonzero, if $hR \ell'^{-1} \geq 2$ RegSol , then it follows that h is in fact a polynomial function, and hence that $\ell \geq 2$ RegSol , as required.

5.3.9. Lemma. If $X \in U(\mathfrak{g}; K)$ and if $\ell \geq 2$ RegSol^0 , then $X \ell \geq 2$ RegSol .

Proof. Fix $\ell \geq 2$ RegSol^0 . We need to prove that $hX \ell' \geq 2$ RegSol for every X and every $\ell' \geq 0$. If $\ell' = 0$, then since

$$hX \ell^0 = eXe \ell;$$

with $eX \in H(g; K)$, the required result follows for every X from Proposition 3.4.6 and Lemma 2.8.3, which together show that eX acts on RegSol^0 as multiplication by a polynomial in λ . The cases of higher ℓ are handled by induction on ℓ using Lemma 5.3.8.

5.3.10. Lemma. If $\lambda \in \text{RegSol}$, then there exists a nonzero polynomial p , some $S^0 \in U(g; K)$ and some $\lambda^0 \in \text{RegSol}^0$, such that $p\lambda = S^0 \lambda^0$.

Proof. It follows from the Peter-Weyl decomposition (3.1.4) and the K -isotypical decomposition of RegSol that there is a family of pairwise orthogonal idempotents f in $R(K)$ such that

$$\text{RegSol} = \sum_M f \text{RegSol}$$

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

$$\lambda = (f \lambda) = (f S^0 \lambda^0)$$

for at least one value of λ , for some $S^0 \in U(g; K)$ and for some $\lambda^0 \in \text{RegSol}^0$. This means, in particular that $f S^0 \lambda^0$ is nonzero, and hence that $f S^0 \lambda$ is nonzero. Since the latter is an element of a free O -module of rank one, of which λ is a generator, we can write

$$f S^0 \lambda = p \lambda$$

for some $p \in O$, as required.

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

$$p S \lambda = S S^0 \lambda^0;$$

and so it follows from Lemma 5.3.9 that $p S \lambda \in \text{RegSol}$. Lemma 5.3.6 now implies that $S \lambda \in \text{RegSol}$, 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 $\ell = 0$, then it may be shown that

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

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_{ℓ} does not depend on the choice of the square root.) If $\ell = 0$, then

$$(5.4.2) \quad F_{\ell}(r) = \frac{(2\ell+1)!}{2^{\ell+1} \ell!} \frac{1}{r^{\ell+1}} J_{2\ell+1}\left(\frac{p}{2}r\right)$$

where $J(z)$ is the Bessel function of the first kind. See for example [LL58, Section 36].

Next, for $\ell = m$, we define $\ell; m \in \text{RegSol}$ by

$$\ell; m = F_{\ell}; Y^{\ell; m};$$

where the functions $Y^{\ell; m}$ are the basis for the spherical harmonic functions of degree ℓ 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

$$(5.4.3) \quad R_{-} \ell; \ell = \frac{p}{2^{p-1}(2^{p-1}+1)} \ell; \ell-1; \ell-1 \\ - \frac{p}{(p+3)(2^{p-1}+1)} \frac{2^{p-1} + (\ell+1)^2 (2^{\ell-1} + 1)}{(\ell+1)(2^{p-1}+3)} \ell+1; \ell-1;$$

The computation involves the explicit form of the functions $F_{\ell};$ 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 $\ell; \ell$ back into RegSol , and hence 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

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

as a $(g; K)$ -module.

5.5.1. Definition. The (modified) Wronskian of two functions ℓ and ℓ' of $r > 0$ is the function

$$\text{wr}(\ell; \ell')(r) = r^2 \frac{d\ell(r)}{dr} (\ell') - \ell(r) \frac{d\ell'(r)}{dr} :$$

The modification ensures that if ℓ and ℓ' are two solutions of the radial equation (5.2.1) for the same ℓ and the same ℓ' , then $\text{wr}(\ell; \ell')$ 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 $\text{Sol}()$ is the bilinear form

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

defined by

$$\text{Wr}(\ell; \ell') = \frac{1}{4} \int_{S^2} \text{wr}(\ell; \ell') d\text{Area} :$$

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

5.5.3. Lemma. If $\ell; \ell' \in \text{RegSol}()$, then $\text{Wr}(\ell; \ell') = 0$.

Proof. If ψ_1 and ψ_2 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.

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

Wr: SingSol() RegSol() ! C:

We shall prove the following result:

5.5.4. Theorem. Let $C \in \mathcal{C}$, and let $X \in \mathcal{G}_j$. If $\gamma \in \text{SingSol}(C)$ and $\gamma \in \text{RegSol}(C)$, then

$$Wr(X'; \quad) + Wr('; (X) \quad) = 0:$$

As a result, the Wronskian induces an isomorphism of $(g; K)$ -modules from $\text{SingSol}()$ to the $-$ -twisted dual of $\text{RegSol}()$.

5.5.5. Corollary. If $2 \in R$, then the Wronskian form induces an isomorphism of $(g; K)$ -modules from $\text{SingSol}()$ to the $-$ -twisted dual of $\text{RegSol}()$.

Proof of the Corollary. The theorem immediately gives

$$\text{Wr}(X'; \overline{}) + \text{Wr}('; (X) \overline{}) = 0$$

for ' 2 SingSol() and 2 RegSol(). But this the same as

$$Wr(X'; \overline{}) + Wr('; \overline{(X)}) = 0;$$

from which the result follows. \square

We shall prove the theorem in a sequence of steps. The first concerns the constituents of the formula

$$(5.5.6) \quad p_{-1}R = C + \frac{1}{r} D + @_r E$$

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

$$A'_k : V^k \rightarrow V'$$

the composition of the restriction of A to the k -isotypical space of V with the projection onto the ℓ -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 $\epsilon \neq 1$, then

$$E'_{-1} = (1 - \epsilon) D'_{-1}$$

and

$$E_i'^{-1} = (1 + \epsilon_i) D_i'^{-1}:$$

Proof. A short computation reveals that

$$\begin{aligned} [\quad; R] &= \frac{1}{r^2} @_r \quad 2E - 2D - [\quad] \\ T &\quad\quad\quad \underline{\quad} \\ ; D] - r^2 \quad D + [&\quad\quad\quad + \frac{1}{r^3} 2[\\ ; C] &\quad\quad\quad ; D] - 2 \\ &\quad\quad\quad D - [\\ &\quad\quad\quad ; E]: \end{aligned}$$

Since $[T; R] = 0$, each of the three terms in parentheses is zero. Our interest is in the first. Since

acts as $'(+1)$ on the $'$ -isotypical space we obtain

$$2E - 2D + '(+1)D - D(' - 1)'_{-1} = 0$$

and after simplification this becomes

$$E - (1 - ')D_{-1} = 0$$

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

$$\int_{S^2} Y DZ \, d\text{Area} = - \int_{S^2} DY Z \, d\text{Area}$$

and

$$\int_{S^2} Y EZ \, d\text{Area} = \int_{S^2} EY Z \, d\text{Area} - 2 \int_{S^2} DY Z \, d\text{Area} :$$

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

5.5.9. Lemma. If $' \geq 2$ $\text{SingSol}()$ and $' \geq 2$ $\text{RegSol}()$, then

$$\text{Wr}(R';) - \text{Wr}('; R) = 0 :$$

Proof. First, we compute that

$$\text{wr}(R';) = (2'^2 + ')r^0 DY Z - (2' + 1)r^0 EY Z + \text{positive-order terms in } r ;$$

for some spherical harmonic functions Y and Z of degrees $' - 1$ and $'$, respectively.

Hence

$$\text{Wr}(R';) = (2'^2 + ') \int_{S^2} DY Z \, d\text{Area} - (2' + 1) \int_{S^2} EY Z \, d\text{Area} ;$$

and similarly

$$\text{Wr}('; R) = -(2'^2 - ') \int_{S^2} Y DZ \, d\text{Area} - (2' - 1) \int_{S^2} Y EZ \, d\text{Area} :$$

It follows that

$$\text{Wr}(R';) - \text{Wr}('; R) = (2' - 2) \int_{S^2} DY Z \, d\text{Area} - 2 \int_{S^2} EY Z \, d\text{Area} ;$$

and to complete the proof we need only apply Lemma 5.5.7.

Proof of Theorem 5.5.4. The Wronskian pairing determines a K -equivariant vector space isomorphism

$$(5.5.10) \quad \text{SingSol}() \xrightarrow{\sim} \text{RegSol}()'$$

(the right-hand side is the $-$ -twisted dual). Moreover this isomorphism is compatible with the action of the Runge-Lenz operators R from $(' - 1)$ - to $'$ -isotypical components, for all $' > 0$, thanks to Lemma 5.5.9.

Now, for all but countably many $'$, the $(g; K)$ -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 $'$,

(5.5.10) can differ from an isomorphism of $(g; K)$ -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 $(g; K)$ -modules. This proves the lemma when the modules in (5.5.10) are irreducible. The general case follows by a continuity argument.

5.6. The algebraic family of singular solutions. In view of the preceding section it is natural to organize the modules $\text{SingSol}()$ 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 $\text{SingSol}()$.

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

$$C^3 \rightarrow \text{SingSol}()$$

that are representable in the form

$$= p(r)G_{\ell'}; Y_{\ell'} \in \text{Sol}()$$

where $p(r)$ is a polynomial function of r and where $G_{\ell'}$ 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

$$\text{SingSol} \times \text{RegSol} \rightarrow \mathcal{O}$$

induces an isomorphism of algebraic families from SingSol to the ℓ' -twisted dual of RegSol .

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 $\psi = G_{\ell'}; Y_{\ell'}$, then

$$R \psi = -(\ell'+1)r^{-(\ell'+2)} D Y_{\ell'} + r^{-(\ell'+2)} E Y_{\ell'} + \text{higher-order terms in } r;$$

Thus

$$hR \psi = \ell' + 1 = G_{\ell'+1}; Z_{\ell'+1}$$

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 $\text{SingSol}()$ would be reducible. It follows that

$$\text{SingSol}^{\ell'+1} \subset U(g) \text{SingSol}^{\ell'};$$

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

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 $T + \frac{1}{2}I$.

Of course, this result leads to a characterization of RegSol , since it is the $-$ -twisted dual of SingSol .

6. PHYSICAL SOLUTIONS AND JANTZEN QUOTIENTS

In this section we shall examine the solution spaces

$$\text{PhysSol}() \text{ RegSol}()$$

for the Schrödinger equation that are used in physics. The physical solutions are characterized within $\text{RegSol}()$ by boundary conditions at infinity in R_0^3 , 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 $2R$, the space $\text{PhysSol}()$ of physical solutions consists of those functions in $\text{RegSol}()$ that converge to zero at infinity. Computations using explicit formulas show that

- (a) $\text{PhysSol}(-^2=n^2)$ is the finite-dimensional subspace of $\text{RegSol}(-^2=n^2)$ comprised of the $SO(3)$ -types $\ell < n$. It is a Harish-Chandra submodule.
- (b) $\text{PhysSol}() = \text{RegSol}()$ for all 0
- (c) $\text{PhysSol}() = 0$ otherwise.

Moreover in every case the physical solution space has the structure of an irreducible $(g; K)$ -module and carries an invariant inner product. See for example [BI66a], [TdCA98] and [BI66b] for the cases of <0 , $=0$ and >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:

$$(6.2.1) \quad \begin{array}{ccc} \text{SingSol} & \xrightarrow{\quad A \quad} & \text{RegSol} \\ & \searrow \quad \quad \swarrow & \\ & \text{UH}(g; K) & \\ & \text{H}(g; K) \otimes & \end{array}$$

The tensor product at the bottom is that for which the Casimir $TL^2 - R^2$ acts as multiplication by $T + \frac{1}{2}I$ on O . The diagonal morphisms are the classifying morphisms (3.4.8) for SingSol and 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 $-$ -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 $B: \text{SingSol} \rightarrow \text{RegSol}$ 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 $p, q \in \mathbb{C}$ for which

$$pA = qB.$$

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 ℓ -isotypical space RegSol^ℓ as an \mathbb{O} -module and a K -module with \mathbb{O}

$\subset W^\ell$, for example by the mapping

$$\begin{aligned} \text{RegSol}^\ell &\cong F^\ell; Y^\ell \mapsto 1 \\ Y^\ell &\subset \mathbb{O} \\ &\subset W^\ell. \end{aligned}$$

Compare Definition 5.2.5. We can do the same for the ℓ -isotypical subspace of SingSol . After making these identifications, it follows from Schur's lemma that the restriction of A to the ℓ -isotypical parts of our families is multiplication by a diagonal coefficient polynomial function $A^\ell(\cdot)$ that is determined up to multiplication by a nonzero constant. The constant depends on ℓ , 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

$$A^\ell(\cdot) = \text{constant}^\ell \cdot Y^\ell \cdot (n^2 + \ell^2); n=1$$

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 [BHS20b, Sec. 4.1] for further details, which are given in precisely the context we are discussing.

An intertwiner $A: F \rightarrow H$ between algebraic families of Harish-Chandra modules over \mathbb{C} determines 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 $F_j^{(p)}$ is defined to be the image in the fiber F_j of all sections f for which $A(f)$ vanishes to order p or more at \cdot .
- (b) For H the filtration is increasing, and $H_j^{(p)}$ is defined to be the image in the fiber H_j of the space of all sections h such that $(T - \cdot)^p h$ belongs to the image of A .

The map $f \mapsto (T - \cdot)^p A(f)$ induces an isomorphism of $(g_j; K)$ -modules

$$(6.3.1) \quad A^{(p)}: F_j^{(p)} \rightarrow F_j^{(p+1)} \cong H_j^{(p)} \rightarrow H_j^{(p-1)}.$$

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 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 $\lambda = -\frac{1}{2}n^2$, then $\text{RegSol}(\lambda)^{(p)}$ is zero for $p < 0$, it is the direct sum of the λ -isotypical subspaces in the range $\lambda' = 0; 1; 2; \dots; n-1$ for $p=0$, and it is the full space $\text{RegSol}(\lambda)$ for $p \geq 1$. There are therefore exactly two nonzero Jantzen quotients. The first is n^2 -dimensional with K -types

$$\lambda' = 0; 1; 2; \dots; n-1;$$

each with multiplicity one. The second is irreducible and infinite-dimensional, with K -types

$$\lambda' = n; n+1; n+2; \dots;$$

each with multiplicity one.

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

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 $\text{RegSol}(\lambda)$ has a nontrivial Jantzen filtration.

6.4. Non-degenerate invariant Hermitian forms. Here we shall use the fact that SingSol is isomorphic to the λ -twisted dual of RegSol (this follows from Theorem 3.4.4). Intertwiners of the form

$$A: \text{RegSol}(\lambda') \rightarrow \text{RegSol}(\lambda);$$

between a family and its λ -twisted dual were analyzed in [BHS20b, Sec. 4.2], where it was pointed out that for a suitable $c \in \mathbb{C}$ the formula

$$A^{(p)}[\lambda]; [\lambda'] = c (T - \lambda)^{-p} (\lambda')$$

determines an invariant and nondegenerate hermitian form on the p 'th Jantzen quotient. Here λ and λ' determine elements in the p 'th parts of the Jantzen filtrations, as in Subsection 6.3, and $[\lambda]$ and $[\lambda']$ 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 λ .

The Hermitian forms, like the Jantzen quotients themselves, are easy to compute using Proposition 6.2.2. Compare [BHS20b, 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 $\lambda = 0$.
 (b) The finite-dimensional Jantzen quotient when $\lambda = -\frac{1}{2}n^2$, 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 $\text{RegSol}(\lambda)$ has a nonzero infinitesimally unitary Jantzen quotient. There is in this case a unique infinitesimally unitary Jantzen quotient, and it is the submodule $\text{PhysSol}(\lambda)$ of $\text{RegSol}(\lambda)$.

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

$$(7.0.1) \quad T = -\Delta - \frac{2}{r}$$

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 $-2/r$ is locally square-integrable on \mathbb{R}^3 , and therefore the operator (7.0.1) is well-defined as map from $C_c^1(\mathbb{R}^3)$ 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 $C_c^1(\mathbb{R}^3)$ in the norm

$$\|f\|_{H^2(\mathbb{R}^3)}^2 = \|f\|_{L^2(\mathbb{R}^3)}^2 + \|\Delta f\|_{L^2(\mathbb{R}^3)}^2;$$

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 $C_c^1(\mathbb{R}^3)$ into $L^2(\mathbb{R}^3)$ 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 $C_c^1(\mathbb{R}^3)$ into $L^1(\mathbb{R}^3)$ extends to a continuous inclusion of $H^2(\mathbb{R}^3)$ into $L^1(\mathbb{R}^3)$.

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 $C_c^1(\mathbb{R}^3)$. The domain of the unique self-adjoint extension is the Sobolev space $H^2(\mathbb{R}^3) \subset L^2(\mathbb{R}^3)$.

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

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

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 $-2/r$ 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 $\mathbb{R}^3 \setminus \{0\}$. 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

$$\left\{ -\frac{2}{n^2} : n = 1, 2, \dots \right\} \cup [0, \infty).$$

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 $C_c^1(\mathbb{R}^3_0)$ (and indeed on a larger domain). Choose a constant $C_0 > 0$ so that

$$hTf; f_i + C_0 hf; f_i \geq 0$$

for every $f \in C_c^1(\mathbb{R}^3_0)$, and then choose $C > C_0$. Using this choice of C , denote by $F(\mathbb{R}^3)$ the Hilbert space completion of $C_c^1(\mathbb{R}^3_0)$ in the norm associated to the inner product

$$(7.2.1) \quad hf; g_i_{F(\mathbb{R}^3)} = h(T + C)f; g_i_{L^2(\mathbb{R}^3)}.$$

There is a bounded linear map

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

that extends the inclusion of $C_c^1(\mathbb{R}^3_0)$ 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 $C_c^1(\mathbb{R}^3_0)$ to a self-adjoint operator on a domain that is included within the subspace $F(\mathbb{R}^3) \subset L^2(\mathbb{R}^3)$. The extension is characterized by the formula

$$h(T + C)^{-1}f; g_i_{F(\mathbb{R}^3)} = hf; g_i_{L^2(\mathbb{R}^3)}$$

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 $C_c^1(\mathbb{R}^3_0)$ 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

$$H^2(\mathbb{R}^3) \cap F(\mathbb{R}^3) \subset L^2(\mathbb{R}^3):$$

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

$$(hf; fi)_{H^1(\mathbb{R}^3)} = -(hf; fi) + (hf; fi);$$

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

$$H^2(\mathbb{R}^3) \subset H^1(\mathbb{R}^3) \subset L^2(\mathbb{R}^3);$$

Now it may be shown without difficulty that $C_c^1(\mathbb{R}_0^3)$ is dense in $H^1(\mathbb{R}^3)$, and since it is clear from (7.2.1) that

$$(hf; fi)_{F(\mathbb{R}^3)} = \text{constant} (hf; fi)_{H^1(\mathbb{R}^3)}$$

for all $f \in C_c^1(\mathbb{R}_0^3)$, the space $H^1(\mathbb{R}^3)$ is included within $F(\mathbb{R}^3)$. We see therefore that

$$H^2(\mathbb{R}^3) \subset H^1(\mathbb{R}^3) \subset F(\mathbb{R}^3);$$

which proves the theorem.

8. RESOLVENTS OF THE SCHRÖDINGER OPERATOR

In this section we shall work with the self-adjoint rescaled Schrödinger operator T , with $\text{dom}(T) = H^2(\mathbb{R}^3)$, 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 $\chi : \mathbb{R}^3 \rightarrow \mathbb{C}$ 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 $\chi : \mathbb{R}^3 \rightarrow \mathbb{C}$ is a cutoff at 1 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

$$\text{dom}_0(T) = \{f : \mathbb{R}_0^3 \rightarrow \mathbb{C} : f \in \text{dom}(T) \text{ for some cutoff } \chi \text{ at } 0 \text{ and}$$

$$\text{dom}_1(T) = \{f : \mathbb{R}_0^3 \rightarrow \mathbb{C} : f \in \text{dom}(T) \text{ for some cutoff } \chi \text{ at } 1\};$$

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 $\text{dom}_1(T)$.

8.1.4. Definition. We shall write

$$\text{Sol}_0() = \text{Sol}() \setminus \text{dom}_0(T) \quad \text{and} \quad \text{Sol}_1() = \text{Sol}() \setminus \text{dom}_1(T);$$

We shall be most concerned with $\text{Sol}_1()$, which according to the definition consists of those K -finite smooth λ -eigenfunctions of the rescaled Schrödinger operator T that coincide with elements of $\text{dom}(T)$ near infinity in \mathbb{R}_0^3 . 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 $G \in \text{SingSol}()$ there is a unique $V \in \text{Sol}_1()$ such that

$$\text{Wr}(G; F) = \text{Wr}(V; F) \quad \forall F \in \text{RegSol}();$$

Proof. First we shall prove existence, and for this it suffices to consider each ℓ -isotypical component of $\text{SingSol}()$ individually. Suppose that $G \in \text{SingSol}()$ is represented by the product of a ℓ -eigenfunction G_ℓ of the radial operator (5.1.2) and a spherical harmonic Y_ℓ of degree ℓ . Let f be a smooth, compactly supported function on \mathbb{R}^3_0 of the form $r^\ell Y_\ell$, where r^ℓ is a smooth, compactly supported function of $r \in (0; 1)$. The function

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

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

$$U = r^\ell Y_\ell$$

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

$$TU = U + f$$

we see that U is a ℓ -eigenfunction for T outside of the compact set where f is supported, and so r^ℓ is a ℓ -eigenfunction for the radial operator (5.1.2) outside of a compact subset of $(0; 1)$.

Now every solution of the eigenvalue equation (5.2.1) that is defined on a subinterval of $(0; 1)$ may be extended to a solution on $(0; 1)$. So there are ℓ -eigenfunctions u_0 and u_1 that agree with r^ℓ near 0 and near 1, respectively. The corresponding functions

$$U_0 = u_0 Y_\ell \quad \text{and} \quad U_1 = u_1 Y_\ell$$

belong to $\text{Sol}_0()$ and $\text{Sol}_1()$, respectively. Note that since $(T - \lambda)^{-1}$ has dense range, there is at least one f for which U_0 and U_1 are nonzero.

The functions u_0 and u_1 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 ℓ -eigenfunction in $\text{dom}(T)$. This would contradict the assumption that $\lambda \notin \text{Spec}(T)$. So u_0 and u_1 must span the two-dimensional space of ℓ -eigenfunctions of the radial operator (5.1.2).

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

$$F_\ell Y_\ell = a U_0 + b U_1 \quad \text{and} \quad G_\ell Y_\ell = c U_0 + d U_1;$$

for suitable constants $a; b; c; d$. The scalar d must be nonzero because G_ℓ 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_1 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

$$d U_1 = G_\ell Y_\ell - c U_0 = G_\ell Y_\ell - c a F_\ell Y_\ell$$

It follows that we can take $V = d U_1$. This completes the proof of existence.

To prove uniqueness, note first that the above argument shows $F_\ell Y_\ell \in \text{Sol}_0()$, and therefore $\text{RegSol}() \subset \text{Sol}_0()$. Now it suffices to show that if $V \in$

$\text{Sol}_1()$, and if $\text{Wr}(V; F) = 0$ for all $F \in \text{RegSol}()$, then $V = 0$. But if the Wronskians are all 0, then $V \in \text{RegSol}()$, and hence $V \in \text{Sol}_0()$, so that in fact $V \in \text{dom}(T)$. This again contradicts the assumption that $\lambda \notin \text{Spec}(T)$.

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

$$\text{Sol}_0() = \text{RegSol}() \quad \text{and} \quad \text{Sol}() = \text{Sol}_0() \cup \text{Sol}_1():$$

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 $(\mathfrak{g}; K)$ -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 $V \in \text{Sol}_1()$, and if R is any Runge-Lenz operator, then $RV \in \text{Sol}_1()$.

Proof. The only issue is whether or not $RV \in \text{dom}_1(T)$. The smooth, K -finite function V is in the Sobolev space $H^2(\mathbb{R}^3)$ near infinity (that is, $V \in H^2(\mathbb{R}^3)$ for a suitable cutoff at infinity). But V is also an eigenfunction for T , so the function $TV = -V - 2rV$ 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

$$(8.2.2) \quad -\frac{p}{x_r} - TR_i = \frac{i}{x_r} @_i + \sum_{j=i}^X @_j L_j:$$

Each L_j acts as a bounded operator on any ϵ -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 $x_i = r$ maps $H^4(\mathbb{R}^3)$ into itself near infinity.

8.2.3. **Definition.** We shall denote by KodairaSol the complex vector space spanned by functions

$$C^n \text{Spec}(T) \rightarrow \mathbb{R}_0^{-3} \rightarrow C$$

of the form $(\cdot; x) \mapsto V(x)$; where

- (i) $V \in \text{Sol}_1()$, and
- (ii) if $F \in \text{RegSol}$, then $\text{Wr}(F; V)$ is a polynomial function of λ on the complement of $\text{Spec}(T)$.

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

8.2.4. **Lemma.** The usual action of differential operators on functions gives the \mathcal{O} -module the structure of a $(\mathfrak{g}; K)$ -module.

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

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

8.2.5. Theorem. The \mathcal{O} -module morphism

$$\text{SingSol} \rightarrow \text{KodairaSol}$$

that maps each $G \in \text{SingSol}$ to the unique $V \in \text{KodairaSol}$ such that $\text{Wr}(G; F)$

$$= \text{Wr}(V; F) \quad \text{for } F \in \text{RegSol} \quad \text{for } \lambda \notin \text{Spec}(T)$$

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 λ . So the function V defined above is indeed an element of 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.

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 should be expressible as limits, as $\epsilon \rightarrow 0$, of rapidly decaying ($i\epsilon$)-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 $(T - \lambda - i\epsilon)^{-1}$ in some topology as ϵ 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 $\text{Im}(k) > 0$ and $k \neq 0$, then there is a unique K -invariant eigenfunction U_k for the eigenvalue k^2 with

$$U_k(r) \sim \exp\left(-\frac{1}{2}kr\right) + \frac{1}{k} \log(r) \quad \text{as } r \rightarrow \infty.$$

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}_0^3 .

In the numerator in the display is the constant from (2.1.4). Observe that if $\text{Im}(k) > 0$, then $U_k \in \text{dom}_1(T)$.

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.

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

$$(8.3.3) \quad a(k) = \text{Wr}(F_0; U_k);$$

where $a = k^2$.

8.3.4. Lemma. If $k > 0$, and if $\lambda = k^2$, then

$$F_{0;+} = \frac{1}{2ik} a(-k) U_k - a(k) U_{-k} :$$

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 λ -eigenfunctions.

8.3.5. Lemma. If $\text{Im}(k) > 0$ and $a(k)=0$, then $k^2 \notin \text{Spec}(T)$.

Proof. Let $\lambda = k^2$. We can write

$$U_k = a(k)G_{0;+} + b(k)F_{0;+};$$

where $F_{0;+}$ and $G_{0;+}$ are as in the proof of Theorem 8.1.5, except that we view them here as K -invariant functions on \mathbb{R}^3 , and $b(k)$ is some scalar. If $a(k)=0$, then $F_{0;+}$ is a multiple of U_k , and hence belongs to $\text{dom}_1(T)$. It then follows from Remark 8.1.6 that $\lambda \notin \text{Spec}(T)$.

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

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

$$\text{Wr}(V_{0;+}; F_{0;+}) = 1$$

for every $\lambda \notin \text{Spec}(T)$. For every $\epsilon > 0$ the limits

$$V_{0;+}^+ = \lim_{\lambda \rightarrow \lambda_0 + i\epsilon} V_{0;+} \quad \text{and} \quad V_{0;+}^- = \lim_{\lambda \rightarrow \lambda_0 - i\epsilon} V_{0;+}$$

exist in the standard topology on $C^1(\mathbb{R}^3_0)$ of uniform convergence on compact sets of functions and all their derivatives. The limits are λ -eigenfunctions, and moreover

$$V_{0;+}^+ - V_{0;+}^- = \text{Wr}(V; \check{V}) F_{0;+} \text{ for}$$

every $\epsilon > 0$.

Proof. To begin, suppose that $\lambda \notin \text{Spec}(T)$. 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, $U_k \in \text{Sol}_1(\lambda)$. Therefore $V_{0;+}$ and U_k are multiples of one another, since the space of K -invariant functions in $\text{Sol}_1(\lambda)$ is one-dimensional. In fact it follows from (8.3.3) and the Wronskian condition in the statement of the theorem that

$$(8.3.8) \quad V_{0;+} = \frac{1}{a(k)} U_k$$

Once again, this formula holds for $\lambda \notin \text{Spec}(T)$ 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

$$V_{0;+}^+ = \frac{1}{a(\sqrt{\lambda})} U_{\sqrt{\lambda}} \quad \text{and} \quad V_{0;+}^- = \frac{1}{a(-\sqrt{\lambda})} U_{-\sqrt{\lambda}};$$

where in both cases we used the positive square root of λ . The final formula in the statement of the theorem is a consequence of Lemma 8.3.4.

For $\delta > 0$ let us now define

$$(8.3.9) \quad w(\delta) = \text{Wr}(V_{0;\delta}^+, V_{0;\delta}^-) = \frac{2j^p}{j a(\frac{\delta}{2})^j}$$

as in Theorem 8.3.7.

8.3.10. Theorem. For every $V \in \text{KodairaSol}$ and for every $\delta > 0$ the limits

$$V^+ = \lim_{\delta \rightarrow 0^+} V_{+\delta} \quad \text{and} \quad V^- = \lim_{\delta \rightarrow 0^+} V_{-\delta}$$

exist in the standard topology on $C^1(\mathbb{R}^3_0)$ of uniform convergence on compact sets of functions and all their derivatives. The limits are δ -eigenfunctions, and moreover

$$V^+ - V \in \text{RegSol}(\delta): \text{In}$$

fact there is a unique $F \in \text{RegSol}$ such that

$$V^+ - V = w(\delta) F$$

every $\delta > 0$.

Proof. The case where V is spherical is covered by Theorem 8.3.7. Because the limits there exist in the C^1 topology, if $X \in U(\mathfrak{g})$, then in addition the limits

$$(XV_{0;\delta})^+ = \lim_{\delta \rightarrow 0^+} XV_{0;\delta}^+ \quad \text{and} \quad (XV_{0;\delta})^- = \lim_{\delta \rightarrow 0^+} XV_{0;\delta}^-$$

exist, and if $\delta > 0$, then

$$(XV_{0;\delta})^+ - (XV_{0;\delta})^- = w(\delta) XF_{0;\delta}$$

This proves the theorem because 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

$$A: \text{KodairaSol} \rightarrow \text{RegSol}$$

by mapping $V \in \text{KodairaSol}$ to the unique $F \in \text{RegSol}$ for which

$$F = \frac{1}{w(\delta)} (V^+ - V^-) \quad \delta > 0;$$

as in Theorem 8.3.10. This is a morphism of algebraic families of $(\mathfrak{g}; K)$ -modules, and an isomorphism on $\delta \neq 0$ isotypical components.

Using the isomorphism in Theorem 8.2.5 we obtain from Theorem 8.3.11 an intertwining operator from SingSol to 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 $\delta \neq 0$ 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, H_λ , which are Hilbert spaces, carry actions of the visible symmetry group K . We shall prove that for almost every λ in the spectrum, the space of K -finite vectors in H_λ carries a natural action of the hidden symmetry Lie algebra \mathfrak{g}_j , and that the $(\mathfrak{g}_j; K)$ -module so-obtained coincides with the physical solution space for λ .

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 μ on $\text{Spec}(T)$, a μ -measurable field of Hilbert spaces $\{H_\lambda\}_{\lambda \in \text{Spec}(T)}$, and a unitary isomorphism

$$L^2(\mathbb{R}^3) \cong \int_{\text{Spec}(T)}^{\oplus} H_\lambda d\mu(\lambda);$$

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

$$[(T - \lambda I)^{-1} f] = \int_{\text{Spec}(T)}^{\oplus} (\lambda - \mu)^{-1} [f] d\mu(\mu)$$

for almost every λ (we are writing $[f]$ 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_λ for $\lambda < 0$ identify with the λ -eigenspaces for T in $L^2(\mathbb{R}^3)$ via the isomorphism in the theorem, and so are easily analyzed. The situation for 0 is more complicated; it will be explained in the following subsections.

9.2. Visible symmetries. For the sequel, we shall fix a measure μ and a μ -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_λ , 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

$$[g f] = g [f]$$

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

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

$$R: C_c^1(\mathbb{R}_0^3) \rightarrow C_c^1(\mathbb{R}_0^3):$$

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

9.3.1. **Theorem.** There are operators

$$R: H_{\text{fin}} \rightarrow H_{\text{fin}}$$

with the following properties:

- (a) if $f g$ is a measurable section of $f H g$ for some $2 \leq K$, then $f R g$ is a measurable section of $f H g$; and
- (b) if $g \in C_c^1(R_0^3)_{\text{fin}}$, then $[R g] = R[g]$ for μ -almost every x .

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 $C_c^1(R_0^3)_{\text{fin}}$ extends to a continuous linear operator from $F(R^3)_{\text{fin}}$ into $L^2(R^3)_{\text{fin}}$ (the operator is bounded on each isotypical subspace, but not uniformly bounded over all isotypical subspaces). The extension maps the subspace $H^2(R^3)_{\text{fin}} \subset F(R^3)_{\text{fin}}$ into $F(R^3)_{\text{fin}}$.

Proof. From (2.7.1) and Lemma 2.8.3

$$T L^2 - R^2 = T + \frac{1}{2} I$$

on $C_c^1(R_0^3)_{\text{fin}}$. The operator L^2 in this formula is the Casimir for K , and on each isotypical component of $C_c^1(R_0^3)_{\text{fin}}$ it acts as a scalar. Therefore on any such component we have

$$(9.3.3) \quad -\hbar^2 f; f = \text{constant} \hbar T f; f + \text{constant} \hbar f; f:$$

But recall that when viewed as unbounded operators on $L^2(R^3)$ with domain $C_c^1(R_0^3)$, the Runge-Lenz operators are skew-symmetric. So it follows from (9.3.3) that

$$k R_1 f k^2 + k R_2 f k^2 + k R_3 f k^2 = \text{constant} \|k f\|_{F(R^3)}^2:$$

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_j map each isotypical component of $H^2(R^3)$ boundedly into itself. The operators $@_i; @_j$ are bounded as operators from $H^2(R^3)$ into $H^1(R^3)$, and hence as operators from $H^2(R^3)$ into $F(R^3)$; see the proof of Theorem 7.2.3. Finally, $x_i = r$ maps $H^2(R^3)$ continuously into $H^1(R^3)$, and hence into $F(R^3)$. This is a simple direct computation using Lemma 7.1.1.

9.3.4. **Lemma.** If $h \in F(R^3)$ and $g \in C_c^1(R^3)$, then

$$h h; g i_{F(R^3)} = h h; (T + C) g i_{L^2(R^3)}:$$

Proof. In the special case where $h \in C_c^1(R_0^3)$, 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 $F(R^3)$ 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 $C_c^1(R_0^3) \subset L^2(R^3)$. Since both sides of the formula are continuous in $h \in F(R^3)$, the general case follows from the special case.

9.3.5. **Lemma.** If $h \in F(R^3)_{\text{fin}}$ and $g \in C_c^1(R^3)$, then

$$h R_i h; g i_{L^2(R^3)} = -h h; R_i g i_{L^2(R^3)}:$$

Proof. This is obvious for $h \in C_c^1(\mathbb{R}_0^3)$ and follows in general by continuity of the left-hand and right-hand sides in $h \in F(\mathbb{R}^3)_{fin}$.

9.3.6. **Lemma.** The restriction of the operator

$$R_i(T + C)^{-1} : L^2(\mathbb{R}^3)_{fin} \rightarrow F(\mathbb{R}^3)_{fin}$$

to $F(\mathbb{R}^3)_{fin} \subset L^2(\mathbb{R}^3)_{fin}$ is equal to $(T + C)^{-1} R_i$.

Proof. It suffices to prove that

$$h R_i(T + C)^{-1} f; g \rangle_{F(\mathbb{R}^3)} = h(T + C)^{-1} R_i f; g \rangle_{F(\mathbb{R}^3)}$$

for all $f; g \in C_c^1(\mathbb{R}_0^3)_{fin}$. Using Lemmas 9.3.4 and 9.3.5 we compute that

$$\begin{aligned} & \langle (T + C)^{-1} f; g \rangle_{F(\mathbb{R}^3)} \\ &= \langle R_i(T + C)^{-1} f; g \rangle_{F(\mathbb{R}^3)} \\ &= \langle R_i(T + C)^{-1} f; (T + C)g \rangle_{L^2(\mathbb{R}^3)} \\ &= \langle (T + C)^{-1} f; R_i(T + C)g \rangle_{L^2(\mathbb{R}^3)} \\ &= \langle (T + C)^{-1} f; (T + C)R_i g \rangle_{L^2(\mathbb{R}^3)} \\ &= \langle f; R_i g \rangle_{L^2(\mathbb{R}^3)} \\ &= \langle R_i f; g \rangle_{L^2(\mathbb{R}^3)} \end{aligned}$$

The proof is finished by using the characterization in Theorem 7.2.2.

Proof of Theorem 9.3.1. The operators

$$S_i = R_i(T + C)^{-1}$$

are defined on $L^2(\mathbb{R}^3)_{fin}$ 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 $f S_i; g$ on each isotypical part of the measurable family $f H; g$. The operators S_i have the property that if $f \in L^2(\mathbb{R}^3)_{fin}$, then

$$(9.3.7) \quad [S_i f] = S_i[f] \text{ for}$$

λ -almost every λ . Now we define

$$R_i = (T + C) S_i : H_{fin} \rightarrow H_{fin} \text{ if } g$$

$\in C_c^1(\mathbb{R}_0^3)$, and if $f = (T + C)g$, then (9.3.7) implies that

$$[R_i g] = R_i[g];$$

for λ -almost every λ , as required.

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

$$f : C_c^1(\mathbb{R}_0^3) \rightarrow H \quad (f \in \text{Spec}(T))$$

such that

- (a) for every $f \in C_c^1(\mathbb{R}_0^3)$ the family $f''(f)g$ is a measurable and square-integrable section of the field $f H; g$;

- (b) for every $f \in C_c^1(\mathbb{R}^3_0)$, the sections $f[f]g$ and $f''(f)g$ are equal, almost everywhere; and
 (c) for almost every λ the map λ 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

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

$\in C_c(\mathbb{R}_0)$ and all $i = 1; 2; 3$.

Proof. Fix a countable dense set in $C_c^1(\mathbb{R}^3_0)$. For any element of this set, the displayed equations hold almost everywhere. So by redefining λ to be zero on a suitable nullset of values λ , we can arrange for the equations to hold for all λ 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 $D^0(\mathbb{R}^3_0)$ the space of distributions on \mathbb{R}^3_0 ; it is of course the topological dual space of $C_c^1(\mathbb{R}^3_0)$. It acquires by duality an action of the group K and the Lie algebra \mathfrak{g} .

9.4.3. Definition. For decomposition fHg as in Theorem 9.1.1 and a family of evaluation maps $f''g$ as in Theorem 9.4.1 and Lemma 9.4.2, the realization morphisms

$$\lambda : H \rightarrow D^0(\mathbb{R}^3_0)$$

are the complex conjugates of the adjoints of the morphisms λ , and hence are characterized by

$$\langle \lambda(f); v \rangle_{H^*} = \int \overline{f}(v); R_0$$

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 :

$$H \rightarrow D^0(\mathbb{R}^3_0)$$

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

Proof. Injectivity of λ follows from the density of the image of λ . Equivariance and the eigendistribution property follow from the equivariance of λ and compatibility of λ 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 λ -eigenfunctions for T on \mathbb{R}^3_0 , which we shall denote by $C^1(\mathbb{R}^3_0)$. 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

$$\lambda : H_{\text{fin}} \rightarrow C^1(\mathbb{R}^3_0)_{\text{fin}}$$

9.5.1. Theorem. For almost every λ there is an action of \mathfrak{g} on the space H_{fin} such that

- (a) the g_j -action on $H_{;fin}$, together with the K -action, gives $H_{;fin}$ the structure of a $(g_j; K)$ -module; and
 (b) the realization map $: H_{;fin} \rightarrow C^1(R^3)_{;fin}$ is an injective morphism of $(g_j; K)$ -modules.

Proof. The K -action and Theorem 9.3.1 give actions of the individual generators L_i and R_i of g_j on $H_{;fin}$. It follows from Lemma 9.4.2 that these actions commute with the morphism ρ , and hence also with ρ . It follows from the injectivity of ρ that the actions of the individual generators constitute an action of g_j , and indeed a $(g_j; K)$ -module structure.

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

$$H_{;fin} \rightarrow C^1(R^3)_{;fin}$$

is an isomorphism of g_j -modules onto the physical solution space $\text{PhysSol}()$.

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

We have seen that $C^1(R^3)_{;fin}$ is an extension

$$0 \rightarrow \text{PhysSol}() \rightarrow C^1(R^3)_{;fin} \rightarrow C^1(R^3)_{;fin} \rightarrow \text{PhysSol}() \rightarrow 0$$

of one irreducible $(g_j; K)$ -module by a second (which is a copy of the first). We shall show that the composition

$$(9.5.3) \quad H_{;fin} \rightarrow C^1(R^3)_{;fin} \rightarrow C^1(R^3)_{;fin} \rightarrow \text{PhysSol}()$$

is zero for almost every λ . This will show that the realization morphism maps the $(g_j; K)$ -module $H_{;fin}$ injectively into a submodule of $\text{PhysSol}()$ for almost every λ . 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 $H_{;fin}$ is zero. But since the spectrum of T includes the full half line $(0; 1)$, the space $H_{;fin}$, and hence H , 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 $(g_j; K)$ -module is irreducible it suffices to show that the restriction

$$H^0 \rightarrow C^1(R_0^3)^0 \rightarrow C^1(R_0^3)^0 \rightarrow \text{PhysSol}()^0$$

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

The space $\text{Sol}()^0 = C^1(R_0^3)^0$ is spanned by the regular solution F_0 ; in (5.2.3), which spans $\text{PhysSol}()^0$, and the solution G_0 ; in (5.2.4). If $f v g$ is a measurable section of $f H g$ then we may write

$$(v) = a F_0 + b G_0;$$

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

Suppose that for some section $f v g$ the function b is not zero almost everywhere. After multiplying the section by a suitable scalar function of λ , we may assume that $b \neq 0$ for all λ ; that v is square-integrable; that v vanishes outside a compact set in $(0; 1)$; that a and b are bounded functions; but still b is not zero almost everywhere. The square-integrable section $f v g$ corresponds to a function

$g \in L^2(\mathbb{R}^3)$. In fact the function g lies in the domain $H^2(\mathbb{R}^3)$ of the self-adjoint operator T because the section $\overline{f}vg$ is square-integrable. But if $f \in C_c^1(\mathbb{R}^3)$, then

$$\begin{aligned} \int_{\mathbb{R}^3} \overline{f(x)} g(x) dx &= \int_{\text{Spec}(T)} h''(f); v_i d() \\ &= \int_{\text{Spec}(T)} \int_{\mathbb{R}^3_0} \overline{f(v)} d() \\ &= \int_{\text{Spec}(T)} \int_{\mathbb{R}^3} \overline{f(x)} (aF_{0;}(x) + bG_{0;}(x)) dx d() \\ &= \int_{\mathbb{R}^3} \overline{f(x)} \int_{\text{Spec}(T)} (aF_{0;}(x) + bG_{0;}(x)) d() dx: \end{aligned}$$

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

$$x \mapsto \int_{\text{Spec}(T)} (aF_{0;}(x) + bG_{0;}(x)) d():$$

But this is not an L^1 -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 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 $(;) \subset \mathbb{R}$.

$$(9.6.1) \quad P_{(;)} = \lim_{\epsilon \downarrow 0} \frac{1}{2i\epsilon} \int_{\epsilon}^{\epsilon} \frac{1}{T - i\epsilon} - \frac{1}{T + i\epsilon} d:$$

This is valid as long as neither ϵ nor $-\epsilon$ 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:

9.6.2. Lemma. Assume that $\epsilon \notin \text{Spec}(T)$, and that $\epsilon = k^2$, with $\text{Im}(k) > 0$. If f is any smooth and compactly supported K -invariant function on \mathbb{R}^3_0 , then

$$\begin{aligned} \text{Wr}(F_{0;}; U_k) (T - \epsilon)^{-1} f(r) \\ = F_{0;}(r) \int_0^1 U_k(s) f(s) ds + U_k(r) \int_r^\infty F_{0;}(s) f(s) ds: r \end{aligned}$$

Proof. If we denote by $(Kf)(r)$ the right-hand side of the formula in the statement of the lemma, then the formula defines a linear operator K from smooth compactly supported functions on $(0; 1)$ to the vector space of smooth functions in $\text{dom}(T)$. We compute directly from the definition of the Wronskian that

$$(T - \epsilon)Kf = \text{Wr}(F_{0;}; U_k)f;$$

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

Now we apply the lemma with $-i$ in place of i , with $\lambda > 0$. Using our previous notation $a(k)$ for the Wronskian in Lemma 9.6.2 we obtain

$$\begin{aligned} \lim_{\lambda \rightarrow 0^+} (T - i)^{-1} f - (T + i)^{-1} f \\ = F_0(r) \int_0^1 a(k) U_k(s) f(s) ds + a(k) U_k(r) \int_0^1 F_0(s) f(s) ds \\ + F_0(r) \int_1^r a(-k) U_{-k}(s) f(s) ds + a(-k) U_{-k}(r) \int_1^r F_0(s) f(s) ds; \end{aligned}$$

where k is the positive square root of λ . Taking into account Lemma 8.3.4 we obtain

$$\lim_{\lambda \rightarrow 0^+} (T - i)^{-1} f - (T + i)^{-1} f = \frac{2i}{ja(\frac{1}{j})^2} F_0(r) \int_0^1 F_0(s) f(s) ds;$$

We find that on spherical functions that are smooth and compactly supported in \mathbb{R}_0^3 ,

$$(P_{(\cdot)} f)(r) = \frac{1}{j} \int_0^1 F_0(r) F_0(s) f(s) ds \frac{2i}{ja(\frac{1}{j})^2} d\lambda$$

This computation is equivalent to the following result:

9.6.3. Theorem (Compare [Kod49, Theorem 4.1]). If the Hilbert spaces H_λ in Theorem 9.1.1 are normed so that $\|F_0\|_\lambda = 1$ for all $\lambda \in \text{Spec}(T)$, then on $(0; 1)$ the measure in Theorem 9.1.1 is given by the formula

$$2i d\lambda = w(\lambda) d\lambda;$$

with $w(\lambda)$ as in (8.3.9).

9.6.4. Remark. It is possible to compute $w(\lambda)$ by determining the asymptotic behavior of the solutions F_0 ; compare [LL58, (36.27) & (36.28)]. The result is

$$w(\lambda) = 4i(1 - e^{2\pi i \sqrt{\lambda}})^{-1} \quad (\lambda > 0);$$

Observe this has singularities when λ is one of the discrete spectral values $-\lambda^2 = n^2$ for T . The singularities come from zeros of $a(\frac{1}{j})$, 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.

REFERENCES

- [AWH13] G. B. Arfken, H. J. Weber, and F. E. Harris. Mathematical methods for physicists. Academic Press, Boston, Seventh edition, 2013.
- [Bar36] V. Bargmann. Zur Theorie des Wasserstoffatoms. Z. Phys., 99:576–582, 1936.
- [Ber88] J. Bernstein. On the support of Plancherel measure. J. Geom. Phys., 5(4):663–710 (1989), 1988.
- [BHS18] D. Barbasch, N. Higson, and E. M. Subag. Algebraic families of groups and commuting involutions. Internat. J. Math., 29(4):1850030, 18, 2018.
- [BHS20a] J. Bernstein, N. Higson, and E. Subag. Algebraic families of Harish-Chandra pairs. Int. Math. Res. Not. IMRN, (15):4776–4808, 2020.
- [BHS20b] J. Bernstein, N. Higson, and E. Subag. Contractions of representations and algebraic families of Harish-Chandra modules. Int. Math. Res. Not. IMRN, (11):3494–3520, 2020.

- [BI66a] M. Bander and C. Itzykson. Group theory and the hydrogen atom. I. *Rev. Modern Phys.*, 38:330–345, 1966.
- [BI66b] M. Bander and C. Itzykson. Group theory and the hydrogen atom. II. *Rev. Modern Phys.*, 38:346–358, 1966.
- [BL96] J. Bernstein and V. Lunts. A simple proof of Kostant’s theorem that $U(\mathfrak{g})$ is free over its center. *Amer. J. Math.*, 118(5):979–987, 1996.
- [Bou60] N. Bourbaki. *Éléments de mathématique. XXVI. Groupes et algèbres de Lie. Chapitre 1: Algèbres de Lie. Actualités Sci. Ind. No. 1285.* Hermann, Paris, 1960.
- [Dix82] J. Dixmier. *C*-algebras.* North-Holland mathematical library. North-Holland, 1982.
- [DSS96] A. A. Drokin, A. V. Shapovalov, and I. V. Shirokov. Algebra of local symmetries of the Schrödinger equation for the hydrogen atom. *Teoret. Mat. Fiz.*, 106(2):273–284, 1996.
- [Foc35] V. Fock. Zur Theorie des Wasserstoffatoms. *Z. Phys.*, 98:145–154, 1935.
- [Gon88] F. B. Gonzalez. Bi-invariant differential operators on the Euclidean motion group and applications to generalized Radon transforms. *Ark. Mat.*, 26(2):191–204, 1988.
- [GS90] V. Guillemin and S. Sternberg. Variations on a theme by Kepler, volume 42 of *American Mathematical Society Colloquium Publications.* American Mathematical Society, Providence, RI, 1990.
- [Hal13] B. C. Hall. *Quantum theory for mathematicians*, volume 267 of *Graduate Texts in Mathematics.* Springer, New York, 2013.
- [Hei43a] W. Heisenberg. Die “beobachtbaren Größen” in der Theorie der Elementarteilchen. *Z. Phys.*, 120:513–538, 1943.
- [Hei43b] W. Heisenberg. Die beobachtbaren Größen in der Theorie der Elementarteilchen. II. *Z. Phys.*, 120:673–702, 1943.
- [Hei44] W. Heisenberg. Die beobachtbaren Größen in der Theorie der Elementarteilchen. III. *Z. Physik*, 123:93–112, 1944.
- [HT20] N. Higson and Q. Tan. On a spectral theorem of Weyl. *Expo. Math.*, 38(2):180–201, 2020.
- [Kat76] T. Kato. *Perturbation theory for linear operators.* Springer-Verlag, Berlin-New York, second edition, 1976. *Grundlehren der Mathematischen Wissenschaften*, Band 132.
- [Kna86] A. W. Knap. Representation theory of semisimple groups, volume 36 of *Princeton Mathematical Series.* Princeton University Press, Princeton, NJ, 1986. An overview based on examples.
- [KO03a] T. Kobayashi and B. Orsted. Analysis on the minimal representation of $O(p; q)$. I. Realization via conformal geometry. *Adv. Math.*, 180(2):486–512, 2003.
- [KO03b] T. Kobayashi and B. Orsted. Analysis on the minimal representation of $O(p; q)$. II. Branching laws. *Adv. Math.*, 180(2):513–550, 2003.
- [KO03c] T. Kobayashi and B. Orsted. Analysis on the minimal representation of $O(p; q)$. III. Ultrahyperbolic equations on $\mathbb{R}^{p-1; q-1}$. *Adv. Math.*, 180(2):551–595, 2003.
- [Kod49] K. Kodaira. The eigenvalue problem for ordinary differential equations of the second order and Heisenberg’s theory of S-matrices. *Amer. J. Math.*, 71:921–945, 1949.
- [Kos63] B. Kostant. Lie group representations on polynomial rings. *Amer. J. Math.*, 85:327–404, 1963.
- [KV95] A. W. Knap and D. A. Vogan, Jr. Cohomological induction and unitary representations, volume 45 of *Princeton Mathematical Series.* Princeton University Press, Princeton, NJ, 1995.
- [LL58] L. D. Landau and E. M. Lifshitz. *Quantum mechanics: non-relativistic theory.* Course of Theoretical Physics, Vol. 3. Addison-Wesley Series in Advanced Physics. Pergamon Press Ltd., London-Paris; for U.S.A. and Canada: Addison-Wesley Publishing Co., Inc., Reading, Mass., 1958. Translated from the Russian by J. B. Sykes and J. S. Bell.
- [Mac20] G. Jordan Maclay. Dynamical symmetries of the H atom. *Symmetry*, 12(8), 2020.
- [Men10] G. Meng. Generalized MICZ-Kepler problems and unitary highest weight modules, II. *J. Lond. Math. Soc. (2)*, 81(3):663–678, 2010.
- [MPW13] W. Miller, Jr., S. Post, and P. Winternitz. Classical and quantum superintegrability with applications. *J. Phys. A*, 46(42):423001, 97, 2013.
- [MZ11] G. Meng and R. Zhang. Generalized MICZ-Kepler problems and unitary highest weight modules. *J. Math. Phys.*, 52(4):042106, 23, 2011.
- [Nel59] E. Nelson. Analytic vectors. *Ann. of Math. (2)*, 70:572–615, 1959.
- [Pau26] W. Pauli. Über das Wasserstoffspektrum vom Standpunkt der neuen Quantenmechanik. *Z. Phys.*, 36(5):336–363, 1926.
- [Sub18] E. M. Subag. Symmetries of the hydrogen atom and algebraic families. *Journal of Mathematical Physics*, 59(7):071702, 2018.
- [TdCA98] G. F. Torres del Castillo and J.L. Calvario Acócal. On the dynamical symmetry of the quantum Kepler problem. *Revista Mexicana de Física*, 44(4):344–352, 1998.

- [Tes12] G. Teschl. Ordinary differential equations and dynamical systems, volume 140 of Graduate Studies in Mathematics. American Mathematical Society, Providence, RI, 2012.
- [Wal88] N. R. Wallach. Real reductive groups. I, volume 132 of Pure and Applied Mathematics. Academic Press, Inc., Boston, MA, 1988.
- [WW96] E. T. Whittaker and G. N. Watson. A course of modern analysis. Cambridge Mathematical Library. Cambridge University Press, Cambridge, 1996. An introduction to the general theory of infinite processes and of analytic functions; with an account of the principal transcendental functions, Reprint of the fourth (1927) edition.

DEPARTMENT OF MATHEMATICS, PENN STATE UNIVERSITY, UNIVERSITY PARK, PA 16802, USA.
Email address: higson@psu.edu

DEPARTMENT OF MATHEMATICS, BAR ILAN UNIVERSITY, RAMAT-GAN, 5290002, ISRAEL.
Email address: eyal.subag@biu.ac.il