Representations of Lie algebras, Casimir operators and their applications

Libor Šnobl

Lectures presented at *5th Student Colloquium and School on Mathematical Physics*, Stará Lesná, August 29th - September 4th, 2011.

Abstract

We intend to review some basic notions in the representation theory of Lie algebras and focus in particular on the notion of Casimir operator and its generalization.

Outline:

1. representations of Lie algebras, reducibility, Schur's Lemma,
2. universal enveloping algebra (UEA) of a given Lie algebra,
3. Casimir operators as nontrivial central elements of UEA, their essential role in labelling of irreducible representations,
4. generalized Casimir invariants and when they can be expressed in terms of Casimir operators (time permitting),
5. applications: irreducible representations of Lorentz group, hydrogen atom in quantum mechanics.

1 Lie algebras and their representations

A *Lie algebra* $\mathfrak{g}$ is a vector space over a field $\mathbb{F}$ equipped with a multiplication (also called a bracket), i.e. a bilinear map $[\ ,\ ]\colon \mathfrak{g}\times\mathfrak{g}\to\mathfrak{g}$, such that

$$
\begin{aligned}
[y,x] &= -[x,y] \qquad \text{(antisymmetry)} && (1)\\
0 &= \big[x,[y,z]\big]+\big[y,[z,x]\big]+\big[z,[x,y]\big] \qquad \text{(Jacobi identity)} && (2)
\end{aligned}
$$

for all elements $x,y,z\in\mathfrak{g}$. In what follows we shall consider the fields $\mathbb{F}=\mathbb{R}$, $\mathbb{C}$ and finite–dimensional Lie algebras only.

The structure of the Lie algebra $\mathfrak{g}$ can be represented in any chosen basis $(e_j)_{j=1}^{\dim\mathfrak{g}}$ by the corresponding *structure constants* ${c_{jk}}^l$ in the basis $(e_j)_{j=1}^{\dim\mathfrak{g}}$

$$[e_j,e_k]=\sum_{l=1}^{\dim\mathfrak{g}}{c_{jk}}^l e_l. \tag{3}$$

A fundamental theorem due to E. E. Levi [1, 2, 3] provides a general scheme for the structure of Lie algebras.

Theorem 1 (Theorem of Levi) *Let $\mathfrak{g}$ be a finite-dimensional Lie algebra over a field $\mathbb{F}$ and $\mathfrak{r}=R(\mathfrak{g})$ be its radical. Then there exists a semisimple subalgebra $\mathfrak{p}$ of $\mathfrak{g}$ such that*

$$\mathfrak{g}=\mathfrak{p}\dotplus\mathfrak{r}. \tag{4}$$

The subalgebra $\mathfrak{p}$ is isomorphic to the factor algebra $\mathfrak{g}/\mathfrak{r}$ and is unique up to automorphisms of $\mathfrak{g}$.

Because $\mathfrak{r}$ is a solvable ideal and $\mathfrak{p}$ a semisimple subalgebra we have

$$[\mathfrak{p},\mathfrak{p}]=\mathfrak{p},\qquad [\mathfrak{p},\mathfrak{r}]\subseteq\mathfrak{r},\qquad [\mathfrak{r},\mathfrak{r}]\subsetneq\mathfrak{r}.$$

A *representation* ρ of a given Lie algebra $\mathfrak{g}$ on a vector space V is a linear map of $\mathfrak{g}$ into the space $\mathfrak{gl}(V)$ of linear operators acting on V

$$\rho\colon \mathfrak{g}\to\mathfrak{gl}(V)\colon x\to\rho(x)$$

such that for any pair x, y of elements of $\mathfrak{g}$

$$\rho([x,y])=\rho(x)\circ\rho(y)-\rho(y)\circ\rho(x) \tag{5}$$

holds. The field over which the vector space is defined must contain $\mathbb{F}$ in order to have the representation well–defined, i.e. we may have representations of real algebras on complex vector spaces but not vice versa. *Dimension of the representation* ρ is understood to be the same as the dimension of the vector space V.

A subspace W of V is called *invariant* if

$$\rho(\mathfrak{g})W = \{\rho(x)w|\, x \in \mathfrak{g}, w \in W\} \subseteq W.$$

A representation ρ of $\mathfrak{g}$ on V is *reducible* if a proper nonvanishing invariant subspace W of V exists.

A representation ρ of $\mathfrak{g}$ on V is *irreducible* if no nontrivial invariant subspace of V exists.

A representation ρ of $\mathfrak{g}$ on V is *fully reducible* when every invariant subspace W of V has an invariant complement $\tilde{W}$, i.e.

$$V = W \oplus \tilde{W}, \qquad \rho(\mathfrak{g})\tilde{W} \subseteq \tilde{W}. \tag{6}$$

In particular, any irreducible representation is also fully reducible.

An important criterion for irreducibility of a given representations is

Theorem 2 (Schur's Lemma) *Let $\mathfrak{g}$ be a complex Lie algebra and ρ its representation on a finite–dimensional vector space V.*

1. *Let ρ be irreducible. Then any operator A on V which commutes with all $\rho(x)$,*
$$[A, \rho(x)] = 0, \qquad \forall x \in \mathfrak{g},$$
has the form $A = \lambda\mathbf{1}$ for some complex number λ.

2. *Let ρ be fully reducible and such that every operator A on V which commutes with all $\rho(x)$ has the form $A = \lambda\mathbf{1}$ for some complex number λ. Then ρ is irreducible.*

The *adjoint representation* of a given Lie algebra $\mathfrak{g}$ is a linear map of $\mathfrak{g}$ into the space $\mathfrak{gl}(\mathfrak{g})$ of linear operators acting on $\mathfrak{g}$

$$\mathrm{ad}\colon \mathfrak{g} \to \mathfrak{gl}(\mathfrak{g})\colon x \to \mathrm{ad}(x)$$

defined for any pair x, y of elements of $\mathfrak{g}$ via

$$\mathrm{ad}(x)\, y = [x, y]. \tag{7}$$

When convenient we may also use an alternative notation $\mathrm{ad}_x = \mathrm{ad}(x)$. The image of ad is denoted by $\mathrm{ad}(\mathfrak{g})$.

2 Universal enveloping algebras and Casimir operators

Universal enveloping algebra is an important object in the representation theory of Lie algebras. It is defined as a certain factoralgebra of the tensor algebra of a given Lie algebra $\mathfrak{g}$.

The *tensor algebra* (or *free algebra*) of the vector space V over the field $\mathbb{F}$ is the vector space

$$\mathcal{T}(V) = \oplus_{k=0}^{\infty} V^{\otimes k} = \mathbb{F} \oplus V \oplus V \otimes V \oplus \ldots \oplus V^{\otimes k} \oplus \ldots$$

equipped with the associative multiplication generated by the multiplication of decomposable elements

$$(v_1 \otimes v_2 \otimes \ldots \otimes v_k) \cdot (w_1 \otimes \ldots \otimes w_l) = v_1 \otimes v_2 \otimes \ldots \otimes v_k \otimes w_1 \otimes \ldots \otimes w_l.$$

When the vector space V is in addition a Lie algebra $V = \mathfrak{g}$, one may consider a two–sided ideal $\mathcal{J}$ in the associative algebra $\mathcal{T}(\mathfrak{g})$ generated by the elements of the form $x \otimes y - y \otimes x - [x, y]$, i.e.

$$\mathcal{J} = \operatorname{span}\left\{A \otimes (x \otimes y - y \otimes x - [x, y]) \otimes B \,|\, x, y \in \mathfrak{g},\ A, B \in \mathcal{T}(\mathfrak{g})\right\}.$$

The factoralgebra

$$\mathfrak{U}(\mathfrak{g}) = \mathcal{T}(\mathfrak{g})/\mathcal{J} \tag{8}$$

is called the *universal enveloping algebra* of the Lie algebra $\mathfrak{g}$. It is obvious that universal enveloping algebras are associative algebras, i.e. the notion of a universal enveloping algebra allows us to construct an infinite dimensional associative algebra out of any Lie algebra in a canonical way.

The main reason why universal enveloping algebras are useful is the following observation: any representation ρ of a Lie algebra $\mathfrak{g}$ on a (finite–dimensional, for simplicity) vector space V gives rise to a representation $\tilde{\rho}$ of the tensor algebra $\mathcal{T}(\mathfrak{g})$ defined by

$$\tilde{\rho}(x_1 \otimes x_2 \otimes \ldots \otimes x_k) = \rho(x_1) \cdot \rho(x_2) \ldots \rho(x_k).$$

The definition of a representation ρ, equation (5), implies that $\tilde{\rho}(\mathcal{J}) = 0$. Consequently, $\tilde{\rho}$ defines also a representation $\hat{\rho}$ of the universal enveloping algebra $\mathfrak{U}(\mathfrak{g})$ on the vector space V

$$\hat{\rho}(a) = \tilde{\rho}(A), \qquad a = A \bmod \mathcal{J} \in \mathfrak{U}(\mathfrak{g}), \quad A \in \mathcal{T}(\mathfrak{g}).$$

Casimir operators are elements of the center of the universal enveloping algebra $\mathfrak{U}(\mathfrak{g})$ of the Lie algebra $\mathfrak{g}$ [4, 5, 6], i.e. such $c \in \mathfrak{U}(\mathfrak{g})$ that

$$c \cdot a = a \cdot c$$

holds for all $a \in \mathfrak{U}(\mathfrak{g})$. A necessary and sufficient condition for c to be a Casimir operator is

$$c \cdot x = x \cdot c, \qquad \forall x \in \mathfrak{g} \simeq \mathfrak{g}^{\otimes 1}/\mathcal{J}.$$

We shall consider nontrivial Casimir operators only, i.e. those different from elements of $\mathbb{F}/\mathcal{J} \simeq \mathbb{F}$. In order to avoid writing mod $\mathcal{J}$ at all times we adopt a convention that Casimir operators shall be written as totally symmetric expressions in the elements of $\mathfrak{g}$. This can be always accomplished using the identity

$$x \otimes y \bmod \mathcal{J} = \frac{1}{2}\left(x \otimes y + y \otimes x\right) + \frac{1}{2}[x, y] \bmod \mathcal{J}$$

as many times as needed, starting from the highest order terms and proceeding order by order. Such a procedure also implies the uniqueness of such totally symmetric representative of the equivalence class mod $\mathcal{J}$. We shall occasionally suppress the tensor product sign, i.e. $xy \equiv x \otimes y$.

The importance of Casimir operators for the representation theory of complex Lie algebras comes from the Schur's lemma, Theorem 2. In any representation ρ we have

$$[\hat{\rho}(c), \rho(x)] = 0, \qquad \forall x \in \mathfrak{g}.$$

Consequently, if the representation ρ is irreducible, $\hat{\rho}(c)$ must be a multiple of the identity operator, $\lambda\mathbf{1}$. The number λ depends on the choice of the representation ρ and the Casimir operator c. If two irreducible representations ρ_1 on V_1 and ρ_2 on V_2 are *equivalent*, i.e. if a linear transformation $T : V_1 \to V_2$ exists such that

$$\rho_2(x) = T \circ \rho_1(x) \circ T^{-1}, \qquad \forall x \in \mathfrak{g},$$

then necessarily we have $\lambda_1 = \lambda_2$ for the given Casimir invariant c. That means that the eigenvalues of $\hat{\rho}(c)$ can be used to distinguish inequivalent irreducible representations.

If ρ is fully reducible but not irreducible then we may use the knowledge of Casimir operators of $\mathfrak{g}$ in the decomposition of ρ into irreducible components. In particular, we construct common eigenspaces of all known Casimir operators and we know that each of them is an invariant subspace (not necessarily irreducible for general $\mathfrak{g}$).

The existence of nontrivial Casimir operators was established for certain classes of Lie algebras only, e.g. for semisimple ones. Also Lie algebras with nonvanishing center, including all nilpotent ones, do possess nontrivial Casimir operators; namely, the elements of the center themselves. On the other hand some Lie algebras are known to have no nontrivial Casimir invariants.

Let us consider a semisimple complex Lie algebra $\mathfrak{g}$ and its Killing form K. Let us take any basis $(e_1, \ldots, e_{\dim \mathfrak{g}})$ of $\mathfrak{g}$ and find the dual basis $(\tilde{e}^1, \ldots, \tilde{e}^{\dim \mathfrak{g}})$ such that

$$K(e_k, \tilde{e}^j) = \delta^j_k.$$

Let us assume that ${c_{ij}}^k$ are the structure constants (3) of the Lie algebra $\mathfrak{g}$ in the basis $(e_1, \ldots, e_k)$. By the invariance of the Killing form K we have

$$K(e_k, [e_a, \tilde{e}^j]) = -K([e_a, e_k], \tilde{e}^j) = -{c_{ak}}^j = -K(e_k, \sum_{m=1}^{\dim \mathfrak{g}} {c_{am}}^j \tilde{e}^m)$$

which by nondegeneracy of K implies that

$$[e_a, \tilde{e}^j] = \sum_{m=1}^{\dim \mathfrak{g}} {c_{ma}}^j \tilde{e}^m.$$

Let us construct an element of the universal enveloping algebra $\mathfrak{U}(\mathfrak{g})$ of the form

$$C = \sum_{k=1}^{\dim \mathfrak{g}} \tilde{e}^k \otimes e_k = \sum_{k=1}^{\dim \mathfrak{g}} e_k \otimes \tilde{e}^k \tag{9}$$

(its symmetry comes from the fact that the Killing form is symmetric).

Suppressing the tensor product signs and computing $\mod \mathcal{J}$, we have for the commutator between $e_a \in \mathfrak{g}$ and $C \in \mathfrak{U}(\mathfrak{g})$

$$\begin{aligned}
[e_a, C] &= \sum_{k=1}^{\dim \mathfrak{g}} \Big(e_a\, \tilde{e}^k\, e_k - \tilde{e}^k\, e_k\, e_a\Big) = \\
&= \sum_{k=1}^{\dim \mathfrak{g}} \Big((e_a\, \tilde{e}^k - \tilde{e}^k\, e_a)\, e_k + \tilde{e}^k\, (e_a\, e_k - e_k\, e_a)\Big) = \\
&= \sum_{k=1}^{\dim \mathfrak{g}} ([e_a, \tilde{e}^k]\, e_k + \tilde{e}^k\, [e_a, e_k]) = \sum_{k,l=1}^{\dim \mathfrak{g}} ({c_{la}}^k \tilde{e}^l\, e_k + {c_{ak}}^l \tilde{e}^k\, e_l) = 0.
\end{aligned}$$

We conclude that C is a Casimir operator of $\mathfrak{g}$. It is called the *quadratic Casimir operator* [4]. For its application in the proof of Weyl's theorem, see [5].

We remark that the quadratic Casimir operator does not exhaust all independent Casimir operators of the semisimple Lie algebra $\mathfrak{g}$ when we have rank $\mathfrak{g} > 1$. It is known that any semisimple Lie algebra of rank l has l independent Casimir operators which generate the whole center of the universal enveloping algebra $\mathfrak{U}(\mathfrak{g})$ through their products and linear combinations. Their explicit form depends on the details of the structure of the considered algebra $\mathfrak{g}$.

Casimir invariants are of primordial importance in physics. They often represent such important quantities as angular momentum, elementary particle mass and spin, Hamiltonians of various physical systems etc.

Example 1 *Let us consider the angular momentum algebra*

$$\mathfrak{so}(3) = \mathrm{span}\{L_1, L_2, L_3\}$$

with

$$[L_j, L_k] = \sum_{l=1}^{3} \epsilon_{jkl} L_l. \tag{10}$$

The quadratic Casimir operator (9) *is*

$$C = -\frac{1}{2} \sum_{l=1}^{3} L_l^2, \tag{11}$$

i.e. it coincides up to a numerical factor $1/2$ *with the square of angular momentum, familiar from the construction of irreducible representations of the angular momentum algebra in quantum mechanics.*

Notice that the sign of the Casimir operator (11) is in fact the same as used in physics: in quantum mechanics the operators of angular momentum $\hat{L}_j$ (measured in multiples of $\hbar$) satisfy the commutation relations

$$[\hat{L}_j, \hat{L}_k] = \sum_{l=1}^{3} \mathrm{i}\epsilon_{jkl} \hat{L}_l$$

which differ from the ones in equation (10) by an extra imaginary unit. This extra i factor can be traced to the requirement that observables are described by Hermitean operators; the generators of unitary representations of Lie groups are, on the contrary, anti–Hermitean. An obvious remedy is to formally introduce a "physical" basis of a given real Lie algebra

$$\hat{e}_j = \mathrm{i} e_j \tag{12}$$

in which the original real structure constants

$$[e_j, e_k] = \sum_{l} f_{jk}{}^{l} e_l$$

become explicitly purely imaginary

$$[\hat{e}_j, \hat{e}_k] = \sum_l \mathrm{i} f_{jk}{}^l \hat{e}_l.$$

Example 2 *Let us consider the Poincaré algebra* $\mathfrak{iso}(1,3)$ *(a.k.a. inhomogeneous Lorentz algebra) spanned by* $M^{\mu\nu}, P^\mu$, $\mu, \nu = 0, \ldots, 3$ *with the nonvanishing commutation relations*

$$\begin{aligned} [M^{\mu\nu}, P^\rho] &= \eta^{\nu\rho} P^\mu - \eta^{\mu\rho} P^\nu, \\ [M^{\mu\nu}, M^{\rho\sigma}] &= \eta^{\mu\sigma} M^{\nu\rho} + \eta^{\nu\rho} M^{\mu\sigma} - \eta^{\mu\rho} M^{\nu\sigma} - \eta^{\nu\sigma} M^{\mu\rho}, \end{aligned} \tag{13}$$

where η *is the Minkowski metric* $\eta^{\mu\nu} = \eta_{\mu\nu} = diag(1, -1, -1, -1)$. *We shall use the metric* η *to move indices up and down, as is common in the theory of relativity, and denote by* $\epsilon_{\mu\nu\rho\sigma}$ *the covariant totally antisymmetric tensor.*

The Poincaré algebra has a nontrivial Levi decomposition (4)

$$\mathfrak{iso}(1,3) = \mathfrak{so}(1,3) \dotplus \mathfrak{r}$$

with its semisimple factor being the Lorentz algebra

$$\mathfrak{so}(1,3) = \mathrm{span}\{M^{\mu\nu}\}_{\mu,\nu=0,1,2,3}$$

and an Abelian radical

$$\mathfrak{r} = \mathrm{span}\{P^\mu\}_{\mu=0,1,2,3}.$$

There are two independent Casimir operators of this Lie algebra, which are usually expressed as

$$P^2 = \sum_{\mu=0}^{3} \eta_{\mu\nu} P^\mu P^\nu \quad \textit{and} \quad W^2 = \sum_{\mu=0}^{3} \eta_{\mu\nu} W^\mu W^\nu$$

where the quadruplet of quadratic elements of $\mathfrak{U}(\mathfrak{g})$

$$W_\mu = -\frac{1}{2} \epsilon_{\mu\nu\rho\sigma} M^{\nu\rho} P^\sigma$$

is called the Pauli–Lubanski vector. That means that in this case one of the Casimir operators is of second order in generators whereas the other is of fourth order.

These two Casimir operators are essential in the construction of irreducible representations of the Poincaré algebra in relativistic quantum field theory. Notice that in this case one constructs infinite–dimensional unitary representations.

2.1 Energy spectrum of hydrogen atom in quantum mechanics

In order to further demonstrate the relevance of Casimir operators to physics, let us review another application, namely an algebraic determination of the hydrogen spectrum in quantum mechanics. This computation is originally due to Wolfgang Pauli [7].

The Hamiltonian of an electron in hydrogen atom is

$$\hat{H} = \frac{1}{2M} \sum_j \hat{P}_j \hat{P}_j - \frac{Q}{r}, \tag{14}$$

where $\hat{P}_j = -\mathrm{i}\hbar \frac{\partial}{\partial x_j}$ are operators of linear momenta in $\mathbb{R}^3$ with the coordinates x_1, x_2, x_3, $r = \sqrt{x_1^2 + x_2^2 + x_3^2}$, M is the mass of the electron and $Q = \frac{e^2}{4\pi\epsilon_0}$ in SI units.

The Hamiltonian (14) has three obvious integrals of motion, namely the angular momenta

$$\hat{L}_j = \frac{1}{\hbar} \sum_{k,l} \epsilon_{jkl} \hat{X}_k \hat{P}_l,$$

(chosen dimensionless for convenience) and three less obvious integrals of motion, namely the components of the Laplace–Runge–Lenz vector

$$\hat{K}_i = \frac{1}{2MQ} \sum_k \sum_j \epsilon_{ikj} (\hat{P}_k \hat{L}_j + \hat{L}_j \hat{P}_k) - \frac{1}{\hbar} \frac{x_i}{r}. \tag{15}$$

The expression $\frac{x_i}{r}$ should be interpreted as the operator of multiplication by the given function of coordinates. For future reference, let us denote

$$\hat{L}^2 = \sum_{j=1}^{3} \hat{L}_j \hat{L}_j, \qquad \hat{K}^2 = \sum_{j=1}^{3} \hat{K}_j \hat{K}_j.$$

As it turns out, the knowledge of these integrals of motions and their algebraic structure is enough to determine the spectrum of bound states in the hydrogen atom.

The crucial ingredients are the commutators between various components $\hat{L}_j$ and $\hat{K}_j$. By a somewhat lengthy but straightforward calculation we find

$$[\hat{L}_j, \hat{L}_k] = \mathrm{i}\sum_{l=1}^{3} \epsilon_{jkl}\hat{L}_l, \tag{16}$$

$$[\hat{L}_j, \hat{K}_k] = \mathrm{i}\sum_{l=1}^{3} \epsilon_{jkl}\hat{K}_l, \tag{17}$$

$$[\hat{K}_j, \hat{K}_k] = -\frac{2\mathrm{i}}{MQ^2}\sum_{l=1}^{3} \epsilon_{jkl}\hat{L}_l\hat{H}. \tag{18}$$

Another important observation is the operator identity

$$\sum_{j=1}^{3} \hat{K}_j\hat{L}_j = 0. \tag{19}$$

The commutator (18) prevents the operators $\hat{L}_j, \hat{K}_j$ from forming a Lie algebra. Nevertheless, this bothersome property can be circumvented if we consider a given energy level, i.e. a subspace $\mathcal{H}_E$ of the Hilbert space $\mathcal{H}$ consisting of all eigenvectors of $\hat{H}$ with the given energy E. Operators $\hat{L}_j, \hat{K}_j$ can be all restricted to $\mathcal{H}_E$ because they commute with $\hat{H}$. When such restriction is understood, the $\hat{H}$ in equation (18) can be replaced by a numerical factor E and the algebra of $\hat{L}_j, \hat{K}_j$ closes. In particular, when $E < 0$ it is isomorphic to the Lie algebra $\mathfrak{so}(4) = \mathfrak{so}(3) \oplus \mathfrak{so}(3)$. When $E > 0$ the difference in sign leads to a different real form of the same complex Lie algebra, namely to $\mathfrak{so}(1,3)$. We shall be interested in bound states here, i.e. we assume $E < 0$.

Once the energy is fixed we may introduce the operators

$$\hat{L}_{(1)j} = \frac{1}{2}\left(\hat{L}_j + \sqrt{-\frac{MQ^2}{2E}}\hat{K}_j\right)$$

and

$$\hat{L}_{(2)j} = \frac{1}{2}\left(\hat{L}_j - \sqrt{-\frac{MQ^2}{2E}}\hat{K}_j\right)$$

(notice that $-\frac{MQ^2}{2E}$ is by assumption a positive number). The commutators of $\hat{L}_{(1)j}$ and $\hat{L}_{(2)j}$ now become

$$[\hat{L}_{(1)j}, \hat{L}_{(1)k}] = \mathrm{i}\sum_{l=1}^{3} \epsilon_{jkl}\hat{L}_{(1)l},$$

$$[\hat{L}_{(2)j}, \hat{L}_{(2)k}] = \mathrm{i}\sum_{l=1}^{3} \epsilon_{jkl}\hat{L}_{(2)l},$$

$$[\hat{L}_{(1)j}, \hat{L}_{(2)k}] = 0.$$

That means that we have an explicit decomposition of our realization of $\mathfrak{so}(4)$ into the direct sum $\mathfrak{so}(3)\oplus\mathfrak{so}(3)$ and that the two independent Casimir operators of $\mathfrak{so}(4)$ can be expressed as

$$C_1 = \sum_{j=1}^{3} \hat{L}^2_{(1)j}, \qquad C_2 = \sum_{j=1}^{3} \hat{L}^2_{(2)j},$$

or equivalently as

$$C_1 = \frac{1}{4}\sum_{j=1}^{3}\left(\hat{L}_j + \sqrt{-\frac{MQ^2}{2E}}\hat{K}_j\right)^2, \qquad C_2 = \frac{1}{4}\sum_{j=1}^{3}\left(\hat{L}_j - \sqrt{-\frac{MQ^2}{2E}}\hat{K}_j\right)^2. \tag{20}$$

The sum of these two Casimir operators, i.e. $C_1 + C_2$, gives the quadratic Casimir operator (9) of $\mathfrak{so}(4)$.

From the theory of angular momentum, i.e. of representations of the Lie algebra $\mathfrak{so}(3)$, we know that in any irreducible representation of $\mathfrak{so}(4)$ we have

$$C_1 = p(p+1)\mathbf{1}, \qquad C_2 = q(q+1)\mathbf{1}$$

for some nonnegative integer or half–integer values of p and q. The irreducible representation of $\mathfrak{so}(4) = \mathfrak{so}(3)\oplus\mathfrak{so}(3)$ determined by these values of the Casimir operators has dimension equal to $(2p+1)\times(2q+1)$.

When we expand the expressions for the Casimir operators (20) and subtract them, we find that

$$C_1 - C_2 = \sqrt{-\frac{MQ^2}{2E}}\sum_{j=1}^{3}\hat{L}_j\hat{K}_j$$

which vanishes in our representation, as we already know (cf. (19)). Therefore, only irreducible representations of $\mathfrak{so}(4)$ with $p = q$ arise in our problem.

Let us now consider such a representation of $\mathfrak{so}(4)$ with the given values of E and p. The angular momentum $\hat{L}_j$ can be expressed as

$$\hat{L}_j = \hat{L}_{(1)j} + \hat{L}_{(2)j},$$

i.e. we can employ the standard result concerning the composition of two independent angular momenta and conclude that $\hat{L}^2$ takes all integer values between $|p-p| = 0$ and $p+p = 2p$. In particular, the s–state, i.e. the state with $\hat{L}^2 = 0$, exists in our representation and is of interest to us. Let ψ be any s–state, i.e. a vector $\psi \in \mathcal{H}$ such that

$\hat{L}_j\psi = 0$. Obviously, ψ is a function of the radial coordinate r only. We have

$$\hat{L}^2\psi = 0$$

and

$$\hat{K}^2\psi = \frac{2}{MQ^2}\hat{H}\psi + \frac{1}{\hbar^2}\psi$$

by inspection of both sides of the equation when expanded in terms of $\hat{X}_j, \hat{P}_j$ etc.

When ψ in addition belongs to our representation of $\mathfrak{so}(4)$ determined by the values of E and p, we have the following value for the quadratic Casimir operator (9) of $\mathfrak{so}(4)$

$$\begin{aligned} (C_1 + C_2)\psi = 2p(p+1)\psi &= \frac{1}{2}\sum_j \left(\hat{L}_j^2\psi - \frac{MQ^2}{2E}\hat{K}_j^2\psi\right) \\ &= -\frac{MQ^2}{4E}\left(\frac{2E}{MQ^2} + \frac{1}{\hbar^2}\right)\psi. \end{aligned} \tag{21}$$

Thus we have arrived at the condition

$$8p(p+1) = -2 - \frac{MQ^2}{\hbar^2 E}$$

which is just a different formulation of the celebrated Rydberg formula

$$E = -\frac{MQ^2}{2\hbar^2}\frac{1}{(2p+1)^2} \tag{22}$$

where the potentially half–integer valued parameter p is traditionally replaced by the integer $n = 2p+1 > 0$. Once we have established that E is determined by the value of p by equation (22) we also see that $\mathcal{H}_E$ coincides with the representation space of the $\mathfrak{so}(4)$ irreducible representation labelled by p and $q = p$. On $\mathcal{H}_E$ we may also write equation (21) in the form

$$C_1 + C_2 = -\left(\frac{MQ^2}{4\hbar^2\hat{H}} + \frac{1}{2}\right) \tag{23}$$

since both $C_1 + C_2$ and $\hat{H}$ take a constant value on $\mathcal{H}_E$. While it may be tempting to consider this to be an operator identity valid on the whole Hilbert space $\mathcal{H}$, we don't consider such interpretation legitimate. In particular, on scattering states ($E > 0$) we even have a different Lie algebra. Therefore, equation (23) should be considered at most on the bound state sector of our Hilbert space $\mathcal{H}$.

To sum up, we have seen that the spectrum of hydrogen atom can be derived using the theory of Lie algebras, without explicit construction of eigenfunctions. More precisely, we have derived a necessary condition (22) that any energy eigenvalue must satisfy. That this formula is physically relevant for all values of $p \geq 0$ such that $2p \in \mathbb{Z}$ is not a consequence of the computation just shown and shall be established by other means (e.g. by an explicit construction of s–states introduced above). Once the existence of at least one state with the energy $E_n = -\frac{MQ^2}{2\hbar^2}\frac{1}{n^2}$ is shown, the degeneracy n^2 of the energy level E_n also follows directly from algebraic considerations.

3 Generalized Casimir invariants

As was shown by Kirillov in [8] and will be explained below, Casimir operators are in one–to–one correspondence with polynomial invariants characterizing orbits of the coadjoint representation of $\mathfrak{g}$. The search for invariants of the coadjoint representation is algorithmic and amounts to solving a system of linear first order partial differential equations [9, 10, 11, 12, 13, 14, 15, 16, 17]. Alternatively, global properties of the coadjoint representation can be used [13, 18, 19, 20]. In general, solutions are not necessarily polynomials and we shall call the nonpolynomial solutions *generalized Casimir invariants.*

For certain classes of Lie algebras, including semisimple Lie algebras, perfect Lie algebras, nilpotent Lie algebras, and more generally algebraic Lie algebras, all invariants of the coadjoint representation are functions of polynomial ones [9, 10].

On the other hand, in the representation theory of solvable Lie algebras their invariants are not necessarily polynomials, i.e. they can be genuinely generalized Casimir invariants. In addition to their importance in representation theory, they may occur in physics. Indeed, Hamiltonians and integrals of motion of classical integrable Hamiltonian systems are not necessarily polynomials in the momenta [21, 22], though typically they are invariants of some group action.

In order to calculate the (generalized) Casimir invariants we consider some basis $(e_1, \ldots, e_n)$ of $\mathfrak{g}$, in which the structure constants are ${c_{ij}}^k$. The coadjoint representation ad^* of $\mathfrak{g}$ is the representation on $\mathfrak{g}^*$ obtained via transposition of the operators in the adjoint representation

$$\langle \mathrm{ad}^*(x)\phi, y\rangle = -\langle \phi, \mathrm{ad}(x)y\rangle, \qquad \forall x, y \in \mathfrak{g}, \phi \in \mathfrak{g}^*.$$

A basis for the coadjoint representation is given by the first order differential operators acting on functions on $\mathfrak{g}^*$, i.e. vector fields,

$$\widehat{E}_k = \sum_{a,b=1}^{n} e_b {c_{ka}}^b \frac{\partial}{\partial e_a}, \qquad 1 \leq k \leq n. \tag{24}$$

In equation (24) the quantities e_a are commuting independent variables – the coordinates in the basis of the space $\mathfrak{g}^*$, dual to the algebra $\mathfrak{g}$. Using the relation $(\mathfrak{g}^*)^* \simeq \mathfrak{g}$ one can identify them with the basis vectors of $\mathfrak{g}$.

The invariants of the coadjoint representation, i.e. the *generalized Casimir invariants*, are solutions of the following system of partial differential equations

$$\widehat{E}_k I(e_1, \ldots, e_n) = 0, \;\; k = 1, \ldots, n. \tag{25}$$

The relation to Casimir operators, i.e. the 1–1 correspondence between polynomial solutions of equation (25) and the elements of the center of the enveloping algebra comes from the following observations.

Firstly, it is obvious that both the operation on $\mathfrak{U}(\mathfrak{g})$ of taking the commutator with a fixed element $e_k \in \mathfrak{g}$ and the application of the first order differential operator $\widehat{E}_k$ satisfy Leibniz rule

$$\begin{aligned}
[e_k, a_1 a_2] &= [e_k, a_1] a_2 + a_1 [e_k, a_2], \qquad && a_1, a_2 \in \mathfrak{U}(\mathfrak{g}), \\
\widehat{E}_k (F_1 F_2) &= \widehat{E}_k(F_1) F_2 + F_1 \widehat{E}_k(F_2), \qquad && F_1, F_2 \in C^\infty(\mathfrak{g}^*).
\end{aligned}$$

Further ingredient of the proof is the fact that $[e_k, \cdot]$ and $\widehat{E}_k$ give the same answer when applied to e_l, namely

$$[e_k, e_l] = \sum_{m=1}^{n} c_{kl}{}^m e_m, \qquad \widehat{E}_k(e_l) = \sum_{m=1}^{n} c_{kl}{}^m e_m, \tag{26}$$

where it is understood that $e_l \in \mathfrak{g} \subset \mathfrak{U}(\mathfrak{g})$ in the first equality and $e_l \in (\mathfrak{g}^*)^*$ in the second.

Now, let us consider a polynomial function F on $\mathfrak{g}^*$. We express it as a completely symmetric expression in the basis functionals $e_l \in (\mathfrak{g}^*)^*$ – since as functions they commute that does not in fact change anything. Next, we associate to it an element $\tilde{F}$ of the universal enveloping algebra by simply changing the interpretation of the generators $e_k \in (\mathfrak{g}^*)^* \to e_k \in \mathfrak{g} \subset \mathfrak{U}(\mathfrak{g})$. Recalling that the totally symmetric representative of a given element $A \in \mathfrak{U}(\mathfrak{g})$ is unique and observing that $[e_k, \tilde{F}]$ is by construction again a totally symmetric expression in the generators e_l, we find that

$$[e_k, \tilde{F}] = 0 \Leftrightarrow \widehat{E}_k(F) = 0$$

by Leibniz rule and equation (26). Thus, polynomial invariants of the coadjoint representation can indeed be identified with Casimir operators in a bijective way.

Let us first determine the number of functionally independent solutions of the system (25). We can rewrite this system as

$$C \cdot \nabla I = 0 \tag{27}$$

where C is the antisymmetric matrix

$$C = \begin{pmatrix} 0 & {c_{12}}^b e_b & \dots & {c_{1n}}^b e_b \\ -{c_{12}}^b e_b & 0 & \dots & {c_{2n}}^b e_b \\ \vdots & & & \vdots \\ -{c_{1,n-1}}^b e_b & \dots & 0 & {c_{n-1,n}}^b e_b \\ -{c_{1n}}^b e_b & \dots & -{c_{n-1,n}}^b e_b & 0 \end{pmatrix} \tag{28}$$

in which summation over the repeated index b is to be understood in each term and ∇ is the gradient operator $\nabla = (\partial_{e_1}, \dots, \partial_{e_n})^t$ (where t stands for transposition). The number of independent equations in the system (25) is $r(C)$, the generic rank of the matrix C. The number of functionally independent solutions of the system (25) is hence

$$n_I = n - r(C). \tag{29}$$

Since C is antisymmetric, its rank is even. Hence n_I has the same parity as n. Equation (29) gives the number of functionally independent generalized Casimir invariants.

The individual equations in the system of partial differential equations (PDEs) (25) can be solved by the method of characteristics, or, equivalently by integration of the vector fields (24).

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