CHAPTER 5: Lie Differentiation and Angular Momentum

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1 Lie differentiation

Kähler's theory of angular momentum is a specialization of his approach to Lie differentiation. We could deal with the former directly, but we do not want to miss this opportunity to show you both, as they are jewels. As an exercise, readers can at each step specialize the Lie theory to rotations.

1.1 Of Lie differentiation and angular momentum

For rotations around the z axis, we have

$$\frac{\partial}{\partial \phi} = x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}. \tag{1.1}$$

On the left of (1.1), we have a partial derivative. On the right, we have an example of what Kähler defines as a Lie operator, i.e.

$$X = \alpha^i(x^1, x^2, ...x^n)\frac{\partial}{\partial x^i}, \tag{1.2}$$

without explicitly resorting to vector fields and their flows. See section 16 of his 1962 paper. Incidentally, $\partial/\partial x^i$ does not respond to the concept of vector field of those authors. For more on these concepts in Cartan and Kähler, see section 8.1 of my book "Differential Geometry for Physicists and Mathematicians". Contrary to what one may read in the literature, not all concepts of vector field are equivalent.

One would like to make (1.2) into a partial derivative. When I had already written most of this section, I realized that it was not good enough to refer readers to Kähler's 1960 paper in order how to do that; until one gets hold of that paper (in German, by the way), many readers would not be able to understand this section. So, we have added the last subsection of this section to effect such a change into a partial derivative.

Following Kähler, we write the operator (1.1) as χ_3 since we may extend the concept to any plane. We shall later use

$$\chi_k = x^i \frac{\partial}{\partial x^j} - x^j \frac{\partial}{\partial x^i}, \tag{1.3}$$

where (i, j, k) constitutes any of the three cyclic permutations of $(1, 2, 3)$, including the unity. Here, the coordinates are Cartesian.

Starting with chapter 2 posted in this web site (the first one to be taught in the Kähler calculus phases (II and III) of the summer school), we have not used tangent-valued differential forms, not even tangent vector fields. Let us be more precise. We will encounter expressions that can be viewed as components of vector-valued differential 1−forms because of the way they transform when changing bases. But those components are extractions from formulas arising in manipulations, without the need to introduce invariant objects of which those expressions may be viewed as components. The not resorting to tangent-valued quantities will remain the case in this chapter, even when dealing with total angular momentum; the three components will be brought together into just one element of the algebra of scalar-valued differential forms.

1.2 Lie operators as partial derivatives

Cartan and Kähler defined Lie operators by (1.2) (in arbitrary coordinate systems!) and applied them to differential forms. A subreptitious difficulty with this operator is that the partial derivatives take place under different conditions as to what is maintained constant for each of them. This has consequences when applied to differential forms.

In subsection 1.8, we reproduce Kähler's derivation of the Lie derivative as a single partial derivative with respect to a coordinate y^n from other coordinate systems,

$$X = \alpha^i(x) \frac{\partial}{\partial x^i} = \frac{\partial}{\partial y^n}. \tag{1.4}$$

His proof of (1.4) makes it obvious why he chose the notation y^n

Let u be a differential form of grade p,

$$u = \frac{1}{p!} a_{i_1 \ldots i_p} dx^{i_1} \wedge \ldots \wedge dx^{i_p}, \tag{1.5}$$

in arbitrary coordinate systems. Exceptionally, summation does not take place over a basis of differential p−forms, but over all values of the indices. This notation is momentarily used to help readers connect with formulas in in Kähler's 1960 paper.

Our starting point will be

$$Xa_{i_1...i_p} = \alpha^i(x)\frac{\partial a_{i_1...i_p}}{\partial x^i} = \frac{\partial a_{i_1...i_p}}{\partial y^n}. \tag{1.6}$$

1.3 Non-invariant form of Lie differentiation

In subsection 1.8, we derive

$$Xu = \frac{1}{p!}\alpha^i \frac{\partial a_{i_1...i_p}}{\partial x^i} dx^{i_1} \wedge ... \wedge dx^{i_p} + d\alpha^i \wedge e_i u, \tag{1.7}$$

with the operator e_i as in previous chapters.

Assume that the α^i's were constants. The last term would drop out. Hence, for X_i given by $\partial/\partial x^i$ and for u given by $a_{i_1...i_p} dx^{i_1} \wedge ... \wedge dx^{i_p}$, we have

$$X_i(a_{i_1...i_p} dx^{i_1} \wedge ... \wedge dx^{i_p}) = \frac{\partial(a_{i_1...i_p} dx^{i_1} \wedge ... \wedge dx^{i_p})}{\partial x^i} = \frac{\partial a_{i_1...i_p}}{\partial x^i} dx^{i_1...i_p}, \tag{1.8}$$

where $dx^{i_1...i_p}$ stands for $dx^{i_1} \wedge ... \wedge dx^{i_p}$. This allows us to rewrite (1.7) as

$$Xu = \frac{1}{p!}\alpha^i \left[\frac{\partial(a_{i_1...i_p} dx^{i_1...i_p})}{\partial x^i}\right] + d\alpha^i \wedge e_i u, \tag{1.9}$$

It is then clear that

$$Xu = \alpha^i \frac{\partial u}{\partial x^i} + d\alpha^i \wedge e_i u, \tag{1.10}$$

In 1962, Kähler used (1.10) as starting point for a comprehensive treatment of lie differentiation.

The first term on the right of (1.10) may look as sufficient to represent the action of X on u, and then be overlooked in actual computations. In subsection 1.8, we show that this is not so. We now focus on the first term since it is the one with which one can become confused in actual practice with Lie derivatives.

Notice again that, if the α^i's are constants —and the constants $(0, 0, ..1, 0, ...0)$ in particular— the last term in all these equations vanishes. So, we have

$$X(cu) = c\frac{\partial u}{\partial x^i}, \tag{1.11}$$

for a equal to a constant c. But

$$X\left[a(x)u\right] = a(x)\frac{\partial u}{\partial x^i} \qquad \text{(Wrong!)}$$

is wrong. When in doubt with special cases of Lie differentiations, resort to (1.10).

The terms on the right of equations (1.7) to (1.10) are not invariant under changes of bases. So, if u were the state differential form for a particle, none of these terms could be considered as properties of the particle, say its orbital and spin angular momenta.

1.4 Invariant form of Lie differentiation

Kähler subtracted $\alpha^i \omega_i{}^k \wedge e_k u$ from the first term in (1.10) and simultaneously added it to the second term. Thus he obtained

$$Xu = \alpha^i d_i u + (d\alpha)^i \wedge e_i u, \tag{1.12}$$

since

$$\alpha^i \frac{\partial u}{\partial x^i} - \alpha^i \omega_i{}^k \wedge e_k u = \alpha^i d_i u, \tag{1.13}$$

and where we have defined $(d\alpha)^i$ as

$$(d\alpha)^i \equiv d\alpha^i + \alpha^i \omega_i{}^k. \tag{1.14}$$

One may view $d\alpha^i + \alpha^k \omega_k{}^i$ as the contravariant components of what Cartan and Kähler call the exterior derivative of a vector field of components α^i. By "components as vector", we mean those quantities which contracted with the elements of a field of vector bases yield the said exterior derivative. Both differential-form-valued vector field and vector-field-valued differential $1-$form are legitimate terms for a quantity of that type. The corresponding covariant components are

$$(d\alpha)_i = d\alpha_i - \alpha_h \omega_i{}^h. \tag{1.15}$$

If you do not find (1.15) in the sources from which you learn differential geometry, and much more so if your knowledge of this subject is confined to the tensor calculus, please refer again to my book "Differential Geometry for Physicists and Mathematicians". Of course, if you do not need to know things in such a depth, just believe the step from (1.14) to (1.15). We are using Kaehler's notation, or staying very close to it. Nevertheless, there is a more Cartanian way of dealing with the contents of this and the next subsections. See subsection 1.7.

In view of the considerations made in the previous sections, we further have

$$Xu = \alpha^i d_i u + (d\alpha)_i \wedge e^i u \tag{1.16}$$

All three terms in (1.12) and (1.16) are invariant under coordinate transformations. The two terms on the right do not mix when performing a change of basis. This was not the case with the two terms on the right of (1.7) and (1.10), even though their form might induce one to believe otherwise.

1.5 Action of a Lie operator on the metric's coefficients

Following Kähler we introduce the differential 1−form α with components α_i, i.e.

$$\alpha = \alpha_k dx^k = g_{ik}\alpha^i dx^k. \tag{1.17}$$

If the α^i were components of a vector field, the α_k would be its covariant components. But both of them are here components of the differential form α. We define $d_i\alpha_k$ by

$$(d\alpha)_i = (d_i\alpha_k)dx^k. \tag{1.18}$$

Hence, on account of (1.15),

$$d_i\alpha_k \equiv \alpha_{i,k} - \alpha_h \Gamma_i{}^h{}_k. \tag{1.19}$$

Therefore,

$$d_i\alpha_k + d_k\alpha_i = \alpha_{i,k} + \alpha_{k,i} - \alpha_h\Gamma_i{}^h{}_k - \alpha_h\Gamma_k{}^h{}_i \tag{1.20}$$

In a coordinate system where $\alpha^i = 0$ $(i < n)$ and $\alpha^n = 1$, we have

$$\alpha_{i\,,k} = (g_{pi}\alpha^p)_{,k} = g_{pi\,,k}\,\alpha^p = g_{ni\,,k}\,, \tag{1.21}$$

and, therefore,

$$\alpha_{i\,,k} + \alpha_{k\,,i} = g_{ni\,,k} + g_{nk\,,i}\,. \tag{1.22}$$

On the other hand,

$$\alpha^l\Gamma_{ilk} + \alpha^l\Gamma_{kli} = 2\Gamma_{ink} = g_{ni,k} + g_{nk,i} - g_{ik,n}, \tag{1.23}$$

From (1.20), (1.22) and (1.23), we obtain

$$d_k\alpha_i + d_i\alpha_k = \frac{\partial g_{ik}}{\partial x^n}. \tag{1.24}$$

1.6 Killing symmetry and the Lie derivative

When the metric does not depend on x^n, (1.24) yields

$$d_k\alpha_i + d_i\alpha_k = 0. \tag{1.25}$$

We then have that

$$e_i d\alpha = -2(d\alpha)_i. \tag{1.26}$$

Indeed,

$$e_i d\alpha = e_i d(\alpha_k dx^k)] = e_i[(\alpha_{k,m} - \alpha_{m,k})(dx^m \wedge dx^k)] = (\alpha_{k,i} - \alpha_{i,k})dx^k, \tag{1.27}$$

where the parenthesis around $dx^m \wedge dx^k$ is meant to signify that we sum over a basis of differential 2−forms, rather than for all values of i and k. By virtue of (1.18), (1.19) and (1.25), we have

$$2(d\alpha)_i = (d_i\alpha_k - d_k\alpha_i)dx^k = [(\alpha_{i,k} - \alpha_h\Gamma_i{}^h{}_k) - (\alpha_{k,i} - \alpha_h\Gamma_k{}^h{}_i)]dx^k. \tag{1.28}$$

We now use that $\Gamma_i{}^h{}_k = \Gamma_k{}^h{}_i$ in coordinate bases, and, therefore,

$$2(d\alpha)_i = (\alpha_{i,k} - \alpha_{k,i})dx^k = -e_i d\alpha. \tag{1.29}$$

Hence (1.26) follows, and (1.16) becomes

$$Xu = \alpha^i d_i u - \frac{1}{2}e_i d\alpha \wedge e^i u. \tag{1.30}$$

Notice that we have just got Xu in pure terms of differential forms, unlike (1.16), where $(d\alpha)_i$ makes implicit reference to the differentiation of a tensor field.

An easy calculation (See Kähler 1962) yields

$$-2e_i d\alpha = d\alpha \vee u - u \vee d\alpha. \tag{1.31}$$

Hence,

$$Xu = \alpha^i d_i u + \frac{1}{4}d\alpha \vee u - \frac{1}{4}u \wedge d\alpha, \tag{1.32}$$

which is our final expression for the Lie derivative of a differential form if that derivative is associated with a Killing symmetry.

1.7 Remarks for improving the Kähler calculus

The Kähler calculus is a superb calculus, and yet Cartan would have written it if alive. The main concern here is the use of coordinate bases. We saw in chapter one the disadvantage they have when compared with the orthonormal ω^i's; these are differential invariants that define a differentiable manifold endowed with a metric. In this section, the disadvantage lies in that one needs to have extreme care when raising and lowering indices, which is not a problem with orthonormal bases since one simply multiplies by one or minus one. Add to that the fact that dx_i does not make sense since there are not "covariant curvilinear coordinates". On the other hand, ω_i is well defined.

Consider next the Killing symmetry, (1.25). The $d_k\alpha_i$ are associated with the covariant derivative of a vector field. But they could also be associated with the covariant derivatives of a differential 1-form. Indeed, we define $(d_i\alpha)_k$ by

$$d_i\alpha = (\alpha_{k,i} - \alpha_l\Gamma_k{}^l{}_i)dx^k \equiv (d_i\alpha)_k dx^k. \tag{1.33}$$

But

$$d_k\alpha_i \equiv \alpha_{k,i} - \alpha_h \Gamma_k{}^h{}_i. \tag{1.34}$$

Thus

$$(d_i\alpha)_k = d_k\alpha_i \tag{1.35}$$

and the argument of the previous two sections could have been carried out with covariant derivatives of differential forms without invoking components of vector fields.

1.8 Derivation of Lie differentiation as partial differentiation

Because the treatment of vector fields and Lie derivatives in the modern literature is what it is, we now proceed to show how a Lie operator as defined by Kähler (and by Cartan, except that he did not use this terminology but infinitesimal operator) can be reduced to a partial derivative.

Consider the differential system

$$\frac{\partial x^i}{\partial \lambda} = \alpha_i(x^1, \; ... \; x^n), \tag{1.36}$$

the α_i not depending on λ. One of n independent "constant of the motion" (i.e. line integrals) is then additive to λ. It can then be considered to be λ itself. Denote as y^i $(i = 1, \quad n-1)$ a set of $n-1$ such integrals, independent among themselves and independent of λ, to which we shall refer as y^n. The y^i's $(i = 1, \quad n)$ constitute a new coordinate system and we have

$$x^i = x^i(y^1, \quad , \; y^n). \tag{1.37}$$

In the new coordinate system, the Lie operator reads $X = \beta^i\partial/\partial y^i$. Its action on a scalar function is

$$\beta^i \frac{\partial f}{\partial y^i} = \alpha^l \frac{\partial f}{\partial x^l} = \frac{\partial x^l}{\partial \lambda}\frac{\partial f}{\partial x^l} = \frac{\partial f}{\partial y^n}. \tag{1.38}$$

We rewrite u (given by (1.5)), as

$$u = \frac{1}{p!} a_{i_1 ... i_p} \frac{\partial x^{i_1}}{\partial y^{i_1}} \quad \frac{\partial x^{i_p}}{\partial y^{i_p}} dy^{k_1} \wedge ... \wedge dy^{k_p}, \tag{1.39}$$

and then

$$\frac{\partial u}{\partial y^n} = \frac{1}{p!}\frac{\partial a_{i_1 ... i_p}}{\partial y^n}\frac{\partial x^{i_1}}{\partial y^{i_1}} \quad \frac{\partial x^{i_p}}{\partial y^{i_p}} dy^{k_1} \wedge ... \wedge dy^{k_p} + \\ + \frac{1}{(p-1)!} a_{i_1 ... i_p} \frac{\partial}{\partial y^n}\left(\frac{\partial x^{i_1}}{\partial y^{k_1}} dy^{k_1}\right) \frac{\partial x^{i_2}}{\partial y^{k_2}} \quad \frac{\partial x^{i_p}}{\partial y^{k_p}} dy^{k_2} \wedge ... \wedge dy^{k_p}. \tag{1.40}$$

We now use that

$$\frac{\partial a_{i_1...i_p}}{\partial y^n} = \frac{\partial a_{i_1...i_p}}{\partial x^i}\frac{\partial x^i}{\partial y^n} = \alpha^i \frac{\partial a_{i_1...i_p}}{\partial x^i} \tag{1.41}$$

and that

$$\frac{\partial}{\partial y^n}\left(\frac{\partial x^{i_1}}{\partial y^{k_1}} dy^{k_1}\right) = \frac{\partial}{\partial y^{k_1}}\left(\frac{\partial x^{i_1}}{\partial y^n}\right) dy^{k_1} = d\left(\frac{\partial x^{i_1}}{\partial y^n}\right) = d\alpha^{i_1}. \tag{1.42}$$

Hence

$$Xu = \frac{\partial u}{\partial y^n} = \frac{1}{p!}\alpha^i \frac{\partial a_{i_1...i_p}}{\partial x^i} dx^{i_1...i_p} + \frac{1}{p!} a_{i_1...i_p} d\alpha^i \wedge dx^{i_2} \wedge ... \wedge dx^{i_p}. \tag{1.43}$$

and finally

$$Xu = \frac{1}{p!}\alpha^i \frac{\partial u}{\partial x^i} + d\alpha^i \wedge e_i u, \tag{1.44}$$

2 Angular momentum

The components of the angular momentum operators acting on scalar functions are given by (1.3), and therefore

$$\alpha_k = -x^j dx^i + x^i dx^j, \tag{2.1}$$

and

$$d\alpha_k = -dx^j \wedge dx^i + dx^i \wedge dx^j = 2dx^i \wedge dx^j \equiv 2w_k. \tag{2.2}$$

Hence

$$\chi_k u = x^i \frac{\partial u}{\partial x^j} - x^j \frac{\partial u}{\partial x^i} + \frac{1}{2} w_k \vee u - \frac{1}{2} u \wedge w_k. \tag{2.3}$$

The last two terms constitute the component k of the spin operator. It is worth going back to (1.7) and (1.10), where we have the entangled germs of the orbital and spin operator, if we replace $\chi$with χ_k. It does not make sense to speak of spin as intrinsic angular momentum until u represents a particle, which would not be the case at this point.

Kähler denotes the total angular momentum as $K + 1$, which he defines as

$$(K+1)u = \sum_{i=1}^{3} \chi_i u \vee w_i. \tag{2.4}$$

He then shows by straightforward algebra that

$$-K(K+1) = \chi_1^2 + \chi_2^2 + \chi_3^2. \tag{2.5}$$

He also develops the expression for $(K + 1)$ until it becomes

$$(K+1)u = -\sum_i \frac{\partial u}{\partial x^i} \vee dx^i \vee rdr + \sum_i x^i \frac{\partial u}{\partial x^i} + \frac{3}{2}(u - \eta u) + g\eta u \tag{2.6}$$

and also

$$(K+1)u = -\zeta\partial\zeta u \vee rdr + \sum_i x^i \frac{\partial u}{\partial x^i} + \frac{3}{2}(u - \eta u) + g\eta u, \qquad (2.7)$$

where η is as in previous chapters, where ζ reverses the order of all the differential 1−form factors in u and where $g \equiv dx^i \wedge e_i$. This expression for $(K+1)u$ is used in the next section.

3 Harmonic differentials in $E_3 - \{0\}$

As could be expected, the equation $\partial u = 0$ (which in $E_3 - \{0\}$ coincides with $\partial\partial u = 0$) has an infinite variety of solutions. One seeks solutions that are proper functions of the total angular momentum operator. One becomes more specific and specializes to those whose coefficients are harmonic functions of the Cartesian coordinates. One need only focus on those that belong to the even subalgebra, since we can obtain the other ones by product of the even ones with the unit differential form of grade three. One recovers generality by forming linear combinations.

Those from the even subalgebra can be written as $u = a + v$, where a and v are differential 0−form and 2−form respectively. Kähler shows that the action of the differential operator K on these differential forms if homogeneous of degree h is given by

$$Ku = -(h+1)a + (h+1)v - 2da \wedge rdr. \qquad (3.1)$$

Kähler shows that for these u to be proper differentials of K with proper value k it is necessary and sufficient that the following equations be satisfied

$$-(h+1)a = ka, \qquad (h+1)v - 2da \wedge rdr = kv. \qquad (3.2)$$

We stop the argument at this point, having shown a role that the operator K plays in finding the sought solutions.

We may retake the argument at some point in the future.

4 The fine structure of the hydrogen atom

5 Entry point for research in analysis with the Kähler calculus