

BNL-101537-2014-TECH AD/AP 47;BNL-101537-2013-IR

On the Differential Algebra Underlying the COSY INFINITY Computer Code Due to M. Berz

V. Garczynski

July 1992

Collider Accelerator Department

Brookhaven National Laboratory

U.S. Department of Energy

USDOE Office of Science (SC)

Notice: This technical note has been authored by employees of Brookhaven Science Associates, LLC under Contract No.DE-AC02-76CH00016 with the U.S. Department of Energy. The publisher by accepting the technical note for publication acknowledges that the United States Government retains a non-exclusive, paid-up, irrevocable, world-wide license to publish or reproduce the published form of this technical note, or allow others to do so, for United States Government purposes.

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or any third party's use or the results of such use of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof or its contractors or subcontractors. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

Accelerator Development Department Accelerator Physics Division BROOKHAVEN NATIONAL LABORATORY Associated Universities, Inc. Upton, NY 11973

Accelerator Physics Technical Note No. 47

On the Differential Algebra Underlying the COSY INFINITY Computer Code Due to M. Berz

V. Garczynski

On the Differential Algebra Underlying the COSY INFINITY Computer Code Due to M. Berz

V. Garczynski

Accelerator Development Department Brookhaven National Laboratory Upton, NY 11973, USA

The mathematical foundations of the differential algebraic approach to beam optics, due to M. Berz, are described. They are simplified by identifying the underlying algebraic structure with the well known algebra of truncated polynomials. Concrete examples of derivations in this algebra, consistent with the truncation operation, are given.

1. Introduction

There are effective methods for solving systems of differential equations, to any order in z_i , $^{1-4}$

$$z' = F(z, \delta), \quad (\delta - \text{parameters})$$

 $z(s_i) = z_i.$ (1.1)

Here z can be a multidimensional vector like, that used in particle beam optics, for example. The solution of this problem can be stated as a mapping between the initial variables $z_i = z(s_i)$, and the final ones $z_f = z(s_f)$

$$z_f = \mathcal{M}\left(z_i, \delta\right),\tag{1.2}$$

The map \mathcal{M} is of particular interest for accelerator physics as it contains important information about various characteristics of a given ring, (nonlinearities, dependence on external parameters δ), and can be used for fast tracking over many turns. The Taylor expansion coefficients of the map, the derivates, more exactly

$$\frac{\partial^k z_f}{\partial z_i^k} = \frac{\partial^k \mathcal{M}}{\partial z_i^k}, \quad k = 1, 2, \dots, n,$$
(1.3)

2 Introduction

yield the transfer matrix if k = 1, and the higher-order aberrations, if k > 1. The corresponding derivatives of \mathcal{M} with the respect to the parameters δ are called sensitivities of a particle beam optics system.

It is known¹ that it is possible to determine derivatives of a given regular function f(x) of a real variable x, through a given order n, by evaluating the function in the algebra containing elements of the form

$$A = (a_0, a_1, \dots, a_n)$$
 – generic element,
$$e = (1, 0, 0, \dots, 0)$$
 – unit element,
$$d = (0, 1, 0, \dots, 0)$$
 – a differential.
$$(1.4)$$

More exactly, the following formula holds

$$f(xe+d) = \left[f(x), f'(x), f''(x), \dots, f^{(n)}(x) \right], \tag{1.5}$$

which yields the Taylor expansion of the function f around the point x. This permits to avoid using the definition of derivative as a (computer inconvenient) limit

$$f'(x) = \lim_{\Delta x \to 0} \frac{f(x + \Delta x) - f(x)}{\Delta x}.$$
 (1.6)

Moreover, the subsequent elements of the array (1.5) can be easily implemented on a computer, and evaluate in parallel. All that is needed here are rules for the addition, multiplication by a number, and multiplication rules for the (n+1)-tupoles A of real numbers, to which the evaluation of the left-hand side of the formula (1.5) reduces once the function f(x) is given. We will describe this, what is called, the arithmetic of differentiation shortly. It turns out that the algebra D of (n+1)-tupoles is a commutative algebra.⁵ It is also a differentiable algebra because it admits derivations. This means that it is possible to define some linear operations ∂ , acting on the (n+1)-tupoles

$$\partial: A \to \partial A,$$
 (1.7)

and such that the Leibnitz rule is satisfied

$$\partial (A \cdot B) = (\partial A) \cdot B + A \cdot \partial B. \tag{1.8}$$

Essentially this kind of approach to the particle optics, but in a somewhat different formulation, which refers to, so called, Non-Standard Analysis, was recently employed and Introduction 3

developed in a series of papers by Berz.^{7,8} His formulation culminated in the computer code package – COSY INFINITY – which can handle aberrations of any order in seemingly any optical system.⁹

We shall describe here the simplest, in our opinion, formulation of the basic assumptions and rules of this approach. It turns out that the algebra involved is the familiar truncated polynomial algebra.⁵ Also, we will explain how the derivations in the algebra D can be introduced in order to remove the confusion on this point in some of the Berz papers (cf., e.g.⁷ formulae (20) and (21)). The operations ∂ proposed there are not derivations, contrary to what is asserted, they do not satisfy the Leibnitz rule. It seems that suitable verification of the COSY INFINITY code, in its differential algebraic routines, will be required. Besides, this would be a kind of an embarrassment since the very name "differential" is justified only when the algebra does admit some derivations.

We start with, and consider it in great detail, the simplest possible case of n=1 and x being a real number, and the generalize the construction to an arbitrary order n and any amount of the independent variables. We borrow freely, both from the mathematical literature, $^{1-5}$ and from Berz's works $^{7-8}$ while keeping the same unifying approach throughout the paper. Originality rests on our treatment of the derivations and on stressing the main role of the truncated polynomial algebra as the underlying concept of the whole differential algebraic approach. The author has endeavored to make the treatment as simple as possible while maintaining the necessary mathematical rigor.

2. The Algebra D(1,1)

Suppose that one is interested only in the linear approximation to a differentiable function a(x) of a single variable $x \in R$, then

$$a(x) = a_0 + a_1 x + \cdots,$$
 (2.1)

(x always within a region of convergence). Thus the function is completely characterized by its two lowest order Taylor coefficients $a_0 = a(0)$, $a_1 = a'(0)$, forming an ordered pair

$$A = (a_0, a_1) \in D(1, 1).$$
 (2.2)

One may restore the function, up to the linear terms, as a scalar product

$$a(x) = (A, X) + \cdots, \tag{2.3}$$

where the vector X is of the form

$$X = (1, x). (2.4)$$

Hence, the vector A describes the whole equivalence class of functions having the same Taylor expansion through the first order, around x = 0.

The elementary operations on the differentiable functions, expanded through the first order around the origin,

1° Scalar multiplication:

$$\lambda a(x) = \lambda a_0 + \lambda a_1 x + \dots, \lambda - \text{real number},$$
 (2.5)

2° Addition:

$$a(x) + b(x) = a_0 + b_0 + (a_1 + b_1)x + \cdots$$
(2.6)

3° Multiplication:

$$a(x)b(x) = b(x)a(x) = a_0b_0 + (a_0b_1 + a_1b_0)x + \cdots$$
 (2.7)

 4^{o} Division:

$$\frac{a(x)}{b(x)} = \frac{a_0 + a_1 x + \dots}{b_0 + b_1 x + \dots} = \frac{a_0}{b_0} + \frac{a_1 b_0 - a_0 b_1}{b_0^2} x + \dots, \quad b_0 \neq 0,$$
 (2.8)

induce the following operations on the set D(1,1) of ordered pairs:

The Algebra
$$D(1,1)$$

5

1°
$$\lambda A = \lambda (a_0, a_1) = (\lambda a_0, \lambda a_1), \lambda$$
 – real number, (2.9)

$$2^{o} A + B = (a_0, a_1) + (b_0, b_1) = (a_0 + b_0, a_1 + b_1),$$
(2.10)

$$3^{o} A \cdot B = (a_0, a_1) \cdot (b_0, b_1) = (a_0 b_0, a_0 b_1 + a_1 b_0) = B \cdot A, \tag{2.11}$$

$$4^{o} \quad \frac{A}{B} = \frac{(a_0, a_1)}{(b_0, b_1)} = \left(\frac{a_0}{b_0}, \frac{a_1 b_0 - a_0 b_1}{b_0^2}\right), \quad b_0 \neq 0.$$
 (2.12)

Multiplication is distributive across addition

$$A \cdot (B+C) = A \cdot B + A \cdot C. \tag{2.13}$$

Hence, the set D(1,1) is a commutative algebra⁵ which is isomorphic to the algebra of truncated first-order polynomials. It is also a differential algebra since a derivation in D(1,1) can be found. Namely, the operation ∂ defined as follows

$$\partial A = \partial (a_0, a_1) = (0, a_1)$$
 (2.14)

satisfies the Leibnitz rule (due to the multiplication rule 3^{o}),

$$\partial (A \cdot B) = (\partial A) \cdot B + A \cdot \partial B. \tag{2.15}$$

Notice that this derivation corresponds to the following differential operation on the functions

$$\mathcal{D} = x \frac{d}{dx},\tag{2.16}$$

where

$$\mathcal{D}a(x) = a_1 x + \dots = (\partial A \cdot X) + \dots, \tag{2.17}$$

the simple differentiation operation $\frac{d}{dx}$ does not lead to a derivation in D(1,1) when applied in a naive way

$$\frac{d}{dx}a(x) = a_1 + \cdots, \tag{2.18}$$

with the corresponding operation on the algebra D(1,1) given by the equality

$$\partial(a_0, a_1) = (a_1, 0),$$
 (2.19)

as it does not satisfy the Leibnitz rule. In order to produce a derivation in D(1,1), the differential operation \mathcal{D} , must respect the division on the linear part and the higher-order terms which are neglected. This is not the case for simple differentiation $\frac{d}{dx}$ which produces linear term out of the neglected quadratic terms. These and higher-order terms compose what is called an ideal I_1 . Any linear combination of the neglected terms is also of higher-order in x. The product of any function a(x) with any term from the set I_1 yields an element from the set I_1 , again, viz., o(x) + o(x) = o(x), and a(x) o(x) = o(x). These properties are essential for mathematical correctness of the definition of the algebra D(1,1).

The Taylor expansion (2.1) can be written as

$$a(x) = (A, X) + \alpha(x), \qquad (2.20)$$

where $\alpha(x)$ belongs to the ideal I_1 . Omission of the second and of the higher- order terms can also be viewed as the truncation operation T_1 , which yields the pure first-order polynomial,

$$T_1 \{a(x)\} = a_0 + a_1 x = (A, X).$$
 (2.21)

The correct differential operation \mathcal{D} which induces a derivation on D(1,1) must respect the division (2.20) of a function a(x) onto the first-order polynomial and an element from the ideal I_1 . More exactly, the following condition must be satisfied

$$T_1\{\mathcal{D}I_1\} = 0. (2.22)$$

This says that the derivation \mathcal{D} does not produce linear terms out of the neglected terms belonging to the ideal I_1 . However, it may produce higher order terms when acting on first-order polynomials. The algebra of truncated polynomials D(1,1) can be viewed as a quotient algebra of differentiable functions, D(R), over the ideal I_1 , viz., $D(1,1) \sim D(R)/I_1$.

2.1 Special Elements: Zero, Unit Element and a Differential

Notice, that the elements

$$0 = (0,0), \quad e = (1,0) - \text{unit element},$$
 (2.23)

are neutral elements with the respect of addition and multiplication, respectively

$$A + 0 = A, \quad A \cdot e = A.$$
 (2.24)

Another special element, d, has non-zero entry on the second place

$$d = (0,1)$$
, a differential. (2.25)

It is nilpotent element of the algebra D(1,1), i.e.,

$$d^2 = 0. (2.26)$$

Notice that for any real number $r \in R$ one can find an element in the algebra D(1,1)

$$r \to re = (r,0), \tag{2.27}$$

and this element can be considered as an extension of r to the algebra. This comes about because of the property that demonstrates the consistency of the extension procedure

$$rA = r(a_0, a_1) = (ra_0, ra_1) = (r, 0) \cdot (a_0, a_1).$$
 (2.28)

Any element of the algebra can be decomposed as follows

$$A = (a_0, a_1) = (a_0, 0) + (0, a_1) = a_0 e + a_1 d = T_1 a(d) = a(d).$$
(2.29)

In the last expression it is assumed that the scalar appearing in a(x) is replaced by its extension, a_0e , to the algebra.

2.2 Ordering on D(1,1)

A consistent ordering can be defined on D(1,1) as follows: We say that the element A is smaller then element B,

$$A < B$$
 if $a_0 < b_0$, or if $a_0 = b_0$ and $a_1 < b_1$, (2.30)

and similarly for A > B. Two elements A, B are equal

$$A = B$$
 if $a_0 = b_0$ and $a_1 = b_1$. (2.31)

Hence, the first components, when not equal, decide which of the two elements is larger. Only when they coincide do we compare the second components. The ordering has all the natural properties. In particular if

$$A < B$$
,

then for any C

$$A + C < B + C$$
,

and, for C > 0

$$A \cdot C < B \cdot C$$
.

A consequence of the ordering is that the algebra D(1,1) contains infinitely small elements since, for any real $\lambda > 0$

$$0 < \lambda d < (a_0, a_1), \text{ if } a_0 \neq 0.$$
 (2.32)

This justifies the name of element d, differential, which is smaller than any number (having non-zero first component). Infinitely small elements

$$(0, a_1) \in D(1, 1),$$
 (2.33)

form an ideal in D(1,1), which we denote J_1 , i.e.,

1°
$$(0, a_1) + (0, b_1) = (0, a_1 + b_1) \in J_1,$$

2° $a \cdot (0, b_1) = (0, a_0 \cdot b_1) \in J_1$, for any $A \in D(1, 1)$.

An absolute value of A can be defined as follows

$$|A| = \begin{cases} A, & A \ge 0 \\ -A, & A < 0. \end{cases}$$
 (2.34)

It has all the usual properties

$$|A \cdot B| = |A| \cdot |B|,$$

 $|A + B| \le |A| + |B|,$ (2.35)
 $|A| = 0$, if, and only if $A = 0$.

Having the norm one may consider sequences $\{A_n; n = 1, 2, ...\}$ of elements from D(1,1) which are Cauchy-convergent to some limits.

2.3 Functions on D(1,1)

One can extend a real function f(x) on R to a function on D(1,1) as follows

$$f(x) \rightarrow f(xe + hd),$$
 (2.36)

where every constant c appearing in f(x) is replaced by its extension to the algebra

$$c \to (c,0). \tag{2.37}$$

Expanding into the Taylor series yields

$$f(xe + hd) = f(xe) + hf'(xe) d =$$

$$= f(x) e + hf'(x) d =$$

$$= [f(x), hf'(x)].$$
(2.38)

Examples:

$$1^{o} \exp(A) = \exp(a_{0}, a_{1}) =$$

$$= \exp(a_{0}e + a_{1}d)$$

$$= [\exp(a_{0}), a_{1} \exp(a_{0})]$$

$$= \exp(a_{0}) \cdot (1, a_{1}).$$

$$2^{o} \ln A = \ln(a_{0}, a_{1}) = \left(\ln a_{0}, \frac{a_{1}}{a_{0}}\right).$$

$$3^{o} \sin(A) = \sin(a_{0}, a_{1}) = [\sin(a_{0}), a_{1} \cos(a_{0})].$$

$$4^{o} \tan^{-1} A = \tan^{-1}(a_{0}, a_{1}) = \left[\tan^{-1}(a_{0}), \frac{a_{1}}{1 + a_{0}^{2}}\right].$$

$$5^{o} A^{-1} = (a_{0}, a_{1})^{-1} = \frac{1}{a_{0}e + a_{1}d} = \frac{1}{a_{0}e} \frac{1}{1 + \frac{a_{1}}{a_{0}}d} =$$

$$= \frac{1}{a_{0}}e\left(1 - \frac{a_{1}}{a_{0}}d\right) = \frac{1}{a_{0}}e - \frac{a_{1}}{a_{0}^{2}}d$$

$$= \left(\frac{1}{a_{0}}, -\frac{a_{1}}{a_{0}^{2}}\right), \quad a_{0} \neq 0.$$

$$6^{o} \sqrt{A} = \sqrt{(a_{0}, a_{1})} = \sqrt{a_{0}e + a_{1}d} = \sqrt{a_{0}}e\sqrt{1 + \frac{a_{1}}{a_{0}}d}$$

$$= \sqrt{a_{0}e}\left(1 + \frac{a_{1}}{2a_{0}}d\right) = \left(\sqrt{a_{0}}, \frac{a_{1}}{2\sqrt{a_{0}}}\right).$$

$$7^{o} fog(A) = fog(a_{0}, a_{1}) = fo[g(a_{0}), a_{1}g'(a_{0})] =$$

$$= [fog(a_{0}), a_{1}g'(a_{0}) f'og(a_{0})],$$

where $f \circ g$ is the composition of two functions f and g, i.e., $(f \circ g)(x) = f[g(x)]$.

8°
$$f(x) = \frac{1}{x+1} + x^2$$
,
 $f[(1,1)] = f(e+d) = \frac{1}{(2.1)} + (1,1)^2 =$
 $= \left(\frac{1}{2}, -\frac{1}{4}\right) + (1,2) = \left(\frac{3}{2}, \frac{3}{4}\right)$
 $= [f(1), f'(1)]$.

3. A Generalization to Higher-Orders: The Algebra D(n, 1)

The scheme admits an immediate generalization to higher orders which we shall briefly outline. Let a(x) be an infinitely differentiable function of a real variable x, having the Taylor expansion around the origin

$$a(x) = a_0 + a_1 \frac{x}{1!} + \dots + a_n \frac{x^n}{n!} + \dots,$$
 (3.1)

where

$$a_k = a^{(k)}(0), \ k = 0, 1, \dots, n,$$

and the neglected higher order terms form an ideal I_n .

Let T_n denote the truncation operation which preserves the terms through the n-th order

$$T_n \{a(x)\} = \sum_{k=0}^n a_k \frac{x^k}{k!} = (A, X),$$
 (3.2)

where the vector X is

$$X = \left(1, \frac{x}{1!}, \cdots, \frac{x^n}{n!}\right),\tag{3.3}$$

while the vector A, consisting of the coefficients a_k , describe the whole equivalence class of functions having the same Taylor expansion through the n-th order

$$A = (a_0, a_1, \dots, a_n) \in D(n, 1).$$
 (3.4)

The arithmetics rule on D(n,1) are:

$$1^o \quad \lambda A = (\lambda a_0, \lambda a_1, \dots, \lambda a_n), \quad \lambda - \text{real number},$$

$$2^{o}$$
 $A + B = (a_0 + b_0, a_1 + b_1, \dots, a_n + b_n),$

$$3^{\circ} \quad A \cdot B = B \cdot A = C = (c_0, c_1, \dots, c_n),$$

where

$$c_k = k! \sum_{\substack{0 \le i, j \le n \\ (i+j=k)}} \frac{a_i b_j}{i! j!}.$$
(3.5)

The above rules correspond to the multiplication by a scalar, addition and multiplication of the relevant truncated Taylor expansions:

$$T_n \{\lambda a(x)\} = (\lambda A, X), \tag{3.6}$$

$$T_n \{a(x) + b(x)\} = (A, X) + (B, X) = (A + B, X), \tag{3.7}$$

$$T_{n} \{a(x)b(x)\} = T_{n} \{[(A,X) + \alpha(x)][(B,X) + \beta(x)]\}$$

$$= T_{n} \{(A,X)(B,X)\} \equiv (A \cdot B,X) = (B \cdot A,X) =$$

$$= (C,X).$$
(3.8)

This follows because the α and β belong to the ideal I_n . Hence, the set D(n,1) is a commutative algebra. This is also a differentiable algebra as it admits derivations. More precisely, every derivation \mathcal{D} defined in the algebra of differentiable functions, such that

$$T_n\left\{\mathcal{D}I_n\right\} = 0,\tag{3.9}$$

induces corresponding derivation ∂ on the algebra D(n,1) according to the formula

$$T_n\{(A, \mathcal{D}X)\} = (\partial A, X). \tag{3.10}$$

For a proof, see Appendix A. Comparing the coefficients at equal powers of x on both sides of this equality one finds all the components $(\partial A)_k$, $k = 0, 1, \ldots, n$.

Examples: The expressions

$$\mathcal{D}_{\alpha} = x^{\alpha} \frac{d}{dx}, \quad \alpha = 1, 2, \dots, n, \tag{3.11}$$

define the derivations on the algebra of differentiable functions, satisfying the condition (3.9). The corresponding induced derivations ∂_{α} on the algebra D(n,1) are obtained from the formula (3.10),

$$(\partial_{\alpha}A)_{k} = \begin{cases} \frac{k!}{(k-\alpha)!} a_{k-\alpha+1}, & k \ge \alpha, \\ 0, & k < \alpha. \end{cases}$$
(3.12)

One sees from it that for $\alpha \geq n+1$ the derivations become trivial, transforming every element to zero. One gets more derivations by taking linear combinations of the ∂_{α} 's

$$\partial = \sum_{\alpha=1}^{n} \lambda_{\alpha} \partial_{\alpha}, \tag{3.13}$$

where the λ_{α} are arbitrary real numbers.

3.1 Special Elements: Zero, Unit Element and Differentials

One has obviously:

$$0 = (0, 0, \dots, 0), \text{ zero element},$$
 (3.14)

$$e = \begin{pmatrix} 1, 0, \dots, 0 \\ 0 - \text{th place} \end{pmatrix}$$
, unit element, (3.15)

and

$$d_1 = (0, 1, \dots, 0) \equiv d,$$
 1-st differential, (3.16)

and

$$d_k = (0, 0, \dots, 1, \dots, 0), \quad k\text{-th differential}, \tag{3.17}$$

and

$$d_n = (0, 0, \dots, 1),$$
 n-th differential. (3.18)

It follows from the multiplication rule of the algebra that

$$d^k = k!d_k, \quad k = 1, 2, \dots, n,$$
 (3.19)

and

$$d^{n+1} = 0. (3.20)$$

Any element of the algebra D(n,1) can be decomposed as a linear combination of the unit element and the differentials d_k

$$A = (a_0, a_1, \dots, a_n) = (a_0, 0, \dots, 0) +$$

$$+ (0, a_1, \dots, 0) +$$

$$+ (0, 0, \dots, a_k, \dots, 0) +$$

$$+ (0, 0, \dots, a_n) =$$

$$= a_0 e + a_1 d_1 + \dots + a_n d_n = \sum_{k=0}^{n} a_k d_k =$$

$$= \sum_{k=0}^{n} a_k \frac{d^k}{k!} = a(d)$$

$$(3.21)$$

where inside of a(d), the zero element, a_0 , is replaced by its extension a_0e to the algebra.

3.2 Ordering on D(n,1)

We define an ordering on D(n,1) in a similar fashion as on the D(1,1) algebra,

$$A > B$$
 if $a_0 > b_0$, or
if $a_0 = b_0$, if $a_1 > b_1$, or
if $a_0 = b_0$, $a_1 = b_1$, and if $a_2 > b_2$, etc.

$$A = B$$
 if $a_k = b_k$ $k = 0, 1, \dots, n$. (3.24)

The differentials of various orders satisfy the relations

$$\lambda_0 e > \lambda_1 d_1 > \dots > \lambda_k d_k > \dots > \lambda_n d_n \tag{3.25}$$

for any real positive numbers $\lambda_0, \lambda_1, \ldots, \lambda_n$.

Elements of the algebra, generated by the set of differentials $(d_j, d_{j+1}, \ldots, d_n)$ form the ideal J_j in D(n, 1)

$$\sum_{k=j}^{n} a_k d_k \in J_j , \quad j = 1, \dots, n.$$
 (3.26)

The following inclusion relations hold

$$D(n,1) \supset J_1 \supset J_2 \supset \cdots \supset J_n.$$
 (3.27)

3.3 Functions on D(n,1)

An extension of a function f(x) on R to the algebra D(n, 1) can be done in the same way as before. One replaces all constants, c, appearing in f by ce and Taylor expands the expression:

$$f(xe + hd) = f(xe) + f'(xe) hd + \dots + f^{(n)}(xe) h^n d_n$$

= \[\int f(x), hf'(x), \dots, h^n f^{(n)}(x) \]. \((3.28)

For h = 1 one recovers the formula (1.5).

Similarly one defines the function f on a general element of the algebra

$$f\left(xe + h_1d_1 + \dots + h_nd_n\right),\tag{3.29}$$

by expanding into a Taylor series and using the formula (3.16)-(3.20).

Examples:

$$1^{o} \exp(A) = \exp(a_{0}, a_{1}, \dots, a_{n}) =$$

$$= \exp[(a_{0}, 0, \dots, 0) + (0, a_{1}, \dots, a_{n})] =$$

$$= \exp(a_{0}e) \exp(0, a_{1}, \dots, a_{n}) =$$

$$= \exp(a_{0}) \sum_{k=0}^{n} \frac{1}{k!} (0, a_{1}, \dots, a_{n})^{k}.$$

A finite number of steps is required to calculate the exponential. The same is true in general since $d_k^{n+1} = 0, k = 1, 2, ..., n$.

$$2^{o} \quad \log(A) = \log(a_{0}, a_{1}, \dots, a_{n}) =$$

$$= \log\left[a_{0}\left(1, \frac{a_{1}}{a_{0}}, \dots, \frac{a_{n}}{a_{0}}\right)\right] =$$

$$= \log\{a_{0}\left[e + \left(0, \frac{a_{1}}{a_{0}}, \dots, \frac{a_{n}}{a_{0}}\right)\right]\} =$$

$$= [\log(a_{0})] e + \log\left[e + \left(0, \frac{a_{1}}{a_{0}}, \dots, \frac{a_{n}}{a_{0}}\right)\right] =$$

$$= [\log(a_{0})] e + \sum_{k=1}^{n} (-1)^{k+1} \frac{1}{k} \left(0, \frac{a_{1}}{a_{0}}, \dots, \frac{a_{n}}{a_{0}}\right)^{k}, a_{0} > 0.$$

$$3^{o} \quad A^{-1} = (a_{0}, a_{1}, \dots, a_{n})^{-1} = \frac{1}{a_{0}e + (0, a_{1}, \dots, a_{n})} =$$

$$= \frac{1}{a_{0}e} \frac{1}{1 + \left(0, \frac{a_{1}}{a_{0}}, \dots, \frac{a_{n}}{a_{0}}\right)} =$$

$$= \frac{1}{a_{0}}e \left[1 - b + b^{2} - \dots + (-1)^{n+1}b^{n}\right],$$

$$b \equiv \left(0, \frac{a_{1}}{a_{0}}, \dots, \frac{a_{n}}{a_{0}}\right), \quad b^{n+1} = 0, a_{0} \neq 0.$$

$$4^{o} \quad \sqrt{A} = \sqrt{(a_{0}, a_{1}, \dots, a_{n})} = \sqrt{a_{0}e + (0, a_{1}, \dots, a_{n})}$$

$$= \sqrt{a_{0}}e\sqrt{1+b} =$$

$$= \sqrt{a_{0}}e\left(1 + \sum_{k=1}^{n} (-1)^{k-1} \frac{1 \cdot 3 \dots (2k-1)}{2^{k} k!} b^{k}\right), a_{0} > 0.$$

where element b of the previous example, appears again.

4. A Generalization to Two Independent Variables: The Algebra $D\left(2,2\right)$

Let us now consider differentiable functions of two independent variables x and y, and expand them to the second order around the origin

$$a(x,y) = a_0 + a_{10}\frac{x}{1!} + a_{01}\frac{y}{1!} + a_{20}\frac{x^2}{2!} + a_{11}xy + a_{02}\frac{y^2}{2!} + \cdots$$
(4.1)

where a_{kl} , k, l = 0, 1, 2 are partial derivatives of a(x, y) calculated at the origin. We would like to relabel them as a_j , j = 0, 1, 2, ..., 5. For this some ordering of the basic monomials in the expansion will be needed:⁷

Monomial
 its position
 a factor

$$M_0 = 1$$
 $I_1 = 0$
 $F_0 = 1$
 $M_1 = x$
 $I_x = 1$
 $F_1 = 1$
 $M_2 = y$
 $I_y = 2$
 $F_2 = 1$
 $M_3 = x^2$
 $I_{x^2} = 3$
 $F_3 = 2!$
 $M_4 = xy$
 $I_{xy} = 4$
 $F_4 = 1$
 $M_5 = y^2$
 $I_{y^2} = 5$
 $F_5 = 2!$

The function a(x,y) can be written as follows

$$a(x,y) = \sum_{k=0}^{5} a_k \frac{M_k}{F_k} + \dots = (A, X) + \dots,$$
 (4.3)

where

$$A = (a_0, a_1, \dots, a_5), \quad X = \left(1, \frac{x}{1!}, \frac{y}{1!}, \frac{x^2}{2!}, \frac{x}{1!}, \frac{y}{1!}, \frac{y^2}{2!}\right), \tag{4.4}$$

and where the neglected terms are of the third and higher orders in x, y. They form an ideal I_2 in the algebra $D(R^2)$ of all differentiable functions of two variables.

Multiplying two functions of this type, and truncating at the second-order, one finds the multiplication rules

$$a(x,y) \cdot b(x,y) = (A \cdot B, X) + \dots = (C, X) + \dots = c(x,y);$$

where

$$C = A \cdot B = B \cdot A \tag{4.5}$$

and

$$C_{0} = a_{0}b_{0},$$

$$C_{1} = a_{0}b_{1} + a_{1}b_{0},$$

$$C_{2} = a_{0}b_{2} + a_{2}b_{0},$$

$$C_{3} = 2(a_{0}b_{3}/2 + a_{1}b_{1} + a_{3}b_{0}/2),$$

$$C_{4} = a_{0}b_{4} + a_{1}b_{2} + a_{2}b_{1} + a_{4}b_{0},$$

$$C_{5} = 2(a_{0}b_{5}/2 + a_{2}b_{2} + a_{5}b_{0}/2).$$

$$(4.6)$$

There are two special elements, the differentials, besides the unit element

$$e = (1, 0, 0, 0, 0, 0),$$
 (4.7)

$$dx = (0, 1, 0, 0, 0, 0), (4.8)$$

$$dy = (0, 0, 1, 0, 0, 0). (4.9)$$

They have the properties

$$dx \cdot dx = (0, 0, 0, 2, 0, 0),$$

$$dx \cdot dy = (0, 0, 0, 0, 1, 0),$$

$$dy \cdot dy = (0, 0, 0, 0, 0, 2),$$

$$(4.10)$$

and

$$dx \cdot dx \cdot dx = dx \cdot dx \cdot dy = dx \cdot dy \cdot dy = dy \cdot dy \cdot dy = 0. \tag{4.11}$$

Evaluating the expression

$$a\left(xe+dx,\ ye+dy\right),\tag{4.12}$$

where all the constants in a(x, y) are assumed to be extended to the algebra, one finds the result

$$a(xe + dx, ye + dy) = \left(a, \frac{\partial a}{\partial x}, \frac{\partial a}{\partial y}, \frac{\partial^2 a}{\partial x^2}, \frac{\partial^2 a}{\partial x \partial y}, \frac{\partial^2 a}{\partial y \partial y}\right)(x, y). \tag{4.13}$$

Examples: $a(x, y) = x + y^2 + 3$

$$xe + dx = (x, 1, 0, 0, 0, 0),$$

 $ye + dy = (y, 0, 1, 0, 0, 0),$

Let x = 1, y = 2 then one gets

$$a(e + dx, 2e + dy) = (1, 1, 0, 0, 0, 0) + (2, 0, 1, 0, 0, 0)^{2}$$

$$+ (3, 0, 0, 0, 0, 0) =$$

$$= (4, 1, 0, 0, 0, 0) + (4, 0, 4, 0, 0, 2) =$$

$$= (8, 1, 4, 0, 0, 2)$$

which agrees with the easily verifiable results

$$a(1,2) = 8,$$
 $\partial_x a(1,2) = 1,$ $\partial_y a(1,2) = 4,$ $\partial_{xx}^2 a(1,2) = 0,$ $\partial_{xy}^2 a(1,2) = 0,$ $\partial_{yy}^2 a(1,2) = 2.$

Possible derivations on the algebra D(2,2) are induced by the following derivations on the algebra of all differentiable functions, and their linear combinations

$$\mathcal{D}_1 = x\partial_x,$$
 $\mathcal{D}_2 = x^2\partial_x,$ $\mathcal{D}_3 = xy\partial_x,$ $\mathcal{D}_4 = y\partial_y,$ $\mathcal{D}_5 = y^2dy,$ $\mathcal{D}_6 = xy\partial_y.$ (4.14)

For instance, the first derivation \mathcal{D} , acts on a(x,y) as follows

$$\mathcal{D}_1 a(x,y) = (A, \mathcal{D}_1 X) + \dots = (\partial, A, X) + \dots = a_1 x + a_3 x^2 + a_4 x y + \dots$$
 (4.15)

Thus the induced derivation on the algebra D(2,2) is given by the formula

$$\partial_1(a_0, a_1, a_2, a_3, a_4, a_5) = (0, a_1, 0, 2a_3, a_4, 0). \tag{4.16}$$

Similarly, for the \mathcal{D}_2 derivation one finds

$$\mathcal{D}_{2}a\left(x,y\right) =a_{1}x^{2}+\cdots, \tag{4.17}$$

which means that the induced derivation ∂_2 acts as follows

$$\partial_2 (a_0, a_1, a_2, a_3, a_4, a_5) = (0, 0, 0, 2a_1, 0, 0).$$
 (4.18)

As an example of an application of the D(2,2) algebra we consider a midplane motion in a 90° homogeneous bending magnet,⁷ as shown in Fig. 1.

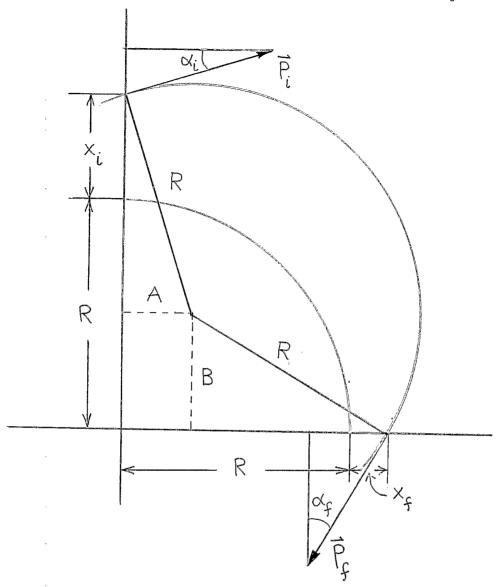


Figure 1.

Denoting

$$a_i = \frac{p_x}{p} \Big|_i = \sin \alpha_i, \tag{4.19}$$

and

$$a_f = \frac{p_x}{p} \Big|_f = \sin \alpha_f, \tag{4.20}$$

one finds the following relations

$$A = R\sin\alpha_i = Ra_i = R + x_f - R\cos\alpha_f, \tag{4.21}$$

and

$$B = R\sin\alpha_f = -Ra_f = R + x_i - R\cos\alpha_i. \tag{4.22}$$

We find the following expressions for the x_f and a_f from here

$$x_f = A - R(1 - \cos \alpha_f) = A - R(1 - \sqrt{1 - a_f^2}),$$
 (4.23)

and

$$a_f = -\frac{B}{R} = \cos \alpha_i - \frac{x_i}{R} - 1 = \sqrt{1 - a_i^2} - \frac{x_i}{R} - 1,$$
 (4.24)

and finally we get

$$x_f = A - R \left\{ 1 - \left[1 - \left(\sqrt{1 - a_i^2} - \frac{x_i}{R} - 1 \right)^2 \right]^{1/2} \right\}. \tag{4.25}$$

Evaluating this map in the algebra D(2,2) spanned by the variables x and a we get all the derivatives of x_f , a_f with the respect to x_i , a_i .

Identifying x_i with dx and a_i with dy we get using the multiplication rules (4.6) we get

$$x_i = (0, 1, 0, 0, 0, 0),$$
 (4.26)

$$a_i = (0, 0, 0, 1, 0, 0, 0),$$
 (4.27)

$$A = Ra_i = (0, 0, R, 0, 0, 0). (4.28)$$

Evaluating the square root we get

$$B = R \left[1 - (1 - a_i)^{1/2} \right] + x_i =$$

$$= R \left[1 - \left(1 - \frac{1}{2} a_i^2 \right) \right] + x_i = x_i + \frac{1}{2} R a_i^2,$$

$$= (0, 1, 0, 0, 0, R),$$
(4.29)

since

and

$$a_i^3 = 0. (4.30)$$

Further, we get

$$a_f = -\frac{B}{R} = \left(0, -\frac{1}{R}, 0, 0, 0, -1\right),$$
 (4.31)

and similarly we get the result

$$x_f = A - \frac{R}{2}a_f^2 = \left(0, 0, R, -\frac{1}{R}, 0, 0\right),$$
 (4.32)

which, according to the formula (4.13) yields the respective derivatives at $x_i = 0$, $a_i = 0$.

5. Generalization to Higher-Orders, & Arbitrary Number of Independent Variables: The Algebra $D(n, \nu)$

We shall now describe the most general case of differentiable functions of ν independent real variables x_k , $k = 1, ..., \nu$ having Taylor expansions through the n-th order

$$a(x_{1},...,x_{j}) = a_{0} + a_{1}x_{1} + ... + a_{\nu}x_{\nu} + ... + + a_{i_{1}...i_{\nu}} \frac{x_{1}^{i_{1}}...x_{\nu}^{i_{\nu}}}{i_{1}!...i_{\nu}!} + ... = (A, X) + ... (i_{1} + ... i_{\nu} = n).$$

$$(5.1)$$

The neglected terms, of order higher than n, form an ideal I_n . The number, $N(n\nu)$, of basic monomials appearing in this expansion is given by the formula, (cf. Appendix B),

$$N(n,\nu) = \frac{(n+\nu)!}{n!\nu!} = \dim(X) = \dim(A).$$
 (5.2)

Let us assume that all $N(n, \nu)$ monomials are arranged in a certain order. For each monomial M we call I_M its position according to the assumed ordering

$$M_I \leftrightarrow I_M,$$
 (5.3)

Conversely, to each I_M we assign the corresponding monomial

$$I_M \to M_I = x_1^{i_1} \cdots x_{\nu}^{i_{\nu}},$$
 (5.4)

and the factor

$$F_I = i_1! \dots i_{\nu}!. \tag{5.5}$$

Hence, we may write the expansion (4.1) as follows

$$a(x_1, \dots, x_{\nu}) = \sum_{I} a_I \frac{M_I}{F_I} + \dots$$
 (5.6)

The usual operations on the differentiable functions, supplemented by the truncation operation T_n at the n-th order polynomials transforms into the algebraic operations on the

N-tupoles formed by the coefficients a_I ,

$$A = (a_0, a_1, \dots, a_{N-1}), \tag{5.7}$$

1°
$$A + B = (a_0 + b_0, \dots, a_{N-1} + b_{N-1}),$$
 (5.8)

$$2^{o} \qquad \lambda A = (\lambda a_0, \dots, \lambda a_{N-1}), \tag{5.9}$$

$$3^{\circ} \quad A \cdot B = B \cdot A = C,$$

$$C_k = F_k \sum_{\substack{0 \le i, j \le N-1}} \frac{a_i b_j}{F_i F_j}$$

$$(M_k = M_i \cdot M_j)$$

$$(5.10)$$

Thus we get the commutative algebra $D(n\nu)$ which is isomorphic to the algebra of truncated polynomials.

As before, one distinguishes special elements

$$d_{N-1} = (0, 0, \dots, 1), \quad (N-1)$$
-th differential,

through which one may express a generic element of the algebra

$$A = (a_0, a_1, \dots, a_{N-1}) = a_0 e + a_1 d_1 + \dots + a_{\nu} d_{\nu} + \dots + a_{N-1} d_{N-1}$$

$$(5.11)$$

Also, one finds using (4.10) that the differentials are nilpotent

$$d_k^N = 0, \quad k = 1, \dots, N - 1.$$
 (5.12)

One may extend a function $f(x_1, \ldots, x_{\nu})$ to the algebra $D(n, \nu)$ as follows

$$f(x_1e + dx_1, \dots, x_{\nu}e + dx_{\nu}) = (f, \nabla f, \dots, \nabla^n f)(x_1, \dots, x_{\nu}),$$
 (5.13)

where

$$\nabla = \left(\frac{\partial}{\partial x_1}, \dots, \frac{\partial}{\partial x_\nu}\right). \tag{5.14}$$

Examples of this extension can be readily supplied in much the same way as in the case of a single variable. One simply follow the multiplication rules (4.10) as applied to the differentials d_1, \ldots, d_{ν} , and takes into account their nilpotency [cf. (5.12)] when expanding a function.

The derivations of differentiable functions

$$\mathcal{D}_{\alpha_1} = x_1^{\alpha_1} \frac{\partial}{\partial x_1}, \cdots, \mathcal{D}_{\alpha_{\nu}} = x_{\nu}^{\alpha_{\nu}} \frac{\partial}{\partial x_{\nu}}, \tag{5.15}$$

where

$$1 \le \alpha_i \le n, \qquad i = 1, \dots, \nu, \tag{5.16}$$

induce the corresponding derivations on the algebra $D(n,\nu)$ through the relations

$$\mathcal{D}_{\alpha_i} a(x_1, \dots, x_{\nu}) = (A, \mathcal{D}_{\alpha_i} X) + \dots = (\partial_{\alpha_i} A, X) + \dots$$
 (5.17)

It is assumed that the truncation to the *n*-th order polynomials is performed in the first terms, after the \mathcal{D}_{α_i} derivation acts on the vector X, viz.,

$$T_n \{ (A, \mathcal{D}_{\alpha_i} X) \} = (\partial_{\alpha_i} A, X), \qquad (5.18)$$

$$i=1,\ldots,\nu,$$
 $\alpha_i=1,\ldots,n.$

All the concepts of the algebraic approach can be readily extended to this general case, at the expense of some notational inconvenience, however. We shall stop at this point as a general scheme is already clear.

6. Concluding Remarks

Solving the differential equations (1.1), through some order n, one finds a map \mathcal{M} , [cf. (1.2)]. Its derivatives, the aberrations of a system, can be found by evaluation of the map on the relevant element of the algebra $D(n, \nu)$.

There are also other applications of the algebraic techniques which yield significant economy of computing time in comparison with more conventional methods, (cf. the Manual,⁹ for examples).

It is rather clear that the algebra of differentiable functions $D\left(R^{\nu}\right)$ is convenient for analytic manipulations while the corresponding algebra $D\left(n,\nu\right)$ of truncated polynomials is well suited for computer handling, $D\left(n,\nu\right) \sim D\left(R^{\nu}\right)/I_{n}$.

It is possible to formulate the whole approach using more advanced mathematical concepts of functional analysis. For instance, the relations (2.3), (3.2), and (4.3) suggest the possible use of, so called, Gelfand duality and triplets.¹⁰ This seems, however, neither necessary nor the practical.

The maximum order n of computed aberrations is limited by the available computer hardware since the dimension, N, of the array A grows drastically with the order n and the number of independent variables, ν , [cf. (5.2)].

Assuming the number $N(n, \nu)$ to be of order 1 million one obtains the limits on the maximum order n for different numbers of the independent variables, shown in the table below.⁷

Number of Variables	Maximum Order
ν	$\max(n)$
6	99
8	30
10	14
12	10

7. Acknowledgments

I would like to thank Dr. M. Berz of Michigan State University, East Lansing, for several clarifying and helpful conversations concerning his approach to the particle beam optics and for providing copies of his papers on the subject, and of his code COSY IN-FINITY. I also thank Dr. Chih-Han Sah and Dr. V. Schechtman from Department of Mathematics of SUNY at Stony Brook for useful discussions about mathematical issues related to the differential algebraic approach. I would like to thank Dr. Johannes Claus for his interest in this work and for correcting my English.

Appendix A.

We shall demonstrate, that the operation ∂ , induced by a derivation \mathcal{D} on the algebra of differentiable functions according to the formula (3.10), is a derivation on the algebra D(n,1).

Proof: Let us consider functions a(x), b(x) which are Taylor expanded around the origin

$$a(x) = (A, X) + \alpha(x), \qquad (A.1)$$

and

$$b(x) = (B, X) + \beta(x), \qquad (A.2)$$

where $\alpha, \beta \in I_n$. Acting with the derivation \mathcal{D} one gets

$$\mathcal{D}a(x) = (A, \mathcal{D}X) + \alpha'(x) =$$

$$= (\partial A, X) + \alpha''(x),$$
(A.3)

and

$$\mathcal{D}b(x) = (B, \mathcal{D}X) + \beta'(x) =$$

$$= (\partial B, X) + \beta''(x),$$
(A.4)

where again $\alpha', \alpha'', \beta', \beta'' \in I_n$, due to the condition (3.9). The relations (A.3) and (A.4) can be written as follows

$$T_n\{(A, \mathcal{D}X)\} = (\partial A, X), \qquad (A.5)$$

and

$$T_n \{(B, \mathcal{D}X)\} = (\partial B, X). \tag{A.6}$$

For the product a(x)b(x) = c(x) one finds similarly

$$a(x)b(x) = (A \cdot B, X) + \gamma(x), \qquad (A.7)$$

and

$$\mathcal{D}\left[a\left(x\right)b\left(x\right)\right] = \left(A \cdot B, \mathcal{D}X\right) + \gamma' =$$

$$= \left(\partial\left(A \cdot B\right), X\right) + \gamma'' \tag{A.8}$$

where $\gamma, \gamma', \gamma'' \in I_n$, as before.

By definition, the derivation \mathcal{D} satisfies the Leibnitz rule

$$\mathcal{D}\left[a\left(x\right)b\left(x\right)\right] = \left[\mathcal{D}a\left(x\right)\right]b\left(x\right) + a\left(x\right)\left[\mathcal{D}b\left(x\right)\right]. \tag{A.9}$$

Applying the truncation operation T_n to both sides of this equality, and taking into account the formulae (A.3), (A.4) and (A.8) we get after using the formula (3.8), the result

$$(\partial (A \cdot B), X) = (\partial A \cdot B, X) + (A \cdot \partial B, X). \tag{A.10}$$

The equality holds for any X which means that the coefficients at equal powers of x, on both sides, coincide

$$\partial (A \cdot B) = \partial A \cdot B + A \cdot \partial B, \tag{A.11}$$

which entails that the operation ∂ is a derivation on D(n, 1).

Appendix B.

The number $N(n,\nu)$, [cf. (4.2)] gives a total amount of the basic monomials in ν variables through order n. It equals the number $N(n-1,\nu)$ of such the monomials through order n-1, plus the number of monomials of exact degree n. The latter can be thought as monomials in $x_1, \ldots, x_{\nu-1}$ variables only multiplied by a power of the variable x_{ν} such that product is of exact degree n. The total number of such the monomials is, clearly, $N(n,\nu-1)$. Hence, one has the recursive relation

$$N(n,\nu) = N(n-1,\nu) + N(n,\nu-1). \tag{B.1}$$

One knows [cf. (2.4), (3.3), (4.2)] that

$$N(1,1) = 2,$$

 $N(n,1) = n + 1,$ (B.2)
 $N(2,2) = 6.$

Moreover, the recursive relation is that for binomial coefficients. Hence, the solution is

$$N(n,\nu) = \binom{n+\nu}{\nu} = \frac{(n+\nu)!}{n!\nu!}.$$
 (B.3)

It satisfies the relations B.1 and the conditions (B.2).

References

- L.B. Rall, The Arithmetic of Differentiation, Mathematics Magazine, 59:275;
 1986.
- G. Corliss and L.B. Rall, Automatic Generation of Taylor Series in Pascal-SC: Basic Applications to Ordinary Differential Equations. In "Transactions of the First Army Conference on Applied Mathematics and Computing", Volume ARO Report 84-1, 1984.
- L.B. Rall, Automatic Differentiation: Techniques and Applications, Lecture Notes in Computer Science No. 120, Springer-Verlag, Berlin-Heidelberg-New York, 1981.
- 4. Y.F. Chang, Automatic Solution of Differential Equations. In "Constructive and Computational Methods for Differential and Integral Equations", D.L. Colton and R.P. Gilbert (Eds.). Lecture Notes in Mathematics, Vol. 430, Springer-Verlag, Berlin-Heidelberg-New York, 1974, 61-94.
- 5. O. Zarisky, P. Samuel, "Commutative Algebra", Vol. 1,2, D. Van Nostrand Co. Inc., 1958.
- J.F. Ritt, "Differential Algebra", American Mathematical Society, Washington, D.C., 1950.
- 7. M. Berz, Differential algebraic description of beam dynamics to very high orders. Particle Accelerators, 24:109, 1989.
- 8. M. Berz, Automatic Differentiation as Nonarchimedean Analysis, MSUCL-809, March 1992.
- 9. M. Berz, Computer Program COSY INFINITY Version 5. User's Guide and Reference Manual, MSU, East Lansing, 1992, and references given there.
- 10. I.M. Gelfand and I.I. Piatecki-Shapiro, Representation Theory and Automorphic Functions. Generalized Functions Vol. VI, Moscow, 1962 (in Russian).