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Ordered operator expansions by comparison

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Abstract. Ordered operator expansions for operators forming physically important low-dimensional Lie algebras are derived in a simple unified way. Starting with the Zassenhaus formula for the disentangling of exponential operators, series expansions of both undisentangled and disentangled exponentials and comparison of the operator coefficients of equal powers of an ordering parameter α leads to ordered operator expansions. This 'comparison method' gives an alternative simple derivation of some already known formulae and a number of new formulae in the physical and chemical applications of the harmonic oscillator and for master equation problems with nearest-neighbour transition probabilities. The 'comparison method' cannot be applied to the angular momentum algebra directly. By a slight modification it can be used to derive from one matrix element or trace of $\hat{J}_x^k\hat{J}_y^l\hat{J}_z^n$ all possible combinations k, l, n by simply comparing powers of ordering parameters.

1. Introduction

It is often necessary to raise a function of non-commuting operators to certain powers or to rearrange operators in a certain order to facilitate calculations of traces and matrix elements.

For operators $\hat{A}$, $\hat{B}$ with the commutator

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} = c\hat{I} \tag{1}$$

where $\hat{I}$ is the identity operator and c a so-called c number, Yamazaki (1952) gave the following formula without proof:

$$(\hat{A}+\hat{B})^m = \sum_{k=0}^{[m/2]} \sum_{s=0}^{m-2k} \frac{(c/2)^k m!\hat{B}^s\hat{A}^{m-2k-s}}{k!s!(m-2k-s)!}. \tag{2}$$

The bracket symbol $[m/2]$ means in this case the integer less than or equal to $(m/2)$. The same formula was derived independently by Cohen (1966) solving an eigenvalue problem and by Wilcox (1967) using normal ordering techniques. A second important formula was also derived by Cohen and by Wilcox:

$$\hat{A}^m\hat{B}^n = \sum_{j=0}^{m} \frac{m!n!c^j\hat{B}^{n-j}\hat{A}^{m-j}}{j!(m-j)!(n-j)!}. \tag{3}$$

In both cases the mathematics is fairly complicated.

The aim of the present paper is to investigate systematically ordered operator expansions from only one formula, the Zassenhaus formula for disentangled exponential operator expressions. The very complex exponential commutator expressions are reduced greatly if the operators form a low-dimensional Lie algebra. The non-ordered and the disentangled exponentials are expanded in series in terms of an ordering scalar α and the operator coefficients of equal powers of α are compared. The method is therefore called the 'comparison method'. Only some formulae of the calculus of non-commuting operators and elementary algebra are needed. The plan of the article is as follows: § 2 gives the Zassenhaus formula, the necessary operator techniques and the comparison method. In § 3 a three- and a four-dimensional Lie algebra, which is essentially the harmonic oscillator algebra, are treated. Section 4 discusses a two-dimensional Lie algebra. In § 5 the limits of the 'comparison method' are shown for the 'split three-dimensional' angular momentum algebra, but by the same method, traces and matrix elements of arbitrary products of angular momentum operators are derived. Section 6 presents a discussion.

As this paper is mainly technical, each section contains a brief sketch on various applications of the results in physics and chemistry.

2. Zassenhaus formula, operator calculus and comparison method

2.1. *Algebra of non-commuting operator*

Magnus (1954) in an excellent review article discussed the Baker–Campbell–Hausdorff (BCH) formula for uniting two exponential operators

$$\exp \hat{A} \exp \hat{B} = \exp\{\hat{A}+\hat{B}+1/2[\hat{A},\hat{B}]+1/12[\hat{A},[\hat{A},\hat{B}]]+1/12[[\hat{A},\hat{B}],\hat{B}]+\dots\}. \tag{4}$$

The commutator series in the exponent was extended by Richtmyer and Greenspan (1965) to order 512 by computer and published to the tenth order. The expansion is not unique due to the existence of the Jacobi identity and higher identities:

$$[[\hat{A},\hat{B}],\hat{C}]+[[\hat{C},\hat{A}],\hat{B}]+[[\hat{B},\hat{C}],\hat{A}] = 0. \tag{5}$$

The dual of the BCH formula, the Zassenhaus formula, has received less attention in the literature.

$$\exp(\hat{A}+\hat{B}) = \exp \hat{A} \exp \hat{B} \exp \hat{C}_2 \dots \exp \hat{C}_m \dots \tag{6}$$

only $\hat{C}_2$ and $\hat{C}_3$ are known, but higher $\hat{C}_m$ can be calculated from a recursion formula given by Wilcox (1967) in his extensive review on exponential operators. For convenience we derived $\hat{C}_4$ and $\hat{C}_5$,

$$\hat{C}_2 = -1/2[\hat{A},\hat{B}] \tag{7}$$

$$\hat{C}_3 = 1/3[\hat{B},[\hat{A},\hat{B}]]+1/6[\hat{A},[\hat{A},\hat{B}]] \tag{8}$$

$$\hat{C}_4 = -1/24\{[\hat{A},[\hat{A},[\hat{A},\hat{B}]]]+3[\hat{B},[\hat{A},[\hat{A},\hat{B}]]]+3[\hat{B},[\hat{B},[\hat{A},\hat{B}]]]\} \tag{9}$$

$$\begin{aligned}\hat{C}_5 = -1/120\{&[\hat{A},[\hat{A},[\hat{A},[\hat{A},\hat{B}]]]]+8[\hat{A},[\hat{A},[\hat{A},\hat{C}_2]]]+24[\hat{A},[\hat{A},[\hat{B},\hat{C}_2]]]\\ &+24[\hat{A},[\hat{B},[\hat{B},\hat{C}_2]]]+8[\hat{B},[\hat{B},[\hat{B},\hat{C}_2]]]+36[\hat{A},[\hat{A},\hat{C}_3]]\\ &+72[\hat{A},[\hat{B},\hat{C}_3]]+36[\hat{B},[\hat{B},\hat{C}_3]]+72[\hat{C}_2,\hat{C}_3]+96[\hat{A},\hat{C}_4]+96[\hat{B},\hat{C}_4]\}\end{aligned} \tag{10}$$

to show the increasing complexity of the $\hat{C}_m$.

For

$$[\hat{A},[\hat{A},\hat{B}]] = [\hat{B},[\hat{A},\hat{B}]] = 0 \tag{11}$$

the $\hat{C}_m$ terminate after $m = 2$ leading to an often used equation in statistical and phonon physics:

$$\exp\{\alpha(\hat{A}+\hat{B})\} = \exp\alpha\hat{A}\exp\alpha\hat{B}\exp(-\alpha^2 c/2). \tag{12}$$

The exponential of an operator is defined by the series expansion:

$$\exp(\alpha\hat{A}) = 1+\alpha\hat{A}+\frac{\alpha^2}{2!}\hat{A}^2+\ldots\frac{\alpha^m}{m!}\hat{A}^m. \tag{13}$$

We need some further formulae of operator calculus, which are treated in detail by Wilcox (1967) and by Louisell (1973):

$$\exp(\alpha\hat{A})\hat{B}\exp(-\alpha\hat{A}) = \hat{B}+\alpha[\hat{A},\hat{B}]+\frac{\alpha^2}{2!}[\hat{A},[\hat{A},\hat{B}]]+\ldots$$

$$= \sum_{k=0}^{\infty}\frac{\alpha^k}{k!}\{\hat{A}^k,\hat{B}\}_- = \tilde{B}(\alpha\hat{A}) \tag{14}$$

$$\exp(\alpha\hat{A})\hat{B}^k\exp(-\alpha\hat{A}) = (\tilde{B}(\alpha\hat{A}))^k \tag{15}$$

$$\exp(\alpha\hat{A})\exp\hat{B}\exp(-\alpha\hat{A}) = \exp(\tilde{B}(\alpha\hat{A})). \tag{16}$$

Instead of the Zassenhaus formula Feynman's (1951) ordering calculus can be used. In a careful investigation Fujiwara (1952) showed that this calculus also leads to high-order exponential operator commutators. Another method of operator calculus is the parameter differentiation technique by Kirzhnits (1967) who gave in the appendix of his book a list of $\hat{K}_m$ which can be related to the $\hat{C}_m$ of the Zassenhaus formula. Though no strict proof can be given, preliminary calculations show that the three approaches to the exponential disentangling problem lead to essentially the same results.

2.2. *The 'comparison method'*

The principle of the comparison method is trivial: the disentangled and the undisentangled forms of equation (6) are expanded in terms of an ordering scalar quantity α and operator coefficients of equal powers of α are compared:

$$\exp\{\alpha(\hat{A}+\hat{B})\} = \exp\alpha\hat{A}\exp\alpha\hat{B}\exp\alpha^2\hat{C}_2\exp\alpha^3\hat{C}_3\ldots \tag{17}$$

$$\sum_{k=0}^{\infty}\frac{\alpha^k}{k!}(\hat{A}+\hat{B})^k = \sum_{r,s,t,u,v,\ldots=0}^{\infty}\frac{\alpha^{r+s+2t+3u\ldots}}{r!s!t!u!}\hat{A}^r\hat{B}^s\hat{C}_2^t\hat{C}_3^u\ldots. \tag{18}$$

Example 1

$$(\hat{A}+\hat{B})^2 = \hat{A}^2+2\hat{A}\hat{B}+\hat{B}^2+2\hat{C}_2 \tag{19}$$

$$(\hat{A}+\hat{B})^3 = \hat{A}^3+3\hat{A}^2\hat{B}+3\hat{A}\hat{B}^2+\hat{B}^3+6\hat{A}\hat{C}_2+6\hat{B}\hat{C}_2+6\hat{C}_3. \tag{20}$$

One sees that the expressions are already in a partial ordered form with the $\hat{A}$ operators standing left from the $\hat{B}$ operators. The difficulty comes from the commutator operators $\hat{C}_m$. It will be shown subsequently that for some low-dimensional Lie algebras of physical interest the $\hat{C}_m$ are operator functions of only one operator type leading to completely ordered forms.

2.3. High-order commutators

It is often difficult to find high-order commutators. Guenin (1968) derived two formulae which can be applied to this and related problems. The formulae are:

$$\hat{A}\hat{B}^n = \sum_{j=0}^{n} \binom{n}{j} (-1)^j \hat{B}^{n-j} \{\hat{B}^j, \hat{A}\}_- \tag{21}$$

and

$$\hat{B}^n\hat{A} = \sum_{j=0}^{n} \binom{n}{j} \{\hat{B}^j, \hat{A}\}_- \hat{B}^{n-j}. \tag{22}$$

We shall give a simple derivation and a slight amplification by the comparison method. Starting with equation (14) we get, after multiplication from the left with $\exp(-\alpha\hat{B})$,

$$\hat{A}\exp(-\alpha\hat{B}) = \exp(-\alpha\hat{B}) \sum_{m=0}^{\infty} \frac{\alpha^m}{m!} \{\hat{B}^m, \hat{A}\}_- \tag{23}$$

series expansion leads to:

$$\sum_{n=0}^{\infty} \frac{(-\alpha)^n}{n!} \hat{A}\hat{B}^n = \sum_{k=0}^{\infty} \sum_{m=0}^{\infty} (-1)^k \frac{\alpha^{k+m}}{k!m!} \hat{B}^k \{\hat{B}^m, \hat{A}\}_- \tag{24}$$

and

$$\sum_{n=0}^{\infty} \frac{\alpha^n}{n!} \hat{B}^n\hat{A} = \sum_{k=0}^{\infty} \sum_{m=0}^{\infty} \frac{\alpha^{k+m}}{k!m!} \{\hat{B}^m, \hat{A}\}_- \hat{B}^k. \tag{25}$$

Because of equation (15) we get:

$$\hat{A}^m \exp(-\alpha\hat{B}) = \exp(-\alpha\hat{B}) \left(\sum_{k=0}^{\infty} \frac{\alpha^k}{k!} \{\hat{B}^k, \hat{A}\}_- \right)^m \tag{26}$$

thus allowing the calculation of general commutators of $\hat{A}^m\hat{B}^n$.

Example 2

$$\hat{A}^2\hat{B}^2 = \hat{A}[\hat{B}, [\hat{B}, \hat{A}]] + 2[\hat{B}, \hat{A}]^2 + [\hat{B}, [\hat{B}, \hat{A}]]\hat{A} - 2\hat{B}\hat{A}[\hat{B}, \hat{A}] - 2\hat{B}[\hat{B}, \hat{A}]\hat{A} + \hat{B}^2\hat{A}^2. \tag{27}$$

3. Three- and four-dimensional Lie algebras

3.1. A three-dimensional Lie algebra

Wei and Norman (1963) in their interesting article on the Lie algebraic solution of linear differential equations discussed several important low-dimensional Lie algebras finding realizations in physics. We make no use of special Lie algebraic properties, but use them only as classification. A Lie algebra is defined as $\{\hat{H}_j, \hat{H}_k, \ldots, \hat{H}_r\}$ with the commutators

$$[\hat{H}_j, \hat{H}_k] = \sum_{r=1}^{n} \gamma_{jk}^r \hat{H}_r \tag{28}$$

where γ_{jk}^r are structure constants. The simplest non-Abelian three-dimensional Lie algebra is formed by $\{\hat{A}, \hat{B}, \hat{I}\}$ with the commutators

$$[\hat{A}, \hat{B}] = c\hat{I}, \qquad [\hat{A}, \hat{I}] = [\hat{B}, \hat{I}] = 0. \tag{29}$$

Ordered operator expansions for this algebra are equations (2) and (3). Using equation (12) and the comparison method leads to

$$\sum_{k=0}^{\infty} \frac{\alpha^k}{k!}(\hat{A}+\hat{B})^k = \sum_{u=0}^{\infty} \sum_{v=0}^{\infty} \sum_{w=0}^{\infty} \frac{\alpha^{u+v+2w}}{u!v!w!}\left(-\frac{c}{2}\right)^w \hat{A}^u \hat{B}^v. \tag{30}$$

Example 3

$$(\hat{A}+\hat{B})^3 = \hat{A}^3 + 3\hat{A}^2\hat{B} + 3\hat{A}\hat{B}^2 + \hat{B}^3 - 3c\hat{A} - 3c\hat{B}. \tag{31}$$

As the comparison presents no difficulties only disentangled operator expressions (DO) are written down in the subsequent sections.

The implicit form of equation (3) is derived from

$$\begin{aligned} \exp(\alpha\hat{A})\exp(\beta\hat{B}) &= \exp(\alpha\hat{A})\exp(\beta\hat{B})\exp(-\alpha\hat{A})\exp(\alpha\hat{A}) \\ &= \exp\{\beta\tilde{B}(\alpha\hat{A})\}\exp\alpha\hat{A}, \qquad (\text{DO}). \end{aligned} \tag{32}$$

An application of equation (32) is the commutator

$$[\hat{A}, \hat{B}^k] = ck\hat{B}^{k-1}. \tag{33}$$

This derivation of equations (2) and (3) has the advantage that it can be repeated immediately from well-known operator formulae. It is more difficult to memorize the compact formulae (2) and (3).

3.2. Derived higher-dimensional algebras

Higher-dimensional algebras can be constructed by: $\{\hat{A}, \hat{B}, \hat{B}^2 \ldots, \hat{B}^k \ldots, \hat{I}\}$ with the commutators

$$[\hat{A}, \hat{B}^k] = ck\hat{B}^{k-1}, \qquad [\hat{A}, \hat{I}] = [\hat{B}^k, \hat{I}] = 0. \tag{34}$$

The $\hat{C}_m$ are up to $m = 4$

$$\hat{C}_2 = -\tfrac{1}{2}ck\hat{B}^{k-1} \tag{35}$$

$$\hat{C}_3 = \tfrac{1}{6}c^2k(k-1)\hat{B}^{k-2} \tag{36}$$

$$\hat{C}_4 = -\tfrac{1}{24}c^3k(k-1)(k-2)\hat{B}^{k-3}. \tag{37}$$

For finite k the Zassenhaus formula terminates leading to a completely ordered expansion.

Example 4

$$(\hat{A}+\hat{B}^3)^2 = \hat{A}^2 + 2\hat{A}\hat{B}^3 - 3c\hat{B}^2 + \hat{B}^6. \tag{38}$$

The algebra can be further enlarged by considering $\{\hat{A}\hat{B}^m, \hat{B}, \hat{B}^2 \ldots, \hat{B}^k \ldots, \hat{I}\}$ with

$$[\hat{A}\hat{B}^m, \hat{B}^k] = kc\hat{B}^{(k+m-1)}. \tag{39}$$

The application to operator products $(\hat{A}\hat{B}^m + \hat{B}^k)^s$ is obvious. The first term is not completely ordered but can be ordered with formula (32).

3.3. *A four-dimensional Lie algebra*

Closely related to the three-dimensional algebra above is the four-dimensional algebra $\{\hat{Q}^2+\hat{P}^2, \hat{Q}, \hat{P}, \hat{I}\}$ with

$$\begin{aligned}
&[\hat{P}^2+\hat{Q}^2, \hat{Q}] = -2i\hbar\hat{P} \\
&[\hat{P}^2+\hat{Q}^2, \hat{P}] = 2i\hbar\hat{Q} \\
&[\hat{Q}, \hat{P}] = i\hbar\hat{I} \\
&[\hat{Q}, \hat{I}] = [\hat{P}, \hat{I}] = [\hat{P}^2+\hat{Q}^2, \hat{I}] = 0.
\end{aligned} \tag{40}$$

This is essentially the harmonic oscillator algebra which can be written in occupation number representation (ONR) (Messiah 1964)

$$\{\hat{a}^+\hat{a}, \hat{a}^+, \hat{a}, \hat{I}\}$$

with

$$\begin{aligned}
&[\hat{a}^+\hat{a}, \hat{a}] = -\hat{a}; \qquad [\hat{a}^+\hat{a}, \hat{a}^+] = \hat{a}^+ \\
&[\hat{a}, \hat{a}^+] = \hat{I}; \qquad [\hat{a}, \hat{I}] = [\hat{a}^+, \hat{I}] = [\hat{a}^+\hat{a}, \hat{I}] = 0.
\end{aligned} \tag{41}$$

The diagonal number operator $\hat{a}^+\hat{a}$ with eigenvalues n from zero to infinity is very important. It is often necessary to write $(\hat{a}^+\hat{a})^k$ in normal or antinormal ordered form with the $\hat{a}^+$ operators standing left or right from all $\hat{a}$ operators. This cannot be achieved directly using a formula given by Schwinger (1965)

$$\exp(\alpha\hat{a}^+\hat{a}) = \sum_{k=0}^{\infty} \frac{(e^{\alpha}-1)^k}{k!}\hat{a}^{+k}\hat{a}^k \tag{42}$$

as the exponentials in the sum lead to difficulties†. We treat the more general case of the commutator (1) and derive some auxiliary formulae:

$$\begin{aligned}
&\exp(\alpha\hat{A}\hat{B})\exp(\beta\hat{A}) = \exp(\beta\hat{A}\exp(-\alpha c))\exp(\alpha\hat{A}\hat{B}), \qquad (\text{DO}) \\
&\exp(\alpha\hat{A}\hat{B})\exp(\beta\hat{B}) = \exp(\beta\hat{B}\exp(\alpha c))\exp(\alpha\hat{A}\hat{B}), \qquad (\text{DO})
\end{aligned} \tag{43}$$

by means of equation (16). Arbitrary powers $(\hat{A}\hat{B})^k$ can be commuted with arbitrary powers $\hat{A}^m$, $\hat{B}^n$.

Example 5

$$(\hat{A}\hat{B})^4\hat{A}^4 = \hat{A}^4((\hat{A}\hat{B})^4 - 16c(\hat{A}\hat{B})^3 + 96c^2(\hat{A}\hat{B})^2 - 256c^3(\hat{A}\hat{B}) + 256c^4). \tag{44}$$

Writing

$$(\hat{A}\hat{B})^k = (\hat{A}\hat{B})^{k-1}\hat{A}\hat{B} \tag{45}$$

and commuting $(\hat{A}\hat{B})^{k-1}$ with $\hat{A}$ leads after repetitions to the expressions wanted.

Example 6

$$(\hat{A}\hat{B})^4 = \hat{A}^4\hat{B}^4 - 6c\hat{A}^3\hat{B}^3 + 7c^2\hat{A}^2\hat{B}^2 - c^3\hat{A}\hat{B}. \tag{46}$$

The reverse equations for ONR operators were derived by Bloch and De Dominicis (1958).

† After completion of this article a very recent note came to my attention: J Katriel 1974 *Lett. Nuovo Cim.* **10** 565–6 where he proved the disentangling of powers of $\hat{n}$.

3.4. Applications

We list some applications of the operator formulae given above. The harmonic oscillator as an exactly solvable quantum system finds wide applications from atoms to nuclei and quarks (Moshinsky 1969). It is furthermore important for coherent states in quantum optics (Cahill and Glauber 1969) and in solid state physics (Kohn and Sherrington 1970). Excitations in solids like phonons (Haken 1973), excitons and polarons (Kuper and Whitfield 1963, Devreese 1971) and magnons (Mattis 1965) can be treated in this framework. Molecular vibrations including vibrational and rotational resonances can be handled easily (Birss and Choi 1970).

4. A two-dimensional Lie algebra

4.1. Sack's identity

The only non-Abelian two-dimensional Lie algebra was discussed by Sack (1958) in connection with the 'quantum mechanical shift operator'. The algebra $\{\hat{X}, \hat{Y}\}$ has the commutator

$$[\hat{X}, \hat{Y}] = y\hat{Y}, \tag{47}$$

with y a c number.

The DO given by Sack can also be derived by Kirzhnits' (1967) parameter differentiation technique:

$$\begin{aligned} \exp\{\alpha(\hat{X}+\beta\hat{Y})\} &= \exp(\alpha\hat{X})\exp\left(\frac{\beta\hat{Y}}{y}(1-\exp(-\alpha y)\right) \\ &= \exp\left(\frac{\beta\hat{Y}}{y}(\exp(\alpha y)-1)\right)\exp(\alpha\hat{X}), \qquad \text{DO.} \end{aligned} \tag{48}$$

A further derivation is also possible by a straightforward application of the Zassenhaus formula. The commutators up to $m = 5$ are:

$$\begin{aligned} C_2 &= -\frac{\beta y}{2}\hat{Y} \\ C_3 &= \frac{\beta y^2}{6}\hat{Y} \\ C_4 &= -\frac{\beta y^3}{24}\hat{Y} \\ C_5 &= \frac{\beta y^4}{120}\hat{Y}. \end{aligned} \tag{49}$$

The exponentials $\hat{C}_m$ can be summed up and written as equation (48). It can be applied to the calculation of ordered expressions of $(\hat{X}+\beta\hat{Y})^k$.

Example 7

$$(\hat{X}+\hat{Y})^3 = \hat{X}^3 + 3\hat{X}^2\hat{Y} - 3y\hat{X}\hat{Y} - 3y\hat{Y}^2 + y^2\hat{Y} + \hat{Y}^3. \tag{50}$$

Using the second form of (48) the reverse ordering can be performed with all $\hat{Y}$ operators standing left of all $\hat{X}$ operators. Commutations of $\hat{X}^k\hat{Y}^m$ are tedious in straight forward calculations. They can be calculated easily from the DO

$$\begin{aligned}\exp(\alpha\hat{X})\exp(\beta\hat{Y}) &= \exp(\alpha\hat{X})\exp(\beta\hat{Y})\exp(-\alpha\hat{X})\exp(\alpha\hat{X})\\ &= \exp(\beta\exp(\alpha y)\hat{Y})\exp(\alpha\hat{X}).\end{aligned} \tag{51}$$

Example 8

$$\hat{X}^4\hat{Y}^4 = \hat{Y}^4\hat{X}^4+16\hat{Y}^4\hat{X}^3+96y^2\hat{Y}^4\hat{X}^2+256y^3\hat{Y}^4\hat{X}+256y^4\hat{Y}^4. \tag{52}$$

4.2. Derived Lie algebras

From the two-dimensional Lie algebra some related Lie algebras can be derived and used in ordered expansions. It is $\{\hat{X}, \hat{X}\hat{Y}\}$ with

$$[\hat{X}, \hat{X}\hat{Y}] = y\hat{X}\hat{Y} \tag{53}$$

two-dimensional allowing application of Sack's identity (48) to expressions $(\hat{X}+\hat{X}\hat{Y})^k$. For similar expansions $(\hat{X}\hat{Y}+\hat{Y})^k$ the full Zassenhaus formula must be used because of the commutator

$$[\hat{X}\hat{Y}, \hat{Y}] = y\hat{Y}^2. \tag{54}$$

The first $\hat{C}_m$ are:

$$\begin{aligned}\hat{C}_2 &= -\frac{y}{2}\hat{Y}^2\\ \hat{C}_3 &= \frac{y^2}{6}\hat{Y}^3.\end{aligned} \tag{55}$$

A further two-dimensional Lie algebra is $\{\hat{X}, \hat{Y}^k\}$ with

$$[\hat{X}, \hat{Y}^k] = ky\hat{Y}^k \tag{56}$$

allowing the ordered expansion of $(\hat{X}+\hat{Y}^k)^m$ by means of the equations above.

4.3. Applications

Wei and Norman (1963) gave two applications in chemical physics. They showed that the Landau–Teller transition probabilities of a system of simple harmonic oscillators are a realization of the above algebra in an infinite dimensional space. By a suitable definition of raising and lowering operators an isomorphism between these operators and those of the abstract algebra can be proved. A second realization is provided by the kinetics of the deuterium exchange reaction. It seems that further problems in statistical mechanics with nearest-neighbour transition probabilities can be reduced to the algebraic problem discussed above. Moreover, generating functions and addition theorems for special functions can be treated in terms of operators forming low-dimensional Lie algebras (Kaufman 1966).

5. Angular momentum algebra

5.1. Failure of the comparison method for angular momentum

As angular momentum algebra is important in many physical applications, one is especially interested in the 'simple split three-dimensional' Lie algebra $\{\hat{E}, \hat{F}, \hat{H}\}$ with the commutators

$$[\hat{E}, \hat{F}] = \hat{H}; \qquad [\hat{E}, \hat{H}] = 2\hat{E}; \qquad [\hat{F}, \hat{H}] = -2\hat{F}. \tag{57}$$

This algebra is a special case of

$$[\hat{A}, \hat{B}] = \hat{C}; \qquad [\hat{A}, \hat{C}] = -b\hat{A}; \qquad [\hat{B}, \hat{C}] = b\hat{B} \tag{58}$$

($b = c$ number).

Kirzhnits (1967) gave a DO of $\exp(\alpha(\hat{A} + \hat{B}))$ which he found by parameter differentiation and comparison of the coefficients of identical operators. The same result can be also derived by repeated application of equation (48):

$$\exp\{\alpha(\hat{A} + \hat{B})\} = \exp(g_1\hat{B})\exp(g_2\hat{C})\exp(g_3\hat{A}) \tag{59}$$

with

$$\begin{aligned} g_1 = g_3 &= (2/b)^{1/2}\tanh((b/2)^{1/2}\alpha) \\ g_2 &= (2/b)\ln\cosh((b/2)^{1/2}\alpha). \end{aligned} \tag{60}$$

The difficulty arises from g_2, as in the expansion of $\ln\cosh((b/2)^{1/2}\alpha)$ the coefficients cannot be compared. A similar problem arose in equation (42). Thus, the 'comparison method' cannot be applied directly to the angular momentum algebra.

5.2. Some ordering formulae for angular momentum

Calculations with angular momentum operators in the spherical and cartesian basis are simplified in the coupled boson representation (CBR), introduced by Schwinger (1965):

$$\hat{J}_+ = \hat{a}_+^\dagger\hat{a}_-; \qquad \hat{J}_- = \hat{a}_-^\dagger\hat{a}_+; \qquad \hat{J}_z = (1/2)(\hat{a}_+^\dagger\hat{a}_+ - \hat{a}_-^\dagger\hat{a}_-) = (1/2)(\hat{n}_+ - \hat{n}_-). \tag{61}$$

The $\hat{a}_\pm^\dagger$, $\hat{a}_\pm$ are two-dimensional harmonic oscillator creation and annihilation operators with

$$[\hat{a}_\pm, \hat{a}_\pm^\dagger] = 1; \qquad [\hat{a}_+, \hat{a}_-] = [\hat{a}_+^\dagger, \hat{a}_-^\dagger] = [\hat{a}_+, \hat{a}_-^\dagger] = [\hat{a}_-, \hat{a}_+^\dagger] = 0. \tag{62}$$

The following DO are useful in the comparison method and are derived by means of equation (16):

$$\begin{aligned} \exp(\alpha\hat{J}_+)\exp(\beta\hat{a}_+^\dagger)\exp(\gamma\hat{a}_+) &= \exp(\beta\hat{a}_+^\dagger)\exp(\gamma\hat{a}_+)\exp(-\alpha\gamma\hat{a}_-)\exp(\alpha\hat{J}_+) \\ \exp(\alpha\hat{J}_+)\exp(\beta\hat{a}_-^\dagger)\exp(\gamma\hat{a}_-) &= \exp(\beta\hat{a}_-^\dagger)\exp(\alpha\beta\hat{a}_+^\dagger)\exp(\gamma\hat{a}_-)\exp(\alpha\hat{J}_+) \\ \exp(\alpha\hat{J}_-)\exp(\beta\hat{a}_+^\dagger)\exp(\gamma\hat{a}_+) &= \exp(\beta\hat{a}_+^\dagger)\exp(\alpha\beta\hat{a}_-^\dagger)\exp(\gamma\hat{a}_+)\exp(\alpha\hat{J}_-) \\ \exp(\alpha\hat{J}_-)\exp(\beta\hat{a}_-^\dagger)\exp(\gamma\hat{a}_-) &= \exp(\beta\hat{a}_-^\dagger)\exp(\gamma\hat{a}_-)\exp(-\alpha\gamma\hat{a}_+)\exp(\alpha\hat{J}_-) \end{aligned} \tag{63}$$

$$\begin{aligned} \exp(\alpha\hat{n}_+)\exp(\beta\hat{J}_+) &= \exp(\beta\hat{J}_+\exp\alpha)\exp(\alpha\hat{n}_+) \\ \exp(\alpha\hat{n}_-)\exp(\beta\hat{J}_+) &= \exp(\beta\hat{J}_+\exp(-\alpha))\exp(\alpha\hat{n}_-) \\ \exp(\alpha\hat{n}_+)\exp(\beta\hat{J}_-) &= \exp(\beta\hat{J}_-\exp(-\alpha))\exp(\alpha\hat{n}_+) \\ \exp(\alpha\hat{n}_-)\exp(\beta\hat{J}_-) &= \exp(\beta\hat{J}_-\exp(\alpha))\exp(\alpha\hat{n}_-). \end{aligned} \tag{64}$$

These expressions can be used for the commutation of $\hat{J}_z^k\hat{J}_\pm^l$. An important application is the ordering of $\hat{J}_+^k\hat{J}_-^l$, so that the expression consists of a diagonal part and powers of $\hat{J}_+$ standing right of all other operators. It is with $k > l$

$$\hat{J}_+^k \hat{J}_-^l = \hat{J}_+^{k-l} \hat{J}_+^l \hat{J}_-^l = \hat{J}_+^{k-l} (\hat{a}_+^{+l} \hat{a}_+^l \hat{a}_-^l \hat{a}_-^{+l}) \tag{65}$$

$\hat{J}_+^{k-l}$ is commuted to the right by means of the formulae above. It is a matter of taste whether $\hat{J}_+^{k-l}$ is commuted with individual powers of $\hat{a}_\pm^k$, $(\hat{a}_\pm^+)^m$ or with the number operators $\hat{n}_\pm$. In the latter case the formulae of Bloch and De Dominicis (1958) must be applied in addition.

5.3. *Matrix elements and traces of products of angular momentum operators*

Traces of products of angular momentum operators were calculated in two comprehensive articles by Ambler *et al* (1962a, b) using conventional angular momentum techniques. Rose (1962) used recoupling and graphical methods. The coupled boson representation and operator algebra were used by Witschel (1971). Here the 'comparison method' will be applied. Whereas the calculation of matrix elements of $\hat{J}_+^k \hat{J}_-^l \hat{J}_z^n$ in the spherical basis is simple, it presents many difficulties for $\hat{J}_x^k \hat{J}_y^l \hat{J}_z^n$ in the cartesian basis. We proceed in the same way as for the Lie algebras above using CBR. The essential point is the property of ONR, $\hat{a}_\pm|00\rangle = 0$, which was already used for the calculation of the rotation matrices $d^j_{mm'}(\theta)$ (Grosswendt and Witschel 1972). The angular momentum eigenvectors are

$$|jm\rangle = (j+m)!(j-m)!^{-1/2} (\hat{a}_+^+)^{j+m} (\hat{a}_-^+)^{j-m} |00\rangle. \tag{66}$$

The matrix element to be calculated

$$M = \langle jm| \exp(2\alpha \hat{J}_x) \exp(2\beta \hat{J}_y) \exp(2\gamma \hat{J}_z) |jm'\rangle \tag{67}$$

reads in CBR

$$M = F^{jj}_{mm'} \langle 00| \hat{a}_+^{j+m} \hat{a}_-^{j-m} \exp\{\alpha(\hat{a}_+^+ \hat{a}_- + \hat{a}_-^+ \hat{a}_+)\} \exp\{-\beta \mathrm{i}(\hat{a}_+^+ \hat{a}_- - \hat{a}_-^+ \hat{a}_+)\}$$
$$\times \exp\{\gamma(\hat{a}_+^+ \hat{a}_+ - \hat{a}_-^+ \hat{a}_-)\} (\hat{a}_+^+)^{j+m'} (\hat{a}_-^+)^{j-m'} |00\rangle \tag{68}$$

$$F^{jj}_{mm'} = \{(j+m)!(j-m)!(j+m')!(j-m')!\}^{-1/2}. \tag{69}$$

Because of the properties of the Lie algebra discussed in equations (59) and (60) the exponentials cannot be disentangled, but they can be moved to the right and the property of ONR mentioned can be used. The algebra of the transformation is omitted. The final result is:

$$M = F^{jj}_{mm'} \langle 00| \hat{a}_+^{j+m} \hat{a}_-^{j-m} \{(\alpha_1 \hat{a}_+^+ + \alpha_2 \hat{a}_-^+) \exp\gamma\}^{j+m'} \{(\alpha_3 \hat{a}_+^+ + \alpha_4 \hat{a}_-^+) \exp(-\gamma)\}^{j-m'} |00\rangle \tag{70}$$

with

$$\begin{aligned} \alpha_1 &= (1/2)\{(1+\mathrm{i})\cosh(\alpha+\beta) + (1-\mathrm{i})\cosh(\alpha-\beta)\} \\ \alpha_2 &= (1/2)\{(1+\mathrm{i})\sinh(\alpha+\beta) + (1-\mathrm{i})\sinh(\alpha-\beta)\} \\ \alpha_3 &= (1/2)\{(1-\mathrm{i})\sinh(\alpha+\beta) + (1+\mathrm{i})\sinh(\alpha-\beta)\} \\ \alpha_4 &= (1/2)\{(1-\mathrm{i})\cosh(\alpha+\beta) + (1+\mathrm{i})\cosh(\alpha-\beta)\}. \end{aligned} \tag{71}$$

As $\hat{a}_+^+$ and $\hat{a}_-^+$ commute, the operator expressions can be evaluated by the ordinary binomial formula. M is different from zero only for equal powers of the corresponding creation and annihilation operators leading to the remaining matrix element M':

$$M' = \langle 00| (\hat{a}_\pm)^k (\hat{a}_\pm^+)^k |00\rangle = k!. \tag{72}$$

For the comparison method both forms of M, equations (68) and (71) are expanded and the coefficients of equal powers of α, β and γ are compared. Thus it is possible to derive from one $M_{jm}^{jm'}$ all possible matrix elements $\langle jm|\hat{J}_x^k\hat{J}_y^l\hat{J}_z^n|jm'\rangle$ by elementary algebra. The powers of the hyperbolic functions are manipulated by ordinary multiplication and Des Moivres' theorem. For some applications which are summarized below it is necessary to calculate the trace, ie the sum of diagonal elements of these operator products. If the diagonal matrix elements of the $(2j+1)$ m-values are calculated, the trace can be formed by summing up the individual matrix elements. Only book-keeping problems limitate the application of the method. An example will illustrate the technique.

Example 9

$$M_{1,0}^{1,0} = \langle 1,0|\exp(2\alpha\hat{J}_x)\exp(2\beta\hat{J}_y)|1,0\rangle = \alpha_1\alpha_4+\alpha_2\alpha_3$$
$$= 1+2\alpha^2+2\beta^2+2/3\alpha^4+4\alpha^2\beta^2+2/3\beta^4+4/45\alpha^6+4/3\alpha^4\beta^2$$
$$+4/3\alpha^2\beta^4+4/45\beta^6+\ldots \quad (73)$$

$$M_{1,1}^{1,1} = \langle 1,1|\exp(2\alpha\hat{J}_x)\exp(2\beta\hat{J}_y)|1,1\rangle = \alpha_1^2$$
$$= 1+\alpha^2+2\mathrm{i}\alpha\beta+\beta^2+1/3\alpha^4+4\mathrm{i}/3\alpha^3\beta+4\mathrm{i}/3\alpha\beta^3+1/3\beta^4+2/45\alpha^6$$
$$+4\mathrm{i}/15\alpha^5\beta+8\mathrm{i}/9\alpha^3\beta^3+4\mathrm{i}/15\alpha\beta^5+2/45\beta^6+\ldots \quad (74)$$

$$M_{1,-1}^{1,-1} = \langle 1,-1|\exp(2\alpha\hat{J}_x)\exp(2\beta\hat{J}_y)|1,-1\rangle = \alpha_4^2$$
$$= 1+\alpha^2-2\mathrm{i}\alpha\beta+\beta^2+1/3\alpha^4-4/3\mathrm{i}\alpha^3\beta-4\mathrm{i}/3\alpha\beta^3+1/3\beta^4+2/45\alpha^6$$
$$-4\mathrm{i}/15\alpha^5\beta-8\mathrm{i}/9\alpha^3\beta^3-4\mathrm{i}/15\alpha\beta^5+2/45\beta^6+\ldots. \quad (75)$$

If we abbreviate the trace by $\langle\!\langle\ \ \rangle\!\rangle_j$ it is:

$$\begin{array}{ll}
\langle\!\langle\hat{J}_x^2\rangle\!\rangle_1 = \langle\!\langle J_y^2\rangle\!\rangle_1 = 2 & \langle\!\langle\hat{J}_x^6\rangle\!\rangle_1 = \langle\!\langle\hat{J}_y^6\rangle\!\rangle_1 = 2 \\
\langle\!\langle J_xJ_y\rangle\!\rangle_1 = 0 & \langle\!\langle\hat{J}_x^5\hat{J}_y\rangle\!\rangle_1 = \langle\!\langle\hat{J}_x\hat{J}_y^5\rangle\!\rangle_1 = 0 \\
\langle\!\langle J_x^3J_y\rangle\!\rangle_1 = \langle\!\langle\hat{J}_x\hat{J}_y^3\rangle\!\rangle_1 = 0 & \langle\!\langle\hat{J}_x^4\hat{J}_y^2\rangle\!\rangle_1 = \langle\!\langle\hat{J}_x^2\hat{J}_y^4\rangle\!\rangle_1 = 1 \\
\langle\!\langle\hat{J}_x^4\rangle\!\rangle_1 = \langle\!\langle\hat{J}_y^4\rangle\!\rangle_1 = 2 & \langle\!\langle\hat{J}_x^3\hat{J}_y^3\rangle\!\rangle_1 = 0 \\
\langle\!\langle\hat{J}_x^2\hat{J}_y^2\rangle\!\rangle_1 = 1. &
\end{array} \quad (76)$$

From general invariance properties of angular momentum traces it follows that they are different from zero only if:

$\hat{J}_a^k$	with $a = x, y, z$;	k even	
$\hat{J}_a^k\hat{J}_b^l$	with $a, b = x, y, z$;	k, l both even	
$\hat{J}_a^k\hat{J}_b^l\hat{J}_c^n$	with $a, b, c = x, y, z$;	k, l, n all even	k, l, n all odd.

Comparison with these restrictions and the extended tables by Ambler *et al* (1962a, b) shows agreement.

5.4. Applications

Biedenharn and Van Dam (see Schwinger 1965) give in their reprint collection a comprehensive bibliography on angular momentum and its application to physics and chemistry. Traces of products of angular momentum operators are important for the computation of thermodynamic properties of paramagnetic salts, especially at low temperature. This and related topics are covered in the authoritative monograph by Abragam and Bleaney (1970). Applications to magnetic problems together with an introduction to CBR are discussed by Mattis (1965). An application in molecular spectroscopy is the calculation of asymmetric top sum rules without (Louck 1963), and with centrifugal distortion (Witschel 1971).

6. Conclusion

Starting with the Zassenhaus formula for disentangling of exponential operator expressions a number of ordering formulae could be derived in an elementary unified way using comparison. This technique thus supplements more sophisticated operator orderings. Some formulae are only rederived but some are apparently new. The advantage of the method is that only four operator formulae and elementary algebra is needed to avoid cumbersome and error proned operator commutations.

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