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A LIST-PROCESSING APPROACH TO QUANTUM MECHANICS

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Abstract

On the basis of several earlier papers and in view of the current availability of logic-programming facilities, the authors propose a list-processing approach to the modelling of algebraic quantum field theory methods in which the noncommutative algebra of quantum-mechanical operators is emulated by lists. The processing produces reordered sequences of elements of a ring with a unit commutator and generates dynamic structures which for some initial arrangements correspond to partially ordered graphs characterized by recurrence relations and combinatorial identities. The approach is illustrated by reviewing the simple case of a forced harmonic oscillator. The programming aspects are briefly described.

1. Introduction

Some years ago, in a paper entitled "Transition probability of a linearly forced harmonic oscillator system" [1], a binomial expansion for non-commuting operators was used, in a time-dependent perturbation calculation in the interaction representation, to expand the evolution operator and obtain the transition probabilities expressed in terms of the generalized Laguerre polynomials. The standard S-matrix calculation was closely followed, except that it was possible to bypass the T ordering and the Wick theorem. The calculation hinged on the application of several algebraic expansion theorems, in the ring generated by two elements with unit commutator, established by the same authors in one of their earlier papers [2].

The aim of the present work is to closely reexamine the algebraic features of these expansion theorems and to attempt to formulate a list-processing approach for calculating various quantum-mechanical queries by computer-implemented logic programming of dynamic lists. It turns out that the implied list-processing corresponds to generating partially ordered graphs from the appropriate initial binary-tree structures, which in some situtations, possessing a certain measure of symmetry of form, leads to recurrence relations and integer-valued coefficients related to combinatorial identities and special functions.

2. Algebraic reordering methods

Let R denote an associative ring with unit 1 of characteristic zero. For any two elements $A, B \in R$ obeying the commutation relation

$$[A, B] = 1, \tag{1}$$

each of the following two sequences

$$\left.\begin{array}{l} 1,\ BA,\ (BA)^2,\ (BA)^3, \ldots, (BA)^n, \ldots \\ 1,\ BA,\ B^2A^2,\ B^3A^3, \ldots,\ B^nA^n, \ldots \end{array}\right\} \tag{2}$$

is linearly independent over the ring of integers [2].

With respect to prospective quantum-mechanical applications, in which the ring would be implemented as an algebra of operators over the vector space of physical states (with B and A in the role of creation and annihilation operators, respectively [3]), the elements of the first sequence $(BA)^n$ would have the basis vectors $|k\rangle$ as eigenvectors, while the elements of the second sequence B^nA^n, appearing as members in the calculation of expectation values of physical operators over a state vector, would produce either 0 or 1. Thus, the decomposition of an arbitrary element of the ring into normal products, in which all B operators appear on the left of A operators, is physically significant. (This, of course, is also implicit in the usual formulation of Wick's theorem in quantum field theory [4].)

In some cases of physical interest, the rearrangements can be achieved algebraically. The procedure is based on the repetitive application of the commutation relation (1), or some of its immediate implications like

$$[A^n, B] = nA^{n-1}, \tag{3}$$

$$[A, B^n] = nB^{n-1}, \tag{4}$$

or some more involved relations, e.g.

$$[A, (BA)^n] = \sum_{q=0}^{n-1} \binom{n}{q} (BA)^q A, \tag{5}$$

or, equivalently,

$$[A, (BA)^n] = (BA)^{n-1}A + (BA)^{n-2}A(BA) + \ldots + (BA)A(BA)^{n-2}. \tag{6}$$

The associated reordering prescriptions take the form of transformation expansions with integer-valued coefficients, subject to certain recurrence relations. The most useful are the following:

(a) $$(AB)^n = \sum_{q=0}^{n} C(n, q)(BA)^q, \tag{7}$$

which is a straightforward consequence of the commutation relation (1), i.e. of replacing AB with $BA + 1$, noting that powers of BA commute, and using Newton's binomial theorem. Coefficients $C(n, q)$, therefore, are recognized as binomial coefficients

$$C(n,q) = \binom{n}{q} \tag{8}$$

and satisfy the recurrence relation

$$C(n, q) = C(n-1, q-1) + C(n-1, q), \tag{9}$$

which, in the context of (7), follows from expressing its left-hand side as $(BA + 1)(AB)^{n-1}$, expanding the second factor and equating the coefficients with equal powers of $(BA)^q$ on both sides.

(b) $$A^n B^n = \sum_{q=0}^{n} L(n, q) B^q A^q, \tag{10}$$

where coefficients $L(n, q)$ satisfy the recurrence relation

$$L(n, q) = L(n-1, q-1) + (n+q) L(n-1, q), \tag{11}$$

with the stopping rule $L(0, 0) = 1$, and $L(n, q) = 0$ for $n < 0$, as well as for $q < 0$ or $q > n$.

The coefficients can be expressed explicitly as

$$L(n,q) = \frac{n!}{q!} \binom{n}{q} \tag{12}$$

and can be recognized as absolute values of the coefficients of Laguerre polynomials $L_n(x)$ [5]:

(c) $$(BA)^n = \sum_{q=1}^{n} \sigma(n, q) B^q A^q, \tag{13}$$

which implies the recurrence relation

$$\sigma(n, q) = \sigma(n-1, q-1) + q\, \sigma(n-1, q), \tag{14}$$

with $\sigma(1, 1) = 1$ and $\sigma(n, q) = 0$ for $n < 0$, as well as for $q < 0$ or $q > n$.

The coefficients are the Stirling numbers of the second kind [5], satisfying the relation

$$\sigma(n+1, q+1) = \sum_{p=q}^{n} \binom{n}{p} \sigma(p, q) \tag{15}$$

and having the explicit expression

$$\sigma(n,q)=\frac{1}{q!}\sum_{k=0}^{q}(-1)^{q-k}\binom{q}{k}k^{n}. \tag{16}$$

(d)

$$B^nA^n=\sum_{q=1}^{n}S(n,q)(BA)^q, \tag{17}$$

where coefficients $S(n, q)$ are defined for any positive integer n and for $q = 1, 2, \ldots, n$, so as to satisfy the following recurrence relation:

$$S(n,q)=S(n-1,q-1)-(n-1)S(n-1,q). \tag{18}$$

Coefficients $S(n, q)$ are known as the Stirling numbers of the first kind, and are generated by the relation

$$x(x-1)\ldots(x-n+1)=\sum_{q=0}^{n}S(n,q)x^q \tag{19}$$

and can be expressed explicitly in the form

$$S(n,q)=\sum_{k=0}^{n-q}\sum_{l=0}^{k}\frac{(-1)^l}{k!}\binom{k}{l}\binom{n-1+k}{n-q+k}\binom{2n-q}{n-q-k}l^{n-q-k}. \tag{20}$$

(e)

$$A^nB^n=\sum_{q=0}^{n}N(n,q)(BA)^q, \tag{21}$$

with the recurrence relation

$$N(n,q)=N(n-1,q-1)+nN(n-1,q) \tag{22}$$

and $N(0, 0) = 1$.

By making use of (3), we obtain

$$A^nB^n=(BA+n)A^{n-1}B^{n-1} \tag{23}$$

and, consequently,

$$A^nB^n=(BA+1)(BA+2)\ldots(BA+n). \tag{24}$$

This implies

$$(x+1)(x+2)\ldots(x+n)=\sum_{q=0}^{n}N(n,q)x^q. \tag{25}$$

By comparison with (19), we note

$$N(n, q) = (-1)^{n-q} S(n+1, q+1). \tag{26}$$

The normal-product expansion of the nth power of $B + A$ has the form

(f) $$(B + A)^n = \sum_{p=0}^{n} \sum_{q=0}^{p} H(n, p) \binom{p}{q} B^q A^{p-q}, \tag{27}$$

with coefficients $H(n, p)$ defined for n, any positive integer or zero, and for $q = 0, 1, 2, 3, \ldots, n$, so as to satisfy the following recurrence relation

$$H(n, q) = H(n-1, q-1) + (q+1) H(n-1, q+1) \tag{28}$$

and the stopping rule $H(0, 0) = 1$.

Coefficients $H(n, q)$ are given explicitly as

$$\begin{aligned} &H(n, n-(2k+1)) = 0, \\ &H(n, n-2k) = \frac{n!}{2^k k! (n-2k)!} \end{aligned} \tag{29}$$

and can be recognized as absolute values of the coefficients of Hermite polynomials, normalized to unit values of the leading coefficient.

Introducing the symbol $[B + A]^n$ to denote the would-be normal-product expansion of $(B + A)^n$, if A and B were mutually commuting operators, namely

$$[B + A]^n \equiv \sum_{q=0}^{n} \binom{n}{q} B^q A^{n-q}, \tag{30}$$

the expansion (27) assumes the form

$$(B + A)^n = \sum_{q=0}^{n} H(n, q) [B + A]^q \tag{31}$$

and can be considered a noncommutative algebra generalization of the usual binomial expansion.

In connection with the generalized binomial expansion, it is interesting to note that the limit

$$\sum_{n=0}^{\infty} \frac{(B + A)^n}{n!} = \sqrt{\mathrm{e}}\, \mathrm{e}^B \mathrm{e}^A, \tag{32}$$

which follows from (31), (29) and some combinatorics, agrees with the well-known formula

$$e^{A+B} = e^{A}e^{B}e^{-1/2[A,B]}, \tag{33}$$

valid whenever the commutator of two operators commutes with each of them [6], and frequently used in quantum mechanics.

The recurrence relations (11), (14), (18), (23) and (28) can be verified by total induction and the use of elementary combinatorics. The recurrence relations, however, are not unique and their form depends on algebraic manipulations applied to the considered operator product. For example, relation (11) for $L(n, q)$ results from using (22) and then applying the identity

$$(BA)B^{n}A^{n} = B^{n}(BA + n)A^{n}, \tag{34}$$

while, on the other hand, considering $A^{n}B^{n}$ as $AA^{n-1}B^{n-1}B$ and using the identity

$$AB^{n}A^{n}B = B^{n+1}A^{n+1} + (2n+1)B^{n}A^{n} + n^{2}B^{n-1}A^{n-1} \tag{35}$$

leads to another recurrence relation for $L(n, q)$

$$L(n, q) = L(n-1, q-1) + (2q+1)L(n-1, q) + (q+1)^{2}L(n-1, q+1). \tag{36}$$

In making a comparison between the noncommutative ring algebraic manipulations and the generating function approach in combinatorics, one should note that algebraic treatment pertains to individual coefficients, while generating functions deal with corresponding polynomials. The polynomial recurrence relations generally relate polynomials and their derivatives, for different neighbouring index values, can in some cases be combined in such a way as to yield a differential equation and turn combinatorial investigation into an application of special functions theory. Alternatively, the noncommutative algebra can be used as a source for obtaining and analyzing combinatorial identities [7].

3. Linearly perturbed harmonic oscillator

The generalized binomial expansion (27) had been utilized in a derivation of the transition probability of a linearly forced harmonic oscillator system [1], where the S-matrix exponential expansion assumed the form

$$S = \sum_{n=0}^{\infty} \frac{(if)^{n}}{n!}(B + A)^{n}, \tag{37}$$

with B and A representing creation and annihilation operators, respectively, and f denoting a constant related to the time dependence of the displacement-proportional perturbation.

Application of (27) to the corresponding matrix element gives

$$S_{jk} = \sum_{n=0}^{\infty} \frac{(if)^n}{n!} \sum_{p=0}^{n} \sum_{q=0}^{p} H(n,p) \binom{p}{q} \langle j|B^q A^{p-q}|k\rangle, \tag{38}$$

and after some algebraic manipulation yields

$$S_{jk} = \sum_{2r=0}^{\infty} \sum_{2q=0}^{2r} \frac{(2r+p)!(k!j!)^{1/2}(if)^{2r+p}}{r!\,2^r q!\,(p-q)!\,(j-q)!\,(2r+p)!}, \tag{39}$$

with $p = 2q + k - j$. The summation can be interchanged with due care to the limits, and the series in $2r$ can be summed to obtain $\exp(-f^2/2)$.

Thus,

$$S_{jk} = \sum_{2q=0}^{\infty} \frac{(k!j!)^{1/2}(if)^{2q+k-j}}{q!\,(q+k-j)!\,(j-q)!} \exp(-f^2/2), \tag{40}$$

or, equivalently,

$$S_{jk} = L_j^{k-j}(f^2) f^{k-j} (j!/k!)^{1/2} \exp(-f^2/2), \tag{41}$$

and, finally,

$$P_{jk} = S_{jk}^2 = \frac{j!}{k!} f^{2(k-j)} \left(L_j^{k-j}(f^2)\right)^2 \exp(-f^2). \tag{42}$$

From the point of view of the noncommutative algebra and the proposed list-processing approach, this represents a very special case in which the interaction has a simple form and the corresponding operator-product manipulation can be dealt with algebraically. In more complicated cases, however, and especially in prospective applications to the many-body problems and to quantum field theory, the algebraic treatment will have to be replaced by computer-implemented symbolic processing.

4. List-processing prescription and graph-related aspects

In order to emulate algebraic manipulations via list-processing, we map a general element of the noncommutative ring to a set of corresponding lists, which possesses an equivalence relation collecting identical elements and providing appropriate coefficients. The term list, as used in the text, complies with the usual computer-science parlance denoting an ordered sequence of arbitrary length, where each element has its predecessor and its successor, while the ordinal position of an element within a list is inessential. The empty list ( ) is also included and corresponds to the unit element 1 of the ring. (Note the distinction between an array and a list, the former possessing a fixed length and explicit values of the position index.)

The transition to normal ordering requires the following list-processing steps:

(a) for each element of the list, a suitable predicate should detect the presence of the ordered pair (A, B);

(b) starting with the first detected pair, the element in the list should be replaced by two new elements, one differing from the original element by an exchange of the (A, B) for a pair (B, A), the other being obtained by deleting the (A, B);

(c) the process should be repeated until there are no (A, B) pairs within the elements of the list;

[d) if in the resulting new list some equal elements appear, they should be collected and the appropriate number placed into the corresponding integer-field.

With respect to computer implementation, one can choose between an imperative or a descriptive programming language, the obvious favorites being LISP and PROLOG, respectively. It is important to note, additionally, that algebraic list-processing relies crucially on recursive procedures [9] and, in particular, on recursive combinatorial algorithms [10].

To provide a feeling for the proposed approach, we explicitly present an elementary version of the normal-reordering part of the query database displayed in the Edinburgh dialect of micro-PROLOG:

```
NORMAL-REORDERING:
    ((collect (X| Y) (x| y))
      (multiplicity X (X| Y) x)
      (remove-all X Y z)
      (collect z Z y))
    ((collect (X) (X) (1)))
    ((multiplicity X () 0))
    ((multiplicity X (X| Y) Z)
      (multiplicity X Y x)
      (SUM x 1 Z))
    ((multiplicity X (Y| Z) x)
      (NOT EQ X Y)
      (multiplicity X Z x))
    ((normorder (X| Y) Z)
      (abba X x y)
      (/)
      (normorder (x) z)
      (normorder (y) X1)
```

```
    (normorder Y Y1)
    (union z X1 Z1)
    (union Y1 Z1 Z))
  ((normorder X X))
  ((abba X Y Z)
    (union x (A B | y) X)
    (sorted y)
    (union x (B A | y) Y)
    (union x y Z)
    (/))
```

extended with rather obvious clauses needed for the predicates: "`remove-all`", "`union`" and "`sorted`".

On the level of associated graphs, the described procedure corresponds to building a binary tree with a new node added at each subsequent replacement of AB by $BA + 1$ in the list. The root of the tree corresponds to the initial operator-product and the leaves of the tree to the elements of the transformed list generated by the removal of all ordered pairs (A, B) from the list.

The presence of identical leaves in the tree, which initiates the collection procedure, is often brought about by some partial ordering implicit in the list-processing. This is reflected in the existence of recurrence relations which, when interpreted as rules connecting respective nodes with weighted edges, transform trees into network structures.

The resulting graphs can be treated by trajectory counting procedures to provide an independent control mechanism. Conversely, suitable graph transformation methods may be used as a means of investigating combinatorial properties of the noncommutative algebra.

To illustrate the possibilities, we include a few elementary examples:

(a) A normal-ordering query performed on the $(A\ A\ B\ B\ B\ A\ B\ A\ A)$ passes through a search sequence

$(AABBB(AB)AA)$,

$(A(AB)BBBBAAA\ A(AB)BBAA)$,

$((AB)ABBBAAA\ (AB)BBAAA\ (AB)ABBAA\ (AB)BAA)$,

$(BA(AB)BBAAA\ (AB)BBAAA\ B(AB)BAAA\ BBAAA\ BA(AB)BAA$
$(AB)BAA\ B(AB)AA\ BAA)$, . . . , etc.,

and after ten binary tree levels, completes reordering and yields the response

$((B\ A\ A)\ (B\ B\ A\ A\ A)\ (B\ B\ B\ A\ A\ A\ A)\ (B\ B\ B\ B\ A\ A\ A\ A\ A\ ))\ (6\ 18\ 9\ 1)$, i.e.

$$AABBBABAA = BBBBAAAAA + 9\,BBBAAAA + 18\,BBAAA + 6\,BAA.$$

The search procedure, therefore, may be viewed as a sequential list manipulation in accordance with the previously stated list-processing steps.

(b) Querying the list $(A\ A\ B\ A\ B)$, we obtain

$$((A)\ (B\ A\ A\ )\ (B\ B\ A\ A\ A\ ))\ (4\ 5\ 1),$$

which, alternatively, may be envisaged as being brought about by collecting leaves on the corresponding binary tree (see fig. 1).

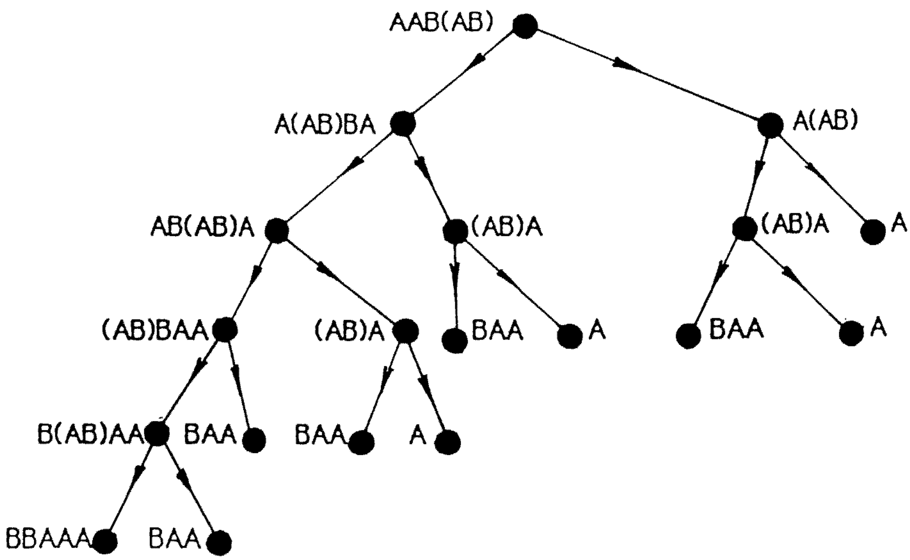

Fig. 1.

If, instead, the collection of equal nodes were introduced at each subsequent level of the calculation, the process could be represented as a graph (see fig. 2) in which the normal-ordered terms correspond to the terminal nodes (i.e. nodes with no exiting lines $B\ B\ A\ A\ A$, $B\ A\ A$, A) and the appropriate expansion coefficients can be obtained via trajectory counting.

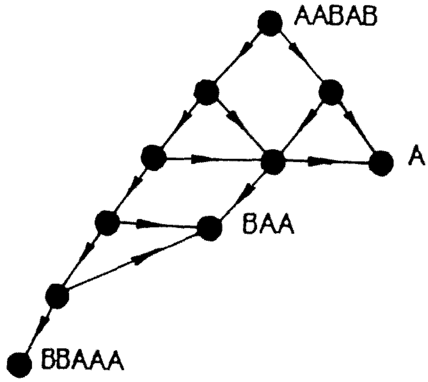

Fig. 2.

(c) A request for normal-ordering of the list $(B\ A\ B\ A\ B\ A\ B\ A)$ yields

$$((B\ A)\ (B\ B\ A\ A)\ (B\ B\ B\ A\ A\ A)\ (B\ B\ B\ B\ A\ A\ A\ A))\ (1\ 7\ 6\ 1),$$

which complies with (13), the coefficients being the Stirling numbers of the second kind $\sigma(4, 1)$, $\sigma(4, 2)$, $\sigma(4, 3)$, $\sigma(4, 4)$.

It is interesting to make a detailed examination of the corresponding binary tree produced by the sequential reapplication of (1), and note that introduction of (4), as a rule in the list-processing, contracts the structure into a weighted Hasse graph (see fig. 3) from which the requested normal ordering can be directly read by trajectory counting.

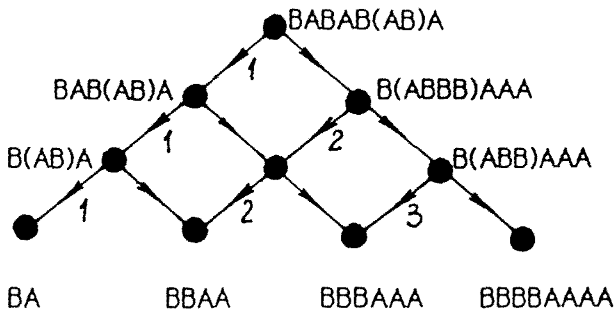

Fig. 3.

In view of (13), the nodes of the Hasse graph appear as values of the Stirling numbers $\sigma(n, q)$. Note that a general node (n, q) receives inputs from two preceding nodes: from $(n-1, q-1)$ with weight 1, and from $(n-1, q)$ with weight q, thus implying the recurrence relation (14), now obtained via graph enumeration.

(d) Queries on lists with all A-operators preceding B-operators, e.g. $(A\ A\ B\ B\ B\ B\ B)$, provide the insight into a graph interpretation of the commutator $[A^m, B^n]$. Namely, expanding the terms in accordance with the commutation relation (4), taken as the database rule instead of (1), we obtain

$(A\ (A\ B\ B\ B\ B\ B))$,

$(((A\ B\ B\ B\ B\ B)\ A), 5\ (A\ B\ B\ B\ B))$,

$((B\ B\ B\ B\ B\ A\ A), 10\ (B\ B\ B\ B\ A), 20\ (B\ B\ B))$,

yielding a graph (see fig. 4) from which the corresponding trajectory counting complies with the query result

$(A\ A\ B\ B\ B\ B\ B) \rightarrow ((B\ B\ B)\ (B\ B\ B\ B\ A)\ (B\ B\ B\ B\ B\ A\ A))\ (20\ 10\ 1)$.

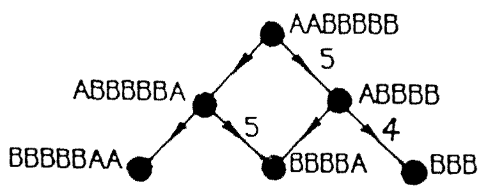

Fig. 4.

Similarly expanding $(A\ A\ A\ A\ A\ B\ B)$, by repeated application of (4), we obtain

$(A\ A\ A\ A\ (A\ B\ B))$,

$((A\ A\ A(A\ B\ B)A)\ 2\ (A\ A\ A(A\ B)))$,

$((A\ A(A\ B\ B)A\ A)\ 4\ (A\ A(A\ B)A)\ 2\ (A\ A\ A))$,

$((A(A\ B\ B)A\ A\ A)\ 6\ (A(A\ B)A\ A)\ 6\ (A\ A\ A))$,

$(((A\ B\ B)A\ A\ A\ A)\ 8\ ((A\ B)A\ A\ A)\ 10\ (A\ A\ A))$,

$((B\ B\ A\ A\ A\ A)\ 10\ (B\ A\ A\ A\ A)\ 20\ (A\ A\ A))$,

correcponding to to the graph of fig. 5, corroborating the query response

$(A\ A\ A\ A\ A\ B\ B)\ ((A\ A\ A)\ (B\ A\ A\ A\ A)\ (B\ B\ A\ A\ A\ A\ A))\ (20\ 10\ 1)$.

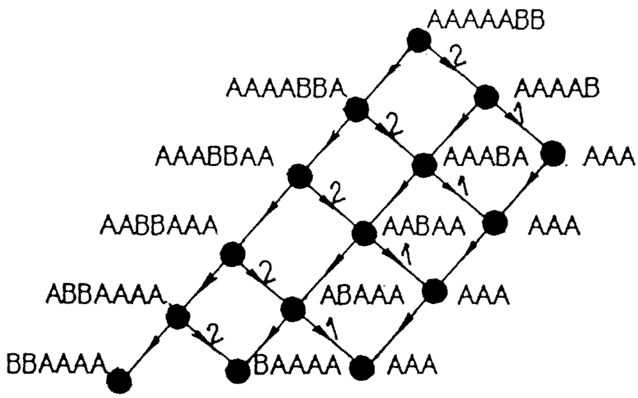

Fig. 5.

One can proceed to the general case of A^mB^n and infer that the corresponding m-leveled weighted digraph would be as given in fig. 6.

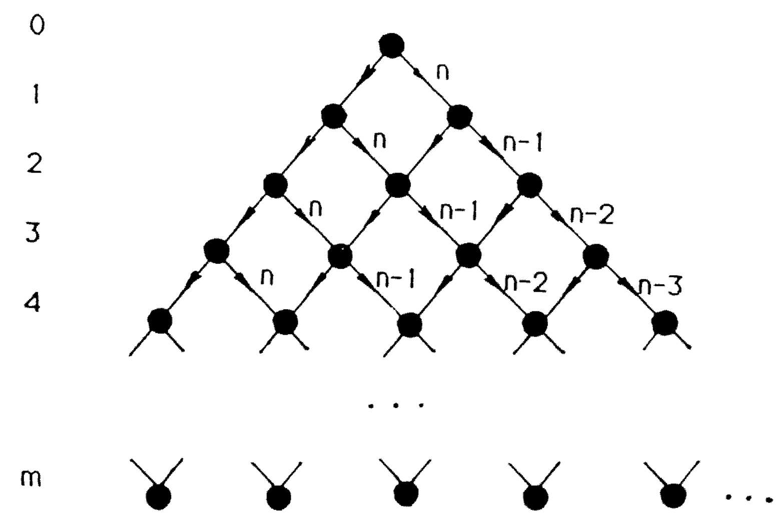

Fig. 6.

Making the observation that for this graph all trajectories which lead to any chosen node carry equal contributions, and taking notice of the fact that the number of trajectories on a Pascal-triangle graph equals the number of corresponding combination, we obtain the general commutation expression:

$$[A^m, B^n] = \sum_{q=1}^{m} q! \binom{m}{q} \binom{n}{q} B^{n-q} A^{m-q}, \tag{44}$$

which is a useful algebraic result.

Comment

More sophisticated future versions of our logic-programming database should use (44) as a basic rule instead of its very special case (1), and thus considerably gain in efficiency when very large lists are normal-order manipulated. This may prove crucial in contemplating real-world quantum mechanical applications.

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